FIRST ORDER OPERATORS AND BOUNDARY TRIPLES

OLAF POST

ABSTRACT. The aim of the present paper is to introduce a first order approach to the abstract concept of boundary triples for Laplace operators. Our main application is the Laplace operator on a manifold with boundary; a case in which the ordinary concept of boundary triples does not apply directly. In our first order approach, we show that we can use the usual boundary operators also in the abstract Green's formula. Another motivation for the first order approach is to give an intrinsic definition of the Dirichlet-to-Neumann map and intrinsic norms on the corresponding boundary spaces. We also show how the first order boundary triples can be used to define a usual boundary triple leading to a Dirac operator. *In memoriam Vladimir A. Geyler (1943-2007)*

1. INTRODUCTION

The concept of boundary triples, originally introduced in [V63], has successfully be applied to the theory of self-adjoint extensions of symmetric operators, for example on quantum graphs, singular perturbations or point interactions on manifolds (see e.g. [BGP08]). For a general treatment of boundary triples we refer to [BGP08, DHMdS06] and the references therein.

Our main purpose here is not to characterise all self-adjoint extensions of a given symmetric operator, but to show that the concept of boundary triples can also be used in the PDE case, namely to Laplacians on a manifold with boundary. The standard theory of boundary triples does not directly apply in this case, since Green's formula

$$\int_X \Delta \overline{f} g \,\mathrm{d}x - \int_X \overline{f} \Delta g \,\mathrm{d}x = \int_{\partial X} (\partial_{\mathrm{n}} \overline{f} g - \overline{f} \partial_{\mathrm{n}} g)\restriction_{\partial X}$$

does not extend to f, g in the maximal operator domain

$$\operatorname{dom} \Delta^{\max} = \{\, f \in \mathsf{L}_2(X) \mid \Delta^{\max} f \in \mathsf{L}_2(X) \text{ (distributional sense)} \,\}$$

(cf. Remark 4.2 for details). A solution to overcome this problem is either to modify the boundary operators (restriction of the function and the normal derivative onto ∂X) as e.g. in [BMNW07, Pc07], or to introduce the concept of *quasi* boundary triples as in [BL07] (cf. also the references therein for further treatments of boundary triples in the PDE case).

Here, we use a different approach: we start with *first order* operators, namely the exterior derivative d taking functions (0-forms) to 1-forms and its adjoint, the *divergence operator* δ, mapping 1-forms into functions, since the first order operator domains are simpler. The Laplacian (on functions) is then defined as $\Delta_0 := \delta\mathrm{d}$. Certainly, in our approach we do not cover all self-adjoint extensions of the minimal Laplacian.

The abstract approach also allows to define the Dirichlet-to-Neumann map in an intrinsic manner, and also the norm of $\mathscr{G}^{1/2} = \mathsf{H}^{1/2}(\partial X)$ is defined intrinsicly. This might be a great advantage when dealing with parameter-depending manifolds, as it is the case for graph-like manifolds (see e.g. [EP07, P06]). We will treat this question in a forthcoming publication. Our approach is related to the recent works of Arlinskii [A00], Behrndt and Langer [BL07], Posilicano [Pc07] and Brown et al. [BMNW07], where also a PDE example is treated in the context of boundary triples.

Date: February 21, 2008.

To precise our idea of the first order approach we sketch the construction here. The given data are[1]

$$\mathscr{H}_0, \quad \mathscr{H}_1, \qquad \mathrm{d}\colon \mathscr{H}_0 \dashrightarrow \mathscr{H}_1, \quad \mathscr{H}_0^1 := \operatorname{dom} \mathrm{d},$$

where $\mathscr{H}_p$ are Hilbert spaces ("p-forms"), and $\mathscr{H}_0^1$ carries the graph norm. Guided by our main application (a manifold with boundary), we call d an *exterior derivative.*

A boundary map (of order 0) is a bounded operator

$$\gamma_0 \colon \mathscr{H}_0^1 \longrightarrow \mathscr{G}, \qquad \mathscr{G}^{1/2} := \operatorname{ran} \gamma_0$$

with dense range $\mathscr{G}^{1/2} \subset \mathscr{G}$, where $\mathscr{G}$ is another Hilbert space (usually over the boundary).

For these data, we define $\mathrm{d}_0 := \mathrm{d}$ restricted to $\mathring{\mathscr{H}}_0^1 := \ker \gamma_0$ and the *divergence* operator $\delta := \mathrm{d}_0^*$ with domain $\mathscr{H}_1^1 := \operatorname{dom} \delta$. Furthermore, we can define a natural norm on $\mathscr{G}^{1/2}$ using γ_0.

In addition, we have a boundary operator of order 1, namely, $\gamma_1 \colon \mathscr{H}_1^1 \longrightarrow \mathscr{G}$, with the same range $\operatorname{ran} \gamma_1 = \operatorname{ran} \gamma_0 = \mathscr{G}^{1/2}$. Moreover, an abstract Green's formula is valid, i.e.,

$$\langle \mathrm{d} f_0, g_1 \rangle - \langle f_0, \delta g_1 \rangle = \langle \gamma_0 f_0, \gamma_1 g_1 \rangle_{\mathscr{G}^{1/2}}.$$

Finally, $h_p = \beta_p^z \varphi$ is the solution of the Dirichlet and Neumann problem

$$\Delta_p h_p = z h_p, \qquad \gamma_p h_p = \varphi,$$

respectively; we call β_p^z also a *Krein* Γ*-field of order* p.

The *Krein Q-function* is defined as

$$Q_0^z \varphi := \gamma_1 \mathrm{d} \beta_0^z;$$

a bounded operator (on the boundary space $\mathscr{G}^{1/2}$), closely related to the usual Dirichlet-to-Neumann map $\Lambda(z)$ on a manifold with boundary defined in Eq. (4.1).

The main idea here is to consider the Laplacian $\Delta_0 f_0 := \delta \mathrm{d} f_0$ on the space

$$\mathscr{H}_0^2 := \operatorname{dom} \delta \mathrm{d} := \{\, f_0 \in \operatorname{dom} \mathrm{d} \,\big|\, \mathrm{d} f_0 \in \operatorname{dom} \delta \,\}$$

instead of the maximal domain $\operatorname{dom} \Delta_0^{\max} = \{\, f_0 \in \mathscr{H}_0 \,|\, \Delta_0 f_0 \in \mathscr{H}_0 \,\}$. Although Δ_0 is not closed on $\mathscr{H}_0^2$, we can develop a suitable theory of boundary spaces. In particular, for a bounded and self-adjoint operator B in $\mathscr{G}^{1/2}$ we can show that the Laplacian Δ_0 restricted to

$$\operatorname{dom} \Delta_0^B := \{\, f_0 \in \mathscr{H}_0^2 \,|\, \gamma_1 \mathrm{d} f_0 = B \gamma_0 f_0 \,\}$$

(Robin-type boundary conditions) is self-adjoint under a suitable condition on the domain of the adjoint (fulfilled in our example of the Laplacian on a manifold with boundary). Our main result is Krein's resolvent formula for the resolvents of Δ_0^B and the Dirichlet Laplacian Δ_0^{D}; and a spectral relation between the operators Δ_0^B and $Q_0^z - B$, namely

$$\sigma(\Delta_0^B) \setminus \sigma(\Delta_0^{\mathrm{D}}) = \{\, z \notin \sigma(\Delta_0^{\mathrm{D}}) \,|\, 0 \in \sigma(Q_0^z - B) \,\}.$$

(see Theorem 2.30). The main advantage of our approach is that it can almost immediately be applied to the case of the Laplacian on a manifold with boundary, using the standard boundary operator (restriction of a function to the boundary and restriction of the normal component of a 1-form to the boundary).

The paper is organised as follows: In the next section, we develop the concept of first order boundary triples. In Section 3 we show how this concept fits into the usual theory of boundary triples. Section 4 contains our motivating example, namely, the Laplacian on a manifold with boundary.

[1]Here and in the sequel, $A\colon \mathscr{H}_0 \dashrightarrow \mathscr{H}_1$ denotes a partial map, i.e., a map (a linear operator) which is defined only on a subset $\operatorname{dom} A \subset \mathscr{H}_0$.

Acknowledgements. The author would like to dedicate this contribution to his dear colleague at the Humboldt University, Vladimir A. Geyler, who passed away very suddenly. The author acknowledges the financial support of the Collaborative Research Center SFB 647 "Space – Time – Matter. Analytic and Geometric Structures" in which Vladimir Geyler also was a member. Finally, the author would like to thank Y. Arlinskii for drawing his attention to the article [A00], where a very similar approach was used.

2. First order approach

In this section, we develop the concept of boundary triples for operators acting in different Hilbert spaces; guided by our main example of the exterior derivative on a manifold with boundary.

Definition 2.1. Let $\mathscr{H} = \mathscr{H}_0 \oplus \mathscr{H}_1$ and $\mathscr{G}$ be Hilbert spaces.

(i) Elements of $\mathscr{H}_p$ are referred to as *p-forms*.

(ii) A partial map $\mathrm{d}\colon \mathscr{H}_0 \dashrightarrow \mathscr{H}_1$ is called an *exterior derivative* if d is a closed map with dense domain $\mathscr{H}_0^1 := \operatorname{dom} \mathrm{d} \subset \mathscr{H}_0$. We endow $\mathscr{H}_0^1$ with the natural norm defined by

$$\|f_0\|^2_{\mathscr{H}_0^1} := \|f_0\|^2 + \|\mathrm{d} f_0\|^2.$$

(iii) We call $\gamma_0\colon \mathscr{H}_0^1 \longrightarrow \mathscr{G}$ a *boundary map (of degree* 0*)* associated to d iff γ_0 is bounded with dense image, and if $\mathring{\mathscr{H}}_0^1 := \ker \gamma_0 \subset \mathscr{H}_0^1 = \operatorname{dom} \mathrm{d}$ is dense in $\mathscr{H}_0$. The auxiliary Hilbert space is also referred to as a *boundary space*. We say that γ_0 is *proper*, if γ_0 is not surjective, i.e., if $\mathscr{G}^{1/2} := \gamma_0(\mathscr{H}_0^1) \subsetneq \mathscr{G}$.

(iv) The data $(\mathscr{H}, \mathscr{G}, \gamma_0)$ define a *first order boundary triple* for the exterior derivative $\mathrm{d}\colon \mathscr{H}_0 \dashrightarrow \mathscr{H}_1$ if γ_0 a boundary map associated to d.

Definition 2.2. We set $\mathrm{d}_0 := \mathrm{d}\restriction_{\mathring{\mathscr{H}}_0^1}$, and call $\delta := \mathrm{d}_0^*\colon \mathscr{H}_1 \dashrightarrow \mathscr{H}_0$ the *divergence operator* with domain $\mathscr{H}_1^1 := \operatorname{dom} \delta$ and $\mathring{\mathscr{H}}_1^1 := \operatorname{dom} \mathrm{d}^*$ (clearly, $\mathring{\mathscr{H}}_1^1 \subset \mathscr{H}_1^1$, and $\mathring{\mathscr{H}}_1^1$ is dense in $\mathscr{H}_1$ since d is densely defined). We endow $\mathscr{H}_1^1$ with the natural norm

$$\|f_1\|^2_{\mathscr{H}_1^1} := \|f_1\|^2 + \|\delta f_1\|^2.$$

Definition 2.3.

(i) We call $\Delta_0 := \delta\mathrm{d}$ the *Laplacian of degree* 0 with domain

$$\mathscr{H}_0^2 := \operatorname{dom} \delta\mathrm{d} := \big\{\, f_0 \in \operatorname{dom} \mathrm{d} \,\big|\, \mathrm{d} f_0 \in \operatorname{dom} \delta \,\big\}$$

Similarly, $\Delta_1 := \mathrm{d}\delta$ is called the *(maximal) Laplacian of degree* 1 with domain

$$\mathscr{H}_1^2 := \operatorname{dom} \mathrm{d}\delta := \big\{\, f_1 \in \operatorname{dom} \delta \,\big|\, \delta f_1 \in \operatorname{dom} \mathrm{d} \,\big\}.$$

We endow $\mathscr{H}_p^2$ with the norms

$$\|f_0\|^2_{\mathscr{H}_0^2} := \|f_0\|^2 + \|\mathrm{d} f_0\|^2 + \|\delta\mathrm{d} f_0\|^2,$$
$$\|f_1\|^2_{\mathscr{H}_0^2} := \|f_1\|^2 + \|\delta f_1\|^2 + \|\mathrm{d}\delta f_1\|^2.$$

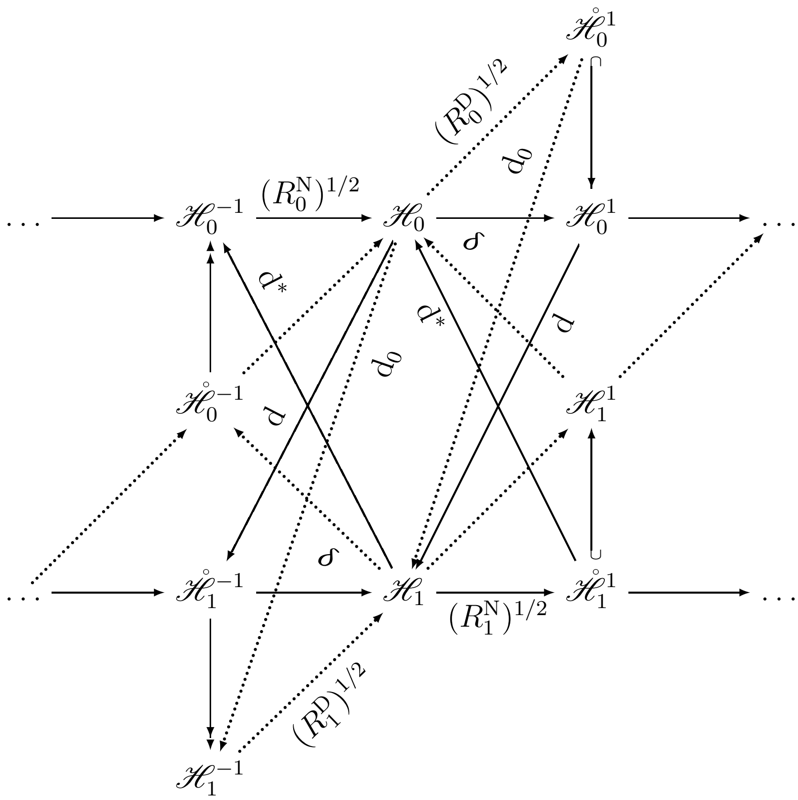
We denote the eigenspaces by $\mathscr{N}_p^z := \ker(\Delta_p - z) \subset \mathscr{H}_p^2$. For $z = -1$, we set $\mathscr{N}_p := \mathscr{N}_p^{-1}$.

(ii) We call

$$\Delta_0^{\mathrm{D}} := \mathrm{d}_0^*\mathrm{d}_0, \qquad \Delta_0^{\mathrm{N}} := \mathrm{d}^*\mathrm{d},$$
$$\Delta_1^{\mathrm{D}} := \mathrm{d}_0\mathrm{d}_0^*, \qquad \Delta_1^{\mathrm{N}} := \mathrm{d}\mathrm{d}^*$$

with the appropriate domains the *Dirichlet Laplacian of degree* $p = 0, 1$ and the *Neumann Laplacian of degree* $p = 0, 1$, respectively. Clearly, all these operators are self-adjoint and non-negative. We denote the corresponding resolvents by $R_p^{\mathrm{D}} := (\Delta_p^{\mathrm{D}} + 1)^{-1}$ and $R_p^{\mathrm{N}} := (\Delta_p^{\mathrm{N}} + 1)^{-1}$.

The following diagram tries to illustrate the two scales of Hilbert spaces associated to d, d^* and d_0, $\mathrm{d}_0^* = \delta$ (dotted arrows). Note that only at order 1, 0 and -1, we have relations between the two scales:



(2.1)

Remark 2.4.

(i) The spaces $\mathscr{H}_p^2$ are complete, i.e., Hilbert spaces with their natural norms.

(ii) Note that Δ_p is a bounded operator on $\mathscr{H}_p^2$. However, Δ_p with $\operatorname{dom} \Delta_p = \mathscr{H}_p^2$ is *not* closed. Although we call Δ_p the *maximal* Laplacian, it is not the maximal operator $\Delta_p^{\max}$ in the usual sens (which is the operator closure of Δ_p with domain

$$\operatorname{dom} \Delta_p^{\max} := \left\{ f_p \in \mathscr{H}_p \,\middle|\, \Delta_p f_p \in \mathscr{H}_p \right\} \tag{2.2}$$

in the distributional sense). In general, $\mathscr{H}_p^2 \subsetneq \operatorname{dom} \Delta_p^{\max}$. This observation is one of the motivations for our first order approach (see Section 4).

Lemma 2.5. *We have* $\mathscr{H}_p^1 = \mathring{\mathscr{H}}_p^1 \oplus \mathscr{N}_p$ *(orthogonal sum).*

Proof. Let $p = 0$ and $f_0 \in \mathscr{H}_0^1$. In this case, $f_0 \in (\mathring{\mathscr{H}}_0^1)^\perp$ is equivalent to

$$0 = \langle f_0, g_0 \rangle_{\mathscr{H}_0^1} = \langle f_0, g_0 \rangle_{\mathscr{H}_0} + \langle \mathrm{d} f_0, \mathrm{d} g_0 \rangle_{\mathscr{H}_1}, \qquad \forall\, g_0 \in \mathring{\mathscr{H}}_0^1. \tag{2.3}$$

However, by definition of the adjoint operator $\delta = \mathrm{d}_0^*$, we have $h_1 \in \operatorname{dom} \mathrm{d}_0^*$ iff there exists $h_0 \in \mathscr{H}_0$ such that

$$\langle h_1, \mathrm{d}_0 g_0 \rangle_{\mathscr{H}_0} = \langle h_0, g_0 \rangle_{\mathscr{H}} \qquad \forall\, g_0 \in \mathring{\mathscr{H}}_0^1. \tag{2.4}$$

Choosing $h_0 = -f_0$, the orthogonality relation (2.3) reads $h_1 = \mathrm{d} f_0 \in \operatorname{dom} \mathrm{d}_0^*$ and $\mathrm{d}_0^* \mathrm{d} f_0 = -f_0$, i.e., $f_0 \in \mathscr{N}_0^z$. The argument for $p = 1$ is similar. $\square$

Lemma 2.6. *The maps* $\mathrm{d} \colon \mathscr{N}_0 \longrightarrow \mathscr{N}_1$ *and* $\delta \colon \mathscr{N}_1 \longrightarrow \mathscr{N}_0$ *are unitary.*

Proof. If $f_0 \in \mathscr{N}_0$ then $\mathrm{d}\delta\mathrm{d} f_0 = -\mathrm{d} f_0$, i.e, $\mathrm{d} f_0 \in \mathscr{N}_1$. Similarly, $f_1 \in \mathscr{N}_1$ implies $\delta f_1 \in \mathscr{N}_0$. Furthermore, $-\delta \mathrm{d} f_0 = f_0$ and $\mathrm{d}(-\delta f_1) = f_1$ implies that $-\delta$ is the inverse of d. Finally, d is an isometry because

$$\|\mathrm{d} f_0\|^2_{\mathscr{H}_1^1} = \|\mathrm{d} f_0\|^2_{\mathscr{H}_1} + \|\delta \mathrm{d} f_0\|^2_{\mathscr{H}_0} = \|\mathrm{d} f_0\|^2_{\mathscr{H}_1} + \|f_0\|^2_{\mathscr{H}_0} = \|f_0\|^2_{\mathscr{H}_0^1}.$$

Since d is surjective, it is therefore unitary with unitary inverse $-\delta$. $\square$

Lemma 2.7. *Assume that the boundary map γ_0 is proper (i.e., $\mathscr{G}^{1/2} = \operatorname{ran}\gamma_0 \subsetneq \mathscr{G}$). Define $\hat\gamma_0 := \gamma_0\restriction_{\mathscr{N}_0}$, then $\hat\gamma_0$ is invertible and $(\hat\gamma_0)^{-1}\colon \mathscr{G} \dashrightarrow \mathscr{N}_0$ is an unbounded operator with domain $\operatorname{dom}(\hat\gamma_0)^{-1} = \mathscr{G}^{1/2}$. Furthermore, $(\hat\gamma_0)^{-1}\varphi = h_0$ is the (unique) solution of the Dirichlet problem*

$$(\Delta_0 + 1)h_0 = 0, \qquad \gamma_0 h_0 = \varphi.$$

Proof. The operator $\hat\gamma_0$ is invertible since $(\ker\gamma_0)^\perp = (\mathring{\mathscr{H}}_0^1)^\perp = \mathscr{N}_0$ by Lemma 2.5. If $(\hat\gamma_0)^{-1}$ were be bounded, then $\hat\gamma_0$ would be a topological isomorphism of $\mathscr{N}_0$ and $\operatorname{ran}\gamma_0 = \mathscr{G}^{1/2}$, in particular, $\mathscr{G}^{1/2}$ would be closed in $\mathscr{G}$, and by the density, we would have $\mathscr{G}^{1/2} = \mathscr{G}$ — a contradiction. The last assertion is an immediate consequence of Lemma 2.5 and the definition of the inverse map $(\hat\gamma_0)^{-1}$. $\square$

Definition 2.8. We endow $\mathscr{G}^{1/2}$ with the norm

$$\|\varphi\|_{\mathscr{G}^{1/2}} := \|(\hat\gamma_0)^{-1}\varphi\|_{\mathscr{H}_0^1}.$$

Lemma 2.9. *Assume that the boundary map γ_0 is proper (i.e., $\mathscr{G}^{1/2} = \operatorname{ran}\gamma_0 \subsetneq \mathscr{G}$), then the following assertions hold:*

(i) *We have $\|\varphi\|_{\mathscr{G}} \le \|\gamma_0\|\,\|\varphi\|_{\mathscr{G}^{1/2}}$ for $\varphi \in \mathscr{G}^{1/2}$.*

(ii) *The operator $\gamma_0\gamma_0^* \ge 0$ is invertible in $\mathscr{G}$, and*

$$\Lambda := (\gamma_0\gamma_0^*)^{-1} = ((\hat\gamma_0)^{-1})^*(\hat\gamma_0)^{-1} \ge \frac{1}{\|\gamma_0\|^2}.$$

We define the associated scale of Hilbert spaces by

$$\mathscr{G}^s := \operatorname{dom}\Lambda^s, \qquad \|\varphi\|_{\mathscr{G}^s} := \|\Lambda^s\varphi\|_{\mathscr{G}}$$

for $s \ge 0$ (and the dual with respect to $(\cdot,\cdot)_{\mathscr{G}}$ for $s < 0$).

(iii) *The operator $((\hat\gamma_0)^{-1})^*\colon \mathscr{N}_0 \dashrightarrow \mathscr{G}$ is unbounded with domain*

$$\operatorname{dom}((\hat\gamma_0)^{-1})^* = \{\, f_0 \in \mathscr{N}_0 \mid \gamma_0 f_0 \in \operatorname{dom}\Lambda = \mathscr{G}^1 \,\}.$$

(iv) *The operator $\gamma_0^*\colon \mathscr{G} \longrightarrow \mathscr{H}_0^1$ is bounded, and $\gamma_0^*\varphi = h_0$ is the unique Neumann solution, i.e.,*

$$(\Delta_0 + 1)h_0 = 0, \qquad \gamma_0 h_0 \in \mathscr{G}^1, \quad \Lambda\gamma_0 h_0 = \varphi.$$

Remark 2.10. If γ_0 is not proper (i.e., if γ_0 is surjective, i.e., $\mathscr{G}^{1/2} = \mathscr{G}$), then all the above assertions remain valid except for the fact that $(\hat\gamma_0)^{-1}$, $((\hat\gamma_0)^{-1})^*$ and Λ are *bounded* operators.

Proof. The first assertion follows from

$$\|\varphi\|_{\mathscr{G}} = \|\hat\gamma_0(\hat\gamma_0)^{-1}\varphi\|_{\mathscr{G}} \le \|\gamma_0\|\,\|(\hat\gamma_0)^{-1}\varphi\|_{\mathscr{H}^1} = \|\gamma_0\|\,\|\varphi\|_{\mathscr{G}^{1/2}}.$$

To prove the second, note that $\gamma_0\gamma_0^* = \hat\gamma_0\hat\gamma_0^*$ is bijective and

$$\langle\varphi,\varphi\rangle_{\mathscr{G}^{1/2}} = \langle(\hat\gamma_0)^{-1}\varphi, (\hat\gamma_0)^{-1}\varphi\rangle_{\mathscr{H}^1} = \langle\varphi, ((\hat\gamma_0)^{-1})^*(\hat\gamma_0)^{-1}\varphi\rangle_{\mathscr{G}} = \langle\varphi,\Lambda\varphi\rangle_{\mathscr{G}}$$

if $(\hat\gamma_0)^{-1}\varphi \in \operatorname{dom}((\hat\gamma_0)^{-1})^*$, i.e, $\varphi \in \operatorname{dom}\Lambda$. Furthermore, $\|\Lambda^{-1}\| \le \|\gamma_0\|^2$.

The third assertion is a consequence of Lemma 2.7, and the domain characterisation can be seen readily. To prove the fourth assertion, take $h_0 = \gamma_0^*\varphi \in \operatorname{ran}\gamma_0^* \subset (\ker\gamma_0)^\perp = \mathscr{N}_0$; in this case

$$\langle h_0, f_0\rangle_{\mathscr{H}_0^1} = \langle\varphi, \gamma_0 f_0\rangle_{\mathscr{G}}$$

for all $f_0 \in \mathscr{H}_0^1$. If $f_0 \in \mathscr{N}_0$, then

$$\langle h_0, f_0\rangle_{\mathscr{H}_0^1} = \langle\gamma_0 h_0, \gamma_0 f_0\rangle_{\mathscr{G}^{1/2}}$$

by definition of the norm on $\mathscr{G}^{1/2}$. But the latter term equals $\langle\Lambda\gamma_0 h_0, \gamma_0 f_0\rangle_{\mathscr{G}}$ if $\gamma_0 h_0 \in \operatorname{dom}\Lambda$, and thus $\varphi = \Lambda\gamma_0 h_0$. $\square$

Remark 2.11. Note that $\mathscr{G}^{-1/2}$ is the completion of $\mathscr{G}$ with respect to the norm $\|\varphi\|_{\mathscr{G}^{-1/2}} = \|\gamma_0\varphi\|_{\mathscr{H}^1_0}$.

Definition 2.12. We define the *boundary map of order* 1 as

$$\gamma_1 \colon \mathscr{H}^1_1 \longrightarrow \mathscr{G}, \qquad \gamma_1 := -\gamma_0 \delta P_1$$

where P_p is the orthogonal projection in $\mathscr{H}^1_p$ onto the subspace $\mathscr{N}_p$.

Lemma 2.13. *We have* $\ker \gamma_1 = \mathring{\mathscr{H}}^1_1$*, and* $\gamma_1 \colon \mathscr{H}^1_1 \longrightarrow \mathscr{G}$ *is bounded with norm* $\|\gamma_1\| = \|\gamma_0\|$*. Furthermore,* $\operatorname{ran}\gamma_1 = \mathscr{G}^{1/2}$ *and* $\hat\gamma_1 := \gamma_1\restriction_{\mathscr{N}_1}$ *is a unitary map from* $\mathscr{N}_1$ *onto* $\mathscr{G}^{1/2}$*.*

Proof. If $f_1 \in \mathring{\mathscr{H}}^1_1 = (\mathscr{N}_1)^\perp$, then $\gamma_1 f_1 = 0$ since $P_1 f_1 = 0$. If $f_1 \in \mathscr{N}_1$, then $\gamma_1 f_1 = -\gamma_0\delta f_1 = 0$ iff $f_1 = 0$ since δ is unitary from $\mathscr{N}_1$ onto $\mathscr{N}_0 = (\ker\gamma_0)^\perp$.

The boundedness follows from

$$\|\gamma_1 f_1\|_{\mathscr{G}} \le \|\gamma_0\delta P_1 f_1\|_{\mathscr{G}} \le \|\gamma_0\|\,\|\delta P_1 f_1\|_{\mathscr{H}^1_0} = \|\gamma_0\|\,\|P_1 f_1\|_{\mathscr{H}^1_1} \le \|\gamma_0\|\,\|f_1\|_{\mathscr{H}^1_1}$$

by Lemma 2.6. Furthermore, for $f_0 \in \mathscr{N}_0$ set $f_1 := \mathrm{d} f_0$, then $\gamma_1 f_1 = -\gamma_0\delta\mathrm{d} f_0 = \gamma_0 f_0$. In particular, $\|\gamma_1\| = \|\gamma_0\|$. Finally,

$$\|\hat\gamma_1 f_1\|_{\mathscr{G}^{1/2}} = \|\gamma_0\delta f_1\|_{\mathscr{G}^{1/2}} = \|\delta f_1\|_{\mathscr{H}^1_0} = \|f_1\|_{\mathscr{H}^1_1}$$

for $f_1 \in \mathscr{N}_1$, since $\delta f_1 \in \mathscr{N}_0$ and by Lemma 2.6. □

Lemma 2.14. *The (abstract) Green's formula holds, namely,*

$$\langle \mathrm{d} f_0, g_1\rangle - \langle f_0, \delta g_1\rangle = \langle \gamma_0 f_0, \gamma_1 g_1\rangle_{\mathscr{G}^{1/2}} = (\gamma_0 f_0, \widetilde\gamma_1 g_1)_{\mathscr{G}}$$

where $\widetilde\gamma_1 := \Lambda\gamma_1 \colon \mathscr{H}^1_1 \longrightarrow \mathscr{G}^{-1/2}$*.*

Proof. If $f_0 \in \mathring{\mathscr{H}}^1_0$, then the LHS vanishes since $\delta = \mathrm{d}_0^*$, and so is the RHS, since $\gamma_0 f_0 = 0$. Similarly, if $g_1 \in \mathring{\mathscr{H}}^1_1 = \operatorname{dom}\mathrm{d}^*$, then the LHS vanishes since $\delta g_1 = \mathrm{d}^* g_1$ and so is the RHS, because $\gamma_1 g_1 = 0$ by Lemma 2.13. For $f_0 \in \mathscr{N}_0$ and $g_1 \in \mathscr{N}_1$, we have

$$\begin{aligned}\langle \mathrm{d} f_0, g_1\rangle - \langle f_0, \delta g_1\rangle &= -\langle \mathrm{d} f_0, \mathrm{d}\delta g_1\rangle - \langle f_0, \delta g_1\rangle \\ &= -\langle f_0, \delta g_1\rangle_{\mathscr{H}^1_0} = \langle \gamma_0 f_0, -\gamma_0\delta g_1\rangle_{\mathscr{G}^{1/2}}\end{aligned}$$

by Definition 2.8. The last assertion is obvious. □

Corollary 2.15. *We have*

$$\begin{aligned}\langle \Delta_0 f_0, g_0\rangle - \langle f_0, \Delta_0 g_0\rangle &= \langle \gamma_0 f_0, \gamma_1 \mathrm{d} g_0\rangle_{\mathscr{G}^{1/2}} - \langle \gamma_1 \mathrm{d} f_0, \gamma_0 g_0\rangle_{\mathscr{G}^{1/2}} \\ &= \langle \gamma_0 f_0, \widetilde\gamma_1 \mathrm{d} g_0\rangle_{\mathscr{G}} - \langle \widetilde\gamma_1 \mathrm{d} f_0, \gamma_0 g_0\rangle_{\mathscr{G}}\end{aligned}$$

for $f_0, g_0 \in \mathscr{H}^2_0$*.*

The following lemma shows that $\Lambda = \Lambda(-1)$ is the Dirichlet-to-Neumann map for the operator $\Delta_0 + 1$:

Lemma 2.16. *For* $\varphi \in \mathscr{G}^{1/2}$ *and* $h_0 := (\hat\gamma_0)^{-1}\varphi$ *we have*

$$\Lambda\varphi = \widetilde\gamma_1 \mathrm{d} h_0.$$

Proof. By Lemma 2.14, we have

$$\langle \mathrm{d} f_0, \mathrm{d} h_0\rangle - \langle f_0, \Delta_0 h_0\rangle = (\gamma_0 f_0, \widetilde\gamma_1 \mathrm{d} h_0)_{\mathscr{G}}.$$

On the other hand, we have

$$\langle \mathrm{d} f_0, \mathrm{d} h_0\rangle - \langle f_0, \Delta_0 h_0\rangle = \langle f_0, h_0\rangle_{\mathscr{H}^1_0} = \langle \gamma_0 f_0, \gamma_0 h_0\rangle_{\mathscr{G}^{1/2}} = \langle \gamma_0 f_0, \varphi\rangle_{\mathscr{G}^{1/2}} = (\gamma_0 f_0, \Lambda\varphi)_{\mathscr{G}}.$$

for $f_0, h_0 \in \mathscr{N}_0$. □

Remark 2.17. The map $\widetilde{\gamma}_1$ is indeed the boundary map occuring in the applications (see Section 4). Namely, the Green's formula is usually formulated with a boundary integral given as an inner product of $\mathscr{G}$ rather than $\mathscr{G}^{1/2}$. In particular, $\widetilde{\gamma}_1 \mathrm{d} h_0$ is the "normal derivative at the boundary" (in the case of a manifold with boundary).

The boundary maps are also bounded as maps with target space $\mathscr{G}^{1/2}$:

Lemma 2.18. *The operators $\gamma_p \colon \mathscr{H}^1_p \longrightarrow \mathscr{G}^{1/2}$ are bounded with norm bounded by* 1.

Proof. For $p = 0$, we have

$$\|\gamma_0 f_0\|_{\mathscr{G}^{1/2}} = \|(\hat{\gamma}_0)^{-1}\gamma_0 f_0\|_{\mathscr{H}^1_0} = \|(\hat{\gamma}_0)^{-1}\gamma_0 P_0 f_0\|_{\mathscr{H}^1_0} = \|P_0 f_0\|_{\mathscr{H}^1_0} \le \|f_0\|_{\mathscr{H}^1_0},$$

since $\gamma_0 f_0 = \gamma_0 P_0 f_0$. For $p = 1$, we obtain

$$\|\gamma_1 f_1\|_{\mathscr{G}^{1/2}} = \|(\hat{\gamma}_0)^{-1}\gamma_0 \delta P_1 f_1\|_{\mathscr{H}^1_0} = \|\delta P_1 f_1\|_{\mathscr{H}^1_0} = \|P_1 f_1\|_{\mathscr{H}^1_1} \le \|f_1\|_{\mathscr{H}^1_1}$$

using Lemmas 2.6–2.7. □

In order to define the Dirichlet-to-Neumann map also for other resolvent values z, we need to provide results similar to those in Lemmas 2.5–2.7 for general z. Write

$$\Sigma_0 := \sigma(\Delta_0^{\mathrm{D}}), \qquad \Sigma_1 := \sigma(\Delta_1^{\mathrm{N}}). \tag{2.5}$$

Lemma 2.19. *For $z \notin \Sigma_p$, we have $\mathscr{H}^1_p = \mathring{\mathscr{H}}^1_p \dotplus \mathscr{N}^z_p$ (topological direct sum). In particular, $\hat{\gamma}^z_p := \gamma_p \restriction_{\mathscr{N}^z_p}$ is a topological isomorphism from $\mathscr{N}^z_p$ onto $\mathscr{G}^{1/2}$.*

Proof. For $z \notin \sigma(\Delta_0^{\mathrm{D}})$, we define

$$P^z_0 := 1 - \iota_0(\Delta^{\mathrm{D}}_0 - z)^{-1}(\Delta_0 - z) \colon \mathscr{H}^1_0 \longrightarrow \mathscr{H}^1_0$$

where

$$\Delta_0 = \delta \mathrm{d} \colon \mathscr{H}^1_0 \longrightarrow \mathring{\mathscr{H}}^{-1}_0, \qquad (\Delta^{\mathrm{D}}_0 - z)^{-1} = (\delta \mathrm{d}_0 - z)^{-1} \colon \mathring{\mathscr{H}}^{-1}_0 \longrightarrow \mathring{\mathscr{H}}^1_0$$

and $\iota_0 \colon \mathring{\mathscr{H}}^1_0 \hookrightarrow \mathscr{H}^1_0$. A simple calculation shows that $(1 - P^z_0)^2 = (1 - P^z_0)$, i.e., $1 - P^z_0$ and therefore P^z_0 are projections. Furthermore, $f_0 = P^z_0 f_0$ is equivalent to $\Delta_0 f_0 = z f_0$. In order to show that $f_0 = P^z_0 f_0 \in \mathscr{N}^z_0$ let us first show that $f_0 \in \mathscr{H}^2_0$, i.e., that $h_1 := \mathrm{d} f_0 \in \mathscr{H}^1_1 = \operatorname{dom} \delta$. To this end, recall the definition of the domain $\operatorname{dom} \delta = \operatorname{dom} \mathrm{d}_0^*$ in (2.4). We have here

$$\langle \mathrm{d} f_0, \mathrm{d}_0 g_0 \rangle = \langle \delta \mathrm{d} f_0, g_0 \rangle = \langle z f_0, g_0 \rangle$$

by Lemma 2.14 (note that $\gamma_0 g_0 = 0$) and the fact that $\delta \mathrm{d} f_0 = z f_0$; we can choose $h_0 = z f_0$ and therefore $f_0 \in \mathscr{H}^2_0$. A straightforward calculation shows now that $(\Delta_0 - z) f_0 = 0$, and finally, $f_0 \in \mathscr{N}^z_0$.

By the definition of P^z_0, it is also clear that $\operatorname{ran}(1 - P^z_0) \subset \mathring{\mathscr{H}}^1_0$, and therefore $\mathscr{H}^1_0$ splits into the direct sum. The direct sum is also a topological sum, since $1 - P^z_0$ and P^z_0 are bounded maps. Therefore $f_0 \mapsto ((1 - P^z_0) f_0, P^z_0 f_0)$ is a bounded bijection, and also a topological isomorphism. The argument for 1-forms is similar, using

$$P^z_1 := 1 - \iota_1(\Delta^{\mathrm{N}}_1 - z)^{-1}(\Delta_1 - z) \colon \mathscr{H}^1_1 \longrightarrow \mathscr{H}^1_1$$

where

$$\Delta_1 = \mathrm{d} \delta \colon \mathscr{H}^1_1 \longrightarrow \mathring{\mathscr{H}}^{-1}_1, \qquad (\Delta^{\mathrm{N}}_1 - z)^{-1} = (\mathrm{d}\mathrm{d}^* - z)^{-1} \colon \mathring{\mathscr{H}}^{-1}_1 \longrightarrow \mathring{\mathscr{H}}^1_1$$

and $\iota_1 \colon \mathring{\mathscr{H}}^1_1 \hookrightarrow \mathscr{H}^1_1$.

For the last assertion, note that $\ker \gamma_p = \mathring{\mathscr{H}}^1_p$ and that $\operatorname{ran} \gamma_p = \mathscr{G}^{1/2}$ (see Lemma 2.13); in particular, $\hat{\gamma}^z_p$ is bijective. Furthermore, $\hat{\gamma}^z_p$ is bounded as restriction of the bounded map $\gamma_p \colon \mathscr{H}^1_p \longrightarrow \mathscr{G}^{1/2}$ (cf. Lemma 2.18), and therefore, $\hat{\gamma}^z_p$ is a topological isomorphism. □

Lemma 2.20. *For $z \neq 0$, the maps* $\mathrm{d}\colon \mathscr{N}_0^z \longrightarrow \mathscr{N}_1^z$ *and* $\delta\colon \mathscr{N}_1^z \longrightarrow \mathscr{N}_0^z$ *are topological isomorphisms.*

Proof. If $f_0 \in \mathscr{N}_0^z$ then $\mathrm{d}\delta\mathrm{d} f_0 = z\mathrm{d} f_0$, i.e, $\mathrm{d} f_0 \in \mathscr{N}_1^z$. Similarly, $f_1 \in \mathscr{N}_1^z$ implies $\delta f_1 \in \mathscr{N}_0^z$. Furthermore, $\frac{1}{z}\delta\mathrm{d} f_0 = f_0$ and $\mathrm{d}(\frac{1}{z}\delta f_1) = f_1$ implies that $\frac{1}{z}\delta$ is the inverse of d. Finally, d is bounded on $\mathscr{N}_0^z$, since

$$\|\mathrm{d} f_0\|^2_{\mathscr{H}_1^1} = \|\mathrm{d} f_0\|^2_{\mathscr{H}_1} + \|\delta\mathrm{d} f_0\|^2_{\mathscr{H}_0} = \|\mathrm{d} f_0\|^2_{\mathscr{H}_1} + |z|^2\|f_0\|^2_{\mathscr{H}_0} \le (1+|z|^2)\|f_0\|^2_{\mathscr{H}_0^1}$$

and therefore a topological isomorphism. The assertion for δ follows similarly. ☐

Definition 2.21. We call $z \mapsto \beta_0^z := (\hat\gamma_0^z)^{-1}$, $z \notin \Sigma_0$ the *Dirichlet solution map* or the *Krein Γ-field of order* 0 associated to the first order boundary triple $(\mathscr{H}, \mathscr{G}, \gamma_0)$. Similarly, we call $z \mapsto \beta_1^z := (\hat\gamma_1^z)^{-1}$, $z \notin \Sigma_1$ the *Neumann solution map* or the *Krein Γ-field of order* 1.

Remark 2.22.

(i) We prefer to use the symbol β instead of γ for the Krein Γ-field in order to avoid confusion with our boundary maps γ_p.

(ii) The maps $\beta_p^z\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{N}_p^z \subset \mathscr{H}_p^1$ are topological isomorphisms, since the inverses $\hat\gamma_p^z$ are.

(iii) The names "Dirichlet/Neumann solution map" are due to the following fact: The p-form $h_p := \beta_p^z\varphi$ is the solution of $(\Delta_p - z)h_p = 0$, and $\gamma_p h_p = \varphi$. For $p = 0$, this is the solution of the "Dirichlet problem" ($\gamma_0 h_0$ prescribed), and for $p = 1$, the solution of the "Neumann problem" ($\gamma_1 h_1$ prescribed). We will see in Lemma 3.7 that the Krein Γ-fields are related to a Krein Γ-field in the sense of an ordinary boundary triple.

(iv) The map $\beta_0^z\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{H}_0^1$ regarded as an operator $\beta_0^z\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{H}_0$ into $\mathscr{H}_0$ is bounded, as well as its adjoint, denoted by $(\beta_0^{\bar z})^*\colon \mathscr{H}_0 \longrightarrow \mathscr{G}^{1/2}$.

Lemma 2.23. *We have* $\gamma_1\mathrm{d} f_0 = (\beta_0^{\bar z})^*(\Delta_0 - z)f_0$ *for* $f_0 \in \operatorname{dom}\Delta_0^{\mathrm{D}} = \mathscr{H}_0^2 \cap \mathring{\mathscr{H}}_0^1$ *where* $(\beta_0^{\bar z})^*$ *is the adjoint of* $\beta_0^{\bar z}$ *as operator* $\beta_0^z\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{H}_0$. *Furthermore,* $\operatorname{ran}(\beta_0^{\bar z})^* = \mathscr{G}^{1/2}$.

Proof. The assertion follows from (see also [BGP08, Thm. 1.23 (2d)])

$$\begin{aligned}\langle \varphi, (\beta_0^{\bar z})^*(\Delta_0 - z)f_0\rangle_{\mathscr{G}^{1/2}} &= \langle \beta_0^z\varphi, (\Delta_0 - z)f_0\rangle_{\mathscr{H}} \\ &= \langle (\Delta_0 - z)\beta_0^z\varphi, f_0\rangle_{\mathscr{H}} + \langle \gamma_0\beta_0^z\varphi, \gamma_1\mathrm{d} f_0\rangle_{\mathscr{G}^{1/2}} - \langle \gamma_1\mathrm{d}\beta_0^z\varphi, \gamma_0 f_0\rangle_{\mathscr{G}^{1/2}} \\ &= \langle \varphi, \gamma_1\mathrm{d} f_0\rangle_{\mathscr{G}^{1/2}}\end{aligned}$$

by Corollary 2.15 for the second equality. As far as the third equality is concerned, note that the first term vanishes since $\beta_0^z\varphi$ solves the eigenvalue equation; the same holds for the third term since $\gamma_0 f_0 = 0$ for $f_0 \in \mathring{\mathscr{H}}_0^1$. For the second term, we have $\gamma_0\beta_0^z\varphi = \varphi$ by the definition of β_0^z. The last assertion follows from $\operatorname{ran}(\beta_0^{\bar z})^* = (\ker\beta_0^{\bar z})^\perp$ and from the fact that $\beta_0^{\bar z}\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{H}_0$ is injective. ☐

We can now define the Dirichlet-to-Neumann map and a closely related map for arbitrary resolvent values z:

Definition 2.24. The *Krein Q-function* associated to the first order boundary triple $(\mathscr{H}, \mathscr{G}, \gamma_0)$ is the map

$$z \mapsto Q_0^z := \gamma_1\mathrm{d}(\hat\gamma_0^z)^{-1} = \gamma_1\mathrm{d}\beta_0^z, \qquad z \notin \Sigma_0 = \sigma(\Delta_0^{\mathrm{D}}).$$

For $z \notin \Sigma_0$, the *abstract Dirichlet-to-Neumann map at z* is defined by

$$\Lambda(z) := \Lambda Q_0^z = \Lambda\gamma_1\mathrm{d}\beta_0^z = \widetilde\gamma_1\mathrm{d}\beta_0^z\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{G}^{-1/2}.$$

Remark 2.25.

(i) We shall see in Section 3 that Q_0^z is indeed a Krein Q-function for an ordinary boundary triple. Note that $Q_0^z\colon \mathscr{G}^{1/2} \longrightarrow \mathscr{G}^{1/2}$ is a bounded map (cf. Lemmas 2.18–2.20). In addition, we have

$$Q_0^{-1} = \gamma_1 \mathrm{d}(\hat{\gamma}_0)^{-1} = -\gamma_0 \delta P_1 \mathrm{d}(\hat{\gamma}_0)^{-1} = \gamma_0(\hat{\gamma}_0)^{-1} = \mathrm{id}_{\mathscr{G}^{1/2}}$$

at $z = -1$.

(ii) Note that $\Lambda(z)$ is indeed the Dirichlet-to-Neumann map: We solve the Dirichlet problem $h_0 = \beta_0^z \varphi$, i.e,

$$\Delta_0 h_0 = z h_0, \qquad \gamma_0 h_0 = \varphi;$$

and the Dirichlet-to-Neumann map is the "normal derivative at the boundary" of h_0 (cf. Remark 2.17), i.e., $\Lambda(z)\varphi = \widetilde{\gamma}_1 \mathrm{d} h_0$.

Let us now define self-adjoint restrictions of Δ_0.

Definition 2.26. Let B be a bounded operator in $\mathscr{G}^{1/2}$. We set

$$\begin{aligned} \operatorname{dom} \Delta_0^B &:= \{\, f_0 \in \mathscr{H}_0^2 \mid \gamma_1 \mathrm{d} f_0 = B \gamma_0 f_0 \,\} \\ \operatorname{dom} \Delta_1^B &:= \{\, f_1 \in \mathscr{H}_1^2 \mid \gamma_1 f_1 = B \gamma_0 \delta f_1 \,\} \end{aligned}$$

and denote by Δ_p^B the restriction of Δ_p onto $\operatorname{dom} \Delta_p^B$.

Lemma 2.27. *Assume that* $\operatorname{dom}(\Delta_0^B)^* \subset \mathscr{H}_0^1$*, then the operator* Δ_0^B *is self-adjoint iff* B *is self-adjoint in* $\mathscr{G}^{1/2}$.

Remark 2.28. The domain condition does not seem to follow from abstract ("soft") arguments; in our manifold example, it follows from elliptic regularity ("hard" arguments). Note that in general, $\operatorname{dom} \Delta_0^{\max}$ defined in (2.2) is even not a subset of $\mathscr{H}_0^1$ (see Remark 2.4 (ii) and Remark 4.2).

Proof. The graph of the operator $(\Delta_0^B)^*$ is given as

$$\begin{aligned} \operatorname{graph}(\Delta_0^B)^* = \Big\{ (f_0, \Delta_0 f_0) \,\Big|\, & f_0 \in \operatorname{dom} \Delta_0^{\max}, \\ & \forall\, g_0 \in \operatorname{dom} \Delta_0^B \colon \langle \Delta_0^{\max} f_0, g_0 \rangle = \langle f_0, \Delta_0^{\max} g_0 \rangle \Big\} \subset \mathscr{H}_0^1 \times \mathscr{H}_0, \end{aligned}$$

and the latter inclusion holds by our assumption on the domain of the adjoint. In particular, $f_0, g_0 \in \mathscr{H}_0^2$ and we can apply Corollary 2.15, namely,

$$\begin{aligned} \langle \Delta_0^{\max} f_0, g_0 \rangle - \langle f_0, \Delta_0^{\max} g_0 \rangle &= \langle \gamma_0 f_0, \gamma_1 \mathrm{d} g_0 \rangle_{\mathscr{G}^{1/2}} - \langle \gamma_1 \mathrm{d} f_0, \gamma_0 g_0 \rangle_{\mathscr{G}^{1/2}} \\ &= \langle \gamma_0 f_0, B \gamma_0 g_0 \rangle_{\mathscr{G}^{1/2}} - \langle B \gamma_0 f_0, \gamma_0 g_0 \rangle_{\mathscr{G}^{1/2}}, \end{aligned}$$

and the latter equality follows from $f_0, g_0 \in \operatorname{dom} \Delta_0^B$. The assertion is now obvious. □

The self-adjointness of B in $\mathscr{G}^{1/2}$ can be shown as follows:

Lemma 2.29. *Let* $\widetilde{B}$ *be a bounded and self-adjoint operator on* $\mathscr{G}$*. In this case,* $B := \Lambda^{-1} \widetilde{B}$ *is bounded and self-adjoint as operator on* $\mathscr{G}^{1/2}$.

Proof. We have

$$\|B\|_{\mathscr{B}(\mathscr{G}^{1/2})} = \|\Lambda^{1/2} B \Lambda^{-1/2}\|_{\mathscr{B}(\mathscr{G})} = \|\Lambda^{-1/2} \widetilde{B} \Lambda^{-1/2}\|_{\mathscr{B}(\mathscr{G})} \le \|\Lambda^{-1}\|_{\mathscr{B}(\mathscr{G})} \|\widetilde{B}\|_{\mathscr{B}(\mathscr{G})},$$

so that B is bounded on $\mathscr{G}^{1/2}$, and

$$\langle B\varphi, \psi \rangle_{\mathscr{G}^{1/2}} = \langle \Lambda^{1/2} B \varphi, \Lambda^{1/2} \psi \rangle_{\mathscr{G}} = \langle \Lambda^{-1/2} \widetilde{B} \varphi, \Lambda^{1/2} \psi \rangle_{\mathscr{G}} = \langle \widetilde{B} \varphi, \psi \rangle_{\mathscr{G}};$$

and the self-adjointness follows from the self-adjointness of $\widetilde{B}$ and a similar expression with B and $\widetilde{B}$ in the second argument. □

We can now formulate our main result. For brevity, we restrict ourselves here to 0-forms. Similar results hold also for 1-forms.

Theorem 2.30. *Let B be a self-adjoint and bounded operator in $\mathscr{G}^{1/2}$, Δ_0^{D} the self-adjoint Laplacian with Dirichlet boundary conditions (cf. Definition 2.3) and Δ_0^B the self-adjoint restriction of the Laplacian (cf. Definition 2.26). Assume that $\operatorname{dom}(\Delta_0^B)^* \subset \mathscr{H}_0^1$.*

(i) *For $z \notin \sigma(\Delta_0^{\mathrm{D}})$ we have $\ker(\Delta_0^B - z) = \beta_0^z \ker(Q_0^z - B)$.*

(ii) *For $z \notin \sigma(\Delta_0^B) \cup \sigma(\Delta_0^{\mathrm{D}})$ we have $0 \notin \sigma(Q_0^z - B)$ and Krein's formula*
$$(\Delta_0^{\mathrm{D}} - z)^{-1} - (\Delta_0^B - z)^{-1} = \beta_0^z (Q_0^z - B)^{-1} (\beta_0^{\bar z})^*$$
is valid, where $(\beta_0^{\bar z})^*$ is the adjoint of $\beta_0^{\bar z}$ as operator $\beta_0^{\bar z} \colon \mathscr{G}^{1/2} \longrightarrow \mathscr{H}_0$.

(iii) *We have*
$$\sigma(\Delta_0^B) \setminus \sigma(\Delta_0^{\mathrm{D}}) = \{\, z \notin \sigma(\Delta_0^{\mathrm{D}}) \,|\, 0 \in \sigma(Q_0^z - B) \,\}.$$

Proof. The proof is again closely related to the proof for ordinary boundary triples (cf. [BGP08, Thm. 1.29]). For the first assertion, take $\varphi \in \ker(Q_0^z - B)$ and set $f_0 = \beta_0^z \varphi$. By the definition of the solution map β_0^z, we have $(\Delta_0 - z) f_0 = 0$ and $\gamma_0 f_0 = \varphi$. Furthermore, $Q_0^z \varphi = B\varphi$ is equivalent to $\gamma_1 \mathrm{d} f_0 = B \gamma_0 f_0$ by the definition of Q_0^z. However, the last equation shows that $f_0 \in \operatorname{dom} \Delta_0^B$, i.e., $f_0 \in \ker(\Delta_0^B - z)$. The opposite inclusion follows similarly.

To prove the second assertion, take $h_0 \in \mathscr{H}_0$ and $f_0 := (\Delta_0^B - z)^{-1} h_0 \in \operatorname{dom} \Delta_0^B$. By Lemma 2.19 we can decompose $f_0 = f_0^z \dotplus g_0^z \in \mathring{\mathscr{H}}_0^1 \dotplus \mathscr{N}_0^z$. Since $f_0, g_0^z \in \mathscr{H}_0^2$ we also have $f_0^z \in \mathscr{H}_0^2$ and
$$h_0 = (\Delta_0^B - z) f_0 = (\Delta_0 - z) f_0 = (\Delta_0 - z) f_0^z = (\Delta_0^{\mathrm{D}} - z) f_0^z,$$
i.e., $f_0^z = (\Delta_0^{\mathrm{D}} - z)^{-1} h_0$. Furthermore, $\gamma_0 f_0^z = 0$, therefore $\gamma_0 f_0 = \gamma_0 g_0^z$, i.e., $g_0^z = \beta_0^z \gamma_0 f_0$ and we have
$$(\Delta_0^B - z)^{-1} h_0 = f_0 = f_0^z + g_0^z = (\Delta_0^{\mathrm{D}} - z)^{-1} h_0 + \beta_0^z \gamma_0 f_0. \tag{2.6}$$
Now we apply $\gamma_1 \mathrm{d}$ to the decomposition of $f_0 \in \operatorname{dom} \Delta_0^B$ and obtain
$$\begin{aligned} B\gamma_0 f_0 = \gamma_1 \mathrm{d} f_0 &= \gamma_1 \mathrm{d} f_0^z + \gamma_1 \mathrm{d} \beta_0^z \gamma_0 f_0 \\ &= (\beta_0^{\bar z})^* (\Delta_0 - z) f_0^z + Q_0^z \gamma_0 f_0 = (\beta_0^{\bar z})^* h_0 + Q_0^z \gamma_0 f_0. \end{aligned}$$
using the definition of Q_0^z (cf. Definition 2.24) and Lemma 2.23 for the third equality. In particular,
$$(Q_0^z - B)\gamma_0 f_0 = (\beta_0^{\bar z})^* h_0, \tag{2.7}$$
and the RHS covers the entire space $\mathscr{G}^{1/2}$ since h_0 covers $\mathscr{H}_0$ (see again Lemma 2.23). In particular, $(Q_0^z - B)$ is surjective. By (i), this operator is also injective, i.e., $0 \notin \sigma(Q_0^z - B)$. Krein's formula now follows from (2.6)–(2.7). The last assertion is a consequence of (ii). ☐

Returning to the original boundary space $\mathscr{G}$ and the Dirichlet-to-Neumann map $\Lambda(z) = \Lambda Q_0^z$ — regarded as an unbounded operator in $\mathscr{G}$ —, we obtain the following result:

Theorem 2.31. *Let $\widetilde B$ be a self-adjoint and bounded operator in $\mathscr{G}$ and $\Delta_0^{\widetilde B}$ the corresponding self-adjoint restriction of the Laplacian with domain*
$$\operatorname{dom} \Delta_0^B := \{\, f_0 \in \mathscr{H}_0^2 \,|\, \widetilde\gamma_1 \mathrm{d} f_0 = \widetilde B \gamma_0 f_0 \,\}$$
(Robin type boundary conditions). Assume that $\operatorname{dom}(\Delta_0^B)^* \subset \mathscr{H}_0^1$

(i) *For $z \notin \sigma(\Delta_0^{\mathrm{D}})$ we have $\ker(\Delta_0^B - z) = \beta_0^z \Lambda^{-1} \ker(\Lambda(z) - B)$.*

(ii) *For $z \notin \sigma(\Delta_0^B) \cup \sigma(\Delta_0^{\mathrm{D}})$ we have $0 \notin \sigma(\Lambda(z) - \widetilde B)$ and Krein's formula*
$$(\Delta_0^{\mathrm{D}} - z)^{-1} - (\Delta_0^B - z)^{-1} = \beta_0^z (\Lambda(z) - \widetilde B)^{-1} (\widetilde{\beta_0^{\bar z}})^*$$
is valid, where $(\widetilde{\beta_0^{\bar z}})^*$ is the adjoint of $\beta_0^{\bar z} \colon \mathscr{G}^{1/2} \longrightarrow \mathscr{H}_0$ considered as an unbounded operator $\widetilde{\beta_0^{\bar z}} \colon \mathscr{G} \dashrightarrow \mathscr{H}_0$ with domain $\mathscr{G}^{1/2}$.

(iii) *We have*

$$\sigma(\Delta_0^B) \setminus \sigma(\Delta_0^{\mathrm{D}}) = \{\, z \notin \sigma(\Delta_0^{\mathrm{D}}) \,|\, 0 \in \sigma(\Lambda(z) - \widetilde{B}) \,\}.$$

Proof. The proof follows from Theorem 2.30 because $\Lambda(z)-\widetilde{B} = \Lambda(Q_0^z - B)$ and $(\widetilde{\beta}_0^z)^* = \Lambda(\beta_0^z)^*$. □

3. Boundary triples

In this section we show how the first order approach of the last section fits into the setting of boundary triples in the usual sense. We only sketch the ideas here; for more details on boundary triples, we refer to [BGP08, DHMdS06] and the references therein.

Definition 3.1. Let $\mathscr{H}$ be a Hilbert space with a closed operator D in $\mathscr{H}$. Assume furthermore that $\widetilde{\mathscr{G}}$ is another Hilbert space, and $\Gamma_0, \Gamma_1 \colon \operatorname{dom} D \longrightarrow \widetilde{\mathscr{G}}$ are two linear maps. We say that $(\widetilde{\mathscr{G}}, \Gamma_0, \Gamma_1)$ is an *(ordinary) boundary triple for D* iff

$$\langle Df, g\rangle_{\mathscr{H}} - \langle f, Dg\rangle_{\mathscr{H}} = \langle \Gamma_0 f, \Gamma_1 g\rangle_{\widetilde{\mathscr{G}}} - \langle \Gamma_1 f, \Gamma_0 g\rangle_{\widetilde{\mathscr{G}}}, \qquad \forall\, f, g \in \operatorname{dom} D \tag{3.1a}$$

$$\Gamma_0 \overset{\curlyvee}{\oplus} \Gamma_1 \colon \operatorname{dom} D \longrightarrow \widetilde{\mathscr{G}} \oplus \widetilde{\mathscr{G}},\ f \mapsto \Gamma_0 f \oplus \Gamma_1 f \quad \text{is surjective} \tag{3.1b}$$

$$\ker(\Gamma_0 \overset{\curlyvee}{\oplus} \Gamma_1) = \ker \Gamma_0 \cap \ker \Gamma_1 \quad \text{is dense in } \mathscr{H}. \tag{3.1c}$$

Lemma 3.2. *Let $\mathscr{H} := \mathscr{H}_0 \oplus \mathscr{H}_1$ and $(\mathscr{H}, \mathscr{G}, \gamma_0)$ be a first order boundary triple as in Definition 2.1. Write*

$$D := \begin{pmatrix} 0 & \delta \\ \mathrm{d} & 0 \end{pmatrix}, \quad \operatorname{dom} D := \mathscr{H}^1 := \mathscr{H}_0^1 \oplus \mathscr{H}_1^1, \quad \|f\|^2_{\mathscr{H}^1} = \|f\|^2_{\mathscr{H}} + \|Df\|^2_{\mathscr{H}},$$

and $\Gamma_p f := \gamma_p f_p$ for $f = f_0 \oplus f_1 \in \mathscr{H}^1$. Then $(\mathscr{G}^{1/2}, \Gamma_0, \Gamma_1)$ is an ordinary boundary triple for D.

Proof. The Green's formula (3.1a) follows from

$$\begin{aligned}\langle Df, g\rangle_{\mathscr{H}} - \langle f, Dg\rangle_{\mathscr{H}} &= \langle \mathrm{d}f_0, g_1\rangle_{\mathscr{H}_1} - \langle f_0, \delta g_1\rangle_{\mathscr{H}_0} + \langle \delta f_1, g_0\rangle_{\mathscr{H}_0} - \langle f_1, \mathrm{d}g_0\rangle_{\mathscr{H}_1} \\ &= \langle \gamma_0 f_0, \gamma_1 g_1\rangle_{\mathscr{G}^{1/2}} - \langle \gamma_1 f_1, \gamma_0 g_0\rangle_{\mathscr{G}^{1/2}}\end{aligned}$$

by Lemma 2.14. The second condition (3.1b) follows from $\Gamma_0 \overset{\curlyvee}{\oplus} \Gamma_1 = \gamma_0 \oplus \gamma_1$ and the surjectivity of $\gamma_p \colon \mathscr{H}_p^1 \longrightarrow \mathscr{G}^{1/2}$. The last condition (3.1c), i.e., the density of $\mathring{\mathscr{H}}^1 := \mathring{\mathscr{H}}_0^1 \oplus \mathring{\mathscr{H}}_1^1$ in $\mathscr{H}$, is a consequence of Definition 2.1 (iii). □

The next lemma can be proved readily:

Lemma 3.3. *Set $\mathscr{N}^w := \ker(D - w)$. If $w \neq 0$ then $\psi_p^w \colon \mathscr{N}_p^{w^2} \longrightarrow \mathscr{N}^w$ with*

$$\psi_0^w f_0 := \frac{1}{\sqrt{2}} \begin{pmatrix} f_0 \\ \frac{1}{w}\mathrm{d}f_0 \end{pmatrix}, \qquad \psi_1^w f_1 := \frac{1}{\sqrt{2}} \begin{pmatrix} \frac{1}{w}\delta f_1 \\ f_1 \end{pmatrix}$$

are topological isomorphisms. In particular, for $w = \pm\mathrm{i}$, they are unitary.

Corollary 3.4. *The operator D has zero defect index, i.e., $\mathscr{N}^{\mathrm{i}} = \ker(D - \mathrm{i})$ and $\mathscr{N}^{-\mathrm{i}} = \ker(D + \mathrm{i})$ are isomorphic.*

The next lemma is a well known fact; we give a proof for completeness.

Lemma 3.5. *If $w \neq 0$ then $\mathscr{H}^1 = \mathring{\mathscr{H}}^1 \dotplus \mathscr{N}^w \dotplus \mathscr{N}^{-w}$ (topological direct sum), and the projection P^w onto $\mathscr{N}^w$ is given by*

$$P^w = \frac{1}{2} \begin{pmatrix} P_0^{w^2} & \frac{1}{w}\delta P_1^{w^2} \\ \frac{1}{w}\mathrm{d}P_0^{w^2} & P_1^{w^2} \end{pmatrix}.$$

If $w = \pm\mathrm{i}$, then we have $\mathscr{H}^1 = \mathring{\mathscr{H}}^1 \oplus \mathscr{N}^{\mathrm{i}} \oplus \mathscr{N}^{-\mathrm{i}}$ (orthogonal direct sum), and $P^{\pm\mathrm{i}}$ are orthogonal *projections (in $\mathscr{H}^1$).*

Proof. Recall that P_p^z is the projection onto $\mathscr{N}_p^z = \ker(\Delta_p - z)$. Denote by $\mathring{P}_p := 1 - P_p^z$ the projection onto $\mathring{\mathscr{H}}_p^1$ and set $\mathring{P} := \mathring{P}_0 \oplus \mathring{P}_1$. Then we can decompose $f \in \mathscr{H}^1$ as

$$f = \mathring{P} f + P^w f + P^{-w} f,$$

since $P^w + P^{-w} = P_0^{w^2} \oplus P_1^{w^2}$ and $\mathring{P} + (P_0^{w^2} \oplus P_1^{w^2}) = 1$. A simple calculation shows that $DP^w = wP^w$, i.e., that $P^w f \in \mathscr{N}^w$; in addition, $(P^w)^2 = P^w$, i.e., P^w is a projection; and $\mathring{P} f \in \mathring{\mathscr{H}}^1$.

The sum of eigenspaces associated to different eigenvalues is direct, and $\mathscr{N}^w \dot{+} \mathscr{N}^{-w} = \mathscr{N}_0^{w^2} \oplus \mathscr{N}_1^{w^2}$ (Lemma 3.3). Since in addition, $\mathscr{H}_p^1 = \mathring{\mathscr{H}}_p^1 \dot{+} \mathscr{N}_p^{w^2}$, it follows that the sum $\mathscr{H}^1 = \mathring{\mathscr{H}}^1 \dot{+} \mathscr{N}^w \dot{+} \mathscr{N}^{-w}$ is direct. The direct sum is also topological since the projections are bounded operators. The orthogonality for $w = \pm \mathrm{i}$ can be checked easily. ☐

Lemma 3.6. *Let $D^{\min}$ be the restriction of D onto* $\operatorname{dom} D^{\min} = \mathring{\mathscr{H}}^1 := \mathring{\mathscr{H}}_0^1 \oplus \mathring{\mathscr{H}}_1^1 = \ker(\Gamma_0 \overset{\curlyvee}{\oplus} \Gamma_1)$. *Then $(D^{\min})^* = D$.*

Proof. We refer to [BGP08, Thm. 1.13 (1)⇒(4)] for a proof. Note that D has self-adjoint restrictions since the defect index is 0 by Corollary 3.4. ☐

We write $D^{\mathrm{D}} := D{\restriction}_{\ker \Gamma_0}$, the *Dirichlet Dirac operator*, and $D^{\mathrm{N}} := D{\restriction}_{\ker \Gamma_1}$, the *Neumann Dirichlet operator*. Note that $(D^{\mathrm{D}})^2 = \Delta_0^{\mathrm{D}} \oplus \Delta_1^{\mathrm{D}}$ and $(D^{\mathrm{N}})^2 = \Delta_0^{\mathrm{N}} \oplus \Delta_1^{\mathrm{N}}$.

Lemma 3.7. *Let $w \notin \sigma(D^{\mathrm{D}})$. The operator $\Gamma_0{\restriction}_{\mathscr{N}^w} \colon \mathscr{N}^w \longrightarrow \mathscr{G}^{1/2}$ has a bounded inverse β^w, and $w \mapsto \beta^w$ is a* Γ-Krein field, *i.e.,*

$$\beta^w \colon \mathscr{G}^{1/2} \longrightarrow \mathscr{N}^w \quad \text{is a topological isomorphism and} \tag{3.2a}$$

$$\beta^{w_1} = U^{w_1,w_2} \beta^{w_2}, \qquad w_1, w_2 \notin \sigma(D^{\mathrm{D}}), \tag{3.2b}$$

where

$$U^{w_1,w_2} := (D^{\mathrm{D}} - w_2)(D^{\mathrm{D}} - w_1)^{-1} = 1 + (w_1 - w_2)(D^{\mathrm{D}} - w_1)^{-1}.$$

Furthermore, $\beta^w = \sqrt{2}\psi_0^w \beta_0^{w^2}$, where β_0^z is the Krein γ-function of order 0 *associated with the first order boundary triple $(\mathscr{H}, \mathscr{G}, \gamma_0)$ (cf. Definition 2.21) and ψ_0^w is defined in Lemma 3.3.*

Proof. For the proof of the first assertion, we refer again to [BGP08, Thm. 1.23 (2a–b)]. The relation with $\beta_0^{w^2}$ follows from the fact that $\Gamma_0 = \gamma_0 \pi_0$, where $\pi_0 \colon \mathscr{H}^1 \longrightarrow \mathscr{H}_0^1$, $f \mapsto f_0$; and the inverse of $\sqrt{2}\psi_0^w$ is π_0 (restricted to the appropriate subspaces). ☐

Lemma 3.8. *The operator $Q^w := \Gamma_1 \beta^w \colon \mathscr{G}^{1/2} \longrightarrow \mathscr{G}^{1/2}$ defines the Krein Q-function $w \mapsto Q^w$, i.e.,*

$$Q^{w_1} - (Q^{\overline{w}_2})^* = (w_1 - w_2)(\beta^{\overline{w}_2})^* \beta^{w_1} \qquad w_1, w_2 \notin \sigma(D^{\mathrm{D}}).$$

Furthermore, $Q^w = \frac{1}{w} Q_0^{w^2}$, where Q_0^z is the Krein Q-function associated to the first order boundary triple $(\mathscr{H}, \mathscr{G}, \gamma_0)$ (cf. Definition 2.24).

Proof. For the proof of the first assertion, we refer again to [BGP08, Thm. 1.23 (2c)]. The other follows straightforward. ☐

Further results like Krein's resolvent formula or the spectral relation for self-adjoint restrictions D^B of D can be found e.g. in [BGP08]. In particular, if B is bounded and self-adjoint in $\mathscr{G}^{1/2}$ then the restriction of D to

$$\operatorname{dom} D^B := \{\, f \in \mathscr{H}^1 \mid \Gamma_1 f = B \Gamma_0 f \,\} = \{\, f \in \mathscr{H}^1 \mid \gamma_1 f_1 = B \gamma_0 f_0 \,\}$$

defines a self-adjoint operator D^B. The Laplacian $(D^B)^2$ acts on each component as the Laplacian $\Delta_p f_p$, but with domain

$$\begin{aligned}\operatorname{dom}(D^B)^2 &= \{\, f \in \operatorname{dom} D^B \mid Df \in \operatorname{dom} D^B \,\}\\ &= \{\, f \in \mathscr{H}^2 \mid \gamma_1 f_1 = B\gamma_0 f_0, \quad \gamma_1 \mathrm{d} f_0 = B\gamma_0 \updelta f_1 \,\}.\end{aligned}$$

Note that this domain is different from $\operatorname{dom}\Delta_0^B \oplus \operatorname{dom}\Delta_1^B$ (cf. Definition 2.26) since the two components in $\operatorname{dom}(D^B)^2$ are coupled.

4. Manifolds with boundary

In this section we present our main example and show how it fits into the abstract setting of first order boundary triples of Section 2 (see also [A00]).

Let X be a compact Riemannian manifold with boundary ∂X equipped with their natural volume measures. Denote the cotangential bundle (or bundle of 1-forms) by T^*X. The data we need to fix are the following:

$$\mathscr{H}_0 := \mathsf{L}_2(X), \qquad \mathscr{H}_0^1 := \mathsf{H}^1(X),$$
$$\mathscr{H}_1 := \mathsf{L}_2(T^*X), \qquad \mathrm{d}\colon \mathsf{H}^1(X) \longrightarrow \mathsf{L}_2(T^*X),$$

where $\mathsf{L}_2(X)$ and $\mathsf{L}_2(T^*X)$ are the spaces of square-integrable functions and sections over the cotangent (1-form) bundle, and where d stands for the usual exterior derivative with domain $\mathscr{H}_0^1 := \mathsf{H}^1(X)$, the Sobolev space of functions $f \in \mathsf{L}_2(X)$ such that $|\mathrm{d}f| \in \mathsf{L}_2(X)$ (or $\mathrm{d}f \in \mathsf{L}_2(T^*X)$, what is the same).

For the boundary map, we need to fix the boundary space $\mathscr{G} := \mathsf{L}_2(\partial X)$, and we define

$$\gamma_0\colon \mathsf{H}^1(X) \longrightarrow \mathsf{L}_2(\partial X), \qquad \gamma_0 f := f\restriction_{\partial X}.$$

Note that the norm of γ_0 depends on the local geometry of X near ∂X. The range of γ_0 is $\mathscr{G}^{1/2} = \mathsf{H}^{1/2}(\partial X)$ together with the intrinsic norm defined in Section 2, namely

$$\|\varphi\|^2_{\mathsf{H}^{1/2}(\partial X)} := \|f_0\|^2_{\mathsf{H}^1(X)} = \|f_0\|^2_{\mathsf{L}_2(X)} + \|\mathrm{d}f_0\|^2_{\mathsf{L}_2(X)},$$

where f_0 is the solution of the Dirichlet problem $(\Delta_0 + 1)f_0 = 0$ and $\gamma_0 f_0 = \varphi$. Since $\mathsf{H}^{1/2}(\partial X) \neq \mathsf{L}_2(\partial X)$, the boundary map γ_0 is proper.

After defining these data, we obtain $\mathring{\mathscr{H}}_0^1 = \mathring{\mathsf{H}}^1(X) = \ker\gamma_0$ and $\mathrm{d}_0 := \mathrm{d}\restriction_{\mathring{\mathsf{H}}^1(X)}$. Furthermore, $\updelta = \mathrm{d}_0^*$ is the divergence operator. Comparing the abstract Green's formula in Lemma 2.14 with Green's formula

$$\int_X \langle \mathrm{d}f, \eta\rangle_x \,\mathrm{d}x - \int_X \overline{f}\, \updelta\eta \,\mathrm{d}x = \int_{\partial X} (\overline{f}\,\eta_{\mathrm{n}})\restriction_{\partial X},$$

where η_{n} stands for the normal component of the 1-form η near ∂X, we see that

$$\widetilde{\gamma}_1\eta = \eta_{\mathrm{n}}\restriction_{\partial X}$$

Remark 4.1. Note that $\mathscr{H}_1^1 := \operatorname{dom}\updelta \subset \mathsf{L}_2(T^*X)$ is *not* the Sobolev space of order 1 on 1-forms, defined locally via charts. Therefore, $\widetilde{\gamma}_1\colon \operatorname{dom}\updelta \longrightarrow \mathsf{H}^{-1/2}(\partial X)$, and $\widetilde{\gamma}_1$ does not map into $\mathsf{H}^{1/2}(\partial X)$, as one could naively guess.

The Dirichlet-to-Neumann map in this case is

$$\Lambda(z)\varphi = \partial_{\mathrm{n}} h_0, \qquad \text{where} \qquad \Delta_0 h_0 = z h_0, \qquad h_0\restriction_{\partial X} = \varphi \tag{4.1}$$

for $\varphi \in \mathsf{H}^{1/2}(\partial X)$ and $z \notin \sigma(\Delta_0^{\mathrm{D}})$ (cf. Definition 2.24).

Self-adjoint boundary conditions of the Laplacian on 0-forms like *Robin boundary conditions* are now given as follows: Let $\widetilde{B}$ be a smooth, real-valued function on ∂X and set $B := \Lambda^{-1}\widetilde{B}$. Then B is bounded and self-adjoint on $\mathscr{G}^{1/2}$ (Lemma 2.29) and

$$\operatorname{dom}(\Delta_0^B)^* = \{\, f_0 \in \Delta_0^{\max} \mid \partial_{\mathrm{n}} f_0\restriction_{\partial X} = \widetilde{B} f_0\restriction_{\partial X} \,\}$$

is a subset of $\mathscr{H}_0^1 = \mathsf{H}^1(X)$ since a priori, $\partial_{\mathrm{n}} f_0 \restriction_{\partial X} \in \mathsf{H}^{-3/2}(\partial X)$, but by the smoothness of $\widetilde{B}$ and $f_0 \restriction_{\partial X} \in \mathsf{H}^{-1/2}(\partial X)$, we conclude that $\partial_{\mathrm{n}} f_0 \restriction_{\partial X} \in \mathsf{H}^{-1/2}(\partial X)$. By a theorem of Lions and Magnenes (see [G68, Prop. III.5.2] or [LM72, Thm. 7.4]), it follows that $f \in \mathsf{H}^1(X)$. In particular, the domain condition is fulfilled, and the above domain defines a *self-adjoint* Laplace operator (cf. Lemma 2.27).

Note that in general, the Robin boundary conditions cannot be expressed as $(D^B)^2$ where D^B is a self-adjoint restriction of the Dirac operator (cf. the end of Section 3). This is another justification of our first order approach (instead of directly starting from an ordinary boundary triple as in Section 3).

Remark 4.2. The first order approach to boundary triples enables us to use the *natural* boundary maps $\gamma_0 f = f \restriction_{\partial X}$ and $\widetilde{\gamma}_1 \eta = \eta_{\mathrm{n}} \restriction_{\partial X}$, in contrast to the second order approach using the Laplacian as e.g. in [BMNW07, Pc07]. In the second order approach, the maximal domain of the Laplacian

$$\operatorname{dom} \Delta^{\max} = \{\, f \in \mathsf{L}_2(X) \mid \Delta f \in \mathsf{L}_2(X) \,\}$$

is *not* a subset of the Sobolev space $\mathsf{H}^1(X)$. In particular, $f \restriction_{\partial X}$ is not in $\mathsf{L}_2(\partial X)$, but only in $\mathsf{H}^{-1/2}(\partial X)$; and $\partial_{\mathrm{n}} f \restriction_{\partial X} \in \mathsf{H}^{-3/2}(\partial X)$ (see e.g. [G68, G06, LM72]). In particular, Green's formula (cf. (3.1a)) fails to hold with the natural boundary maps.

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