Generalized Q-functions and Dirichlet-to-Neumann maps for elliptic differential operators

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Abstract

The classical concept of Q-functions associated to symmetric and selfadjoint operators due to M.G. Krein and H. Langer is extended in such a way that the Dirichlet-to-Neumann map in the theory of elliptic differential equations can be interpreted as a generalized Q-function. For couplings of uniformly elliptic second order differential expression on bounded and unbounded domains explicit Krein type formulas for the difference of the resolvents and trace formulas in an H^2-framework are obtained.

Key words: Q-function, Nevanlinna function, elliptic operator, Dirichlet-to-Neumann map, Krein's formula, trace formula

1 Introduction

The notion of a Q-function associated to a pair $\{S, A\}$ consisting of a symmetric operator S and a selfadjoint extension A of S in a Hilbert or Pontryagin space was introduced by M.G. Krein and H. Langer in [37,38]. A Q-function contains the spectral information of the selfadjoint extensions of the underlying symmetric operator and therefore these functions play a very important role

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[1] Earl Katz Family Chair in algebraic system theory.

in the spectral and perturbation theory of selfadjoint operators. Q-functions appear also naturally in the description of the resolvents of the selfadjoint extensions of a symmetric operator with the help of Krein's formula and they can be used to construct functional models for selfadjoint operators. In the theory of boundary triplets associated to symmetric operators Q-functions can be interpreted as so-called Weyl functions; cf. [16–19,29]. A prominent example for a Q-function is the classical Titchmarsh-Weyl coefficient in the theory of singular Sturm-Liouville operators.

The main objective of this paper is to extend the concept of Q-functions in such a way that the Dirichlet-to-Neumann map in the theory of elliptic differential equations can be identified as a generalized Q-function. In the abstract part of the paper we introduce the notion of generalized Q-functions and we show that these functions have similar properties as classical Q-functions. Besides a symmetric operator S and a selfadjoint extension A also an operator T whose closure coincides with S^* is used. Some of the ideas here parallel [9], where a more abstract approach with isometric and unitary relations in Krein spaces was used. The main result in the abstract part is Theorem 2.6 which states that an operator function is a generalized Q-function if and only if it coincides up to a possibly unbounded constant on a dense subspace with the restriction of a Nevanlinna function with an invertible imaginary part and a certain asymptotic behaviour.

Section 3 and Section 4 deal with second order elliptic operators on bounded and unbounded domains, and with the coupling of such operators. Suppose first that the domain $\Omega \subset \mathbb{R}^n$, $n > 1$, is bounded with a smooth boundary $\partial\Omega$. Let A_D and A_N be the selfadjoint realizations of an formally symmetric uniformly elliptic differential expression

$$\mathcal{L} = -\sum_{j,k=1}^{n} \frac{\partial}{\partial x_j} a_{jk} \frac{\partial}{\partial x_k} + a \tag{1.1}$$

in $L^2(\Omega)$ defined on $H^2(\Omega)$ and subject to Dirichlet and Neumann boundary conditions, respectively. If T denotes the realization of $\mathcal{L}$ on $H^2(\Omega)$, then the closure of T in $L^2(\Omega)$ coincides with the maximal operator associated to $\mathcal{L}$ in $L^2(\Omega)$, and A_D and A_N are both selfadjoint restrictions of T. For a function $f \in H^2(\Omega)$ denote the trace and the trace of the conormal derivative by $f|_{\partial\Omega}$ and $\frac{\partial f}{\partial \nu}|_{\partial\Omega}$, respectively. Then for each $\lambda \in \rho(A_D)$ the Dirichlet-to-Neumann map

$$Q(\lambda)(f_\lambda|_{\partial\Omega}) := -\frac{\partial f_\lambda}{\partial \nu}\Big|_{\partial\Omega}, \qquad \text{where} \quad T f_\lambda = \lambda f_\lambda, \tag{1.2}$$

is well-defined and will be regarded as an operator in $L^2(\partial\Omega)$ defined on $H^{3/2}(\partial\Omega)$ with values in $H^{1/2}(\partial\Omega)$. The minus sign in (1.2) is used for technical reasons. It turns out that the operator function $\lambda \mapsto Q(\lambda)$ is a generalized

Q-function in the sense of Definition 2.2 and an explicit variant of Krein's formula for the resolvents of A_D and A_N is obtained in Theorem 3.4, see also [9,13,25,26,47–50] for more general problems. In particular, in the case $n = 2$ it follows from results due to M.S. Birman that the difference of these resolvents is a trace class operator. As a consequence we obtain the trace formula

$$\operatorname{tr}\Big((A_D-\lambda)^{-1}-(A_N-\lambda)^{-1}\Big)=\operatorname{tr}\left(\overline{Q(\lambda)^{-1}}\,\frac{d}{d\lambda}\,\widetilde{Q}(\lambda)\right) \tag{1.3}$$

for $\lambda \in \rho(A_D) \cap \rho(A_N)$. Here $\overline{Q(\lambda)^{-1}}$ is the closure of $Q(\lambda)^{-1}$ in $L^2(\partial\Omega)$ and $\widetilde{Q}$ is a Nevanlinna function which differs from the Dirichlet-to-Neumann map by a symmetric constant. Trace formulas for canonical differential expressions and in more abstract situations for finite dimensional resolvent differences can be found in, e.g., [2,3,10].

In Section 4 we consider a so-called coupling of elliptic operators. Such couplings are of great interest in problems of mathematical physics, e.g., in the description of quantum networks; for more details and further references we refer the reader to the recent works [20,21,44–46]. Suppose that $\mathbb{R}^n$, $n > 1$, is decomposed in a bounded domain Ω with smooth boundary $\mathcal{C}$ and the unbounded domain $\Omega' = \mathbb{R}^n\backslash\overline{\Omega}$. The orthogonal sum of the selfadjoint Dirichlet operators A_D and A'_D associated to $\mathcal{L}$ in $L^2(\Omega)$ and $L^2(\Omega')$, respectively, is regarded as a selfadjoint diagonal block operator matrix in $L^2(\mathbb{R}^n)$. The resolvent of $A_D \oplus A'_D$ is then compared with the resolvent of the usual selfadjoint realization $\widetilde{A}$ of $\mathcal{L}$ in $L^2(\mathbb{R}^n)$ defined on $H^2(\mathbb{R}^n)$. In order to express this difference in the Krein type formula

$$\Big((A_D\oplus A'_D)-\lambda\Big)^{-1}-(\widetilde{A}-\lambda)^{-1}=\Gamma(\lambda)Q(\lambda)^{-1}\Gamma(\bar{\lambda})^* \tag{1.4}$$

with a generalized Q-function an analogon of the Dirichlet-to-Neumann map is constructed which measures the jump of the conormal derivative of $L^2(\Omega)$ and $L^2(\Omega')$-solutions of $\mathcal{L}u = \lambda u$ on the boundary $\mathcal{C}$, see (4.21). The operator $\Gamma(\lambda) : L^2(\mathcal{C}) \to L^2(\mathbb{R}^n)$ in (1.4) is closely connected with the generalized Q-function and is identified with a Poisson-type operator solving a certain Dirichlet problem. As a consequence of the representation (1.4) we also obtain a trace formula of the type (1.3) in the coupled case.

Acknowledgements

The authors are grateful to Gerd Grubb for helpful comments and valuable suggestions. Jussi Behrndt thanks the Institute for Advanced Studies in Mathematics at Ben-Gurion University of the Negev for support and hospitality during a research stay in May 2008.

2 Generalized Q-functions

In this section we introduce the notion of generalized Q-functions associated to symmetric operators in Hilbert spaces. The class of generalized Q-functions is characterized in Theorem 2.6, where it turns out that generalized Q-functions are closely connected with operator-valued Nevanlinna or Riesz-Herglotz functions. We also note in advance that for the case of finite deficiency indices of the underlying symmetric operator the concept of generalized Q-functions coincides with the classical notion of (ordinary) Q-functions studied by M.G. Krein and H. Langer in [37,38], see also [35,36].

Let $\mathcal{H}$ be a separable Hilbert space and let S be a densely defined closed symmetric operator with equal (in general infinite) deficiency indices

$$n_{\pm}(S) = \dim \ker(S^* \mp i) \leq \infty$$

in $\mathcal{H}$. It is well known that under this assumption S admits selfadjoint extensions in $\mathcal{H}$. In the following let A be a fixed selfadjoint extension of S in $\mathcal{H}$, so that, $S \subset A = A^* \subset S^*$. Furthermore, let T be a linear operator in $\mathcal{H}$ such that $A \subset T \subset S^*$ and $\overline{T} = S^*$ holds, i.e., the domain $\operatorname{dom} T$ of T is a core of $\operatorname{dom} S^*$ (see [34]), $\operatorname{dom} T$ contains $\operatorname{dom} A$ and $Af = Tf$ holds for all $f \in \operatorname{dom} A$.

For $\lambda \in \mathbb{C}$ belonging to the resolvent set $\rho(A)$ of the selfadjoint operator A define the defect spaces $\mathcal{N}_\lambda(T) = \ker(T - \lambda)$ and $\mathcal{N}_\lambda(S^*) = \ker(S^* - \lambda)$. Then the decompositions

$$\operatorname{dom} S^* = \operatorname{dom} A \dot{+} \mathcal{N}_\lambda(S^*) \quad \text{and} \quad \operatorname{dom} T = \operatorname{dom} A \dot{+} \mathcal{N}_\lambda(T) \tag{2.1}$$

hold for all $\lambda \in \rho(A)$ and the closure $\overline{\mathcal{N}_\lambda(T)}$ of $\mathcal{N}_\lambda(T)$ in $\mathcal{H}$ coincides with $\mathcal{N}_\lambda(S^*)$. Recall that the symmetric operator S is said to be *simple* if there exists no nontrivial subspace $\mathcal{D}$ in $\operatorname{dom} S$ such that S restricted to $\mathcal{D}$ is a selfadjoint operator in the Hilbert space $\overline{\mathcal{D}}$. It is important to note that S is simple if and only if

$$\mathcal{H} = \overline{\operatorname{span}} \left\{ \mathcal{N}_\lambda(S^*) : \lambda \in \mathbb{C} \backslash \mathbb{R} \right\} \tag{2.2}$$

holds; cf. [36]. Here $\overline{\operatorname{span}}$ denotes the closed linear span. As $\overline{\mathcal{N}_\lambda(T)} = \mathcal{N}_\lambda(S^*)$ it is clear that the right hand side in (2.2) coincides with

$$\overline{\operatorname{span}} \left\{ \mathcal{N}_\lambda(T) : \lambda \in \mathbb{C} \backslash \mathbb{R} \right\}.$$

Fix some $\lambda_0 \in \rho(A)$, let $\mathcal{G}$ be a Hilbert space with the same dimension as $\mathcal{N}_{\lambda_0}(T)$ and let Γ_{λ_0} be a densely defined bounded operator from $\mathcal{G}$ into $\mathcal{H}$ such that $\operatorname{ran}\Gamma_{\lambda_0} = \mathcal{N}_{\lambda_0}(T)$ and $\ker\Gamma_{\lambda_0} = \{0\}$ holds. The domain $\operatorname{dom}\Gamma_{\lambda_0}$ of Γ_{λ_0} will be denoted by $\mathcal{G}_0$. Observe that the closure $\overline{\Gamma}_{\lambda_0}$ of the operator Γ_{λ_0} is the bounded extension of Γ_{λ_0} which is defined on $\overline{\mathcal{G}}_0 = \mathcal{G}$. We write $\overline{\Gamma}_{\lambda_0} \in \mathcal{L}(\mathcal{G}, \mathcal{H})$, where $\mathcal{L}(\mathcal{G}, \mathcal{H})$ is the space of bounded linear operators defined on $\mathcal{G}$ with values in $\mathcal{H}$.

Lemma 2.1 *The operator function* $\lambda \mapsto \Gamma(\lambda) := (I + (\lambda - \lambda_0)(A - \lambda)^{-1})\Gamma_{\lambda_0}$ *satisfies* $\Gamma(\lambda_0) = \Gamma_{\lambda_0}$*,*

$$\Gamma(\lambda) = \Big(I + (\lambda - \mu)(A - \lambda)^{-1}\Big)\Gamma(\mu), \qquad \lambda, \mu \in \rho(A),$$

and $\Gamma(\lambda)$ *is a bounded operator from* $\mathcal{G}$ *into* $\mathcal{H}$ *which maps* $\operatorname{dom}\Gamma(\lambda) = \mathcal{G}_0$ *bijectively onto* $\mathcal{N}_\lambda(T)$ *for all* $\lambda \in \rho(A)$*. Moreover,* $\lambda \mapsto \Gamma(\lambda)g$ *is holomorphic on* $\rho(A)$ *for every* $g \in \mathcal{G}_0$*.*

Proof. Let us show that $\operatorname{ran}\Gamma(\lambda) = \mathcal{N}_\lambda(T)$ is true. The other assertions in the lemma are obvious or follow from a straightforward calculation. Since T is an extension of A we have $(T - \lambda)(A - \lambda)^{-1} = I$ for $\lambda \in \rho(A)$ and therefore

$$(T - \lambda)\Gamma(\lambda)h = (T - \lambda)\Big(I + (\lambda - \lambda_0)(A - \lambda)^{-1}\Big)\Gamma_{\lambda_0}h = (T - \lambda_0)\Gamma_{\lambda_0}h = 0$$

shows that $\operatorname{ran}\Gamma(\lambda) \subset \mathcal{N}_\lambda(T)$ holds. Now let $f_\lambda \in \mathcal{N}_\lambda(T)$. Then it follows as above that

$$f_{\lambda_0} := \Big(I + (\lambda_0 - \lambda)(A - \lambda_0)^{-1}\Big)f_\lambda$$

is an element in $\mathcal{N}_{\lambda_0}(T)$ and hence there exists $h \in \mathcal{G}_0$ such that $f_{\lambda_0} = \Gamma_{\lambda_0}h$. Now a simple calculation shows $f_\lambda = \Gamma(\lambda)h$, thus $\operatorname{ran}\Gamma(\lambda) = \mathcal{N}_\lambda(T)$. □

In the following definition the concept of generalized Q-functions is introduced.

Definition 2.2 *Let* S*,* A*,* T*, and* $\Gamma(\cdot)$ *be as above. An operator function* Q *defined on* $\rho(A)$ *whose values* $Q(\lambda)$ *are linear operators in* $\mathcal{G}$ *with* $\operatorname{dom}Q(\lambda) = \mathcal{G}_0$ *for all* $\lambda \in \rho(A)$ *is said to be a* generalized Q-function *of the triple* $\{S, A, T\}$ *if*

$$Q(\lambda) - Q(\mu)^* = (\lambda - \bar{\mu})\Gamma(\mu)^*\Gamma(\lambda), \qquad \lambda, \mu \in \rho(A), \tag{2.3}$$

holds on $\mathcal{G}_0$*. If, in addition,* $\mathcal{G}_0 = \mathcal{G}$ *and* $T = S^*$*, then* Q *is called an* ordinary Q-function *of* $\{S, A\}$*.*

We note that the values $Q(\lambda)$, $\lambda \in \rho(A)$, of a generalized Q-function can be unbounded non-closed operators. The adjoint $Q(\mu)^*$ in (2.3) is well defined since $\operatorname{dom}Q(\mu)$ is dense in $\mathcal{G}$ and by (2.3) also $Q(\mu) \subset Q(\bar{\mu})^*$ holds for all $\mu \in \rho(A)$. In particular, the operators $Q(\lambda)$ are closable in $\mathcal{G}$ and symmetric for $\lambda \in \rho(A) \cap \mathbb{R}$. The real and imaginary parts of the operators $Q(\lambda)$ are defined as usual:

$$\operatorname{Re} Q(\lambda) = \frac{1}{2}\Big(Q(\lambda) + Q(\lambda)^*\Big) \quad \text{and} \quad \operatorname{Im} Q(\lambda) = \frac{1}{2i}\Big(Q(\lambda) - Q(\lambda)^*\Big).$$

Since $(\operatorname{Re} Q(\lambda)h, h)$ and $(\operatorname{Im} Q(\lambda)h, h)$ are real for all $h \in \mathcal{G}_0$ the operators $\operatorname{Re} Q(\lambda)$ and $\operatorname{Im} Q(\lambda)$ are symmetric.

Remark 2.3 *We note that the concept of generalized Q-functions is closely connected with the theory of boundary triplets and associated Weyl functions. The Weyl function of an ordinary or generalized boundary triplet* (*see* [16,18,19,29]) *is also a generalized Q-function, but the converse is not true. The class of generalized Q-functions studied here coincides with the class of Weyl functions of so-called quasi boundary triplets introduced in* [9]. *Furthermore, we note that generalized Q-functions are no subclass of the Weyl families associated to boundary relations, see* [17] *and Theorem* 2.6.

The concept of generalized Q-functions differs from the classical notion of ordinary Q-functions only in the case $n_\pm(S) = \infty$.

Proposition 2.4 *Let Q be a generalized Q-function of the triple $\{S, A, T\}$ and assume, in addition, that the deficiency indices $n_\pm(S)$ are finite. Then $T = S^*$ and Q is an ordinary Q-function of the pair $\{S, A\}$.*

Proof. If the deficiency indices of the closed operator S are finite, then T is a finite dimensional extension of S and hence also T is closed. Therefore $T = \overline{T} = S^*$. Moreover, in this case also $\dim \mathcal{G} = \dim \mathcal{N}_{\lambda_0}(T)$ is finite and hence $\mathcal{G}_0 = \operatorname{dom} \Gamma(\lambda) = \operatorname{dom} Q(\lambda) = \mathcal{G}$, $\lambda \in \mathbb{C}\backslash\mathbb{R}$. □

The representation of a generalized Q-function with the help of the resolvent of A in the next proposition is formally the same as for ordinary Q-functions, see [37–39].

Proposition 2.5 *Let Q be a generalized Q-function of the triple $\{S, A, T\}$ and let $\lambda_0 \in \rho(A)$. Then Q can be written as the sum of the possibly unbounded operator $\operatorname{Re} Q(\lambda_0)$ and a bounded holomorphic operator function,*

$$Q(\lambda) = \operatorname{Re} Q(\lambda_0) + \Gamma_{\lambda_0}^*\Big((\lambda - \operatorname{Re} \lambda_0) + (\lambda - \lambda_0)(\lambda - \bar{\lambda}_0)(A - \lambda)^{-1}\Big)\Gamma_{\lambda_0}, \tag{2.4}$$

and, in particular, any two generalized Q-functions of $\{S, A, T\}$ differ by a constant.

Proof. Let $h \in \mathcal{G}_0$ and set $\mu = \lambda_0$ in (2.3). Making use of the definition of

$\Gamma(\lambda)$ in Lemma 2.1 we obtain

$$Q(\lambda)h = Q(\lambda_0)^*h + (\lambda - \bar{\lambda}_0)\Gamma_{\lambda_0}^*\Big(I + (\lambda - \lambda_0)(A - \lambda)^{-1}\Big)\Gamma_{\lambda_0}h.$$

As $Q(\lambda_0)h - Q(\lambda_0)^*h = (\lambda_0 - \bar{\lambda}_0)\Gamma_{\lambda_0}^*\Gamma_{\lambda_0}h$ we see that the above formula can be rewritten as

$$Q(\lambda)h = Q(\lambda_0)h + (\lambda - \lambda_0)\Gamma_{\lambda_0}^*\Gamma_{\lambda_0}h + \Gamma_{\lambda_0}^*(\lambda - \lambda_0)(\lambda - \bar{\lambda}_0)(A - \lambda)^{-1}\Gamma_{\lambda_0}h.$$

The representation (2.4) follows by inserting $Q(\lambda_0)h = \operatorname{Re} Q(\lambda_0)h + i\operatorname{Im} Q(\lambda_0)h$ and $\operatorname{Im} Q(\lambda_0)h = \operatorname{Im}\lambda_0\Gamma_{\lambda_0}^*\Gamma_{\lambda_0}h$ into this expression. □

Generalized Q-functions are closely connected with the class of Nevanlinna functions; cf. Theorem 2.6 below. Let $\mathcal{L}(\mathcal{G})$ be the space of everywhere defined bounded linear operators in $\mathcal{G}$. Recall that an $\mathcal{L}(\mathcal{G})$-valued operator function $\widetilde{Q}$ which is holomorphic on $\mathbb{C}\backslash\mathbb{R}$ and satisfies

$$\frac{\operatorname{Im}\widetilde{Q}(\lambda)}{\operatorname{Im}\lambda} \geq 0 \qquad \text{and} \qquad \widetilde{Q}(\bar{\lambda}) = \widetilde{Q}(\lambda)^* \tag{2.5}$$

for $\lambda \in \mathbb{C}\backslash\mathbb{R}$ is said to be an $\mathcal{L}(\mathcal{G})$-valued *Nevanlinna function*. We note that $\widetilde{Q}$ is an $\mathcal{L}(\mathcal{G})$-valued Nevanlinna function if and only if $\widetilde{Q}$ admits an integral representation of the form

$$\widetilde{Q}(\lambda) = \alpha + \lambda\beta + \int_{\mathbb{R}} \left(\frac{1}{t-\lambda} - \frac{t}{1+t^2}\right) d\Sigma(t), \qquad \lambda \in \mathbb{C}\backslash\mathbb{R}, \tag{2.6}$$

where $\alpha = \alpha^* \in \mathcal{L}(\mathcal{G})$, $0 \leq \beta = \beta^* \in \mathcal{L}(\mathcal{G})$ and $t \mapsto \Sigma(t) \in \mathcal{L}(\mathcal{G})$ is a selfadjoint nondecreasing $\mathcal{L}(\mathcal{G})$-valued function on $\mathbb{R}$ such that

$$\int_{\mathbb{R}} \frac{1}{1+t^2}\, d\Sigma(t) \in \mathcal{L}(\mathcal{G}).$$

It is well known that Nevanlinna functions can be represented with the help of selfadjoint operators or relations in Hilbert spaces in a very similar form as in (2.4). Such operator and functional models for Nevanlinna functions can be found in, e.g., [1,7,12,15,19,27,33,39,41].

In the next theorem we characterize the class of generalized Q-functions. Roughly speaking, it turns out that up to a symmetric constant a generalized Q-function is a restriction of an $\mathcal{L}(\mathcal{G})$-valued Nevanlinna function $\widetilde{Q}$ with invertible imaginary part on $\operatorname{dom} Q(\lambda)$ and $\widetilde{Q}$ satisfies certain limit properties at ∞.

Theorem 2.6 *Let $\mathcal{G}_0$ be a dense subspace of $\mathcal{G}$, $\lambda_0 \in \mathbb{C}\backslash\mathbb{R}$, and let Q be a function defined on $\mathbb{C}\backslash\mathbb{R}$ whose values $Q(\lambda)$ are linear operators in $\mathcal{G}$ with* $\operatorname{dom} Q(\lambda) = \mathcal{G}_0$, $\lambda \in \mathbb{C}\backslash\mathbb{R}$. *Then the following is equivalent:*

(i) *Q is a generalized Q-function of a triple $\{S, A, T\}$, where S is a simple symmetric operator in some separable Hilbert space $\mathcal{H}$, A is a selfadjoint extension of S in $\mathcal{H}$ and $A \subset T \subset S^*$ with $\overline{T} = S^*$;*

(ii) *There exists a unique $\mathcal{L}(\mathcal{G})$-valued Nevanlinna function $\widetilde{Q}$ with the properties (α), (β) and (γ):*

(α) *The relations*

$$Q(\lambda)h - \operatorname{Re} Q(\lambda_0)h = \widetilde{Q}(\lambda)h$$

and

$$Q(\lambda)^*h - \operatorname{Re} Q(\lambda_0)h = \widetilde{Q}(\lambda)^*h$$

hold for all $h \in \mathcal{G}_0$ and $\lambda \in \mathbb{C}\backslash\mathbb{R}$;

(β) $\operatorname{Im} \widetilde{Q}(\lambda)h = 0$ *for some $h \in \mathcal{G}_0$ and $\lambda \in \mathbb{C}\backslash\mathbb{R}$ implies $h = 0$;*

(γ) *The conditions*

$$\lim_{\eta\to+\infty} \frac{1}{\eta}(\widetilde{Q}(i\eta)k, k) = 0 \quad \textit{and} \quad \lim_{\eta\to+\infty} \eta \operatorname{Im}(\widetilde{Q}(i\eta)k, k) = \infty$$

are valid for all $k \in \mathcal{G}$, $k \neq 0$.

Proof. We start by showing that (i) implies (ii). For this, let Q be a generalized Q-function of the triple $\{S, A, T\}$ and suppose that S is simple. Let Γ_{λ_0} be a bounded operator defined on $\operatorname{dom} Q(\lambda) = \mathcal{G}_0$ such that $\operatorname{ran} \Gamma_{\lambda_0} = \mathcal{N}_{\lambda_0}(T)$ and $\ker \Gamma_{\lambda_0} = \{0\}$. According to Proposition 2.5 for each $\lambda \in \mathbb{C}\backslash\mathbb{R}$

$$Q(\lambda) - \operatorname{Re} Q(\lambda_0) = \Gamma_{\lambda_0}^* \Big((\lambda - \operatorname{Re} \lambda_0) + (\lambda - \lambda_0)(\lambda - \bar{\lambda}_0)(A - \lambda)^{-1} \Big) \Gamma_{\lambda_0}$$

is a bounded operator in $\mathcal{G}$ defined on the dense subspace $\mathcal{G}_0$ and hence admits a unique bounded extension onto $\mathcal{G}$ which is given by

$$\widetilde{Q}(\lambda) := \Gamma_{\lambda_0}^* \Big((\lambda - \operatorname{Re} \lambda_0) + (\lambda - \lambda_0)(\lambda - \bar{\lambda}_0)(A - \lambda)^{-1} \Big) \overline{\Gamma}_{\lambda_0}, \tag{2.7}$$

where $\overline{\Gamma}_{\lambda_0} \in \mathcal{L}(\mathcal{G}, \mathcal{H})$ is the closure of Γ_{λ_0}. Obviously we have

$$Q(\lambda)h - \operatorname{Re} Q(\lambda_0)h = \widetilde{Q}(\lambda)h$$

for all $h \in \mathcal{G}_0$ and $\lambda \in \mathbb{C}\backslash\mathbb{R}$, which is the first relation in (α). Recall that for a generalized Q-function $Q(\bar{\lambda})^*$ is an extension of $Q(\lambda)$. This implies $\operatorname{Re} Q(\lambda_0) \subset (\operatorname{Re} Q(\lambda_0))^*$,

$$Q(\lambda)^* - \operatorname{Re} Q(\lambda_0) \subset \Big(Q(\lambda) - \operatorname{Re} Q(\lambda_0) \Big)^* = \widetilde{Q}(\lambda)^*$$

and therefore also $Q(\lambda)^*h - \operatorname{Re} Q(\lambda_0)h = \widetilde{Q}(\lambda)^*h$ is true for all $h \in \mathcal{G}_0$ and $\lambda \in \mathbb{C}\backslash\mathbb{R}$. Hence we have shown (α).

Clearly $\widetilde{Q}$ in (2.7) is a holomorphic $\mathcal{L}(\mathcal{G})$-valued function on $\mathbb{C}\backslash\mathbb{R}$. Denote by $\overline{\Gamma(\lambda)}$ the closure of $\Gamma(\lambda) = (I + (\lambda - \lambda_0)(A - \lambda)^{-1})\Gamma_{\lambda_0}$. Then

$$\overline{\Gamma(\lambda)} = \Bigl(I + (\lambda - \lambda_0)(A - \lambda)^{-1}\Bigr)\overline{\Gamma}_{\lambda_0}, \qquad \lambda \in \mathbb{C}\backslash\mathbb{R},$$

and it is not difficult to see that (2.3) extends to

$$\widetilde{Q}(\lambda) - \widetilde{Q}(\mu)^* = (\lambda - \bar{\mu})\Gamma(\mu)^*\overline{\Gamma(\lambda)}.$$

Hence

$$\Bigl(\operatorname{Im}\widetilde{Q}(\lambda)k, k\Bigr) = (\operatorname{Im}\lambda)\Bigl(\Gamma(\lambda)^*\overline{\Gamma(\lambda)}k, k\Bigr) = (\operatorname{Im}\lambda)\|\overline{\Gamma(\lambda)}k\|^2$$

holds for all $k \in \mathcal{G}$ and this implies that $\widetilde{Q}$ is a Nevanlinna function; cf. (2.5). Furthermore, for $h \in \mathcal{G}_0$ we have

$$\operatorname{Im}\widetilde{Q}(\lambda)h = (\operatorname{Im}\lambda)\Gamma(\lambda)^*\Gamma(\lambda)h$$

and from the property $\ker\Gamma(\lambda) = \{0\}$ (see Lemma 2.1) we conclude that $\operatorname{Im}\widetilde{Q}(\lambda)h = 0$ for $h \in \mathcal{G}_0$ implies $h = 0$, i.e., condition (β) holds. The same arguments as in [39, Theorem 2.4, Corollaries 2.5 and 2.6] together with the assumption that S is a densely defined closed simple symmetric operator show that $\widetilde{Q}$ satisfies the conditions in (γ).

Let us now verify the converse direction. If $\widetilde{Q}$ is a $\mathcal{L}(\mathcal{G})$-valued Nevanlinna function, $\lambda_0 \in \mathbb{C}\backslash\mathbb{R}$ and the first condition in (γ) holds, then it is well known that there exists a Hilbert space $\mathcal{H}$, a selfadjoint operator A in $\mathcal{H}$ and a mapping $\widetilde{\Gamma} \in \mathcal{L}(\mathcal{G}, \mathcal{H})$ such that the representation

$$\widetilde{Q}(\lambda) = \operatorname{Re}\widetilde{Q}(\lambda_0) + \widetilde{\Gamma}^*\Bigl((\lambda - \operatorname{Re}\lambda_0) + (\lambda - \lambda_0)(\lambda - \overline{\lambda}_0)(A - \lambda)^{-1}\Bigr)\widetilde{\Gamma} \tag{2.8}$$

is valid for all $\lambda \in \mathbb{C}\backslash\mathbb{R}$, see, e.g., [33,39]. Furthermore, the space $\mathcal{H}$ can be chosen minimal, i.e.,

$$\mathcal{H} = \overline{\operatorname{span}}\Bigl\{\Bigl(I + (\lambda - \lambda_0)(A - \lambda)^{-1}\Bigr)\widetilde{\Gamma}k : k \in \mathcal{G},\, \lambda \in \mathbb{C}\backslash\mathbb{R}\Bigr\}. \tag{2.9}$$

We define the mapping Γ_{λ_0} to be the restriction of $\widetilde{\Gamma}$ onto $\mathcal{G}_0$. As $\widetilde{\Gamma}$ is bounded the closure $\overline{\Gamma}_{\lambda_0}$ of Γ_{λ_0} coincides with $\widetilde{\Gamma}$. We claim that Γ_{λ_0} is injective. In fact, if $\Gamma_{\lambda_0}h = 0$ for some $h \in \mathcal{G}_0$ then $\widetilde{\Gamma}h = 0$ and by (2.8) we have $\widetilde{Q}(\lambda)h = \operatorname{Re}\widetilde{Q}(\lambda_0)h$. Therefore $\operatorname{Im}\widetilde{Q}(\lambda)h = 0$ and by assumption (β) this implies $h = 0$.

Define the operator S by

$$Sf = Af, \quad \operatorname{dom} S = \Bigl\{f \in \operatorname{dom} A : ((A - \bar{\lambda}_0)f, \Gamma_{\lambda_0}h) = 0 \text{ for all } h \in \mathcal{G}_0\Bigr\}.$$

Then S is a closed symmetric operator and the identities $\operatorname{ran}(S-\bar{\lambda}_0) = (\operatorname{ran}\Gamma_{\lambda_0})^\perp$ and $\ker(S^*-\lambda_0) = \overline{\operatorname{ran}\Gamma_{\lambda_0}}$ hold. Let

$$\Gamma(\lambda) = (I + (\lambda-\lambda_0)(A-\lambda)^{-1})\Gamma_{\lambda_0}, \qquad \lambda \in \mathbb{C}\backslash\mathbb{R}. \tag{2.10}$$

It is not difficult to check that $\operatorname{ran}(S-\bar{\lambda}) = (\operatorname{ran}\Gamma(\lambda))^\perp$ is true for all $\lambda \in \mathbb{C}\backslash\mathbb{R}$ and the conditions in (γ) together with (2.9) now yield in the same way as in [39, Theorem 2.4, Corollaries 2.5 and 2.6] that S is densely defined and simple.

Note that $\operatorname{dom} A \cap \operatorname{ran}\Gamma_{\lambda_0} = \{0\}$ since $\lambda_0 \in \rho(A)$ and $\operatorname{ran}\Gamma_{\lambda_0} \subset \mathcal{N}_{\lambda_0}(S^*)$. Let us define a linear operator T in $\mathcal{H}$ on $\operatorname{dom} T := \operatorname{dom} A \dot{+} \operatorname{ran}\Gamma_{\lambda_0}$ by

$$T(f+f_{\lambda_0}) := Af + \lambda_0 f_{\lambda_0}, \qquad f \in \operatorname{dom} A,\ f_{\lambda_0} \in \operatorname{ran}\Gamma_{\lambda_0}.$$

Obviously T is an extension of A and since $\mathcal{N}_{\lambda_0}(T) = \operatorname{ran}\Gamma_{\lambda_0}$ and $\operatorname{ran}\Gamma_{\lambda_0}$ is dense in $\mathcal{N}_{\lambda_0}(S^*)$ we obtain from $\operatorname{dom} S^* = \operatorname{dom} A \dot{+} \mathcal{N}_{\lambda_0}(S^*)$ (see (2.1)) that $T \subset S^*$ and $\overline{T} = S^*$ holds.

According to condition (α) the Nevanlinna function $\widetilde{Q}$ and the function Q are related by

$$Q(\lambda)h = \widetilde{Q}(\lambda)h + \operatorname{Re} Q(\lambda_0)h \quad \text{and} \quad Q(\lambda)^*h = \widetilde{Q}(\lambda)^*h + \operatorname{Re} Q(\lambda_0)h$$

for all $h \in \mathcal{G}_0$ and $\lambda \in \mathbb{C}\backslash\mathbb{R}$. It remains to show that Q satisfies (2.3). Observe first that for $\lambda,\mu \in \mathbb{C}\backslash\mathbb{R}$ we have

$$Q(\lambda)h - Q(\mu)^*h = \widetilde{Q}(\lambda)h - \widetilde{Q}(\mu)^*h. \tag{2.11}$$

Denote the closures of the operators $\Gamma(\lambda)$, $\lambda \in \mathbb{C}\backslash\mathbb{R}$, in (2.10) by $\widetilde{\Gamma}(\lambda)$. Then

$$\widetilde{\Gamma}(\lambda) = \overline{\Gamma(\lambda)} = \Big(I + (\lambda-\lambda_0)(A-\lambda)^{-1}\Big)\overline{\Gamma}_{\lambda_0} = \Big(I + (\lambda-\lambda_0)(A-\lambda)^{-1}\Big)\widetilde{\Gamma}$$

and it follows from (2.8) with a straightforward calculation that

$$\widetilde{Q}(\lambda) - \widetilde{Q}(\mu)^* = (\lambda-\bar{\mu})\widetilde{\Gamma}(\mu)^*\widetilde{\Gamma}(\lambda), \qquad \lambda,\mu \in \mathbb{C}\backslash\mathbb{R}, \tag{2.12}$$

holds. As $\widetilde{\Gamma}(\mu)^* = \overline{\Gamma(\mu)}^* = \Gamma(\mu)^*$ we conclude

$$Q(\lambda)h - Q(\mu)^*h = (\lambda-\bar{\mu})\Gamma(\mu)^*\Gamma(\lambda)h, \qquad h \in \mathcal{G}_0,$$

from (2.11). Therefore Q is a generalized Q-function of the triple $\{S, A, T\}$. □

Remark 2.7 *The definition of a generalized Q-function can be extended to the case that A is a selfadjoint relation, S is a non-densely defined symmetric operator or relation and T is a linear relation which is dense in the relation S^*. We refer to* [39] *for ordinary Q-functions in this more general situation. In this case the condition (γ) in Theorem* 2.6 *can be dropped.*

For ordinary Q-functions Theorem 2.6 reads as follows; cf. [39, Theorem 2.2 and Theorem 2.4].

Theorem 2.8 *A $\mathcal{L}(\mathcal{G})$-valued Nevanlinna function $\widetilde{Q}$ is an ordinary Q-function of some pair $\{S, A\}$, where S is a densely defined closed simple symmetric operator in some Hilbert space $\mathcal{H}$ and A is a selfadjoint extension of S in $\mathcal{H}$, if and only if condition (γ) in Theorem 2.6 and $0 \in \rho(\operatorname{Im}\widetilde{Q}(\lambda))$ holds for some, and hence for all, $\lambda \in \mathbb{C}\backslash\mathbb{R}$.*

Corollary 2.9 *Let Q be a generalized Q-function of $\{S, A, T\}$ and let $\widetilde{Q}$ be the $\mathcal{L}(\mathcal{G})$-valued Nevanlinna function in Theorem 2.6. Then for all $\lambda \in \mathbb{C}\backslash\mathbb{R}$ and $h \in \mathcal{G}_0$ we have*

$$\frac{d}{d\lambda}\,Q(\lambda)h = \frac{d}{d\lambda}\,\widetilde{Q}(\lambda)h = \Gamma(\bar{\lambda})^*\Gamma(\lambda)h.$$

Proof. It follows from (2.12) that

$$\frac{d}{d\lambda}\,\widetilde{Q}(\lambda) = \lim_{\bar{\mu}\to\lambda} \frac{\widetilde{Q}(\lambda) - \widetilde{Q}(\mu)^*}{\lambda - \bar{\mu}} = \widetilde{\Gamma}(\bar{\lambda})^*\widetilde{\Gamma}(\lambda)$$

holds. Hence condition (α) in Theorem 2.6 and $\widetilde{\Gamma}(\lambda) = \overline{\Gamma(\lambda)}$ imply

$$\frac{d}{d\lambda}\,Q(\lambda)h = \lim_{\bar{\mu}\to\lambda} \frac{Q(\lambda)h - Q(\mu)^*h}{\lambda - \bar{\mu}} = \lim_{\bar{\mu}\to\lambda} \frac{\widetilde{Q}(\lambda)h - \widetilde{Q}(\mu)^*h}{\lambda - \bar{\mu}} = \Gamma(\bar{\lambda})^*\Gamma(\lambda)h$$

for $h \in \mathcal{G}_0$. □

3 Elliptic operators and the Dirichlet-to-Neumann map

Let $\Omega \subset \mathbb{R}^n$ be a bounded or unbounded domain with compact C^∞-boundary $\partial\Omega$. Let $\mathcal{L}$ be the "formally selfadjoint" uniformly elliptic second order differential expression

$$(\mathcal{L}f)(x) := -\sum_{j,k=1}^{n} \left(\frac{\partial}{\partial x_j} a_{jk} \frac{\partial f}{\partial x_k}\right)(x) + a(x)f(x), \tag{3.1}$$

$x \in \Omega$, with bounded infinitely differentiable real valued coefficients $a_{jk} \in C^\infty(\overline{\Omega})$ satisfying $a_{jk}(x) = a_{kj}(x)$ for all $x \in \overline{\Omega}$ and $j, k = 1, \dots, n$; the function $a \in L^\infty(\Omega)$ is real valued and

$$\sum_{j,k=1}^{n} a_{jk}(x)\xi_j\xi_k \geq C \sum_{k=1}^{n} \xi_k^2 \tag{3.2}$$

holds for some $C > 0$, all $\xi = (\xi_1, \dots, \xi_n)^\top \in \mathbb{R}^n$ and $x \in \overline{\Omega}$. We note that the assumptions on the domain Ω and the coefficients of $\mathcal{L}$ can be relaxed but it is not our aim to treat the most general setting here. We refer the reader to e.g. [30,40,43,52] for possible generalizations.

In the following we consider the selfadjoint realizations of $\mathcal{L}$ in $L^2(\Omega)$ subject to Dirichlet and Neumann (or oblique Neumann) boundary conditions. For a function f in the Sobolev space $H^2(\Omega)$ we denote the trace by $f|_{\partial\Omega}$ and the trace of the conormal derivative is defined by

$$\frac{\partial f}{\partial \nu}\Big|_{\partial\Omega} := \sum_{j,k=1}^{n} a_{jk} n_j \frac{\partial f}{\partial x_k}\Big|_{\partial\Omega};$$

here $n(x) = (n_1(x), \dots, n_n(x))^\top$ is the unit vector at the point $x \in \partial\Omega$ pointing out of Ω. Recall that the mapping $C^\infty(\overline{\Omega}) \ni f \mapsto \left\{ f|_{\partial\Omega}, \frac{\partial f}{\partial \nu}\big|_{\partial\Omega} \right\}$ extends by continuity to a continuous surjective mapping

$$H^2(\Omega) \ni f \mapsto \left\{ f|_{\partial\Omega}, \frac{\partial f}{\partial \nu}\Big|_{\partial\Omega} \right\} \in H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega). \tag{3.3}$$

The kernel of this map is

$$H_0^2(\Omega) = \left\{ f \in H^2(\Omega) : f|_{\partial\Omega} = \frac{\partial f}{\partial \nu}\Big|_{\partial\Omega} = 0 \right\}$$

which coincides with the closure of $C_0^\infty(\Omega)$ in $H^2(\Omega)$. We refer the reader to the monographs [40,43,52] for more details. In the following the scalar products in $L^2(\Omega)$ and $L^2(\partial\Omega)$ are denoted by $(\cdot,\cdot)_\Omega$ and $(\cdot,\cdot)_{\partial\Omega}$, respectively. Then Green's identity

$$(\mathcal{L}f, g)_\Omega - (f, \mathcal{L}g)_\Omega = \left(f|_{\partial\Omega}, \frac{\partial g}{\partial \nu}\Big|_{\partial\Omega} \right)_{\partial\Omega} - \left(\frac{\partial f}{\partial \nu}\Big|_{\partial\Omega}, g|_{\partial\Omega} \right)_{\partial\Omega} \tag{3.4}$$

holds for all functions $f, g \in H^2(\Omega)$. We note that (3.4) is even true for $f \in H^2(\Omega)$ and g belonging to the domain of the maximal operator associated to $\mathcal{L}$ in $L^2(\Omega)$ if the $(\cdot,\cdot)_{\partial\Omega}$ scalar product in $L^2(\partial\Omega)$ is extended by continuity to $H^{3/2}(\partial\Omega) \times H^{-3/2}(\partial\Omega)$ and $H^{1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$, respectively, see [40,52]. However, we shall make use of (3.4) only for the case $f, g \in H^2(\Omega)$.

It is known that the realizations A_D and A_N of $\mathcal{L}$ subject to Dirichlet and Neumann boundary conditions defined by

$$\begin{aligned} A_D f &= \mathcal{L}f, \quad \operatorname{dom} A_D = \left\{ f \in H^2(\Omega) : f|_{\partial\Omega} = 0 \right\}, \\ A_N f &= \mathcal{L}f, \quad \operatorname{dom} A_N = \left\{ f \in H^2(\Omega) : \frac{\partial f}{\partial \nu}\Big|_{\partial\Omega} = 0 \right\}, \end{aligned} \tag{3.5}$$

are selfadjoint operators in $L^2(\Omega)$. The following statement is known and can be found in, e.g., [40]. It can be proved with similar methods as Theorem 4.1 in the next section.

Proposition 3.1 *Let $\mathcal{L}$ be the elliptic differential expression in* (3.1)*. Then the operator*

$$Sf = \mathcal{L}f, \qquad \operatorname{dom} S = H_0^2(\Omega), \tag{3.6}$$

is a densely defined closed symmetric operator in $L^2(\Omega)$ with infinite deficiency indices $n_\pm(S)$ and the adjoint S^* of S coincides with the maximal operator associated to $\mathcal{L}$,

$$S^* f = \mathcal{L}f, \qquad \operatorname{dom} S^* = \Big\{ f \in L^2(\Omega) : \mathcal{L}f \in L^2(\Omega) \Big\}.$$

The operator

$$Tf = \mathcal{L}f, \qquad \operatorname{dom} T = H^2(\Omega),$$

is not closed as an operator in $L^2(\Omega)$ and T satisfies $\overline{T} = S^*$ and $T^* = S$. Furthermore, the selfadjoint operators A_D and A_N in (3.5) *are extensions of S and restrictions of T.*

In order to define a mapping Γ_{λ_0} for the definition of a generalized Q-function associated to the triple $\{S, A_D, T\}$ we make use of the decomposition (2.1) in the present situation. More precisely, for all points λ in the resolvent set $\rho(A_D)$ of the selfadjoint Dirichlet operator A_D we have the direct sum decomposition of $\operatorname{dom} T = H^2(\Omega)$:

$$H^2(\Omega) = \operatorname{dom} A_D \dot{+} \mathcal{N}_\lambda(T) = \Big\{ f \in H^2(\Omega) : f|_{\partial\Omega} = 0 \Big\} \dot{+} \mathcal{N}_\lambda(T), \tag{3.7}$$

where

$$\mathcal{N}_\lambda(T) = \ker(T - \lambda) = \Big\{ f_\lambda \in H^2(\Omega) : \mathcal{L}f_\lambda = \lambda f_\lambda \Big\}.$$

Let now φ be a function in $H^{3/2}(\partial\Omega)$ and let $\lambda_0 \in \rho(A_D)$. Then it follows from (3.3) and (3.7) that there exists a unique function $f_{\lambda_0} \in H^2(\Omega)$ which solves the equation $\mathcal{L}f_{\lambda_0} = \lambda_0 f_{\lambda_0}$, i.e., $f_{\lambda_0} \in \mathcal{N}_{\lambda_0}(T)$, and satisfies $f_{\lambda_0}|_{\partial\Omega} = \varphi$. We shall denote the mapping that assigns f_{λ_0} to φ by Γ_{λ_0},

$$H^{3/2}(\partial\Omega) \ni \varphi \mapsto \Gamma_{\lambda_0}\varphi := f_{\lambda_0} \in \mathcal{N}_{\lambda_0}(T), \tag{3.8}$$

and we regard Γ_{λ_0} as an operator from $L^2(\partial\Omega)$ into $L^2(\Omega)$ with $\operatorname{dom} \Gamma_{\lambda_0} = H^{3/2}(\partial\Omega)$ and $\operatorname{ran} \Gamma_{\lambda_0} = \mathcal{N}_{\lambda_0}(T)$.

Proposition 3.2 *Let $\lambda_0 \in \rho(A_D)$, let Γ_{λ_0} be as in* (3.8) *and let $\lambda \in \rho(A_D)$. Then the following holds:*

(i) Γ_{λ_0} *is a bounded operator from* $L^2(\partial\Omega)$ *in* $L^2(\Omega)$ *with dense domain* $H^{3/2}(\partial\Omega)$*;*

(ii) *The operator* $\Gamma(\lambda) = (I + (\lambda - \lambda_0)(A_D - \lambda)^{-1})\Gamma_{\lambda_0}$ *is given by*

$$\Gamma(\lambda)\varphi = f_\lambda, \quad \textit{where} \quad f_\lambda \in \mathcal{N}_\lambda(T) \quad \textit{and} \quad f_\lambda|_{\partial\Omega} = \varphi;$$

(iii) *The mapping* $\Gamma(\bar\lambda)^* : L^2(\Omega) \to L^2(\partial\Omega)$ *satisfies*

$$\Gamma(\bar\lambda)^*(A_D - \lambda)f = -\frac{\partial f}{\partial \nu}\Big|_{\partial\Omega}, \qquad f \in \operatorname{dom} A_D.$$

Proof. Statement (i) will be a consequence of (iii). We prove assertion (ii). Recall that by Lemma 2.1 the range of the operator $\Gamma(\lambda)$, $\lambda \in \rho(A_D)$, is $\mathcal{N}_\lambda(T)$. Let $\varphi \in \operatorname{dom}\Gamma(\lambda) = H^{3/2}(\partial\Omega)$ and choose elements $f_\lambda \in \mathcal{N}_\lambda(T)$ and $f_{\lambda_0} \in \mathcal{N}_{\lambda_0}(T)$ such that

$$f_\lambda|_{\partial\Omega} = \varphi = f_{\lambda_0}|_{\partial\Omega}$$

holds. According to (3.7) the functions f_λ and f_{λ_0} are unique. Then $\Gamma_{\lambda_0}\varphi = f_{\lambda_0}$ and hence we obtain

$$\Gamma(\lambda)\varphi = \Gamma_{\lambda_0}\varphi + (\lambda - \lambda_0)(A_D - \lambda)^{-1}\Gamma_{\lambda_0}\varphi = f_{\lambda_0} + (\lambda - \lambda_0)(A_D - \lambda)^{-1}\Gamma_{\lambda_0}\varphi.$$

Since $(\lambda - \lambda_0)(A_D - \lambda)^{-1}\Gamma_{\lambda_0}\varphi$ belongs to $\operatorname{dom} A_D$ it is clear that the trace of this element vanishes. Therefore, the traces of the functions $\Gamma(\lambda)\varphi \in \mathcal{N}_\lambda(T)$ and f_{λ_0} coincide,

$$(\Gamma(\lambda)\varphi)|_{\partial\Omega} = f_{\lambda_0}|_{\partial\Omega} = \varphi = f_\lambda|_{\partial\Omega}.$$

Thus we have that the traces of $\Gamma(\lambda)\varphi \in \mathcal{N}_\lambda(T)$ and $f_\lambda \in \mathcal{N}_\lambda(T)$ coincide and from (3.7) we conclude $\Gamma(\lambda)\varphi = f_\lambda$.

(iii) Let $\varphi \in H^{3/2}(\partial\Omega)$ and choose the unique function $g_{\bar\lambda} \in \mathcal{N}_{\bar\lambda}(T)$ with the property $g_{\bar\lambda}|_{\partial\Omega} = \varphi$. Hence we have $\Gamma(\bar\lambda)\varphi = g_{\bar\lambda}$ and for $f \in \operatorname{dom} A_D$ it follows

$$\Big(\Gamma(\bar\lambda)\varphi, (A_D - \lambda)f\Big)_\Omega = (g_{\bar\lambda}, A_D f)_\Omega - (\bar\lambda g_{\bar\lambda}, f)_\Omega = (g_{\bar\lambda}, A_D f)_\Omega - (T g_{\bar\lambda}, f)_\Omega.$$

Making use of Green's identity (3.4) we find

$$(g_{\bar\lambda}, A_D f)_\Omega - (T g_{\bar\lambda}, f)_\Omega = \left(\frac{\partial g_{\bar\lambda}}{\partial \nu}\Big|_{\partial\Omega}, f|_{\partial\Omega}\right)_{\partial\Omega} - \left(g_{\bar\lambda}|_{\partial\Omega}, \frac{\partial f}{\partial \nu}\Big|_{\partial\Omega}\right)_{\partial\Omega}$$

and since the trace of $f \in \operatorname{dom} A_D$ vanishes the first summand on the right hand side is zero. Therefore

$$\Big(\Gamma(\bar\lambda)\varphi,(A_D-\lambda)f\Big)_\Omega = -\left(g_{\bar\lambda}|_{\partial\Omega},\frac{\partial f}{\partial\nu}\Big|_{\partial\Omega}\right)_{\partial\Omega} = \left(\varphi,-\frac{\partial f}{\partial\nu}\Big|_{\partial\Omega}\right)_{\partial\Omega}$$

holds for all $\varphi\in\operatorname{dom}\Gamma(\bar\lambda)=H^{3/2}(\partial\Omega)$. This gives $(A_D-\lambda)f\in\operatorname{dom}\Gamma(\bar\lambda)^*$ and

$$\Gamma(\bar\lambda)^*(A_D-\lambda)f = -\frac{\partial f}{\partial\nu}\Big|_{\partial\Omega}.$$

Moreover, as $\lambda\in\rho(A_D)$ and $f\in\operatorname{dom}A_D$ was arbitrary we see that $\Gamma(\bar\lambda)^*$ is defined on the whole space $L^2(\Omega)$. This together with the fact that $\Gamma(\bar\lambda)^*$ is closed implies

$$\Gamma(\bar\lambda)^*\in\mathcal{L}\Big(L^2(\Omega),L^2(\partial\Omega)\Big)$$

for $\lambda\in\rho(A_D)$ and, in particular, $\Gamma(\bar\lambda)\subset\overline{\Gamma(\bar\lambda)}=\Gamma(\bar\lambda)^{**}$ is bounded. Inserting $\lambda_0=\bar\lambda$ this yields assertion (i). □

In the study of elliptic differential operators the so-called Dirichlet-to-Neumann map plays an important role, we mention only [4,14,22–26,31,42,44–49,51]. Roughly speaking this operator maps the Dirichlet boundary value $f_\lambda|_{\partial\Omega}$ of an $H^2(\Omega)$-solution of the equation $\mathcal{L}u=\lambda u$ onto the Neumann boundary value $\frac{\partial f_\lambda}{\partial\nu}|_{\partial\Omega}$ of this solution. In the following definition also a minus sign arises, which is needed to obtain a generalized Q-function in Theorem 3.4. Otherwise $-Q$ would turn out to be a generalized Q-function.

Definition 3.3 *Let $\lambda\in\rho(A_D)$ and assign to $\varphi\in H^{3/2}(\partial\Omega)$ the unique function $f_\lambda\in\mathcal{N}_\lambda(T)$ such that $f_\lambda|_{\partial\Omega}=\varphi$, see* (3.3) *and* (3.7)*. The operator $Q(\lambda)$ in $L^2(\partial\Omega)$ defined by*

$$Q(\lambda)\varphi = Q(\lambda)(f_\lambda|_{\partial\Omega}) := -\frac{\partial f_\lambda}{\partial\nu}\Big|_{\partial\Omega},\qquad \varphi\in\operatorname{dom}Q(\lambda)=H^{3/2}(\partial\Omega),\qquad(3.9)$$

is called the Dirichlet-to-Neumann map *associated to $\mathcal{L}$.*

Note that by (3.3) the range of the Dirichlet-to-Neumann map $Q(\lambda)$, $\lambda\in\rho(A_D)$, lies in $H^{1/2}(\partial\Omega)$. We remark that the Dirichlet-to-Neumann map can be extended, e.g., to an operator from $H^1(\partial\Omega)$ in $L^2(\partial\Omega)$ if instead of $H^2(\Omega)$ the operator T is defined on a suitable subspace of $H^{3/2}(\Omega)$; cf. [4–6,9,32,40]. However, for our purposes this is not necessary since A_D and A_N are defined on subspaces of $H^2(\Omega)$.

In the next theorem we show that the Dirichlet-to-Neumann map is a generalized Q-function and we illustrate the usefulness of this object in the representation of the difference of the resolvents of the Dirichlet and Neumann operators A_D and A_N in (3.5). Similar Krein type resolvent formulas can also be found in [9,13,25,26,47–50]. The fact that the difference of the resolvents belongs to some von Neumann-Schatten class depending on the dimension of the space is well-known and goes back to M.S. Birman; cf. [11].

Theorem 3.4 *Let $\mathcal{L}$ be the elliptic differential expression in* (3.1) *and let A_D and A_N be the selfadjoint realizations of $\mathcal{L}$ in* (3.5)*. Denote by S the minimal operator associated to $\mathcal{L}$ and let $T = \mathcal{L} \upharpoonright H^2(\Omega)$ be as in Proposition* 3.1*. Define $\Gamma(\lambda)$ as in Proposition* 3.2 *and let $Q(\lambda)$, $\lambda \in \rho(A_D)$, be the Dirichlet-to-Neumann map. Then the following holds:*

(i) *Q is a generalized Q-function of the triple $\{S, A_D, T\}$;*
(ii) *The operator $Q(\lambda)$ is injective for all $\lambda \in \rho(A_D) \cap \rho(A_N)$ and the resolvent formula*

$$(A_D - \lambda)^{-1} - (A_N - \lambda)^{-1} = \Gamma(\lambda) Q(\lambda)^{-1} \Gamma(\bar{\lambda})^* \tag{3.10}$$

holds;
(iii) *For $p > \frac{n-1}{2}$ the difference of the resolvents in* (3.10) *belongs to the von Neumann-Schatten class $\mathfrak{S}_p(L^2(\Omega))$.*

Proof. In order to prove assertion (i) we have to check the relation

$$Q(\lambda) - Q(\mu)^* = (\lambda - \bar{\mu}) \Gamma(\mu)^* \Gamma(\lambda), \qquad \lambda, \mu \in \rho(A_D), \tag{3.11}$$

on $\operatorname{dom} Q(\lambda) = H^{3/2}(\partial\Omega)$. For this it will be first shown that $H^{3/2}(\partial\Omega)$ is a subset of $\operatorname{dom} Q(\mu)^*$ and that $Q(\mu)^*$ is an extension of $Q(\bar{\mu})$. Let $\psi \in H^{3/2}(\partial\Omega)$ and choose the unique function $f_{\bar{\mu}} \in \mathcal{N}_{\bar{\mu}}(T)$ such that $f_{\bar{\mu}}|_{\partial\Omega} = \psi$. For an arbitrary $\varphi \in \operatorname{dom} Q(\mu) = H^{3/2}(\partial\Omega)$ let $f_\mu \in \mathcal{N}_\mu(T)$ be the unique function that satisfies $f_\mu|_{\partial\Omega} = \varphi$. By the definition of the Dirichlet-to-Neumann map we have

$$Q(\mu)\varphi = -\frac{\partial f_\mu}{\partial \nu}\Big|_{\partial\Omega} \quad \text{and} \quad Q(\bar{\mu})\psi = -\frac{\partial f_{\bar{\mu}}}{\partial \nu}\Big|_{\partial\Omega}$$

and hence Green's identity (3.4) shows

$$\begin{aligned}
(Q(\mu)\varphi, \psi)_{\partial\Omega} &= \left(-\frac{\partial f_\mu}{\partial \nu}\Big|_{\partial\Omega}, f_{\bar{\mu}}|_{\partial\Omega} \right)_{\partial\Omega} \\
&= \left(f_\mu|_{\partial\Omega}, \frac{\partial f_{\bar{\mu}}}{\partial \nu}\Big|_{\partial\Omega} \right)_{\partial\Omega} - \left(\frac{\partial f_\mu}{\partial \nu}\Big|_{\partial\Omega}, f_{\bar{\mu}}|_{\partial\Omega} \right)_{\partial\Omega} + \left(\varphi, -\frac{\partial f_{\bar{\mu}}}{\partial \nu}\Big|_{\partial\Omega} \right)_{\partial\Omega} \\
&= (Tf_\mu, f_{\bar{\mu}})_\Omega - (f_\mu, Tf_{\bar{\mu}})_\Omega + \left(\varphi, -\frac{\partial f_{\bar{\mu}}}{\partial \nu}\Big|_{\partial\Omega} \right)_{\partial\Omega}.
\end{aligned}$$

Since $f_\mu \in \mathcal{N}_\mu(T)$ and $f_{\bar{\mu}} \in \mathcal{N}_{\bar{\mu}}(T)$ it is clear that $(Tf_\mu, f_{\bar{\mu}})_\Omega = (f_\mu, Tf_{\bar{\mu}})_\Omega$

holds and therefore we obtain

$$(Q(\mu)\varphi,\psi)_{\partial\Omega} = \left(\varphi, -\frac{\partial f_{\bar\mu}}{\partial\nu}\Big|_{\partial\Omega}\right)_{\partial\Omega}$$

for all $\varphi \in \operatorname{dom} Q(\mu)$. Thus $\psi \in \operatorname{dom} Q(\mu)^*$ and

$$Q(\mu)^*\psi = -\frac{\partial f_{\bar\mu}}{\partial\nu}\Big|_{\partial\Omega} = Q(\bar\mu)\psi.$$

Next we prove the relation (3.11). Let $\varphi,\psi \in H^{3/2}(\partial\Omega)$ and choose the functions $f_\lambda \in \mathcal{N}_\lambda(T)$ and $g_\mu \in \mathcal{N}_\mu(T)$ such that $f_\lambda|_{\partial\Omega} = \varphi$ and $g_\mu|_{\partial\Omega} = \psi$. Hence we have

$$Q(\lambda)\varphi = -\frac{\partial f_\lambda}{\partial\nu}\Big|_{\partial\Omega}, \quad Q(\mu)\psi = -\frac{\partial g_\mu}{\partial\nu}\Big|_{\partial\Omega}, \quad \Gamma(\lambda)\varphi = f_\lambda \quad\text{and}\quad \Gamma(\mu)\psi = g_\mu.$$

Note that $\varphi \in H^{3/2}(\Omega)$ belongs to $\operatorname{dom} Q(\mu)^*$ by the above considerations. With the help of Green's identity (3.4) we find

$$\begin{aligned}
\Big((Q(\lambda) - Q(\mu)^*)\varphi,\psi\Big)_{\partial\Omega} &= -\left(\frac{\partial f_\lambda}{\partial\nu}\Big|_{\partial\Omega}, g_\mu|_{\partial\Omega}\right)_{\partial\Omega} + \left(f_\lambda|_{\partial\Omega}, \frac{\partial g_\mu}{\partial\nu}\Big|_{\partial\Omega}\right)_{\partial\Omega} \\
&= (Tf_\lambda, g_\mu)_\Omega - (f_\lambda, Tg_\mu)_\Omega = (\lambda-\bar\mu)(f_\lambda, g_\mu)_\Omega \\
&= (\lambda-\bar\mu)(\Gamma(\lambda)\varphi, \Gamma(\mu)\psi)_\Omega = \Big((\lambda-\bar\mu)\Gamma(\mu)^*\Gamma(\lambda)\varphi,\psi\Big)_{\partial\Omega}.
\end{aligned}$$

This holds for all ψ in the dense subset $H^{3/2}(\partial\Omega)$ of $L^2(\partial\Omega)$ and therefore (3.11) is valid on $\operatorname{dom} Q(\lambda) = \operatorname{dom}\Gamma(\lambda) = H^{3/2}(\partial\Omega)$, i.e., the Dirichlet-to-Neumann map is a generalized Q-function of the triple $\{S, A_D, T\}$.

(ii) Let $\lambda \in \rho(A_D) \cap \rho(A_N)$ and suppose that we have $Q(\lambda)\varphi = 0$ for some $\varphi \in H^{3/2}(\partial\Omega)$. There exists a unique $f_\lambda \in \mathcal{N}_\lambda(T)$ such that $f_\lambda|_{\partial\Omega} = \varphi$ and for this f_λ by assumption we have $\frac{\partial f_\lambda}{\partial\nu}|_{\partial\Omega} = 0$. Hence $f_\lambda \in \operatorname{dom} A_N \cap \mathcal{N}_\lambda(T)$ and from $\lambda \in \rho(A_N)$ we conclude $f_\lambda = 0$, that is, $\varphi = f_\lambda|_{\partial\Omega} = 0$.

Therefore $Q(\lambda)^{-1}$, $\lambda \in \rho(A_D) \cap \rho(A_N)$ exists and, roughly speaking, $Q(\lambda)^{-1}$ maps the negative Neumann boundary values of $H^2(\Omega)$-solutions of $\mathcal{L}u = \lambda u$ onto their Dirichlet boundary values. Let us prove the formula (3.10) for the difference of the resolvents of A_D and A_N. Observe first, that the right hand side in (3.10) is well defined. In fact, by Proposition 3.2 (iii) and (3.3) the range of $\Gamma(\bar\lambda)^*$ lies in $H^{1/2}(\partial\Omega)$ and it follows from the surjectivity of the mapping in (3.3) that $Q(\lambda)^{-1}$ is defined on the whole space $H^{1/2}(\partial\Omega)$ and maps $H^{1/2}(\partial\Omega)$ onto $H^{3/2}(\partial\Omega)$, the domain of $\Gamma(\lambda)$.

Let now $f \in L^2(\Omega)$. We claim that the function

$$g = (A_D - \lambda)^{-1} f - \Gamma(\lambda) Q(\lambda)^{-1} \Gamma(\bar{\lambda})^* f \tag{3.12}$$

belongs to $\operatorname{dom} A_N$. It is clear that g is in $H^2(\Omega)$ since $(A_D - \lambda)^{-1} f \in \operatorname{dom} A_D$ and the second term on the right hand side belongs to $\mathcal{N}_\lambda(T)$, the range of $\Gamma(\lambda)$. In order to verify $\frac{\partial g}{\partial \nu}|_{\partial\Omega} = 0$ we choose $f_D \in \operatorname{dom} A_D$ such that $f = (A_D - \lambda) f_D$, so that (3.12) becomes

$$g = f_D - \Gamma(\lambda) Q(\lambda)^{-1} \Gamma(\bar{\lambda})^* (A_D - \lambda) f_D = f_D + \Gamma(\lambda) Q(\lambda)^{-1} \frac{\partial f_D}{\partial \nu}\Big|_{\partial\Omega}, \tag{3.13}$$

where we have used Proposition 3.2 (iii). Let $f_\lambda := \Gamma(\lambda) Q(\lambda)^{-1} \frac{\partial f_D}{\partial \nu}|_{\partial\Omega}$. Then $f_\lambda \in \mathcal{N}_\lambda(T)$ and the trace of f_λ is given by

$$f_\lambda|_{\partial\Omega} = Q(\lambda)^{-1} \frac{\partial f_D}{\partial \nu}\Big|_{\partial\Omega}.$$

Hence $Q(\lambda) f_\lambda|_{\partial\Omega} = \frac{\partial f_D}{\partial \nu}|_{\partial\Omega}$, but on the other hand, by the definition of the Dirichlet-to-Neumann map $Q(\lambda) f_\lambda|_{\partial\Omega} = -\frac{\partial f_\lambda}{\partial \nu}|_{\partial\Omega}$. Therefore, the sum of the Neumann boundary value of the function f_λ and the Neumann boundary value of f_D is zero and we conclude from (3.13)

$$\frac{\partial g}{\partial \nu}\Big|_{\partial\Omega} = \frac{\partial f_D}{\partial \nu}\Big|_{\partial\Omega} + \frac{\partial}{\partial \nu}\left(\Gamma(\lambda) Q(\lambda)^{-1} \frac{\partial f_D}{\partial \nu}\Big|_{\partial\Omega}\right)\Big|_{\partial\Omega} = \frac{\partial f_D}{\partial \nu}\Big|_{\partial\Omega} + \frac{\partial f_\lambda}{\partial \nu}\Big|_{\partial\Omega} = 0.$$

We have shown that g in (3.12) belongs to $\operatorname{dom} A_N$. As T is an extension of A_N and A_D, and $\operatorname{ran} \Gamma(\lambda) = \ker(T - \lambda)$ we obtain

$$(A_N - \lambda) g = (T - \lambda)(A_D - \lambda)^{-1} f - (T - \lambda) \Gamma(\lambda) Q(\lambda)^{-1} \Gamma(\bar{\lambda})^* f = f.$$

Together with (3.12) we find

$$(A_N - \lambda)^{-1} f = (A_D - \lambda)^{-1} f - \Gamma(\lambda) Q(\lambda)^{-1} \Gamma(\bar{\lambda})^* f$$

for all $\lambda \in \rho(A_D) \cap \rho(A_N)$ and $f \in L^2(\Omega)$, and therefore the resolvent formula (3.10) is valid.

Up to some small modifications assertion (iii) was proved in [11]. $\square$

We mention that for $\lambda, \lambda_0 \in \rho(A_D)$ the Dirichlet-to-Neumann map is connected with the resolvent of A_D via

$$Q(\lambda) = \operatorname{Re} Q(\lambda_0) + \Gamma_{\lambda_0}\Big((\lambda - \operatorname{Re}\lambda_0) + (\lambda - \lambda_0)(\lambda - \bar{\lambda}_0)(A_D - \lambda)^{-1}\Big)\Gamma_{\lambda_0}.$$

This follows from the fact that Q is a generalized Q-function and Proposition 2.5. The following two corollaries collect some properties of the Dirichlet-to-Neumann map and its inverse.

Corollary 3.5 *For $\lambda, \lambda_0 \in \rho(A_D)$ the Dirichlet-to-Neumann map $Q(\lambda)$ has the following properties.*

(i) *$Q(\lambda)$ is a non-closed unbounded operator in $L^2(\partial\Omega)$ defined on $H^{3/2}(\partial\Omega)$ with* $\operatorname{ran} Q(\lambda) \subset H^{1/2}(\partial\Omega)$*;*
(ii) *$Q(\lambda) - \operatorname{Re} Q(\lambda_0)$ is a non-closed bounded operator in $L^2(\partial\Omega)$ defined on $H^{3/2}(\partial\Omega)$;*
(iii) *the closure $\widetilde{Q}(\lambda)$ of the operator $Q(\lambda) - \operatorname{Re} Q(\lambda_0)$ in $L^2(\partial\Omega)$ satisfies*

$$\frac{d}{d\lambda}\widetilde{Q}(\lambda) = \Gamma(\bar{\lambda})^* \overline{\Gamma(\lambda)}$$

and $\widetilde{Q}$ is a $\mathcal{L}(L^2(\partial\Omega))$-valued Nevanlinna function.

Proof. Besides the statement that $Q(\lambda)$ is a non-closed unbounded operator the assertions follow from the fact that Q is a generalized Q-function and the results in Section 2. In Corollary 3.6 it will turn out that $\overline{Q(\lambda)^{-1}}$ is a compact operator and that $Q(\lambda)^{-1}$ is not closed. This implies that $\overline{Q(\lambda)}$ and $Q(\lambda)$ are unbounded and that $Q(\lambda)$ is not closed. □

Corollary 3.6 *For $\lambda \in \rho(A_D) \cap \rho(A_N)$ the inverse $Q(\lambda)^{-1}$ of the Dirichlet-to-Neumann map $Q(\lambda)$ has the following properties.*

(i) *$Q(\lambda)^{-1}$ is a non-closed bounded operator in $L^2(\partial\Omega)$ defined on $H^{1/2}(\partial\Omega)$ with* $\operatorname{ran} Q(\lambda)^{-1} = H^{3/2}(\partial\Omega)$*;*
(ii) *the closure $\overline{Q(\lambda)^{-1}}$ is a compact operator in $L^2(\partial\Omega)$;*
(iii) *the function $\lambda \mapsto -\overline{Q(\lambda)^{-1}}$ is a $\mathcal{L}(L^2(\partial\Omega))$-valued Nevanlinna function.*

Proof. It is clear that (i) is an immediate consequence of (ii). Statement (iii) follows from Theorem 2.6 and general properties of the Nevanlinna class. Assertion (ii) is essentially a consequence of the classical results in [40], see also [32, Theorem 2.1]. Namely, for $\lambda \in \rho(A_D) \cap \rho(A_N)$ the operator $Q(\lambda) : H^{3/2}(\partial\Omega) \to H^{1/2}(\partial\Omega)$ is an isomorphism and can be extended to an isomorphism $\widehat{Q}(\lambda) : H^1(\partial\Omega) \to L^2(\partial\Omega)$ which acts as in (3.9). Therefore $Q(\lambda)^{-1} \subset \widehat{Q}(\lambda)^{-1}$ is a densely defined operator in $L^2(\partial\Omega)$ which is bounded as an operator in $H^1(\partial\Omega)$ and hence also bounded when considered as an operator in $L^2(\partial\Omega)$. Its closure $\overline{Q(\lambda)^{-1}}$ in $L^2(\partial\Omega)$ is a bounded everywhere defined operator in $L^2(\partial\Omega)$ with values in $H^1(\partial\Omega)$ and coincides with $\widehat{Q}(\lambda)^{-1}$. As $H^1(\partial\Omega)$ is compactly embedded in $L^2(\partial\Omega)$ it follows that $\overline{Q(\lambda)^{-1}}$ is a compact operator in $L^2(\partial\Omega)$. □

The next corollary is a simple consequence of Theorem 3.4 for the case that the difference of the resolvents is a trace class operator.

Corollary 3.7 *Let the assumptions be as in Theorem* 3.4*, let* $\widetilde{Q}$ *be the Nevanlinna function from Corollary* 3.5 *and suppose, in addition,* $n = 2$*. Then*

$$\operatorname{tr}\Big((A_D - \lambda)^{-1} - (A_N - \lambda)^{-1}\Big) = \operatorname{tr}\left(\overline{Q(\lambda)^{-1}}\,\frac{d}{d\lambda}\,\widetilde{Q}(\lambda)\right) \tag{3.14}$$

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

Proof. The resolvent formula (3.10) can be written in the form

$$(A_D - \lambda)^{-1} - (A_N - \lambda)^{-1} = \overline{\Gamma(\lambda)}\,\overline{Q(\lambda)^{-1}}\,\Gamma(\bar{\lambda})^*, \tag{3.15}$$

where the closures $\overline{\Gamma(\lambda)}$ and $\overline{Q(\lambda)^{-1}}$ are everywhere defined bounded operators; cf. Corollary 3.6 (ii). In the case $n = 2$ it follows from Theorem 3.4 (iii) that (3.15) is a trace class operator and from Corollaries 2.9, 3.5 (iii) and well known properties of the trace of bounded operators (see [28]) we conclude (3.14). □

4 Coupling of elliptic differential operators

In this section we study the uniformly elliptic second order differential expression $\mathcal{L}$ from (3.1) on two different domains and a coupling of the associated Dirichlet operators. More precisely, let $\Omega \subset \mathbb{R}^n$ be a simply connected bounded domain with C^∞-boundary $\mathcal{C} := \partial\Omega$ and let $\Omega' = \mathbb{R}^n \backslash \overline{\Omega}$ be the complement of the closure of Ω in $\mathbb{R}^n$. Clearly, Ω' is an unbounded domain with the compact C^∞-boundary $\partial\Omega' = \mathcal{C}$. Let again $\mathcal{L}$ be given by

$$\mathcal{L}h = -\sum_{j,k=1}^{n} \frac{\partial}{\partial x_j}\, a_{jk} \frac{\partial h}{\partial x_k} + ah \tag{4.1}$$

with bounded real valued coefficients $a_{jk} \in C^\infty(\mathbb{R}^n)$ satisfying $a_{jk}(x) = a_{kj}(x)$ for all $x \in \mathbb{R}^n$ and $j, k = 1, \ldots, n$; the function $a \in L^\infty(\mathbb{R}^n)$ is real valued and suppose that $\mathcal{L}$ is uniformly elliptic; cf. (3.2). The restriction of $\mathcal{L}$ on functions f defined on Ω or functions f' defined on Ω' will be denoted by $\mathcal{L}_\Omega$ and $\mathcal{L}_{\Omega'}$, respectively. Then it is clear that the differential expressions $\mathcal{L}_\Omega$ and $\mathcal{L}_{\Omega'}$ are of the type as in Section 3.

In the following we will usually denote functions defined on $\mathbb{R}^n$ by h or k, and we denote functions defined on Ω or Ω' by f, g or f', g', respectively. The scalar products of $L^2(\Omega)$ and $L^2(\Omega')$ are indexed with Ω and Ω', respectively, whereas the scalar product of $L^2(\mathbb{R}^n)$ is just denoted by $(\cdot,\cdot)$. For the trace of a function $f \in H^2(\Omega)$ and $f' \in H^2(\Omega')$ we write $f|_\mathcal{C}$ and $f'|_\mathcal{C}$, and the trace of the conormal derivatives are

$$\frac{\partial f}{\partial \nu}\Big|_\mathcal{C} = \sum_{j,k=1}^n a_{jk} n_j \frac{\partial f}{\partial x_k}\Big|_\mathcal{C} \quad \text{and} \quad \frac{\partial f'}{\partial \nu'}\Big|_\mathcal{C} = \sum_{j,k=1}^n a_{jk} n_j' \frac{\partial f}{\partial x_k}\Big|_\mathcal{C}; \tag{4.2}$$

here $n(x) = (n_1(x), \ldots, n_n(x))^\top$ and $n'(x) = -n(x)$ are the unit vectors at the point $x \in \mathcal{C} = \partial\Omega = \partial\Omega'$ pointing out of Ω and Ω', respectively. Note also that the coefficients a_{jk} in (4.2) are the restrictions of the coefficients in (4.1) onto Ω and Ω', respectively. The Dirichlet operators

$$\begin{aligned} A_\Omega f &= \mathcal{L}_\Omega f, & \operatorname{dom} A_\Omega &= \Big\{ f \in H^2(\Omega) : f|_\mathcal{C} = 0 \Big\}, \\ A_{\Omega'} f' &= \mathcal{L}_{\Omega'} f', & \operatorname{dom} A_{\Omega'} &= \Big\{ f' \in H^2(\Omega') : f'|_\mathcal{C} = 0 \Big\}, \end{aligned}$$

are selfadjoint operators in $L^2(\Omega)$ and $L^2(\Omega')$, respectively. Hence the orthogonal sum

$$A = \begin{pmatrix} A_\Omega & 0 \\ 0 & A_{\Omega'} \end{pmatrix}, \qquad \operatorname{dom} A = \operatorname{dom} A_\Omega \oplus \operatorname{dom} A_{\Omega'}, \tag{4.3}$$

is a selfadjoint operator in $L^2(\mathbb{R}^n) = L^2(\Omega) \oplus L^2(\Omega')$. Observe that

$$\begin{aligned} A(f \oplus f') &= \mathcal{L}(f \oplus f') = \mathcal{L}_\Omega f \oplus \mathcal{L}_{\Omega'} f', \\ \operatorname{dom} A &= \Big\{ f \oplus f' \in H^2(\Omega) \oplus H^2(\Omega') : f|_\mathcal{C} = 0 = f'|_\mathcal{C} \Big\}, \end{aligned} \tag{4.4}$$

and that A is not a usual second order elliptic differential operator on $\mathbb{R}^n$ since for a function $f \oplus f' \in \operatorname{dom} A$ the traces of the conormal derivatives $\frac{\partial f}{\partial \nu}|_\mathcal{C}$ and $-\frac{\partial f'}{\partial \nu'}|_\mathcal{C}$ at the boundary $\mathcal{C}$ of the domains Ω and Ω' in general do not coincide.

Besides the operator A we consider the usual selfadjoint operator associated to $\mathcal{L}$ in $L^2(\mathbb{R}^n)$ defined by

$$\widetilde{A} h = \mathcal{L} h, \qquad h \in \operatorname{dom} \widetilde{A} = H^2(\mathbb{R}^n), \tag{4.5}$$

and our aim is to prove a formula for the difference of the resolvents of $\widetilde{A}$ and A with the help of a generalized Q-function in a similar form as in the previous section.

The following theorem indicates how S and T in the triple $\{S, A, T\}$ for the definition of a generalized Q-function can be chosen.

Theorem 4.1 *The operator*

$$Sh = \mathcal{L} h, \quad \operatorname{dom} S = \Big\{ h = f \oplus f' \in H^2(\mathbb{R}^n) : f|_\mathcal{C} = 0 = f'|_\mathcal{C} \Big\}, \tag{4.6}$$

is a densely defined closed symmetric operator in $L^2(\mathbb{R}^n)$ *with infinite deficiency indices* $n_\pm(S)$*. The operator*

$$\begin{aligned} T(f\oplus f') &= \mathcal{L}(f\oplus f'),\\ \operatorname{dom} T &= \bigl\{ f\oplus f' \in H^2(\Omega)\oplus H^2(\Omega') : f|_{\mathcal{C}} = f'|_{\mathcal{C}} \bigr\}, \end{aligned} \tag{4.7}$$

is not closed as an operator in $L^2(\mathbb{R}^n)$ *and* T *satisfies* $\overline{T} = S^*$ *and* $T^* = S$*. Furthermore, the selfadjoint operators* A *and* $\widetilde{A}$ *in* (4.3), (4.4) *and* (4.5) *are extensions of* S *and restrictions of* T*.*

Proof. The operator S is a restriction of the selfadjoint operator A and hence S is symmetric. The fact that $\operatorname{dom} S$ is dense follows, e.g., from the fact that $H^2_0(\Omega)$ and $H^2_0(\Omega')$ are dense subspaces of $L^2(\Omega)$ and $L^2(\Omega')$, respectively, and

$$H^2_0(\Omega)\oplus H^2_0(\Omega') \subset \operatorname{dom} S.$$

Since for any function $h\in H^2(\mathbb{R}^n)$ decomposed as $h = f\oplus f'$, where $f\in H^2(\Omega)$, $f'\in H^2(\Omega')$, we have $f|_{\mathcal{C}} = f'|_{\mathcal{C}} \in H^{3/2}(\mathcal{C})$ it follows that $\widetilde{A}$ is an extension of S and a restriction of the operator T. Moreover, $S\subset A\subset T$ is obvious.

Let us verify that $S = T^*$ holds. In particular this implies that S is closed and that $\overline{T} = S^*$ is true. We start with the inclusion $S\subset T^*$. Let $h = f\oplus f' \in \operatorname{dom} S$ and $k = g\oplus g'\in \operatorname{dom} T$, where $f, g\in H^2(\Omega)$ and $f', g'\in H^2(\Omega')$. First of all we have

$$(Tk,h) - (k,Sh) = (\mathcal{L}_\Omega g, f)_\Omega - (g,\mathcal{L}_\Omega f)_\Omega + (\mathcal{L}_{\Omega'} g', f')_{\Omega'} - (g',\mathcal{L}_{\Omega'} f')_{\Omega'}$$

and Green's identity (3.4) shows that this is equal to

$$\left(g|_{\mathcal{C}}, \frac{\partial f}{\partial\nu}\Big|_{\mathcal{C}} \right)_{\mathcal{C}} - \left(\frac{\partial g}{\partial\nu}\Big|_{\mathcal{C}}, f|_{\mathcal{C}} \right)_{\mathcal{C}} + \left(g'|_{\mathcal{C}}, \frac{\partial f'}{\partial\nu'}\Big|_{\mathcal{C}} \right)_{\mathcal{C}} - \left(\frac{\partial g'}{\partial\nu'}\Big|_{\mathcal{C}}, f'|_{\mathcal{C}} \right)_{\mathcal{C}}.$$

Since $h = f\oplus f'\in \operatorname{dom} S$ we have

$$f|_{\mathcal{C}} = f'|_{\mathcal{C}} = 0 \qquad \text{and} \qquad \frac{\partial f}{\partial\nu}\Big|_{\mathcal{C}} = -\frac{\partial f'}{\partial\nu'}\Big|_{\mathcal{C}},$$

and for $k = g\oplus g'\in \operatorname{dom} T$ by definition $g|_{\mathcal{C}} = g'|_{\mathcal{C}}$ holds. Hence we conclude

$$(Tk,h) - (k,Sh) = 0$$

and therefore every $h\in\operatorname{dom} S$ belongs to $\operatorname{dom} T^*$ and $T^*h = Sh$, i.e., $S\subset T^*$. Let us now prove the converse inclusion $T^*\subset S$. For this it is sufficient to check that every function $h\in \operatorname{dom} T^*$ belongs to $\operatorname{dom} S$. From the fact that

T is an extension of the selfadjoint operators A and $\widetilde{A}$ we conclude

$$T^* \subset A^* = A \subset T \qquad \text{and} \qquad T^* \subset \widetilde{A}^* = \widetilde{A} \subset T,$$

so that T^* is a restriction of A and $\widetilde{A}$. Hence every function h in $\operatorname{dom} T^*$ belongs also to $\operatorname{dom} A$ and $\operatorname{dom} \widetilde{A}$. Thus $h = f \oplus f' \in H^2(\mathbb{R}^n)$ and $f \in H^2(\Omega)$ and $f' \in H^2(\Omega')$ satisfy $f|_{\mathcal{C}} = f'|_{\mathcal{C}} = 0$. Therefore $\operatorname{dom} T^* \subset \operatorname{dom} S$ and we have shown $T^* = S$.

Next it will be verified that T is not closed. The arguments are similar as in [8, Proof of Proposition 4.5] and could also be formulated in terms of unitary relations between Krein spaces; cf. [17]. Assume that T is closed, i.e., $T = \overline{T}$, and consider the subspace

$$\mathcal{M} = \left\{ \begin{bmatrix} f \oplus f' \\ T(f \oplus f') \\ f|_{\mathcal{C}} \\ \frac{\partial f}{\partial \nu}|_{\mathcal{C}} + \frac{\partial f'}{\partial \nu'}|_{\mathcal{C}} \end{bmatrix} : f \oplus f' \in \operatorname{dom} T \right\} \subset L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C}).$$

Observe that by (3.3) and the definition of T the mapping

$$\operatorname{dom} T \ni f \oplus f' \;\mapsto\; \left\{ f|_{\mathcal{C}}, \frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}} \right\} \in H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C}) \tag{4.8}$$

is onto. Setting $\mathcal{N} = L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus \{0\} \oplus \{0\}$ it is clear that the sum of the subpaces $\mathcal{M}$ and $\mathcal{N}$ is

$$\mathcal{M} + \mathcal{N} = L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus \Big(H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C}) \Big). \tag{4.9}$$

We will calculate the orthogonal complements of $\mathcal{M}$ and $\mathcal{N}$ in $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$ and show that $\mathcal{M}^\perp + \mathcal{N}^\perp$ is closed. First of all we have

$$\mathcal{N}^\perp = \{0\} \oplus \{0\} \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C}) \tag{4.10}$$

and in order to determine $\mathcal{M}^\perp$ suppose that

$$\begin{bmatrix} l \oplus l' \\ g \oplus g' \\ \varphi \\ \psi \end{bmatrix} \in \mathcal{M}^\perp, \qquad g, l \in L^2(\Omega),\; g', l' \in L^2(\Omega'),\; \varphi, \psi \in L^2(\mathcal{C}), \tag{4.11}$$

is an element in $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$ which is orthogonal to $\mathcal{M}$. Then we have

$$\big(T(f \oplus f'), g \oplus g'\big) + \big(f \oplus f', l \oplus l'\big) = -\big(f|_{\mathcal{C}}, \varphi\big)_{\mathcal{C}} - \left(\frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}}, \psi\right)_{\mathcal{C}} \tag{4.12}$$

for all $f \oplus f' \in \operatorname{dom} T$. In particular, for $f \oplus f' \in \operatorname{dom} S$ we have

$$\frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} = -\frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}} \quad \text{and} \quad f|_{\mathcal{C}} = f'|_{\mathcal{C}} = 0,$$

so that (4.12) becomes

$$\big(T(f \oplus f'), g \oplus g'\big) = \big(S(f \oplus f'), g \oplus g'\big) = -\big(f \oplus f', l \oplus l'\big)$$

and hence $g \oplus g' \in \operatorname{dom} S^*$ and $S^*(g \oplus g') = -l \oplus l'$. But we have assumed that T is closed and hence from $S = T^*$ we conclude $S^* = T^{**} = \overline{T} = T$, so that

$$g \oplus g' \in \operatorname{dom} T \qquad \text{and} \quad T(g \oplus g') = -l \oplus l'. \tag{4.13}$$

From Green's identity we then obtain

$$\begin{aligned}
&\big(T(f \oplus f'), g \oplus g'\big) - \big(f \oplus f', T(g \oplus g')\big) \\
&\quad = (\mathcal{L}_\Omega f, g)_\Omega - (f, \mathcal{L}_\Omega g)_\Omega + (\mathcal{L}_{\Omega'} f', g')_{\Omega'} - (f', \mathcal{L}_{\Omega'} g')_{\Omega'} \\
&\quad = \left(f|_{\mathcal{C}}, \frac{\partial g}{\partial \nu}\Big|_{\mathcal{C}}\right)_{\mathcal{C}} - \left(\frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}}, g|_{\mathcal{C}}\right)_{\mathcal{C}} + \left(f'|_{\mathcal{C}}, \frac{\partial g'}{\partial \nu'}\Big|_{\mathcal{C}}\right)_{\mathcal{C}} - \left(\frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}}, g'|_{\mathcal{C}}\right)_{\mathcal{C}} \\
&\quad = \left(f|_{\mathcal{C}}, \frac{\partial g}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial g'}{\partial \nu'}\Big|_{\mathcal{C}}\right)_{\mathcal{C}} - \left(\frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}}, g|_{\mathcal{C}}\right)_{\mathcal{C}},
\end{aligned}$$

where we have used that $f \oplus f'$, $g \oplus g' \in \operatorname{dom} T$ satisfy $f|_{\mathcal{C}} = f'|_{\mathcal{C}}$ and $g|_{\mathcal{C}} = g'|_{\mathcal{C}}$. Inserting (4.13) in (4.12) and comparing this with the above relation shows that the identity

$$\left(f|_{\mathcal{C}}, \frac{\partial g}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial g'}{\partial \nu'}\Big|_{\mathcal{C}} + \varphi\right)_{\mathcal{C}} = \left(\frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}}, g|_{\mathcal{C}} - \psi\right)_{\mathcal{C}} \tag{4.14}$$

holds for all $f \oplus f' \in \operatorname{dom} T$. As the mapping (4.8) is surjective and $H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C})$ is dense in $L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$ we conclude from (4.14) that

$$\varphi = -\left(\frac{\partial g}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial g'}{\partial \nu'}\Big|_{\mathcal{C}}\right) \qquad \text{and} \qquad \psi = g|_{\mathcal{C}}$$

holds. Hence we have seen that the element (4.11) in $\mathcal{M}^\perp$ is of the form

$$\begin{bmatrix} -T(g \oplus g') \\ g \oplus g' \\ -\frac{\partial g}{\partial \nu}|_{\mathcal{C}} - \frac{\partial g'}{\partial \nu'}|_{\mathcal{C}} \\ g|_{\mathcal{C}} \end{bmatrix} \tag{4.15}$$

for some $g \oplus g' \in \operatorname{dom} T$. It is not difficult to check that conversely an element as in (4.15) belongs to $\mathcal{M}^\perp$. Therefore the orthogonal complement of $\mathcal{M}$ is given by

$$\mathcal{M}^\perp = \left\{ \begin{bmatrix} -T(g \oplus g') \\ g \oplus g' \\ -\frac{\partial g}{\partial n}\Big|_{\mathcal{C}} - \frac{\partial g'}{\partial \nu'}\Big|_{\mathcal{C}} \\ g|_{\mathcal{C}} \end{bmatrix} : g \oplus g' \in \operatorname{dom} T \right\} \subset L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$$

and together with (4.10) we find that the sum of $\mathcal{M}^\perp$ and $\mathcal{N}^\perp$ is

$$\mathcal{M}^\perp + \mathcal{N}^\perp = \left\{ \begin{bmatrix} -T(g \oplus g') \\ g \oplus g' \end{bmatrix} : g \oplus g' \in \operatorname{dom} T \right\} \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C}).$$

The assumption that T is closed implies that $\mathcal{M}^\perp + \mathcal{N}^\perp$ is a closed subspace of $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$. But then according to [34, IV Theorem 4.8] also $\mathcal{M} + \mathcal{N}$ is a closed subspace of $L^2(\mathbb{R}^n) \oplus L^2(\mathbb{R}^n) \oplus L^2(\mathcal{C}) \oplus L^2(\mathcal{C})$ which is a contradiction to (4.9). Thus T can not be closed. □

The following lemma will be useful later in this section.

Lemma 4.2 *Let S and T be as in Theorem 4.1 and let $\widetilde{A}$ be the selfadjoint realization of $\mathcal{L}$ in $L^2(\mathbb{R}^n)$ defined on $H^2(\mathbb{R}^n)$. For a function $f \oplus f' \in \operatorname{dom} T$, where $f \in H^2(\Omega)$ and $f' \in H^2(\Omega')$, we have*

$$f \oplus f' \in \operatorname{dom} \widetilde{A} \qquad \textit{if and only if} \qquad \frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} = -\frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}}.$$

Proof. For a function $f \oplus f' \in \operatorname{dom} \widetilde{A} = H^2(\mathbb{R}^n)$ it is clear that $\frac{\partial f}{\partial \nu}|_{\mathcal{C}} = -\frac{\partial f'}{\partial \nu'}|_{\mathcal{C}}$ holds. Conversely, let $f \oplus f' \in \operatorname{dom} T$ and assume

$$\frac{\partial f}{\partial \nu}\Big|_{\mathcal{C}} = -\frac{\partial f'}{\partial \nu'}\Big|_{\mathcal{C}}. \tag{4.16}$$

Then also $f|_\mathcal{C} = f'|_\mathcal{C}$ and since every $g \oplus g' \in \operatorname{dom} \widetilde{A}$ satisfies

$$g|_\mathcal{C} = g'|_\mathcal{C} \qquad \text{and} \qquad \frac{\partial g}{\partial \nu}\Big|_\mathcal{C} = -\frac{\partial g'}{\partial \nu'}\Big|_\mathcal{C}$$

Green's identity implies

$$\begin{aligned} &\Big(\widetilde{A}(g \oplus g'), f \oplus f'\Big) - \Big(g \oplus g', T(f \oplus f')\Big) \\ = &\left(g|_\mathcal{C}, \frac{\partial f}{\partial \nu}\Big|_\mathcal{C}\right)_\mathcal{C} - \left(\frac{\partial g}{\partial \nu}\Big|_\mathcal{C}, f|_\mathcal{C}\right)_\mathcal{C} + \left(g'|_\mathcal{C}, \frac{\partial f'}{\partial \nu}\Big|_\mathcal{C}\right)_\mathcal{C} - \left(\frac{\partial g'}{\partial \nu}\Big|_\mathcal{C}, f'|_\mathcal{C}\right)_\mathcal{C} = 0. \end{aligned}$$

Therefore $f \oplus f' \in \operatorname{dom} \widetilde{A}^* = \operatorname{dom} \widetilde{A}$. □

Next we define a mapping Γ_{λ_0} which satisfies the assumptions in the definition of a generalized Q-function. For this let A be the selfadjoint operator in $L^2(\mathbb{R}^n)$ in (4.3) and (4.4) which is the orthogonal sum of the Dirichlet operators A_Ω and $A_{\Omega'}$ in $L^2(\Omega)$ and $L^2(\Omega')$, respectively. For $\lambda \in \rho(A)$ the domain of the operator T in Theorem 4.1 can be decomposed in

$$\begin{aligned} \operatorname{dom} T &= \operatorname{dom} A \dot{+} \mathcal{N}_\lambda(T) \\ &= \Big\{f \oplus f' \in H^2(\Omega) \oplus H^2(\Omega') : f|_\mathcal{C} = f'|_\mathcal{C} = 0\Big\} \dot{+} \mathcal{N}_\lambda(T); \end{aligned} \tag{4.17}$$

cf. (2.1). Let us fix some $\lambda_0 \in \rho(A)$. The decomposition (4.17) and the surjectivity of the map

$$\operatorname{dom} T \ni f \oplus f' \;\mapsto\; \left\{f|_\mathcal{C}, \frac{\partial f}{\partial \nu}\Big|_\mathcal{C} + \frac{\partial f'}{\partial \nu'}\Big|_\mathcal{C}\right\} \in H^{3/2}(\mathcal{C}) \times H^{1/2}(\mathcal{C}) \tag{4.18}$$

(see (3.3) and (4.8)) imply that for a given function $\varphi \in H^{3/2}(\mathcal{C})$ there exists a unique function $f_{\lambda_0} \oplus f'_{\lambda_0} \in \mathcal{N}_{\lambda_0}(T)$ such that $f_{\lambda_0}|_\mathcal{C} = f'_{\lambda_0}|_\mathcal{C} = \varphi$. Let Γ_{λ_0} be the mapping that assigns $f_{\lambda_0} \oplus f'_{\lambda_0}$ to φ,

$$H^{3/2}(\mathcal{C}) \ni \varphi \mapsto \Gamma_{\lambda_0}\varphi := f_{\lambda_0} \oplus f'_{\lambda_0}. \tag{4.19}$$

Similarly as in the previous section Γ_{λ_0} will be regarded as an operator from $L^2(\mathcal{C})$ to $L^2(\mathbb{R}^n)$ with $\operatorname{dom} \Gamma_{\lambda_0} = H^{3/2}(\mathcal{C})$ and $\operatorname{ran} \Gamma_{\lambda_0} = \mathcal{N}_{\lambda_0}(T)$. Observe that the function $\Gamma_{\lambda_0}\varphi = f_{\lambda_0} \oplus f'_{\lambda_0}$ consists of an $H^2(\Omega)$-solution f_{λ_0} of $\mathcal{L}_\Omega u = \lambda_0 u$ and an $H^2(\Omega')$-solution f'_{λ_0} of $\mathcal{L}_{\Omega'} u' = \lambda_0 u'$ satisfying the boundary conditions $\varphi = f_{\lambda_0}|_\mathcal{C} = f'_{\lambda_0}|_\mathcal{C}$.

The following proposition parallels Proposition 3.2.

Proposition 4.3 *Let $\lambda_0 \in \rho(A)$, let Γ_{λ_0} be as in* (4.19) *and let $\lambda \in \rho(A)$. Then the following holds:*

(i) Γ_{λ_0} *is a bounded operator from* $L^2(\mathcal{C})$ *in* $L^2(\mathbb{R}^n)$ *with dense domain* $H^{3/2}(\mathcal{C})$*;*

(ii) *The operator* $\Gamma(\lambda) = (I + (\lambda - \lambda_0)(A - \lambda)^{-1})\Gamma_{\lambda_0}$ *is given by*

$$\Gamma(\lambda)\varphi = f_\lambda \oplus f'_\lambda, \quad \textit{where} \quad f_\lambda \oplus f'_\lambda \in \mathcal{N}_\lambda(T) \quad \textit{and} \quad f_\lambda|_\mathcal{C} = \varphi = f'_\lambda|_\mathcal{C};$$

(iii) *The mapping* $\Gamma(\bar\lambda)^* : L^2(\mathbb{R}^n) \to L^2(\mathcal{C})$ *satisfies*

$$\Gamma(\bar\lambda)^*(A - \lambda)h = -\frac{\partial f}{\partial \nu}\Big|_\mathcal{C} - \frac{\partial f'}{\partial \nu'}\Big|_\mathcal{C}, \qquad h = f \oplus f' \in \operatorname{dom} A.$$

Proof. We start with the proof (ii). Let $\varphi \in H^{3/2}(\mathcal{C})$ and choose the unique elements $f_\lambda \oplus f'_\lambda \in \mathcal{N}_\lambda(T)$ and $f_{\lambda_0} \oplus f'_{\lambda_0} \in \mathcal{N}_{\lambda_0}(T)$ such that

$$f_\lambda|_\mathcal{C} = f'_\lambda|_\mathcal{C} = \varphi = f_{\lambda_0}|_\mathcal{C} = f'_{\lambda_0}|_\mathcal{C}$$

holds. By definition $\Gamma_{\lambda_0}\varphi = f_{\lambda_0} \oplus f'_{\lambda_0}$ and therefore

$$\begin{aligned}\Gamma(\lambda)\varphi &= \Gamma_{\lambda_0}\varphi + (\lambda - \lambda_0)(A - \lambda)^{-1}\Gamma_{\lambda_0}\varphi \\ &= f_{\lambda_0} \oplus f'_{\lambda_0} + (\lambda - \lambda_0)(A - \lambda)^{-1}\Gamma_{\lambda_0}\varphi.\end{aligned}$$

Since $(\lambda - \lambda_0)(A - \lambda)^{-1}\Gamma_{\lambda_0}\varphi$ is a function belonging to $\operatorname{dom} A$ we have

$$\Big((\lambda - \lambda_0)(A - \lambda)^{-1}\Gamma_{\lambda_0}\varphi\Big)\Big|_\mathcal{C} = 0;$$

cf. (4.4). This implies

$$(\Gamma(\lambda)\varphi)|_\mathcal{C} = (\Gamma_{\lambda_0}\varphi)|_\mathcal{C} = \Big(f_{\lambda_0} \oplus f'_{\lambda_0}\Big)|_\mathcal{C} = f_{\lambda_0}|_\mathcal{C} = f'_{\lambda_0}|_\mathcal{C} = \varphi$$

and since $\operatorname{ran}\Gamma(\lambda) = \mathcal{N}_\lambda(T)$ (see Lemma 2.1) and $f_\lambda \oplus f'_\lambda$ is the unique function in $\mathcal{N}_\lambda(T)$ with $f_\lambda|_\mathcal{C} = f'_\lambda|_\mathcal{C} = \varphi$ we conclude $\Gamma(\lambda)\varphi = f_\lambda \oplus f'_\lambda$.

Next we verify (iii). Observe that then $\Gamma(\bar\lambda)^*$, $\lambda \in \rho(A)$, is a closed operator which is defined on the whole space, i.e., $\Gamma(\bar\lambda)^*$ is bounded and hence assertion (i) follows by setting $\lambda_0 = \bar\lambda$. Let $\varphi \in H^{3/2}(\mathcal{C})$ and choose the unique function $f_{\bar\lambda} \oplus f'_{\bar\lambda} \in \mathcal{N}_{\bar\lambda}(T)$ such that

$$f_{\bar\lambda}|_\mathcal{C} = f'_{\bar\lambda}|_\mathcal{C} = \varphi \tag{4.20}$$

holds. Then $\Gamma(\bar\lambda)\varphi = f_{\bar\lambda} \oplus f'_{\bar\lambda}$ and for each $h = f \oplus f' \in \operatorname{dom} A$, where $f \in H^2(\Omega)$, $f' \in H^2(\Omega')$, we have

$$\begin{aligned}\Big(\Gamma(\bar\lambda)\varphi, (A - \lambda)h\Big) &= \Big(f_{\bar\lambda} \oplus f'_{\bar\lambda}, A(f \oplus f')\Big) - \Big(T(f_{\bar\lambda} \oplus f'_{\bar\lambda}), f \oplus f'\Big) \\ &= (f_{\bar\lambda}, \mathcal{L}_\Omega f)_\Omega - (\mathcal{L}_\Omega f_{\bar\lambda}, f)_\Omega + (f'_{\bar\lambda}, \mathcal{L}_{\Omega'} f')_{\Omega'} - (\mathcal{L}_{\Omega'} f'_{\bar\lambda}, f')_{\Omega'}.\end{aligned}$$

With the help of Green's identity this can be rewritten as

$$\left(\frac{\partial f_{\bar\lambda}}{\partial\nu}\Big|_{\mathcal C}, f|_{\mathcal C}\right)_{\mathcal C} - \left(f_{\bar\lambda}|_{\mathcal C}, \frac{\partial f}{\partial\nu}\Big|_{\mathcal C}\right)_{\mathcal C} + \left(\frac{\partial f'_{\bar\lambda}}{\partial\nu'}\Big|_{\mathcal C}, f'|_{\mathcal C}\right)_{\mathcal C} - \left(f'_{\bar\lambda}|_{\mathcal C}, \frac{\partial f'}{\partial\nu'}\Big|_{\mathcal C}\right)_{\mathcal C}.$$

Since for $h = f \oplus f' \in \operatorname{dom} A$ we have $f|_{\mathcal C} = f'|_{\mathcal C} = 0$ we conclude from the above calculation and (4.20) that

$$\big(\Gamma(\bar\lambda)\varphi, (A-\lambda)h\big) = -\left(\varphi, \frac{\partial f}{\partial\nu}\Big|_{\mathcal C} + \frac{\partial f'}{\partial\nu'}\Big|_{\mathcal C}\right)_{\mathcal C}$$

holds for every $\varphi \in H^{3/2}(\mathcal C) = \operatorname{dom}\Gamma(\bar\lambda)$. Hence $(A-\lambda)h \in \operatorname{dom}\Gamma(\bar\lambda)^*$ and

$$\Gamma(\bar\lambda)^*(A-\lambda)h = -\frac{\partial f}{\partial\nu}\Big|_{\mathcal C} - \frac{\partial f'}{\partial\nu'}\Big|_{\mathcal C}, \qquad h = f \oplus f' \in \operatorname{dom} A.$$

Furthermore, for $\lambda \in \rho(A)$ we have $\operatorname{ran}(A-\lambda) = L^2(\mathbb R^n)$, so that $\Gamma(\bar\lambda)^*$ is a bounded operator defined on $L^2(\mathbb R^n)$. □

Next we define a function Q in a similar way as the Dirichlet-to-Neumann map in Definition 3.3. For this we make use of the decomposition (4.17). Namely, for $\lambda \in \rho(A)$ and $\varphi \in H^{3/2}(\mathcal C)$ there exists a unique function $f_\lambda \oplus f'_\lambda \in \mathcal N_\lambda(T)$ such that $f_\lambda|_{\mathcal C} = f'_\lambda|_{\mathcal C} = \varphi$. The operator $Q(\lambda)$ in $L^2(\mathcal C)$ is now defined by

$$Q(\lambda)\varphi := -\frac{\partial f_\lambda}{\partial\nu}\Big|_{\mathcal C} - \frac{\partial f'_\lambda}{\partial\nu'}\Big|_{\mathcal C}, \qquad \varphi \in \operatorname{dom} Q(\lambda) = H^{3/2}(\mathcal C). \tag{4.21}$$

Observe that $\operatorname{ran} Q(\lambda) \subset H^{1/2}(\mathcal C)$ holds. Roughly speaking, up to a minus sign $Q(\lambda)$ maps the Dirichlet boundary value of the H^2-solutions of $\mathcal L_\Omega u = \lambda u$ and $\mathcal L_{\Omega'} u' = \lambda u'$, $u|_{\mathcal C} = u'|_{\mathcal C}$, onto the sum of the Neumann boundary values of these solutions. We mention that in the analysis of so-called intermediate Hamiltonians a modified form of such a Dirichlet-to-Neumann map has been used in [44].

In the following theorem it turns out that Q can be interpreted as a generalized Q-function and the difference of the resolvents of A and $\widetilde A$ is expressed with the help of Q.

Theorem 4.4 *Let $\mathcal L$ be the elliptic differential expression in* (4.1) *and let A and $\widetilde A$ be the selfadjoint realizations of $\mathcal L$ in* (4.3)-(4.4) *and* (4.5), *respectively. Let S and T be the operators in Theorem* 4.1, *define $\Gamma(\lambda)$ as in Proposition* 4.3 *and let $Q(\lambda)$, $\lambda \in \rho(A)$, be as in* (4.21). *Then the following holds:*

(i) *Q is a generalized Q-function of the triple $\{S, A, T\}$;*

(ii) *The operator $Q(\lambda)$ is injective for all $\lambda \in \rho(A) \cap \rho(\widetilde{A})$ and the resolvent formula*

$$(A-\lambda)^{-1} - (\widetilde{A}-\lambda)^{-1} = \Gamma(\lambda)Q(\lambda)^{-1}\Gamma(\bar{\lambda})^* \tag{4.22}$$

holds;

(iii) *For $p > \frac{n-1}{2}$ the difference of the resolvents in* (4.22) *belongs to the von Neumann-Schatten class $\mathfrak{S}_p(L^2(\mathbb{R}^n))$.*

Proof. Let us prove assertion (i). Before the defining relation (2.3) for a generalized Q-function will be verified we show that the operator $Q(\mu)^*$ is an extension of $Q(\bar{\mu})$, $\mu \in \rho(A)$. For this let $\psi \in H^{3/2}(\mathcal{C})$ and choose the unique element $f_{\bar{\mu}} \oplus f'_{\bar{\mu}} \in \mathcal{N}_{\bar{\mu}}(T)$ with the property $f_{\bar{\mu}}|_{\mathcal{C}} = f'_{\bar{\mu}}|_{\mathcal{C}} = \psi$. For $\varphi \in H^{3/2}(\mathcal{C})$ let $f_\mu \oplus f'_\mu \in \mathcal{N}_\mu(T)$ be such that $f_\mu|_{\mathcal{C}} = f'_\mu|_{\mathcal{C}} = \varphi$ holds. By the definition of Q in (4.21) we have

$$Q(\mu)\varphi = -\frac{\partial f_\mu}{\partial \nu}\Big|_{\mathcal{C}} - \frac{\partial f'_\mu}{\partial \nu'}\Big|_{\mathcal{C}} \quad \text{and} \quad Q(\bar{\mu})\psi = -\frac{\partial f_{\bar{\mu}}}{\partial \nu}\Big|_{\mathcal{C}} - \frac{\partial f'_{\bar{\mu}}}{\partial \nu'}\Big|_{\mathcal{C}}.$$

From $(f_\mu|_{\mathcal{C}}, \frac{\partial f_{\bar{\mu}}}{\partial \nu}|_{\mathcal{C}})_{\mathcal{C}} = (\frac{\partial f_\mu}{\partial \nu}|_{\mathcal{C}}, f_{\bar{\mu}}|_{\mathcal{C}})_{\mathcal{C}}$ and $(f'_\mu|_{\mathcal{C}}, \frac{\partial f'_{\bar{\mu}}}{\partial \nu'}|_{\mathcal{C}})_{\mathcal{C}} = (\frac{\partial f'_\mu}{\partial \nu'}|_{\mathcal{C}}, f'_{\bar{\mu}}|_{\mathcal{C}})_{\mathcal{C}}$ we then conclude

$$(Q(\mu)\varphi, \psi) = -\left(\frac{\partial f_\mu}{\partial \nu}\Big|_{\mathcal{C}}, f_{\bar{\mu}}|_{\mathcal{C}}\right)_{\mathcal{C}} - \left(\frac{\partial f'_\mu}{\partial \nu'}\Big|_{\mathcal{C}}, f'_{\bar{\mu}}|_{\mathcal{C}}\right)_{\mathcal{C}} = -\left(\varphi, \frac{\partial f_{\bar{\mu}}}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'_{\bar{\mu}}}{\partial \nu'}\Big|_{\mathcal{C}}\right)_{\mathcal{C}}$$

and therefore $\psi \in \operatorname{dom} Q(\mu)^*$ and $Q(\mu)^*\psi = Q(\bar{\mu})\psi$.

Let $\Gamma(\cdot)$ be as in Proposition 4.3. We prove now that

$$Q(\lambda) - Q(\mu)^* = (\lambda - \bar{\mu})\Gamma(\mu)^*\Gamma(\lambda), \qquad \lambda, \mu \in \rho(A) \tag{4.23}$$

holds on $\operatorname{dom}\Gamma(\lambda) = H^{3/2}(\mathcal{C})$. For this let $\varphi, \psi \in H^{3/2}(\mathcal{C})$ and choose the unique elements $f_\lambda \oplus f'_\lambda \in \mathcal{N}_\lambda(T)$, $f_\mu \oplus f'_\mu \in \mathcal{N}_\mu(T)$ with the properties

$$f_\lambda|_{\mathcal{C}} = f'_\lambda|_{\mathcal{C}} = \varphi \quad \text{and} \quad f_\mu|_{\mathcal{C}} = f'_\mu|_{\mathcal{C}} = \psi. \tag{4.24}$$

Then according to Proposition 4.3 (ii) $\Gamma(\lambda)\varphi = f_\lambda \oplus f'_\lambda$ and $\Gamma(\mu)\psi = f_\mu \oplus f'_\mu$ and the definition of $Q(\cdot)$ in (4.21) shows

$$\big((Q(\lambda) - Q(\mu)^*)\varphi, \psi\big)_{\mathcal{C}} = -\left(\frac{\partial f_\lambda}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'_\lambda}{\partial \nu'}\Big|_{\mathcal{C}}, \psi\right)_{\mathcal{C}} + \left(\varphi, \frac{\partial f_\mu}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'_\mu}{\partial \nu'}\Big|_{\mathcal{C}}\right)_{\mathcal{C}}.$$

By inserting (4.24) and making use of Green's identity we obtain

$$\begin{aligned}
&\big((Q(\lambda)-Q(\mu)^*)\varphi,\psi\big)_{\mathcal{C}}\\
&\qquad=(\mathcal{L}_\Omega f_\lambda,f_\mu)_\Omega-(f_\lambda,\mathcal{L}_\Omega f_\mu)_\Omega+(\mathcal{L}_{\Omega'}f'_\lambda,f'_\mu)_{\Omega'}-(f'_\lambda,\mathcal{L}_{\Omega'}f'_\mu)_{\Omega'}\\
&\qquad=(\lambda-\bar\mu)\big((f_\lambda,f_\mu)_\Omega+(f'_\lambda,f'_\mu)_{\Omega'}\big)=(\lambda-\bar\mu)\big(f_\lambda\oplus f'_\lambda,f_\mu\oplus f'_\mu\big)\\
&\qquad=(\lambda-\bar\mu)(\Gamma(\lambda)\varphi,\Gamma(\mu)\psi)=\big((\lambda-\bar\mu)\Gamma(\mu)^*\Gamma(\lambda)\varphi,\psi\big)_{\mathcal{C}},
\end{aligned}$$

i.e., (4.23) holds and Q is a generalized Q-function for the triple $\{S,A,T\}$.

(ii) We check first that $\ker Q(\lambda)=\{0\}$ holds for $\lambda\in\rho(A)\cap\rho(\widetilde{A})$. Assume that $Q(\lambda)\varphi=0$ for some $\varphi\in H^{3/2}(\mathcal{C})$ and let $f_\lambda\oplus f'_\lambda\in\mathcal{N}_\lambda(T)$ be the unique element with the property $f_\lambda|_{\mathcal{C}}=f'_\lambda|_{\mathcal{C}}=\varphi$. Then the definition of Q and the assumption $Q(\lambda)\varphi=0$ imply

$$\frac{\partial f_\lambda}{\partial\nu}\Big|_{\mathcal{C}}=-\frac{\partial f'_\lambda}{\partial\nu'}\Big|_{\mathcal{C}}.$$

According to Lemma 4.2 this yields $f_\lambda\oplus f'_\lambda\in\operatorname{dom}\widetilde{A}\cap\mathcal{N}_\lambda(T)$. But as $\lambda\in\rho(\widetilde{A})$ we conclude $f_\lambda=0$ and $f'_\lambda=0$, and hence $\varphi=0$.

Now we prove the formula (4.22) for the difference of the resolvents of A and $\widetilde{A}$. By the above argument $Q(\lambda)^{-1}$ exists for $\lambda\in\rho(A)\cap\rho(\widetilde{A})$. Furthermore, (4.18) implies $\operatorname{ran}Q(\lambda)=H^{1/2}(\mathcal{C})$ and it follows from Proposition 4.3 that the right hand side in (4.22) is well defined. Let $h\in L^2(\mathbb{R}^n)$ and define the function k as

$$k=(A-\lambda)^{-1}h-\Gamma(\lambda)Q(\lambda)^{-1}\Gamma(\bar\lambda)^*h. \tag{4.25}$$

We show $k\in\operatorname{dom}\widetilde{A}$. First of all it is clear that $k\in\operatorname{dom}T$ since $(A-\lambda)^{-1}h\in\operatorname{dom}A\subset\operatorname{dom}T$ and $\Gamma(\lambda)$ maps into $\mathcal{N}_\lambda(T)$. Therefore $k=g\oplus g'$, where $g\in H^2(\Omega)$, $g'\in H^2(\Omega')$, and $g|_{\mathcal{C}}=g'|_{\mathcal{C}}$. According to Lemma 4.2 for $k\in\operatorname{dom}\widetilde{A}$ it is sufficient to check

$$\frac{\partial g}{\partial\nu}\Big|_{\mathcal{C}}+\frac{\partial g'}{\partial\nu'}\Big|_{\mathcal{C}}=0. \tag{4.26}$$

We proceed in a similar way as in the proof of Theorem 3.4. Let $h_A=f_A\oplus f'_A\in\operatorname{dom}A$ be such that $h=(A-\lambda)h_A$. Making use of Proposition 4.3 (iii) we obtain

$$k=h_A+f_\lambda\oplus f'_\lambda,\quad f_\lambda\oplus f'_\lambda:=\Gamma(\lambda)Q(\lambda)^{-1}\left(\frac{\partial f_A}{\partial\nu}\Big|_{\mathcal{C}}+\frac{\partial f'_A}{\partial\nu'}\Big|_{\mathcal{C}}\right)\in\mathcal{N}_\lambda(T), \tag{4.27}$$

from (4.25). Then Proposition 4.3 (ii) together with the definition of $Q(\lambda)$ in

(4.21) implies

$$\frac{\partial f_A}{\partial \nu}\Big|_{\mathcal{C}} + \frac{\partial f'_A}{\partial \nu'}\Big|_{\mathcal{C}} = Q(\lambda)(f_\lambda|_{\mathcal{C}}) = Q(\lambda)(f'_\lambda|_{\mathcal{C}}) = -\frac{\partial f_\lambda}{\partial \nu}\Big|_{\mathcal{C}} - \frac{\partial f'_\lambda}{\partial \nu'}\Big|_{\mathcal{C}}.$$

Hence we conclude that the function $k = g \oplus g'$ in (4.27) fulfils (4.26), i.e., $k \in \operatorname{dom} \widetilde{A}$. From (4.25) and $A, \widetilde{A} \subset T$ we obtain

$$(\widetilde{A} - \lambda)k = (T - \lambda)(A - \lambda)^{-1}h - (T - \lambda)\Gamma(\lambda)Q(\lambda)^{-1}\Gamma(\bar{\lambda})^* h = h$$

and now $k = (\widetilde{A} - \lambda)^{-1}h$ and (4.25) imply (4.22).

Assertion (iii) is a direct consequence of [11, Theorem 1.3]. □

The following corollaries can be proved in the same way as Corollary 3.5 and Corollary 3.6.

Corollary 4.5 *For $\lambda, \lambda_0 \in \rho(A)$ the following holds.*

(i) *$Q(\lambda)$ is a non-closed unbounded operator in $L^2(\mathcal{C})$ defined on $H^{3/2}(\mathcal{C})$ with* $\operatorname{ran} Q(\lambda) \subset H^{1/2}(\mathcal{C})$*;*
(ii) *$Q(\lambda) - \operatorname{Re} Q(\lambda_0)$ is a non-closed bounded operator in $L^2(\mathcal{C})$ defined on $H^{3/2}(\mathcal{C})$;*
(iii) *the closure $\widetilde{Q}(\lambda)$ of the operator $Q(\lambda) - \operatorname{Re} Q(\lambda_0)$ in $L^2(\mathcal{C})$ satisfies*

$$\frac{d}{d\lambda}\widetilde{Q}(\lambda) = \Gamma(\bar{\lambda})^* \overline{\Gamma(\lambda)}$$

and $\widetilde{Q}$ is a $\mathcal{L}(L^2(\mathcal{C}))$-valued Nevanlinna function.

Corollary 4.6 *For $\lambda \in \rho(A) \cap \rho(\widetilde{A})$ the following holds.*

(i) *$Q(\lambda)^{-1}$ is a non-closed bounded operator in $L^2(\mathcal{C})$ defined on $H^{1/2}(\mathcal{C})$ with* $\operatorname{ran} Q(\lambda)^{-1} = H^{3/2}(\mathcal{C})$*;*
(ii) *the closure $\overline{Q(\lambda)^{-1}}$ is a compact operator in $L^2(\mathcal{C})$;*
(iii) *the function $\lambda \mapsto -\overline{Q(\lambda)^{-1}}$ is a $\mathcal{L}(L^2(\mathcal{C}))$-valued Nevanlinna function.*

As a corollary of Theorem 4.4 we obtain a trace formula for the difference of the resolvents of A and $\widetilde{A}$.

Corollary 4.7 *Let the assumptions be as in Theorem* 4.4*, let $\widetilde{Q}$ be the Nevanlinna function from Corollary* 4.5 *and suppose, in addition, $n = 2$. Then*

$$\operatorname{tr}\Big((A - \lambda)^{-1} - (\widetilde{A} - \lambda)^{-1}\Big) = \operatorname{tr}\left(\overline{Q(\lambda)^{-1}}\frac{d}{d\lambda}\widetilde{Q}(\lambda)\right)$$

holds for all $\lambda \in \rho(A) \cap \rho(\widetilde{A})$.

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