Boundary pairs associated with quadratic forms

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We introduce an abstract framework for elliptic boundary value problems in a variational form. Given a non-negative quadratic form in a Hilbert space, a boundary pair consists of a bounded operator, the boundary operator, and an auxiliary Hilbert space, the boundary space, where the boundary operator (usually, the restriction of a function to a subset) is bounded from the quadratic form domain into the auxiliary Hilbert space.

These data determine a Neumann and Dirichlet operator, a Dirichlet solution and a Dirichlet-to-Neumann operator. The basic example we have in mind is a manifold with boundary, where the quadratic form is the integral over the squared derivative, and the boundary map is the restriction of a function to (a subset of) the boundary of the manifold.

As one of the main theorems, we derive a Krein’s type resolvent formula relating the difference of the resolvents of the Neumann and Dirichlet operator with the Dirichlet solution and the Dirichlet-to-Neumann operator. From this, we deduce a spectral characterisation for a point being in the spectrum of the Neumann resp. Dirichlet operator.

We relate our concept with existing concepts such as boundary triples including conditions expressed purely in terms of boundary pairs. We illustrate the theory by many examples including Jacobi operators, Laplacians on manifolds with (non-smooth) boundary and the Zaremba (mixed boundary conditions) problem.

Contents

1 Introduction 2
2 Boundary pairs associated with quadratic forms 6
  2.1 Boundary pairs, Dirichlet solution operators and Dirichlet-to-Neumann operators . . . . . . . . 6
  2.2 The Dirichlet solution operator at arbitrary points . . . . . . . . . . . . . . . . . . . . . . . . 9
  2.3 The Dirichlet-to-Neumann form at arbitrary points . . . . . . . . . . . . . . . . . . . . . . . . 11
  2.4 The Neumann-to-Dirichlet operator . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 13
3 Boundary pairs with additional properties 15
  3.1 Elliptically regular boundary pairs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 15
  3.2 Uniformly positive boundary pairs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 18
4 Krein’s resolvent formula and spectral relations 19
  4.1 Krein’s resolvent formula for boundary pairs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 19
  4.2 Spectral relations for the Dirichlet-to-Neumann operator . . . . . . . . . . . . . . . . . . . . . . . . 20
5 Boundary pairs constructed from other boundary pairs 25
  5.1 Robin boundary conditions . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 25
  5.2 Coupled boundary pairs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 26
  5.3 Direct sum of boundary pairs . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 27
5.4 Making a boundary pair bounded .......................................... 28

6 Relation to boundary triples and other concepts .......................... 28
  6.1 Relation to boundary triples ................................................. 28
  6.2 Relation to extension theory .................................................. 32
  6.3 Relation to generalised elliptic forms and associated operators ....... 34

7 Examples .................................................................................. 35
  7.1 Trivial examples ........................................................................ 35
  7.2 Examples with finite-dimensional boundary space ......................... 36
  7.3 Examples with Jacobi operators .................................................. 36
  7.4 Laplacian on a manifold with Lipschitz boundary ........................ 39
  7.5 Laplacian on a non-compact cylindrical manifold ......................... 40
  7.6 Dirichlet-to-Neumann operator supported on a metric graph .......... 41
  7.7 Laplacian with mixed boundary conditions: the Zaremba problem .... 42
  7.8 Example with large boundary space: discrete Laplacians ............... 43

1 Introduction

Probably the best way to illustrate the main subject of this article is to start with a basic example, from which we borrow the names for the abstract setting: Let $X$ be a manifold with (possibly non-smooth, but Lipschitz) boundary $\partial X$. We set

$$\mathcal{H} := L_2(X), \ h(u) := \|u\|^2, \ u \in \text{dom } h = \mathcal{H}^1 = H^1(X),$$

where $H^1(X)$ is the completion of the set of smooth function with respect to the norm given by $\|u\|^2_{H^1} := \|u\|^2_{H^2} + h(u)$. The operator $H$ associated with $h$ is the usual Neumann Laplacian on $X$. As boundary space and operator we set

$$\mathcal{G} := L_2(Y) \quad \text{and} \quad \Gamma u := u|_{\partial Y},$$

respectively, where $Y = \partial X$ (or a suitable subset).

In the abstract setting, a boundary pair $(\Gamma, \mathcal{G})$ associated with a non-negative closed quadratic form $h$ consists of a bounded operator $\Gamma : \mathcal{H}^1 \to \mathcal{G}$ (the boundary map) and an auxiliary Hilbert space $\mathcal{G}$ such that $\ker \Gamma \subset \mathcal{H}$ and $\text{ran } \Gamma \subset \mathcal{G}$ are dense.

In the concrete manifold example, these conditions are fulfilled and we say that $(\Gamma, \mathcal{G})$ is the boundary pair associated with $(X, Y)$. Moreover, $\Gamma$ is the Sobolev trace operator and not surjective. We call such a boundary pair unbounded. The operator $H^D$ associated with the form $h^D := h|_{\ker \Gamma}$ is the usual Dirichlet Laplacian (or, if $Y \subseteq \partial X$, a mixed boundary value problem, also called Zaremba problem if $\partial X$ is smooth). The Sobolev space $\mathcal{H}$ decomposes into the sum of $\mathcal{H}^{1, D} := \ker \Gamma$ and $\mathcal{A}^1(z)$, where $\mathcal{A}^1(z)$ is the space of weak solutions, i.e.,

$$\mathcal{A}^1(z) := \{ h \in \mathcal{H} \mid \langle h, f \rangle = z(h, f)_{\mathcal{G}} \quad \forall f \in \ker \Gamma \},$$

and the sum is direct if $z \in \mathbb{C}$ is not in the spectrum of the Dirichlet operator $H^D$. On this weak solution space, we can invert the boundary operator and call

$$S(z) := (\Gamma|_{\mathcal{A}^1(z)})^{-1} : \mathcal{G}^{1/2} \to \mathcal{H}^1$$

the (weak) Dirichlet solution operator or Poisson operator, because $h = S(z)\varphi$ is the (unique) weak solution of the Dirichlet problem $h \in \mathcal{A}^1(z)$ with $\Gamma h = \varphi$. The Dirichlet-to-Neumann operator $\Lambda(z)$ is now defined as the operator associated with the sesquilinear form

$$I_z(\varphi, \psi) = \langle h - z1, S(z)\varphi, S(-1)\psi \rangle.$$

Applying the (first) Green’s formula for sufficiently regular $\varphi$ one can see that $\Lambda(z)\varphi = \partial_n h|_{\partial Y}$, i.e., that $\Lambda(z)$ acts as the usual Dirichlet-to-Neumann operator associating the normal derivative of the Dirichlet solution of a boundary value $\varphi$ (see Proposition 6.8 for details).

As one of the main theorems of the abstract theory, we derive a Krein’s type resolvent formula

$$R(z) - R^D(z) = S(z)\Lambda(z)^{-1}S(\overline{z})^*, \quad (1.1)$$
relating the difference of the resolvents of the Neumann and Dirichlet operator with the Dirichlet solution and the Dirichlet-to-Neumann operator (Theorem 4.4). From this, we deduce a second main theorem, a spectral characterisation for a point being in the spectrum of the Neumann operator (Theorems 4.9 and 4.18), namely
\[ \lambda \in \sigma(H) \iff 0 \in \sigma(\Lambda(\lambda)), \] (1.2)
provided \( \lambda \notin \sigma(H^D) \). This spectral relation extends known results for (ordinary) boundary triples to our general context (see e.g. [M10], [BGW09, Cor. 2.3, Sec. 2.2], [BGP08, BMN02], going back to ideas already contained in [V52] and [Gr68]). We would like to stress that our approach here allows the natural boundary operators and Dirichlet-to-Neumann operator in this context.

The concept of boundary pairs associated with a non-negative quadratic form is in some sense a generalisation of the concept of boundary triples (also called boundary value spaces) associated with a closed operator \( H^{\text{max}} \). Boundary triples are often used to describe all possible self-adjoint extensions of \( H^{\text{min}} = (H^{\text{max}})^* \), see e.g. [GG91, DM91, DM95, BMN02] or [BGP08] for an overview. In our context, \( H^{\text{min}} = H^D \cap H \) (i.e., \( \text{dom} \ H^{\text{min}} = \text{dom} \ H^D \cap \text{dom} \ H \)).

Extension theory for operators in Hilbert spaces is a subject with a long history. Possibly the first treatment goes back to von Neumann [vN30] and Friedrichs [Fr34]. Further contributions are given by Krein [Kr47], and Birman [Bi56]. Later on, Vishik [V52], Grubb [Gr68, Gr70] and many other authors contributed to the subject in the context of elliptic boundary value problems, see e.g. [BGW09, BL10, Gr11] for a more up-to-date reference list.

Only recently (although there are many earlier attempts), these two subjects have been combined, and successfully applied to elliptic boundary value problems, see [Gr12, Gr11, BL10, Gr10, M10, BGW09, BHM09, BMN02, GM09, PsR09, Gr08, BMNW08, P08, Ry07, P07, BL07] and references therein.

In this article, we use a slightly different approach. Instead of starting with a symmetric operator \( H^{\text{min}} \), we start with a non-negative quadratic form \( \mathfrak{h} \) and only one boundary operator \( \Gamma \), a bounded operator from the quadratic form domain \( \mathcal{H}^1 = \text{dom} \mathfrak{h} \) into an auxiliary Hilbert space \( \mathcal{G} \). The data \((\Gamma, \mathcal{G})\) and \( \mathfrak{h} \) determine a Neumann operator \( H \) (the operator associated with the quadratic form itself), a Dirichlet operator \( H^D \) (the operator associated with the restriction of the quadratic form to the kernel of the boundary operator), a Dirichlet solution \( S(z) \) associated to a boundary value \( \varphi \in \text{ran} \Gamma =: \mathcal{G}^{1/2} \) the (weak) solution \( h = S(z)\varphi \) of the Dirichlet problem and finally, a Dirichlet-to-Neumann operator \( \Lambda(z) \) in \( \mathcal{G} \) \((z \in \mathbb{C} \setminus \sigma(H^D))\).

The form approach has already been used in the context of extension theory in [Gr70] and [Ar96] going back to results of Krein [Kr47] and Birman [Bi56], see also the nice review [Ar09]. We would like to stress that our main motivation is not to describe all possible extensions, but rather to show Krein’s resolvent formula (1.1) and the spectral characterisation (1.2), see also the next subsection for further motivations.

Let us now relate our concept of boundary pairs with the concept of boundary triples (and related concepts). Namely, we can associate a boundary triple \((\Gamma, \Gamma', \mathcal{G})\) with a boundary pair \((\Gamma, \mathcal{G})\) (fulfilling some mild conditions), where the second boundary operator \( \Gamma' \) maps from a subspace of \( \mathcal{H}^1 \) into \( \mathcal{G} \) such that the (first) Green’s formula
\[ \mathfrak{h}(f, g) = \langle H^{\text{max}} f, g \rangle_{\mathcal{H}^1} + \langle \Gamma' f, \Gamma g \rangle_{\mathcal{G}} \]
holds. In the manifold example above, this is the usual Green’s formula where \( \Gamma' \) is the normal derivative restricted to the boundary (see Section 6.1).

The choice of “Neumann” and “Dirichlet” conditions for boundary pairs is not as restricted as it looks like at first glance: one can replace the quadratic form \( \mathfrak{h} \) by \( \mathfrak{h}_L \), where \( \mathfrak{h}_L(u) := \mathfrak{h}(u) + \langle L' u, u \rangle \) for some operator \( L \) in \( \mathcal{G} \). It can then be shown that \((\Gamma, \mathcal{G})\) is also a boundary pair associated with \( \mathfrak{h}_L \) (for suitable operators \( L \)), and that the associated Neumann operator is of Robin-type, i.e., functions in its domain fulfill \( \Gamma' u + L' u = 0 \) (see Section 5.1).

Another main result of this article is to identify properties in terms of the boundary pair to assure that the associated boundary triple is an ordinary, generalised or quasi-boundary triple introduced by other authors (see e.g. [BL10, BGP08, BL07, BMN02, DM95] and references therein). We call these additional properties of a boundary pair elliptic regularity and uniform positiveness, expressed in terms of the Dirichlet solution operator \( S := S(-1) \): A boundary pair is elliptically regular (resp. uniformly positive) if there is a constant \( c \in (0, \infty) \) such that
\[ \| S \varphi \|_{\mathcal{H}^1} \leq c \| \varphi \|_{\mathcal{G}} \quad \text{ (resp. } \| S \varphi \|_{\mathcal{H}^1} \geq c \| \varphi \|_{\mathcal{G}} \text{)} \]
for all \( \varphi \in \mathcal{G}^{1/2} = \text{ran} \Gamma \), see Theorems 3.5 and 3.14 for equivalent characterisations and justifications of the names. Let us just mention here that the notation “elliptic regularity” is very closely related to the same notion for elliptic partial differential operators (see the proofs of Theorems 7.12, 7.25 and 7.27).

To our knowledge, these conditions are new; only the condition of elliptic regularity appears in the works of Brasche et al. [BD05, BAB08, BBAB11] in order to have an optimal convergence speed for Robin-type resolvents (see Remark 3.7).
1 Introduction

We have the following (classes of) examples showing that the above properties of boundary pairs are relevant (see Definition 6.3 for the notion of ordinary, generalised and quasi-boundary triples). Note that a boundary pair \((\Gamma, \mathcal{G})\) with finite-dimensional boundary space is automatically bounded (i.e., \(\text{ran} \Gamma = \Gamma(\mathcal{H}) = \mathcal{G}\)), and that a bounded boundary pair is automatically elliptically regular.

<table>
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<tr>
<th>boundary pair is</th>
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<td>fin bdd ell pos</td>
<td>o-bd3 g-bd3 q-bd3</td>
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- yes; \(\times\) no.
- fin: finite dimensional boundary space \(\mathcal{G}\);
- bdd: bounded boundary pair (\(\text{ran} \Gamma = \mathcal{G}\));
- ell: elliptically regular boundary pair;
- pos: uniformly positive boundary pair.
- o-bd3: the associated boundary triple is an ordinary boundary triple;
- g-bd3: ...generalised boundary triple;
- q-bd3: ...quasi-boundary triple.

As an example, the elliptic regularity of the boundary pair associated with \((X, Y)\) described at the beginning is equivalent with the condition that \(\Gamma' u \in \mathcal{G} = L^2(Y)\) for all \(u \in \text{dom} H^D\), where \(\Gamma' u = \partial_n u\) is the normal derivative in a weak form (see Theorem 6.9). For the Zaremba problem (see Section 7.7 and Theorem 7.27), \(Y\) is a proper subset of the smooth boundary \(\partial X\). The corresponding “Dirichlet” operator \(H^D\) fulfills Dirichlet conditions on \(Y\) and Neumann conditions on \(\partial X \setminus Y\). It can be seen that there are functions \(u \in \text{dom} H^D\) such that \(\partial_n u \notin L^2(Y)\), hence the corresponding boundary pair is not elliptic. Nevertheless we have a (weak) formulation of Krein’s resolvent formula (1.1).

Purpose of this article

Let us explain here why we believe that our approach is useful:

- Boundary pairs give a simple and unified language bringing together very different approaches such as boundary triples, Weyl-Titchmarsh functions, Jacobi operators, elliptic boundary value problems (even with low regularity as for the Zaremba problem or with non-smooth Robin boundary conditions), Dirichlet-to-Neumann operators, boundary conditions for differential form Laplacians, non-negative form perturbations, Dirichlet forms, discrete Laplacians;
- The concept of boundary pairs uses only very little information on the model, but still allows to develop a reasonable spectral analysis of the problem and to include a wide variety of examples. This is useful for example in problems with low regularity or with parameter-depending spaces such as manifolds shrinking to a metric graph.
- We provide conditions under which a boundary pair fits into existing concepts such as boundary triples; and in what sense it is more general than existing concepts.
- We see our approach as a starting point for ongoing research (see the outlook below), and this article is meant to provide the basic tools.

It is clear that such a general concept cannot avoid deep analysis on certain classes of problems such as elliptic regularity questions for partial differential operators (“there is no free lunch . . . ”). But we believe that we can provide interesting new links between very different subjects; e.g. the property of a boundary pair to be elliptically regular is equivalent in the Schrödinger operator model with infinitely many point interactions with a certain optimality of the resolvent convergence (see Remark 3.7).

Related works

The closest link to abstract boundary value problems is possibly the concept of quasi-boundary triples; and it turns out that precisely the *elliptically regular* boundary pairs have an associated quasi-boundary triple (see Theorem 6.9). For an overview concerning quasi-boundary triples we refer to [BL10]. A related (generalised) concept is considered by Ryzhov in [Ry07], where he solves the inverse problem: if two families \((A(z)_z)\) of Dirichlet-to-Neumann operators...
agree in a neighbourhood of $z = 0$, then the associated boundary triples are (in a certain sense) “isomorphic”. Both concepts are formulated on the operator level.

Moreover, the notion of boundary pairs appears also in works of Arlinskii [Ar96, Ar99, Ar00] (see also the survey [Ar12] and references therein), but with the Krein extension as Neumann operator and the additional condition that ran $\Gamma = \mathcal{G}$ (what we call bounded boundary pair here, see Remark 6.17). Arlinskii was mainly interested in characterising all possible variational extensions of the associated minimal operator (for related works by Grubb [Gr68] see also Section 6.2). Arlinskii [Ar99] also associates a boundary triple with a boundary pair in the same spirit as we do in Section 6.1.

Lyantse and Storozh [LS83] use a similar notion for operators (see Remark 6.13). There is another approach for first order systems in [Mo12]. Malamud and Mogilevskii [MM02] discuss the extension theory for dual pairs of operators or even relations and also provide a Krein-type formula for the resolvents.

Posilicano [P08] considers (in our notation) a self-adjoint extension $H^D$ and a bounded operator $\Gamma'$: dom $H^D \rightarrow \mathcal{G}$ (dom $H^D$ with its graph norm) which is surjective and has dense kernel. He then describes all self-adjoint extensions of the associated minimal operator $H_{\text{min}}^\alpha := H^D|_{\ker \Gamma'}$ via a Krein-type formula. Other results on Krein-type resolvent formulas are also considered in [DHMdS09, Ps01].

Abstract formulations of elliptic boundary value problems have already been considered by Grubb in [Gr70] where she considers self-adjoint extensions of a non-negative, closed operator (see Section 6.2 for details). There is also an extensive literature of applications of boundary triples to elliptic partial differential operators (see [Gr11, BL10, M10, GM09, Ry09, BGW09, Gr08, P08, BL07, Ry07, Pa06, Ar00, Gr68, V52] and references therein). In most of these articles, one either has to use different boundary operators than $\Gamma u = u|_\partial$ and $\Gamma' u = \partial_h u$ in $L_2(\partial X)$, change the boundary space $L_2(\partial X)$ using some non-local identifications, or one has to use a generalised concept for boundary triples (see the discussion in [P12a, Sec. 1.2.9]).

Arendt and ter Elst [AtE08] define a generalised notion for sesquilinear forms and associated operators, using an operator playing the role of our boundary operator $\Gamma$. Their concept allows to define a Dirichlet-to-Neumann operator even on very rough domains, see [AtE11]. We relate their results with ours in Section 6.3.

A different approach using the notion of Dirichlet forms is used in the works of Brasche et al [BD05, BAB08, BBAB11]. Their concept is called non-negative form perturbations and can equivalently be given (in our notation) by a non-negative closed quadratic form $\mathcal{H}$ in $\mathcal{H}$ with domain $\mathcal{H}':=\text{dom}\mathcal{H}$, an auxiliary Hilbert space $\mathcal{G}$ and an identification operator $\Gamma$, closed as operator $\mathcal{H}' \rightarrow \mathcal{G}$ and densely defined in $\mathcal{H}'$ with dense range ran $\Gamma$ ([BBAB11, Ex. 2.1 and Lem. 2.2]). It is more general than our concept since $\Gamma$ is not assumed to be bounded as operator $\mathcal{H}' \rightarrow \mathcal{G}$ and since ker $\Gamma$ is not assumed to be dense in $\mathcal{H}$ (we have one example where we also drop the latter density condition, see Section 7.8). We would like to stress that Brasche et al. only consider (what we call) the Dirichlet-to-Neumann operator $\Lambda = \Lambda(-1)$ at $z = -1$ and not families of Dirichlet-to-Neumann operators $(\Lambda(z))_z$ as we do.

One of the main examples in [BBAB11] is the Laplacian on $\mathbb{R}$ with infinitely many delta interactions on it (in the terminology above, Robin-type perturbations of the Neumann Laplacian on $\mathbb{R}$, see Remark 3.7), a case also treated in detail in [KM10].

**Outlook**

Let us describe here further ideas and concepts serving as starting points for ongoing research:

1. **Boundary pairs:**
   - consider differences of powers of resolvents, trace formulae and relative determinants;
   - consider more general Robin-type conditions than the ones in Section 5.1 ($L = a \geq 0$), apply this to the manifold case where $L$ is the multiplication with a low regular function on the boundary or some other operator; allow negative operators $L$;
   - couplings of building blocks (encoded by boundary pairs) according to a graph, relate global with local properties;
   - convergence of operators in different Hilbert spaces and boundary pairs (see the forthcoming publication on graph-like manifolds [BP12]);
   - inverse problem: isomorphy of boundary pair; given an operator-valued Herglotz function $-\Lambda(\cdot)$, can we reconstruct a boundary pair with $\Lambda(\cdot)$ as Dirichlet-to-Neumann operator? What information is contained in the Dirichlet-to-Neumann operator? What operator-valued Herglotz families can be obtained by general boundary pairs (in the spirit of [DM95] or [AB09])?
   - analyse the non-elliptically regular case and extend the spectral analysis for such boundary pairs, consider also $\Lambda(\cdot)$ as operator pencil;
2 Boundary pairs associated with quadratic forms

- generalise the concept to boundary operators $\Gamma$ which are only closed as operators $\mathcal{H}^1 \rightarrow \mathcal{G}$ (in the spirit of [BBAB11] and [AtE08]);
- relate the concept to the theory of Dirichlet forms; assuming that $\mathcal{H} = \mathcal{L}_2(X)$ and $\mathcal{G} = \mathcal{L}_2(Y)$, and $\Gamma$ is compatible with the lattice structure of the $L_2$-spaces.

• Boundary triples:
  - given a boundary triple associated with $(H^{\min})^*, H^{\min} \geq 0$, when is there an associated boundary pair?
  - characterise the Dirichlet spectrum via the Neumann-to-Dirichlet operator $\Lambda(z)^{-1}$; consider the absolutely and singular continuous spectrum.

Structure of this article

Section 2 contains the basic notion of a boundary pair, Dirichlet solution operator and Dirichlet-to-Neumann operator. In Section 3 we find additional properties of boundary pairs needed in order to prove certain Krein-type resolvent formulas and spectral relations in Section 4 and to relate our concept to boundary triples and others in Section 6. Section 5 consists of boundary pairs constructed from others, such as the Robin-type perturbation in Section 5.1 and coupled boundary pairs in Section 5.2; and a construction how to turn an unbounded boundary pair in a bounded one in Section 5.4. In Section 7 we provide many examples including Laplacians on intervals, Jacobi operators, Laplacians on manifolds with Lipschitz boundary, a Dirichlet-to-Neumann operator supported on an embedded metric graph, the Zaremba problem and discrete Laplacians.

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2 Boundary pairs associated with quadratic forms

2.1 Boundary pairs, Dirichlet solution operators and Dirichlet-to-Neumann operators

We start with our basic object, using only quadratic form domains for the moment.

Definition 2.1. Let $h$ be a closed non-negative and densely defined quadratic form in the Hilbert space $\mathcal{H}$ with domain $\mathcal{H}^1 := \text{dom} \ h$. We endow $\mathcal{H}^1$ with its natural norm given by the quadratic form, i.e.,

\[
\|f\|^2_{\mathcal{H}^1} := \|f\|^2_{\mathcal{H}} + h(f).
\]

Moreover, let

$\Gamma: \mathcal{H}^1 \rightarrow \mathcal{G}$

be a bounded map, where $\mathcal{G}$ is another Hilbert space. We denote the norm of the operator $\Gamma$ by $\|\Gamma\|_{1 \rightarrow 0}$.

i. We say that $(\Gamma, \mathcal{G})$ is a boundary pair (or $\Gamma$ is a boundary map) associated with the quadratic form $h$ if the following conditions are fulfilled:

a) $\mathcal{H}^{1,D} := \ker \Gamma$ is dense in $\mathcal{H}$.

b) $\mathcal{G}^{1/2} := \text{ran} \Gamma$ is dense in $\mathcal{G}$.

If the first condition is not fulfilled, i.e., if $\ker \Gamma$ is not dense in $\mathcal{H}$ then we say that the boundary space is large in $\mathcal{H}$ or shortly, that the boundary pair has a large boundary space.

ii. If $\mathcal{G}^{1/2} \neq \mathcal{G}$, then we call the boundary pair $(\Gamma, \mathcal{G})$ unbounded. Otherwise, if the boundary map is surjective, then we call the boundary pair bounded.
2.1 Boundary pairs, Dirichlet solution operators and Dirichlet-to-Neumann operators

iii. We call the self-adjoint and non-negative operator $H$ associated with $\mathfrak{g}$ (see [Kat66, Thm. VI.2.1]) the Neumann operator. Its resolvent is denoted by $R(z) := (H - z)^{-1}$ and $R := R(-1)$ for $z \in \mathbb{C} \setminus \sigma(H)$. The associated scale of Hilbert spaces is $\mathcal{H}^k := \text{dom}(H^{k/2})$ with norm $\|u\|_{k,1} := \|H^{k/2}u\|$. For negative $k$, we set $\mathcal{H}^{-k,1} := (\mathcal{H}^{k,1})^*$, where $(\cdot)^*$ refers to the pairing induced by the inner product of $\mathcal{H}$. In particular, we can interpret $\mathcal{H}^{-k,1}$ as the completion of $\mathcal{H}$ with respect to the norm $\|\cdot\|_{-k,1}$. Note that $\mathcal{H}^1 = \mathcal{H}^{-1,1}$; for details on scales of Hilbert spaces, see [P12a, Sec. 3.2], see also the beginning of Section 4.2.

iv. Denote by $\mathfrak{g}^D := \mathfrak{g}|_{\mathcal{H}^k}$ the form¹ restricted to $\mathcal{H}^{1,D}$. Denote by $\mathfrak{g}^{0,D}$ the closure² of ker $\Gamma = \mathcal{H}^{1,D}$ in $\mathcal{H}$. Moreover, we call the self-adjoint and non-negative operator $H^D$ associated with $\mathfrak{g}^D$ in $\mathcal{H}^{0,D}$ the Dirichlet operator. We denote its resolvent by $R^D(z) := (H^D - z)^{-1}$ and $R^D := R^D(-1)$ for $z \in \mathbb{C} \setminus \sigma(H^D)$. The associated scale of Hilbert spaces in $\mathcal{H}^{0,D}$ is denoted by $\mathcal{H}^{k,D} := \text{dom}(H^{D,k/2})$ with norm $\|u\|_{k,D} := \|(H^D + 1)^{k/2}u\|$ and $\mathcal{H}^{-k,D} := (\mathcal{H}^{k,D})^*$ for $k \geq 0$.

For consistency, we extend $R^D(z)$ by 0 on $(\mathcal{H}^{0,D})^*$, and denote the extended resolvent by the same symbol, i.e., we set $R^D(z)f := (H^D - z)^{-1}f^D \oplus 0$ for $f = f^D \oplus f^\perp$ (see e.g. [We84] for the concept of a resolvent for a non-densely defined operator and the related concept of a quasi-inverse).

We sometimes use the notation $A^{k+m,D}$ (or similar ones) to indicate that $B: \mathcal{H}^k \to \mathcal{H}^{m,D}$ is a bounded operator. If $a$ is a quadratic form associated from below and closed, with domain $\mathcal{H}^k$, and if $m = -k$, then we also write $\tilde{A} := A^{k+m,D}$, where $(\tilde{A}u)v := a(u,v)$ (see also the beginning of Section 4.2).

Remark 2.3.

i. If ran $\Gamma$ is not dense in $\mathfrak{g}$, then we can replace $\mathfrak{g}$ by $\mathfrak{g}_0 := \text{ran} \Gamma$.

ii. In most of our examples, ker $\Gamma$ is dense in $\mathcal{H}$, but it is sometimes useful to drop the condition that ker $\Gamma$ is dense, i.e., to allow that the boundary pair $(\Gamma, \mathfrak{g})$ has a large boundary space. If we want to stress that we mean a boundary pair such that ker $\Gamma$ is dense in $\mathcal{H}$, we say that $(\Gamma, \mathfrak{g})$ has a small boundary space.

An example of a boundary pair with large boundary space is presented in Example 2.4 and in Sections 7.1 and 7.8.

iii. We mostly work with unbounded quadratic forms $\mathfrak{g}$. In Section 7.8, we present an example with a bounded form $\mathfrak{g}$ related to a discrete Laplacian on a graph; in this case, $\mathcal{H} = \mathcal{H}^1$.

iv. Note that if the boundary pair $(\Gamma, \mathfrak{g})$ associated with $\mathfrak{g}$ is not bounded (i.e., ran $\Gamma \subseteq \mathfrak{g}$), then we can turn it into a bounded boundary pair $(\tilde{\Gamma}, \mathfrak{g})$ (i.e., ran $\tilde{\Gamma} = \mathfrak{g}$) associated with $\mathfrak{g}$ as shown in Proposition 5.9.

Nevertheless, after this modification, the boundary space is less natural in many applications.

Example 2.4. Let us illustrate the above setting by a prototype we have in mind (see also [BBAB11] and references therein): Assume that $(X, \mu)$ is a measured space. As quadratic form we usually choose an “energy form”, i.e., $b(f) = \int_X |f|^2 \, d\mu$, where $|f|^2 = (f)^2$ is usually a sort of “derivative” on $X$. Moreover, we assume that $Y \subseteq X$ is measurable (the “boundary” of $X$) and $\nu$ is a measure on $Y$. We set $\mathcal{H} := L_2(X,\mu)$ and $\mathfrak{g} := L_2(Y,\nu)$. As boundary map we choose $\Gamma f := f|_Y$. One has to check now that $\Gamma$ is bounded as operator $\mathcal{H}^1 \to \mathfrak{g}$, i.e., that there is a constant $C > 0$ such that

$$\int_Y |f|^2 \, d\nu \leq C \int_X (|f|^2 + |f|^2) \, d\mu.$$  

If $\mu(Y) > 0$, then the boundary space is large, and we may take as measure $\nu$ the measure induced by $X$ (i.e., $\nu(B) := \mu(B)$ for measurable sets $B \subseteq Y$). Here, in this article, we mostly are interested in the case when $\mu(Y) = 0$, i.e., $\nu$ is supported on a set of $\mu$-measure 0 only. This leads to a boundary map for which ker $\Gamma$ is dense in $\mathcal{H} = L_2(X,\mu)$, i.e., to a small boundary space.

Definition 2.5. Let $\mathcal{N}$ be the orthogonal complement of ker $\Gamma$ in $\mathcal{H}^1$. We call the inverse

$$S := (\Gamma|_{\mathcal{N}^1})^{-1} : \mathfrak{g}^{1/2} \to \mathcal{N}^1 \subset \mathcal{H}^1$$

of the bijective map $\Gamma : \mathcal{N}^1 \to \mathfrak{g}^{1/2} := \text{ran} \Gamma$ the (weak) Dirichlet solution map (at the point $z = -1$).

¹Note that $\mathfrak{g}^D$ is a closed form since $\Gamma: \mathcal{H}^1 \to \mathfrak{g}$ is bounded, hence dom $\mathfrak{g}^D = \text{ker} \Gamma$ closed in $\mathcal{H}^1$.

²Note that $\mathfrak{g}^{0,D} \subset \mathcal{H}$ only if the boundary pair has a large boundary space, i.e., if ker $\Gamma$ is not dense in $\mathcal{H}$. This general setting allows us to treat some interesting examples as well.
Clearly, \( h = S\varphi \) with \( \varphi \in \mathcal{G}^{1/2} \) is the weak solution of the Dirichlet problem, i.e.,
\[
(h + 1)(f, h) = h(f, h) + (f, h) = 0 \quad \forall f \in \mathcal{H}^{1, D}, \quad \Gamma h = \varphi.
\]

The Dirichlet solution operator \( S \) allows us to define a natural norm on the range \( \mathcal{G}^{1/2} \) of \( \Gamma \), namely we set
\[
\|\varphi\|_{\mathcal{G}^{1/2}} := \|S\varphi\|_{\mathcal{H}^1}, \quad (2.6)
\]
i.e. the norm of the boundary element \( \varphi \) is given by the \( \mathcal{H}^1 \)-norm of its (weak) Dirichlet solution. Clearly, the operator \( S: \mathcal{G}^{1/2} \to \mathcal{H}^1 \) is isometric and its left inverse \( \Gamma: \mathcal{H}^1 \to \mathcal{G}^{1/2} \) is unitary. In particular, \( \mathcal{G}^{1/2} \) is itself a Hilbert space (with its inner product induced by \( \|\cdot\|_{\mathcal{G}^{1/2}} \)). Moreover, the natural inclusion \( \mathcal{G}^{1/2} \subseteq \mathcal{G} \) is bounded, since
\[
\|\varphi\|_{\mathcal{G}} = \|\Gamma S\varphi\|_{\mathcal{G}} \leq \|\Gamma\|_{1 \to 0} \|S\varphi\|_{\mathcal{H}^1} = \|\Gamma\|_{1 \to 0} \|\varphi\|_{\mathcal{G}^{1/2}}, \quad (2.7)
\]
where \( \|\cdot\|_{1 \to 0} \) is the norm of \( \Gamma \) as operator \( \Gamma: \mathcal{H}^1 \to \mathcal{G} \).

**Proposition 2.8.** Let \((\Gamma, \mathcal{G})\) be a boundary pair associated with \( \mathfrak{h} \), then we have:

i. The Dirichlet solution operator \( S \) is closed and densely defined as operator in \( \mathcal{G} \to \mathcal{H}^1 \). Its domain is given by \( \text{dom} \ S = \mathcal{G}^{1/2} \).

ii. The quadratic form \( l(\varphi) := \|S\varphi\|_{\mathcal{H}^1}^2 \) with \( \text{dom} \ l = \mathcal{G}^{1/2} \) is a closed quadratic form in \( \mathcal{G} \). Moreover,
\[
l(\varphi) \geq \frac{1}{\|\Gamma\|_{1 \to 0}^2} \|\varphi\|_{\mathcal{G}}^2, \quad (2.9)
\]
for \( \varphi \in \mathcal{G}^{1/2} \).

**Proof.** (i) The operator \( S \) has (by definition) a bounded inverse, hence \( S \) is closed.

(ii) The lower bound on \( I \), the optimality and the norm equality for \( \|\Gamma\|_{1 \to 0} \) follow immediately from (2.7). In order to show that \( I \) is closed, let \((\varphi_n)\) be a Cauchy sequence in \( \mathcal{G}^{1/2} \) with respect to \( I \), then \((\varphi_n)\) is also a Cauchy sequence in \( \mathcal{G} \), hence converges in \( \mathcal{G} \) to an element \( \varphi \in \mathcal{G} \). Moreover, \((S\varphi_n)\) is a Cauchy sequence in \( \mathcal{H}^1 \), hence also convergent to \( h \in \mathcal{H}^1 \). Since \( S \) is closed it follows that \( \varphi \in \text{dom} \ S = \mathcal{G}^{1/2} \) and \( S\varphi = h \), i.e., \( \varphi \in \text{dom} \ I \) and \( I(\varphi_n - \varphi) \to 0 \). The lower bound on \( I \) follows from (2.6). \( \square \)

Let us now associate a natural operator \( \Lambda \) to a boundary pair \((\Gamma, \mathcal{G})\). It will turn out later on (cf. Proposition 6.8) that \( \Lambda \) is the Dirichlet-to-Neumann operator, i.e., \( \Lambda \varphi \) associates to a suitable boundary value \( \varphi \) the “normal derivative” of the associated solution of the Dirichlet problem \( h = S\varphi \).

**Definition 2.10.** Let \( \Lambda \) be the operator associated with the quadratic form \( I \). Then \( \Lambda \) is called the **Dirichlet-to-Neumann operator** (at the point \( z = -1 \)) associated with the boundary map \( \Gamma \) and the quadratic form \( I \). We denote by \( \mathcal{G}^k \) the natural scale of Hilbert spaces associated with the self-adjoint operator \( \Lambda \), i.e. we set
\[
\mathcal{G}^k := \text{dom} \Lambda^k, \quad \|\varphi\|_k := \|\Lambda^k \varphi\|_{\mathcal{G}}.
\]

Note that \( \|\varphi\|_{1/2}^2 = \|\Lambda^{1/2} \varphi\|^2 = I(\varphi) = \|\varphi\|_{\mathcal{G}^{1/2}}^2 \), i.e. the setting is compatible with our previously defined norm in (2.6). The exponents in the scale of Hilbert spaces \( \mathcal{H}^k \) and \( \mathcal{G}^k \) will be consistent with the regularity order of Sobolev spaces in our main examples in Section 7.4, a boundary pair associated with a Laplacian on a manifold with (smooth) boundary.

In the following proposition, we denote the adjoints\(^3\) of \( \Gamma: \mathcal{H}^1 \to \mathcal{G} \) w.r.t. the inner products in \( \mathcal{H}^1 \) and \( \mathcal{G} \) by \( \Gamma^* \). Similarly, the adjoint of the operator \( S \) viewed as (possibly unbounded) operator from \( \mathcal{G} \) into \( \mathcal{H}^1 \) with domain \( \mathcal{G}^{1/2} \) is denoted by \( S^* \).

**Theorem 2.11.** Let \( \Gamma \) be a boundary map associated with \( \mathfrak{h} \).

i. We have \( (\mathcal{G} = \mathcal{G}^1) \) \( \text{dom} \ \Lambda = \text{dom} \ S^* S \) and
\[
\Lambda = S^* S \geq \frac{1}{\|\Gamma\|_{1 \to 0}^2}, \quad (2.12)
\]
In particular, \( \Lambda^{-1} = \Gamma^{-1} S^* \) exists and is a bounded operator in \( \mathcal{G} \) with norm bounded by \( \|\Gamma\|_{1 \to 0}^2 \).

\(^3\)It is easy to see that \( \Gamma^* = H^T: \mathcal{G} \to \mathcal{H}^1 \) and \( S^* = S(\bar{H} + 1): \mathcal{H}^1 \to \mathcal{G} \), where \( \Gamma^* : \mathcal{H}^{-1} \to \mathcal{G} \) and \( S^* : \mathcal{G} \to \mathcal{H}^{-1} \) are the duals with respect to the pairing \( \langle \cdot, \cdot \rangle_{-1,1}: \mathcal{H}^{-1} \times \mathcal{H}^1 \to \mathbb{C} \).
ii. We have \( \| \Gamma \|_{1\to 0}^2 = 1/\inf \sigma(\Lambda) \); in particular, the lower bounds in (2.9) and (2.12) are optimal.

iii. The boundary pair is unbounded iff \( \Lambda \) is unbounded.\(^4\)

Proof. (i) The lower bound on \( \Lambda \) follows from (2.9). Moreover, by definition of the associated operator (see e.g. [Kat66, Thm. VI.2.1]) \( \varphi \in \text{dom} \Lambda \) iff
\[
\langle \cdot, \varphi \rangle_{\mathcal{H}^1} = \langle \cdot, S \varphi \rangle_{\mathcal{H}^1} = \langle S \varphi, \cdot \rangle_{\mathcal{H}^1}
\]
extends to a bounded functional \( \mathcal{G} \to \mathbb{C} \), i.e., iff \( S \varphi \in \text{dom} \mathcal{S}^* \). Moreover,
\[
\langle \varphi, S \varphi \rangle_{\mathcal{G}} = \langle \varphi, \varphi \rangle_{\mathcal{G}}^{1/2} = \langle S \varphi, S \varphi \rangle_{\mathcal{H}^1} = \langle \varphi, S^* \mathcal{S} \varphi \rangle_{\mathcal{G}}
\]
for \( \varphi \in \text{dom} \Lambda \). Since \( \mathcal{S} \) is closed, densely defined and \( \mathcal{S}^{-1} = \Gamma: \mathcal{N}^1 \to \mathcal{G} \) is bounded, it follows that \( \mathcal{S}^* \) is invertible and \( \mathcal{S}^*^{-1} = \mathcal{B} = \mathcal{G}^* \) (cf. [Kat66, Thm. III.5.30]), hence \( \Lambda^{-1} = \mathcal{S} \mathcal{S}^* \).

(ii) From (2.12) we conclude immediately the inequality \( \geq \). For the inequality \( \leq \), note that there is a sequence \( h_n \in \mathcal{N}^1 \) such that \( \| h_n \|_{\mathcal{H}^1} = 1 \) and \( \| \Gamma h_n \| \to \| \Gamma \|_{1\to 0} \). Moreover, we can assume that \( h_n \in \mathcal{N}^1 \), since the component in \( \ker \mathcal{B} = \mathcal{H}^1, \mathcal{D} \) does not contribute to the norm of \( \Gamma \). Let \( \varphi_n := \Gamma h_n \), then we have
\[
\frac{\| \varphi_n \|^2_{\mathcal{G}}}{\| \varphi_n \|^2} = \frac{\| h_n \|^2_{\mathcal{H}^1}}{\| \Gamma h_n \|^2} \to \frac{1}{\| \varphi \|^2_{\mathcal{G}}},
\]
hence \( \inf \sigma(\Lambda) \leq 1/\| \Gamma \|^2_{1\to 0} \) by the variational characterisation of the spectrum of \( \Lambda \).

(iii) Assume that \( \text{ran} \Gamma = \mathcal{G} \). Since \( \Gamma \mathcal{N}^1 \to \mathcal{G} \) is bounded and bijective, its inverse \( \mathcal{S} \) is bounded as well by the open mapping theorem. Hence \( \Lambda = \mathcal{S}^* \mathcal{S} \) is bounded. On the other hand, if \( \Lambda \) is bounded, then \( \langle \varphi, \mathcal{S} \varphi \rangle_{\mathcal{G}} = \| \varphi \|_{\mathcal{G}}^2 \). For \( \varphi \in \mathcal{D} \) we then have \( \varphi = \mathcal{S} \varphi \in \text{ran} \Gamma \), i.e., \( \text{ran} \Gamma = \mathcal{G} \).

For a bounded boundary pair, the scale of Hilbert spaces consists of one vector space only, and all norms are equivalent, i.e.
\[
\| \Gamma \|_{1\to 0}^{-2k} \| \varphi \|_{\mathcal{G}} \leq \| \varphi \|_{\mathcal{G}} \leq \| \Lambda \| \| \varphi \|_{\mathcal{G}}.
\] \hfill (2.13)

2.2 The Dirichlet solution operator at arbitrary points

Let us now extend the Dirichlet solution operator to arbitrary spectral points \( z \in \mathbb{C} \setminus \sigma(\mathcal{H}^1) \).

**Definition 2.14.** Let \( z \in \mathbb{C} \).

i. We call
\[
\mathcal{N}^1(z) := \{ h \in \mathcal{N}^1 \ | \ h(h, f) - z(h, f)_{\mathcal{H}} = 0 \ \forall f \in \mathcal{H}^1, \mathcal{D} \}
\]
the set of weak solutions in \( z \in \mathbb{C} \) (with respect to the boundary pair \( (\Gamma, \mathcal{G}) \) and the quadratic form \( h \)).

ii. Let \( \varphi \in \mathcal{G}^1 \). We say that \( h \) is a weak solution of the Dirichlet problem at the point \( z \), if \( h \in \mathcal{N}^1(z) \) and \( \Gamma h = \varphi \).

Note that \( \mathcal{N}^1(-1) = \mathcal{N}^1 \) (see Definition 2.5). Moreover, it is easy to see that \( \mathcal{N}^1(z) \) is a closed subspace of \( \mathcal{H}^1 \).

**Proposition 2.15.** Let \( z \in \mathbb{C} \setminus \sigma(\mathcal{H}^1) \).

i. Let \( h_1, h_2 \in \mathcal{N}^1(z) \) be two weak solutions of the same Dirichlet problem \( \Gamma h_1 = \Gamma h_2 \), then \( h_1 = h_2 \).

ii. The spaces \( \mathcal{H}^1, \mathcal{D} \) and \( \mathcal{N}^1(z) \) are closed as subspaces of \( \mathcal{H}^1 \) and we have the decomposition\(^5\)
\[
\mathcal{H}^1 = \mathcal{H}^1, \mathcal{D} + \mathcal{N}^1(z),
\]
and
\[
P(z) g := S \varphi + (z + 1) R^D(z) S \varphi
\]
is the projection of \( g \) onto \( \mathcal{N}^1(z) \) with respect to the above decomposition. The sum is orthogonal if \( z = -1 \).

---

\(^4\)A similar proof shows that the boundary is unbounded iff \( \Lambda(z) \) is unbounded for some (any) \( z \in \mathbb{C} \setminus \sigma(\mathcal{H}^1) \), see Section 2.3 for the definition of \( \Lambda(z) \).

\(^5\)Here, we denote by \( \mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2 \) the topological sum of \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \), i.e., the sum is direct (but not necessarily orthogonal), and \( \mathcal{H}_1, \mathcal{H}_2 \) are closed in \( \mathcal{H} \).
The choice of $P(z)$ becomes more clear with Theorem 2.21 (i) (choosing $w = -1$).

Proof. (i) Assume that $h_1$ and $h_2$ are two solutions of the Dirichlet problem with $\Gamma h_1 = \Gamma h_2$. Then $h := h_1 - h_2 \in \mathcal{H}^{1,D} \cap \mathcal{N}^1(z)$. Since $h^D - z1$ is non-degenerate on $\mathcal{H}^{1,D} \times \mathcal{H}^{1,D}$ for $z \notin \sigma(H^D)$, we conclude $h = 0$.

(ii) The space $\mathcal{H}^{1,D}$ is closed since $\Gamma$ is bounded, and $\mathcal{N}^1(z)$ is easily seen to be closed as subspace of $\mathcal{H}^1$, too. Moreover, for $g \in \mathcal{H}^1$, we set $g_2 = P(z)g = h + (z + 1)R^D(z)h$ with $h := \Gamma g$ and $g^D := g - g_2$. Then
\[
\Gamma g^D = \Gamma g - \Gamma h = 0 \quad \text{and} \quad (h - z1)(g_2, f) = (h - z1)(h + (z + 1)R^D(z)h, f)
\]
\[
= (h + 1)(h, f) - (z + 1)(h, f) + (z + 1)(h^D - z)(R^D(z)h, f) = 0
\]
for $f \in \mathcal{H}^{1,D}$. Here, the first term vanishes since $\mathcal{N}^1$ and $\mathcal{H}^{1,D}$ are orthogonal in $\mathcal{H}^1$, and the second and third term cancel each other. Therefore, we have shown that $g = g^D + g_2 \in \mathcal{H}^{1,D} + \mathcal{N}^1(z)$. Finally, the sum is direct, since $\mathcal{N}^1(z) \cap \mathcal{H}^{1,D} = \{0\}$ by the uniqueness of the weak Dirichlet solution, cf. (i).

We now define a “solution” operator $S(z)$ as the inverse of the boundary map $\Gamma$, i.e., $h = S(z)v$ is the unique solution of the weak Dirichlet problem $h \in \mathcal{N}^1(z)$ and $\Gamma h = v$ for $z \notin \sigma(H^D)$.

**Definition 2.17.** Let $S(z) : \mathcal{G}^{1/2} \to \mathcal{H}^1$ be given by
\[
S(z) := (\Gamma|_{\mathcal{N}^1(z)})^{-1} : \mathcal{G}^{1/2} \to \mathcal{N}^1(z) \subset \mathcal{H}^1.
\]

Let us now relate the Dirichlet solution operator in different points $z, w \in C \setminus \sigma(H^D)$. For $f \in \mathcal{H}$ we set
\[
U(z, w) f := f + (z - w)R^D(z)f.
\]
Recall the convention $R^D(z)f = (H^D - z)^{-1}f \oplus 0$ if $f = f^D \oplus f^\perp \in \mathcal{H}^{0,D} \oplus (\mathcal{H}^{0,D})^\perp = \mathcal{H}$ if ker $\Gamma$ is not dense in $\mathcal{H}$ (see Definition 2.1 (iv)).

**Proposition 2.19.** Let $z, w \in C \setminus \sigma(H^D)$.

i. The operator $U(z, w) : \mathcal{H} \to \mathcal{H}$ is a topological isomorphism given by
\[
U(z, w) = (H^D - w)R^D(z) \oplus \text{id}_{(\mathcal{H}^{0,D})^\perp},
\]
and $U(z, w)$ extends/restricts to a topological isomorphism
\[
U(z, w) : \mathcal{H}^k \to \mathcal{H}^k, \quad \text{for all } k \text{ with } k \geq 1 \text{ bounded by } C^{D}(z, w), \text{ where}^6
\]
\[
C^{D}(z, w) := \| (H^D - w)(H^D - z)^{-1} \| \leq 1 + \frac{|z - w|}{d(z, \sigma(H^D))},
\]
The inverse is given by $U(w, z)$.

ii. If $f \in \mathcal{H}^1$, then
\[
U(z, w)f = f + (z - w)R^D(z)f \in \mathcal{H}^1,
\]
and $U(z, w)^{-1} : \mathcal{H}^1 \to \mathcal{H}^1$, $f \mapsto U(z, w)f$ is a topological isomorphism (extending $U(z, w)^{1,D-1,D}$), with inverse $U(w, z)^{-1}$, and norm bounded by
\[
C^{1}(z, w) := \|U(z, w)^{-1}\|_{1 \to 1} \leq 1 + |z - w| \sup_{\lambda \in \sigma(H^D)} \frac{(\lambda + 1)^{1/2}}{|\lambda - z|}.
\]

iii. The projection $P(z)$ onto $\mathcal{N}^1(z)$ in $\mathcal{H}^1$ with kernel $\mathcal{H}^{1,D}$ is given by $P(z) = S(z)\Gamma = U^{1,D-1,D}(z, -1)S\Gamma$ and fulfills $\|P(z)\|_{1 \to 1} = C^1(z, -1)$.

Proof. (i) is clear from the spectral calculus. Moreover, an easy calculation using the resolvent equality $R^D(z) - R^D(w) = (z - w)R^D(z)R^D(w)$ shows that $U(z, w)U(w, z)f = f$ for $f \in \mathcal{H}$.

(ii) The fact that $U(z, w)f \in \mathcal{H}^1$ if $f \in \mathcal{H}^1$ is obvious, since $R^D(z)f \in \mathcal{H}^{2,D} \subset \mathcal{H}^1$. Moreover, $U(z, w)U(w, z)f = f$ for $f \in \mathcal{H}^1$ since this equality is already true for $f \in \mathcal{H}^1$. The bound on the norm shows that $U(z, w)$ is a topological isomorphism from $\mathcal{H}^1$ onto $\mathcal{H}^1$ with inverse $U(z, w)$. The bound can be seen by the estimate
\[
\|U^{1,D-1}(z, w)\|_{1 \to 1} = \|1 + (z - w)(H^D)^{1/2}R^D(z)(H^D)^{1/2}\|
\]
\[
\leq \|1 + (z - w)(H^D)^{1/2}R^D(z)\|.
\]

(iii) is obvious from Theorem 2.21 or from (2.16b) and (2.22a). For the norm bound note that $P(z) = U^{1,D-1}(z, -1)P(-1)$ and $P(-1)$ is an orthogonal projection. □

---

6We use the convention $C^D(z, w) := 1$ if $\sigma(H^D) = \emptyset$ in the extreme case $\mathcal{H} = \emptyset$, $\Gamma = \text{id}$ and $\mathcal{H}^{1,D} = \{0\}$, see Section 7.1.
Let us now collect some facts about the Dirichlet solution operator:

**Theorem 2.21.** Let $z, w \in \mathbb{C} \setminus \sigma(H^D)$.

1. We have $U(z,w)^{1-1}S(w) = S(z)$ or equivalently
   \[ S(z) - S(w) = (z-w)R^D(z)^{1-1}S(w) = (z-w)R^D(w)^{1-1}S(z) : \mathcal{G}^{1/2} \rightarrow \mathcal{H}^1. \quad (2.22a) \]

   In particular,
   \[ U(z, w)^{1-1} : \mathcal{H}^{1,D} + \mathcal{A}^1(w) \rightarrow \mathcal{H}^{1,D} + \mathcal{A}^1(z) \]
   respects the splitting and the projection onto $\mathcal{A}^1(z)$ is given by $P(z) = S(z)\Gamma$.

2. The solution operator $S(z) : \mathcal{G}^{1/2} \rightarrow \mathcal{A}^1(z)$ is a topological isomorphism with left inverse given by $\Gamma$. Moreover,
   \[ \frac{1}{C_1(\mathbb{-1}, z)}\|\phi\|_{\mathcal{G}^{1/2}} \leq \|S(z)\phi\|_{\mathcal{H}^1} \leq C_1(z, -1)\|\phi\|_{\mathcal{G}^{1/2}} \quad (2.22b) \]
   with $C_1(\mathbb{-1}, z)$ defined in (2.20b).

3. The solution operator is holomorphic\(^7\) in $z$, and the $k$-th derivative with respect to $z$ is given by
   \[ S^{(k)}(z) = k! R^D(z)^{k}S(z) : \mathcal{G}^{1/2} \rightarrow \left\{ \begin{array}{ll} \mathcal{H}^1 & , k = 0, \\
                   \mathcal{H}^{2k,D} & , k \geq 1. \end{array} \right. \]

**Proof.** (i) Let $f := S(w)\phi \in \mathcal{A}^1(w)$ and $g := U(z, w)^{1-1}f = f + (z-w)R^D(z)f$. We have to show that $g$ is the weak solution of the Dirichlet problem in $z$. The fact that $\Gamma g = \Gamma f = \phi$ is obvious since $\Gamma R^D(z) = 0$. It remains to show that $g \in \mathcal{A}^1(z)$. Let $u \in \mathcal{H}^{1,D}$, then
   \[ (\mathbf{h} - z\mathbf{1})(g, u) = (\mathbf{h} - z\mathbf{1})(f, u) + (z-w)(\mathbf{h} - z\mathbf{1})(R^D(z)f, u). \]
   But the latter summand equals $(z-w)(f, u)$, so that $(\mathbf{h} - z\mathbf{1})(g, u) = (\mathbf{h} - w\mathbf{1})(f, u) = 0$ since $f \in \mathcal{A}^1(w)$. By the definition of $U(z, w)^{1-1}$, we have $U(z, w)^{1-1} \mathcal{H}^{1,D} \subset \mathcal{H}^{1,D}$. Moreover, we have just shown that $U(z, w)^{1-1}$ respects the splitting. Finally, $P(z) = S(z)\Gamma$ follows from (2.16b).

(ii) That $S(z)$ is a topological isomorphism follows already from the fact that $\Gamma$ restricted as map $\mathcal{A}^1(z) \rightarrow \mathcal{G}^{1/2}$ is bounded and bijective. The norm bounds on $S(z)\phi$ follow easily from $S(z) = U^{1-1}(z, -1)S$.

(iii) The formula for the derivative follows immediately from (2.22a).

---

### 2.3 The Dirichlet-to-Neumann form at arbitrary points

Let us now define a sesquilinear form which will be associated with the Dirichlet-to-Neumann operator at $z \in \mathbb{C} \setminus \sigma(H^D)$. We will see later on that this form and the associated operator is indeed what we expect from a Dirichlet-to-Neumann operator: Roughly, $\Lambda(z)\phi$ is the “normal derivative” on the boundary of the Dirichlet solution associated with $\phi$ at $z$, i.e., $\Lambda(z) = \Gamma S(z)\phi$, as we will see in Proposition 6.8.

Let us start first with what we will call the **Dirichlet-to-Neumann form** later on:

**Theorem 2.23.** Let $(\Gamma, \mathcal{G})$ be a boundary pair and $z \in \mathbb{C} \setminus \sigma(H^D)$.

1. The expression
   \[ \mathcal{I}_z(\phi, \psi) := (\mathbf{h} - z\mathbf{1})(S(z)\phi, g), \quad (2.24a) \]
   where $g \in \mathcal{H}^1$ with $\Gamma g = \psi$, is well-defined (i.e., independent of the choice of $g$) and defines a sesquilinear form $\mathcal{I}_z : \mathcal{G}^{1/2} \times \mathcal{G}^{1/2} \rightarrow \mathbb{C}$.

2. The family $(\mathcal{I}_z)_{z \in \mathbb{C} \setminus \sigma(H^D)}$ of sesquilinear forms is symmetric, i.e., $\mathcal{I}_z^* = \mathcal{I}_z$, where $\mathcal{I}_z^*(\phi, \psi) := \mathcal{I}_z(\psi, \phi)$ defines as usual the adjoint form associated with $\mathcal{I}_z$.

3. For $z, w \in \mathbb{C} \setminus \sigma(H^D)$, we have
   \[ \mathcal{I}_z(\phi, \psi) - \mathcal{I}_w(\phi, \psi) = -(z-w)(S(z)\phi, S(\overline{w})\psi) = -(z-w)(S(w)\phi, S(\overline{z})\psi). \quad (2.24b) \]

---

\(^7\) The holomorphy of the operator family does not depend on the topology (weak, strong or operator-norm, see [Kat66, Thm. III.3.12]).
iv. The sesquilinear form $l_z: \mathcal{H}^{1/2} \times \mathcal{H}^{1/2} \to \mathbb{C}$ is bounded, i.e., $|l_z(\varphi, \psi)| \leq L(z)\|\varphi\|_{1/2}\|\psi\|_{1/2}$, where

$$L(z) := 1 + |z + 1|\|S(z)\|_{1/2} \leq 1 + |z + 1|C^4(z,-1).$$

2.24c

v. The Dirichlet-to-Neumann form is holomorphic in $z$, i.e., $z \mapsto l_z(\varphi, \psi)$ depends holomorphically on $z \in \mathbb{C} \setminus \sigma(\mathcal{H})$ for all $\varphi, \psi \in \mathcal{H}^{1/2}$. Its derivative (denoted by $l'_z$) is

$$l'_z(\varphi, \psi) = -\langle S(z)\varphi, S(\overline{\varphi})\psi \rangle,$$

and the $k$-th derivative with respect to $z$ is given by

$$l^{(k)}_z(\varphi, \psi) = -k!(R^D(z))^{k-1}S(z)\varphi, S(\overline{\varphi})\psi,$$

where the sesquilinear forms $l^{(k)}_z$ are bounded as sesquilinear forms on $\mathcal{H}^{1/2} \times \mathcal{H}^{1/2}$.

vi. If $\lambda \in \mathbb{R} \setminus \sigma(\mathcal{H}^D)$, then $l'_z \leq 0$. Moreover, $\lambda_1 \leq \lambda_2$ implies $l_{\lambda_1} \geq l_{\lambda_2}$. In particular, $l_0 \geq 0$ is a non-negative form for $\lambda \leq 0$.

vii. We have

$$(\text{Im} l_z)(\varphi) = -(\text{Im} z)\|S(z)\varphi\|_{\mathcal{H}}^2 \leq 0$$

for $\varphi \in \mathcal{H}^{1/2}$ provided $\text{Im} z \geq 0$. In particular, $-l_z$ is a form-valued Herglotz function.

Proof. (i) Let $g_1, g_2 \in \mathcal{H}^1$ such that $\Gamma g_1 = \Gamma g_2 = \varphi$. Then $g_1 - g_2 \in \mathcal{H}^{1/2}$, and

$$(h - z1)(S(z)\varphi, g_1 - g_2) = 0$$

since $S(z)\varphi \in \mathcal{A}^1(z)$ is a weak solution by Theorem 2.21 (i).

(ii) is obvious.

(iii) Choosing $g = S(\overline{\varphi})\varphi$ and using (2.22a), we have

$$l_z(\varphi, \psi) = (h - z1)(S(z)\varphi, g) = (h - w1)(S(w)\varphi, g) + (z - w)(R^D(z)S(w)\varphi, g) - (z - w)(S(z)\varphi, g) = l_w(\varphi) - (z - w)(S(z)\varphi, g).$$

Note that by this choice of $g$, the middle term in the second line vanishes (by definition of $\mathcal{A}^1(w)$).

For (iv), we set $w = -1$ in (2.24b) and obtain

$$|l_z(\varphi)| \leq \|\varphi\|_{1/2}^2 + |z + 1|\|S(z)\varphi\|_{\mathcal{H}}\|\varphi\|_{\mathcal{H}}.$$  

Using the estimates $\|S(z)\varphi\|_{\mathcal{H}} \leq \|S(z)\varphi\|_{\mathcal{H}^1}$ and $\|S\varphi\|_{\mathcal{H}} \leq \|S\varphi\|_{\mathcal{H}^1} = \|\varphi\|_{1/2}$, we obtain the desired bound.

(v) and (vii) follow by a straightforward calculation from (2.24b). (vi) is a special case of (v) for real $z = \lambda$. 

Definition 2.25. We call the sesquilinear form $l_z$ defined in (2.24a) the Dirichlet-to-Neumann form at $z \in \mathbb{C} \setminus \sigma(\mathcal{H})$ associated with the boundary pair $(\Gamma, \mathcal{G})$.

By the previous proposition, $l_z$ is bounded as form on $\mathcal{H}^{1/2} \times \mathcal{H}^{1/2}$. We therefore can define an operator

$$\tilde{A}(z): \mathcal{H}^{1/2} \to \mathcal{H}^{-1/2}, \quad \varphi \mapsto l_z(\varphi, \cdot),$$

called the weak Dirichlet-to-Neumann operator, i.e.,

$$\langle \tilde{A}(z)\varphi, \psi \rangle_{-1/2,1/2} = l_z(\varphi, \psi) = (h - z1)(S(z)\varphi, S(\overline{\varphi})\psi),$$

or $\tilde{A}(z) = S^*(\hat{H} - z)S(z): \mathcal{H}^{1/2} \to \mathcal{H}^1 \to \mathcal{H}^{-1} \to \mathcal{H}^{-1/2}$ in the scale of Hilbert spaces.

---

*The imaginary part of a sesquilinear form $a$ is defined as $\text{Im } a := \frac{1}{2i}(a - a^*)$, i.e., $(\text{Im } a)(\varphi, \psi) := \frac{1}{2i}(a(\varphi, \psi) - a(\psi, \varphi))$. Note that $(\text{Im } a)(\varphi, \psi) \in \mathbb{C}$ is in general not equal to $\text{Im } (a(\varphi, \psi)) \in \mathbb{R}$. This equality is only true for the associated quadratic form $\text{Im } a(\varphi) := \text{Im } a(\varphi, \varphi)$ (denoted as usual by the same symbol).*
We always have an associated operator with $I_z$, defined by

$$\text{dom } \Lambda(z) := \{ \varphi \in \mathcal{G}^{1/2} \mid \exists \psi \in \mathcal{G} \forall \eta \in \mathcal{G}^{1/2}: I_z(\varphi, \eta) = \langle \psi, \eta \rangle_{\mathcal{G}} \}$$

(2.26)

and $\Lambda(z) \varphi := \psi$, and that the latter definition is well-defined (this is due to the defining equation (2.26), since $\mathcal{G}^{1/2} = \text{ran } \Gamma$ is dense in $\mathcal{G}$ by definition of a boundary pair). We call this operator the (strong) Dirichlet-to-Neumann operator associated with a boundary pair. Actually, $\Lambda(z)$ is the restriction of $\tilde{\Lambda}(z)$ to those $\varphi$ such that $\tilde{\Lambda}(z) \varphi \in \mathcal{G}$. It is easily seen that $\varphi \in \text{dom } \Lambda(z)$ can equivalently expressed by

$$\exists u \in \mathcal{H}^1, \Gamma u = \varphi \exists \psi \in \mathcal{G} \forall \psi \in \mathcal{G}^{1/2}: \langle h - z I \rangle (u, v) = \langle \psi, \Gamma v \rangle_{\mathcal{G}}$$

(2.27)

without referring to the solution operator.

We use the notation $\tilde{\Lambda}(z)$ when we want to stress that we mean the weak Dirichlet-to-Neumann operator, and not the strong Dirichlet-to-Neumann operator. Recall the definition of $\Lambda$ as operator associated with $I$ in Definition 2.10: We have $\Lambda = \Lambda(-1)$ since $I = I_{-1}$.

We state more results on the strong Dirichlet-to-Neumann operator later on (see Theorems 2.29 and 3.8 and Proposition 3.11).

Remark 2.28. Theorem 2.23 (vii) allows us to express the quadratic form $q_\lambda$ defined by $q_\lambda(\varphi) := \|S(z)\varphi\|^2_{\mathcal{G}^*}$ in terms of the Dirichlet-to-Neumann form $I_z$, namely, $q_\lambda = -I_z^* \lambda$ for $\lambda \in \mathbb{C} \setminus \sigma(H^D)$. This is useful in reconstructing a boundary pair from a given form-valued Herglotz function. We will treat this and related questions in a forthcoming publication.

### 2.4 The Neumann-to-Dirichlet operator

Let us first show that the weak Dirichlet-to-Neumann operator $\tilde{\Lambda}(z)$ is invertible if $z$ is not in the Neumann spectrum, and that the function $z \mapsto \Lambda(z)^{-1}$ extends continuously into the Dirichlet spectrum $z \in \sigma(H^D)$.

**Theorem 2.29.** Let $z \in \mathbb{C} \setminus (\sigma(H^D) \cup \sigma(H))$. Then we have:

i. The weak Dirichlet-to-Neumann operator $\tilde{\Lambda}(z): \mathcal{G}^{1/2} \rightarrow \mathcal{G}^{-1/2}$ is bijective with inverse

$$\Lambda(z)^{-1} = \Gamma R(z)\Gamma^*; \mathcal{G}^{-1/2} \rightarrow \mathcal{G}^{1/2}.$$  

(2.30)

ii. The operator-valued function $z \mapsto \Lambda(z)^{-1}$ extends into $z \in \sigma(H^D)$, and the value is again a bounded operator denoted by the same symbol $\Lambda(z)^{-1}$.

iii. The norm of $\Lambda(z)^{-1}$ is bounded by $CN(z, -1)$ where $CN(z, w)$ is defined as in (2.20a) with $H^D$ replaced by $H$.

iv. Denote by $\Lambda(z)^{-1}: \mathcal{G} \rightarrow \mathcal{G}$ the operator $\Lambda(z)^{-1}$ restricted to $\mathcal{G}$ and with range space $\mathcal{G}$, then $\Lambda(z)^{-1}$ is the inverse of the strong operator $\Lambda(z)$: $\text{dom } \Lambda(z) \rightarrow \mathcal{G}$ and $\Lambda(z)^{-1}$ is bounded by $\|\Gamma\|^2_{\mathcal{G}^*}CN(z, -1)$.

v. The strong Dirichlet-to-Neumann operator $\Lambda(z)$ is closed for $z \in \mathbb{C} \setminus (\sigma(H^D) \cup \sigma(H))$.

**Proof.** (i) Let $\varphi \in \text{ker } \tilde{\Lambda}(z)$, i.e., $I_z(\varphi, \eta) = 0$ for all $\eta \in \mathcal{G}^{1/2}$. Therefore,

$$0 = I_z(\varphi, \eta) = (h - z I)(S(z)\varphi, g)$$

for all $g \in \mathcal{H}^1$ with $\Gamma g = \eta$. Since $z \notin \sigma(H)$, the form $h - z I$ is non-degenerative, and therefore $S(z)\varphi = 0$, i.e., $\varphi = 0$. In particular, we have shown that $\Lambda(z)$ is injective.

For the surjectivity, let $\psi \in \mathcal{G}^{-1/2}$. Set $\varphi := \Gamma R(z)\Gamma^* \psi$, then $\varphi \in \mathcal{G}^{1/2}$, and

$$\langle \tilde{\Lambda}(z)\varphi, \eta \rangle_{-1/2, 1/2} = I_z(\varphi, \eta) = (h - z I)(S(z)\Gamma R(z)\Gamma^* \psi, g),$$

where $g \in \mathcal{H}^1$ with $\Gamma g = \eta$. Moreover, $h = \tilde{R}(z)\Gamma^* \psi \in \mathcal{H}^1(z)$, since $(h - z I)(h, f) = \langle \psi, \Gamma f \rangle$ for all $f \in \mathcal{H}^1,D$, hence $h = S(z)\Gamma h$ by Theorem 2.21 (ii), and we have

$$\langle \Lambda(z) \varphi, \eta \rangle_{-1/2, 1/2} = (h - z I)(h, g) = \langle \psi, \eta \rangle_{-1/2, 1/2},$$

i.e., we have shown that $\tilde{\Lambda}(z) \varphi = \psi$ and $\varphi = \Gamma R(z)\Gamma^* \psi$, i.e., that $\Lambda(z)^{-1} = \Gamma R(z)\Gamma^*$. (i)-(iii) are obvious from the representation of $\Lambda(z)^{-1}$, as well as the norm estimate in (iv).

(iv) By the previous results, $\Lambda(z): \text{dom } \Lambda(z) \rightarrow \mathcal{G}$ is bijective and its inverse $\Lambda(z)^{-1}$ is bounded as map $\mathcal{G} \rightarrow \mathcal{G}$ provided $z \notin \sigma(H)$. Note that $\text{dom } \Lambda(z) = \{ \varphi \in \mathcal{G}^{1/2} \mid \tilde{\Lambda}(z) \varphi = 0 \}$.

(v) The inverse of $\Lambda(z)$ is bounded as operator $\mathcal{G} \rightarrow \mathcal{G}$, hence $\Lambda(z)$ is closed. \qed
Definition 2.31. We call \( \Lambda(z)^{-1} : \mathcal{G} \to \mathcal{G} \) the Neumann-to-Dirichlet operator.

For a justification of the name, we refer to Proposition 6.8.

Remark 2.32. For a general boundary pair, it is a priori not clear whether \( \Lambda(\lambda) \) as operator associated with \( I_2 \) is closed also for \( \lambda \in \sigma(H) \). If \( \text{dom} \Lambda(\lambda) \) is dense in \( \mathcal{G}^{1/2} \), then the closedness can be shown. This is e.g. the case for elliptically regular boundary pairs; we will see that \( I_2 \) is a closed and sectorial quadratic form for all \( z \in \mathbb{C} \setminus \sigma(H^D) \); in particular, \( \Lambda(z) \) is the associated operator and hence closed (see Section 3.1 and Theorem 3.8). Moreover, the domain of \( \Lambda(z) \) is independent of \( z \) in this case.

Nevertheless, it may happen that \( I_2 \) is closable, but the closure \( \mathcal{G}^{1/2} \) is strictly larger than \( \mathcal{G}^{1/2} \), i.e., there are embeddings \( \mathcal{G}^{1/2} \hookrightarrow \mathcal{G}^{1/2} \hookrightarrow \mathcal{G} \), and none of the embeddings is surjective (see Example 7.10).

Let us now look at the Neumann-to-Dirichlet operator at different points:

Proposition 2.33. Let \( z, w \in \mathbb{C} \setminus \sigma(H) \),

\[ i. \text{We have} \quad \Lambda(z)^{-1} - \Lambda(w)^{-1} = (z - w)\Gamma R(w)(\Gamma R(\overline{z}))^* = (z - w)\Gamma R(z)(\Gamma R(\overline{w}))^* : \mathcal{G} \to \mathcal{G}. \quad (2.34) \]

\[ ii. \text{We have} \quad \text{Im} \Lambda(z)^{-1} := \frac{1}{2}(\Lambda(z)^{-1} - \Lambda(\overline{z})^{-1}) = (\text{Im} z)(\Gamma R(z))(\Gamma R(\overline{z}))^* \geq 0. \text{ In particular, } \Lambda(z)^{-1} \text{ is an operator-valued Herglotz function.} \]

Proof. (i) follows immediately from (2.30) and the resolvent equation. (ii) is obvious from (i).

Theorem 2.35. The following assertions are equivalent:

\[ i. \Lambda^{-1} : \mathcal{G} \to \mathcal{G} \text{ is compact}, \]

\[ ii. \Lambda(z)^{-1} : \mathcal{G} \to \mathcal{G} \text{ is compact for all } z \in \mathbb{C} \setminus \sigma(H), \]

\[ iii. \Gamma : \mathcal{H}^1 \to \mathcal{G} \text{ is compact} \]

Assume additionally that \( R \) is compact. Then any of the above condition is also equivalent with the following:

\[ iv. \text{For all } z \in \mathbb{C} \setminus \sigma(H^D), \text{ there exists } a \geq 0 \text{ such that } (\Lambda(z) + a)^{-1} \text{ is compact}, \]

\[ v. \text{For all } z \in \mathbb{C} \setminus \sigma(H^D), \text{ the operator } \Lambda(z) \text{ is closed and has purely discrete spectrum.} \]

Proof. (i) \( \Rightarrow \) (ii) \& (iii): We have the factorisation \( \Lambda^{-1} = K^* K \) with \( K = (\Gamma R^{1/2})^* \). Assume now that \( \Lambda^{-1} \) is compact, then \( K \) is compact, and therefore also \( \Gamma = K(H + 1)^{1/2} \) (hence (iii) is shown). Moreover, \( (\Gamma R)^* = R^{1/2} K : \mathcal{G} \to \mathcal{H} \) is compact, too. Now, by (2.34) and the resolvent equation, we have

\[ \Lambda(z)^{-1} = \Lambda^{-1} + (\Gamma R)(1 + (z + 1)R(z))(\Gamma R)^* \]

which shows that \( \Lambda(z)^{-1} \) is compact as operator \( \mathcal{G} \to \mathcal{G} \) for any \( z \in \mathbb{C} \setminus \sigma(H) \).

(ii) \( \Rightarrow \) (i) is obvious. (iii) \( \Rightarrow \) (i): The compactness of \( \Lambda^{-1} \) follows from \( \Lambda^{-1} = \Gamma^{-1} : \mathcal{G} \to \mathcal{G} \) (see Theorem 2.11 (i)).

For the assertions (iv) and (v) we need some material provided in Section 5.1: Introducing the Robin boundary conditions allows us to find a parameter \( a \) such that \( z \) is not in the spectrum of the Neumann operator \( H_a \) for the boundary pair \( (\Gamma, \mathcal{G}) \) associated with the form \( h_a \) (see Section 5.1 for the notation).

(i) \( \Rightarrow \) (iv): Let \( z \notin \sigma(H^D) \). By Proposition 5.3, there exists \( a > 0 \) such that \( z \notin \sigma(H_a) \). By assumption, \( \Lambda^{-1} \) is compact, hence \( \Lambda^{-1} = (\Lambda + a)^{-1} \) is also compact. We can now apply (i) \( \Rightarrow \) (ii) for the boundary pair \( (\Gamma, \mathcal{G}) \) associated with \( h_a \) and obtain that \( \Lambda_a(z)^{-1} = (\Lambda(z) + a)^{-1} \) is compact.

(iv) \( \Rightarrow \) (i): Set \( z = -1 \), then \( \Lambda^{-1} = (1 + a\Lambda^{-1})(\Lambda + a)^{-1} \) and this operator is compact, if \( (\Lambda + a)^{-1} \) is. The equivalence (iv) \( \Leftrightarrow \) (v) is a general fact from operator theory.

Remark 2.36. We want to remark that, in general, the compactness of \( R \) and \( \Lambda^{-1} \) are independent of each other as the following examples show:

i. \( R \) and \( R^D \) non-compact, \( \Lambda^{-1} \) compact: The compactness of \( \Lambda^{-1} \) does not imply the compactness of \( R \), as the following manifold example shows: Let \( \Delta_{\mathbb{R}^n \times Y} \) be the Laplacian on a half-cylinder \( X = [0, \infty) \times Y \) with compact manifold \( Y \) (see Section 7.5), then \( R = (\Delta_{\mathbb{R}^n \times Y} + 1)^{-1} \) and \( R^D \) are non-compact, while \( \Lambda^{-1} = (\Delta_y + 1)^{-1/2} \) is compact.
ii. $R$ and $R^D$ compact, $\Lambda^{-1}$ non-compact: On the other hand, the compactness of $R$ does not imply the compactness of $\Lambda^{-1}$ either (see the bounded modification of a boundary pair associated with a compact manifold in Example 7.21).

iii. $R$ non-compact, $R^D$ compact, $\Lambda^{-1}$ compact: There are boundary pairs for which $R$ is non-compact, while $R^D$ is compact; the associated Dirichlet-to-Neumann operator at $z = 0$ is a Jacobi operator (see Example 7.9 in Section 7.3). If $\alpha > 2$ in the example then $\Lambda(0)$ has purely discrete spectrum and $\Lambda^{-1} \leq \Lambda(0)^{-1}$ is compact; if $\alpha = 2$, then $\Lambda(0)$ has purely absolutely continuous spectrum $[1/4, \infty)$, and hence $\Lambda(0)^{-1}$ is not compact.

3 Boundary pairs with additional properties

Let us now describe further properties of boundary pairs described in terms of the Dirichlet solution operator. It turns out that these properties allow us to relate the concept of boundary pairs to other concepts such as boundary triples (see Section 6.1)

3.1 Elliptically regular boundary pairs

The Dirichlet solution operator $S(z): G^{1/2} \to H^1$ can sometimes be extended to a bounded operator denoted by $\overline{S}(z): G \to H$, or, equivalently, that the dual operator $S(z)^*: H^{-1} \to G^{1/2}$ restricts to a bounded operator $B(z): H \to G$. This property has already been recognised as important in a different context by Brasche et al., see Remark 3.7.

The main consequence of these facts is that the sesquilinear form $t_z$ associated with the Dirichlet-to-Neumann operator is sectorial, and hence, the strong Dirichlet-to-Neumann operator (the operator associated with the form $t_z$) is closed. Moreover, its domain $\text{dom} \Lambda(z)$ is independent of $z$ (see Theorem 3.8).

**Definition 3.1.** Let $(\Gamma, \mathcal{G})$ be a boundary pair. We say that the boundary pair is elliptically regular if there is a constant $C > 0$ such that $\|S\varphi\|_{\mathcal{H}} \leq C\|\varphi\|_{\mathcal{G}}$ for all $\varphi \in G^{1/2}$.

Let us first present a simple consequence:

**Proposition 3.2.** Let $(\Gamma, \mathcal{G})$ be a boundary pair and let $S(z)$ be the corresponding weak Dirichlet solution operator. If the boundary pair $(\Gamma, \mathcal{G})$ is bounded, then it is elliptically regular.

**Proof.** If the boundary pair is bounded, then $\Lambda$ is a bounded operator in $\mathcal{G}$ by Theorem 2.11 (iii). Moreover,

$$\|S\varphi\|_{\mathcal{H}} \leq \|S\varphi\|_{\mathcal{H}^1} = \|\varphi\|_{\mathcal{H}^{1/2}} \leq \|\Lambda\|_{1/2}\varphi,$$

i.e., we can choose $C := \|\Lambda\|^{1/2}$. \qed

**Remark 3.3.**

i. Not all boundary pairs are elliptically regular, see the unbounded Jacobi operator example in Section 7.3 or the Zaremba problem in Theorem 7.27. Moreover, not all elliptic boundary pairs are bounded (see the manifold examples in Sections 7.4–7.6).

ii. The notion “elliptically regular” for boundary pairs is actually inspired by a similar property in one of our main examples presented in Section 7.4.

The name “elliptically regular” is also justified by the following fact (see also Section 6.3):

**Definition 3.4.** We say that the sesquilinear form $t_z: G^{1/2} \times G^{1/2} \to \mathbb{C}$ is elliptic or coercive in $\mathcal{G}$ if there exist $\alpha > 0$ and $\omega(z) \in \mathbb{R}$ such that

$$(\text{Re} t_z)(\varphi) + \omega(z)\|\varphi\|^2_{\mathcal{G}} \geq \alpha\|\varphi\|^2_{G^{1/2}}$$

for all $\varphi \in G^{1/2}$.

Actually, $t_z$ is $J$-elliptic in the sense of Definition 6.21 with $J: G^{1/2} \hookrightarrow \mathcal{G}$ being the embedding map.

Let us now present some equivalent conditions assuring elliptic regularity, we give some more characterisations in Theorem 6.9 (i):

**Theorem 3.5.** Let $(\Gamma, \mathcal{G})$ be a boundary pair and let $S(z)$ be the corresponding weak Dirichlet solution operator for $z \in \mathbb{C} \setminus \sigma(H^D)$. Then the following conditions are equivalent:

\[\text{(i)} \quad \|S\varphi\|_{\mathcal{H}} \leq C\|\varphi\|_{\mathcal{G}} \quad \text{for all } \varphi \in G^{1/2}.
\]

\[\text{(ii)} \quad \text{there exists } \alpha > 0 \text{ such that } (\text{Re} t_z)(\varphi) + \omega(z)\|\varphi\|^2_{\mathcal{G}} \geq \alpha\|\varphi\|^2_{G^{1/2}}\text{ for all } \varphi \in G^{1/2}.
\]

\[\text{(iii)} \quad \text{there exists } \alpha > 0 \text{ such that } (\text{Re} t_z)(\varphi) + \omega(z)\|\varphi\|^2_{\mathcal{G}} \geq \alpha\|\varphi\|^2_{\mathcal{H}^{1/2}}\text{ for all } \varphi \in G^{1/2}.
\]
i. The boundary pair is elliptically regular.

ii. The weak Dirichlet solution operator $S(z)$ extends to a bounded operator $\overline{S}(z): \mathcal{G} \to \mathcal{H}$ for some (any) $z \in \mathbb{C} \setminus \sigma(H^D)$.

iii. There is a constant $c > 0$ such that $|\Gamma h|_G \geq c||h||_\mathcal{H}$ for all $h \in \Lambda^1$.

iv. The dual $S(\overline{\cdot}) : \mathcal{H}^{-1} \to \mathcal{G}^{-1/2}$ of the Dirichlet solution operator $S(\overline{\cdot})$ restricts to a bounded operator $\mathcal{H} \to \mathcal{G}$ (denoted by $B(z)$) for some (any) $z \in \mathbb{C} \setminus \sigma(H^D)$.

v. The quadratic form $q_z$ defined by $q_z(\varphi) := ||S(z)\varphi||^2$ for $\varphi \in \mathcal{G}^{1/2}$ is associated with a bounded operator $Q(z)$ on $\mathcal{G}$ (given by $\text{Im} \Lambda(z) := -(\text{Im} z)Q(z)$) for some (any) $z \in \mathbb{C} \setminus \mathbb{R}$.

vi. The imaginary part $\text{Im} \mathcal{I}_z := \frac{1}{2}(l_z - l_z^*)$ of the form $\mathcal{I}_z$ is associated with a bounded operator on $\mathcal{G}$ (given by $\text{Im} \Lambda(\lambda) := -Q(\lambda)$) for some (any) $\lambda \in \mathbb{R} \setminus \sigma(H^D)$.

vii. For $z \in \mathbb{R}$ in a neighbourhood of $-1$ (resp. for all $z \in \mathbb{C} \setminus \sigma(H^D)$), there exists $\omega(z)$ such that $\omega(-1) = 0$ and $\lim\sup_{a \to -1} \frac{\varphi(a)}{a + 1}$ is finite, and the sesquilinear form $\mathcal{I}_z$ is elliptically regular with constants $\alpha = 1$ and $\omega(z)$.

ix. We have $\Gamma(\text{dom } H) \subset \mathcal{G}^1 = (\text{dom } \Lambda)$.

x. The operator $\Lambda G \Gamma$ maps $\mathcal{H}$ into $\mathcal{G}$ and is bounded as operator $\mathcal{H} \to \mathcal{G}$.

Proof. (i) $\iff$ (ii): By definition, $S$ extends to a bounded operator $\overline{S}: \mathcal{G} \to \mathcal{H}$. Let now $z \in \mathbb{C} \setminus \sigma(H^D)$, then $S(z) = U(z, -1)^{-1}S$ by Theorem 2.21 (i) and $U(z, -1)^{-1}$ extends to a bounded operator $U(z, -1) = 1 + (z + 1)\overline{R}(z): \mathcal{H} \to \mathcal{H}$. The assertion (iii) is just a reformulation of the definition (i) for the inverse. The equivalences (ii) $\iff$ (iv) $\iff$ (v) are simple facts from operator theory. For (vi), note that $\text{Im} \mathcal{I}_z = -(\text{Im} z)q_z$ by Theorem 2.23 (vii), hence (vi) is equivalent with (v). Similarly, for (vii) we note that $\mathcal{I}_z = -q_z$ by Theorem 2.23 (v).

(i) $\implies$ (viii) We have

$$\text{Re} \mathcal{I}_z(\varphi) - \mathcal{I}(\varphi) = -\text{Re} \langle (z + 1)U(z, -1)\overline{S}\varphi, \overline{S}\varphi \rangle \geq -\omega(z)||\varphi||^2$$

for $\varphi \in \mathcal{G}$, where

$$\omega(z) := ||\overline{S}||^2 \max\left\{ \sup_{\lambda \in \sigma(H^D)} \text{Re} \left( \frac{(z + 1)(\lambda + 1)}{\lambda - z} \right), 0 \right\}. \quad (3.6)$$

Note that the inequality holds by the spectral calculus. Since the real part of the fraction as a function in $\lambda \in \sigma(H^D)$ is continuous and has a limit as $\lambda \to \infty$, it attains a maximum $C_+(z) \in \mathbb{R}$ (and a minimum $C_-(z) \in \mathbb{R}$) for $z \in \mathbb{C} \setminus \sigma(H^D)$. In particular, $\omega(z) = ||\overline{S}||^2 \max\{C_+(z), 0\} < \infty$.

If $z = a < 0$, then $C_+(a) = -(a + 1)$ and $C_-(a) = (a + 1)/a$. Moreover, $\omega(a)/(a + 1) = -||\overline{S}||^2$ and the limes superior is finite.

(viii) $\implies$ (i) From Theorem 2.23 (v) we know that $\mathcal{I}_z = -q_z$. Moreover, from the assumption, we have $-(\mathcal{I}_z(\varphi) - \mathcal{I}(\varphi)) \leq \omega(\varphi)||\varphi||^2$ for $a < 0$ near $-1$ and $\varphi \in \mathcal{G}^{1/2}$. Therefore, we conclude

$$0 \leq ||S\varphi||^2 = q_{-1}(\varphi) = -\lim_{a \to -1} \frac{I_a(\varphi) - \mathcal{I}(\varphi)}{a + 1} \leq \limsup_{a \to -1} \frac{\omega(a)}{a + 1} ||\varphi||^2,$$

hence the boundary pair is elliptically regular with $C^2 = \lim\sup_{a \to -1} \omega(a)/(a + 1)$.

(ii) $\implies$ (x) By assumption, $\Lambda \Gamma \mathcal{H} = \Lambda \Gamma \mathcal{H} \subset \mathcal{G}$. Assume that $f_n \to f$ in $\mathcal{H}$ and $\psi_n := \Lambda \Gamma f_n \to \psi$ in $\mathcal{G}$, and the convergence also holds in $\mathcal{G}^{-1/2}$. Moreover, $\psi_n = \Lambda \Gamma f_n \to \Lambda \Gamma f$ in $\mathcal{G}^{-1/2}$ since $\Lambda \Gamma$ is bounded as operator $\mathcal{H} \to \mathcal{H}^{-1} \to \mathcal{G}^{-1/2}$. Since limits in $\mathcal{G}^{-1/2}$ are unique, we have $\Lambda \Gamma f = \psi \in \mathcal{G}$. In particular, $\Lambda \Gamma: \mathcal{H} \to \mathcal{G}$ is closed, hence bounded by the closed graph theorem.

(x) $\implies$ (ix) Since $\Lambda \Gamma(\text{dom } H) = \Lambda \Gamma \mathcal{H} \subset \mathcal{G}$ by assumption, we have $\Gamma(\text{dom } H) \subset \mathcal{G}^1 = \text{dom } \Lambda$.

(i) $\iff$ (x) We have $(\Lambda \Gamma)^* = S: \mathcal{G}^{1/2} \to \mathcal{H}^1$, hence $S$ extends to a bounded operator $\mathcal{G} \to \mathcal{H}$ iff $\Lambda \Gamma$ restricts to a bounded operator $\mathcal{H} \to \mathcal{G}$. 

There is another equivalent characterisation of elliptic regularity:
Remark 3.7. The characterisations Theorem 3.5 (ix) and (x) are due to Ben Amor and Brasche [BAB08] (see also [BBBAB11, Thm. 2.7] and the references therein). They showed that elliptic regularity (more precisely, that Theorem 3.5 (ix) and (x)) are also equivalent to
\[
\lim_{a \to \infty} a |R_a - R^D| < \infty,
\]
where \( R_a = (H_a + 1)^{-1} \) and where \( H_a \) is the operator associated with the quadratic form \( h_a(f) := h(f) + a\|f\|^2_H \) for \( a \geq 0 \). We can now interpret the boundary pair \((\Gamma, \mathcal{J})\) as been associated with the quadratic form \( h_a \) (see Section 5.1).

Here are some consequences of elliptic regularity:

**Theorem 3.8.** Let \((\Gamma, \mathcal{J})\) be an elliptically regular boundary pair and \( z \in \mathbb{C} \setminus \sigma(H^D) \), then the following assertions are true:

i. The norms \( \| \cdot \|_1 \) and \( \| \cdot \|_{\mathcal{J}^{1/2}} \) are equivalent, i.e.,
\[
\| \varphi \|_{\mathcal{J}^{1/2}}^2 \leq \| \varphi \|_{1}^2 := \text{Re} I_1(\varphi + \omega(z))|\varphi|_H^2 \leq (L(z) + \omega(z)||\Gamma||^2_{1 \to 0})|\varphi|_H^2,
\]
where \( L(z) \) is defined in (2.24c).

ii. The form \( I_1 \) resp. the associated operator \( \Lambda(\lambda) \) is bounded from below for all \( \lambda \in \mathbb{R} \setminus \sigma(H^D) \).

iii. The form \( I_2 \) is closed and sectorial, i.e., \( I_2(\varphi) \in \Sigma_\vartheta - \omega(z) \) for all \( \varphi \in \mathcal{J}^{1/2} \), where
\[
\Sigma_\vartheta := \{ w \in \mathbb{C} \mid |\text{arg } w| \leq \vartheta \}
\]
for \( \vartheta = \vartheta_2 := \arctan L(z) \).

iv. The associated operator family \( \Lambda(z) \) is self-adjoint, i.e., \( \Lambda(z)^* = \Lambda(\overline{z}) \). In particular, \( \Lambda(z) \) is closed and self-adjoint for \( z \in \mathbb{R} \setminus \sigma(H^D) \). Moreover, the domain is \( \text{dom} \Lambda(z) = \mathcal{J}^1 \), i.e., independent of \( z \), and \( \Lambda(z) \) considered as operator \( \Lambda(z)^{1-\alpha} : \mathcal{J}^1 \to \mathcal{J} \) is bounded.

v. The operator \( \Lambda(z) \) is sectorial, i.e., we have \( \sigma(\Lambda(z)) \subset \Sigma_\vartheta - \omega(z) \), i.e., the spectrum of the Dirichlet-to-Neumann map is contained in the sector \( \Sigma_\vartheta - \omega(z) \) for \( \vartheta = \vartheta_2 \).

vi. The operator \( \Lambda(z) \) is \( m \)-sectorial in the sense of Kato, i.e.,
\[
\|(\Lambda(z) - w)^{-1}\|_\mathcal{J} \leq \frac{1}{|w + \omega(z)| \sin(\vartheta_0 - \vartheta)}
\]
for \( \vartheta_0 \in (\vartheta, \pi) \) and \( w \in \mathbb{C} \setminus (\Sigma_{\vartheta_0} - \omega(z)) \).

**Proof.** (i) follows from the ellipticity of \( L_2 \) shown in Theorem 3.5 (viii), (2.7) and Theorem 2.23. (ii) follows immediately from (i). (iii) The Closeness of \( I_1 \) on \( \mathcal{J}^{1/2} \) follows from (i). Moreover, for \( \varphi \in \mathcal{J}^{1/2} \setminus \{0\} \) we have
\[
\frac{|\text{Im} I_2(\varphi)|}{\text{Re} I_2(\varphi + \omega(z))|\varphi|_H^2} \leq \frac{L(z)}{\alpha} = L(z)
\]
using again Theorem 2.23. In particular, \( I_2(\varphi) \) lies in the sector \( \Sigma_\vartheta - \omega(z) \).

(iv) Note that \( \Lambda(z) \) is the operator associated with \( L_2 \) in the sense of sesquilinear forms [Kat66, Thm. VI.2.1]; in particular, \( \Lambda(z) \) is closed and sectorial, and dom \( \Lambda(z) \) is a form core (i.e., dense in \( \mathcal{J}^{1/2} \)). Moreover, \( \Lambda(z) \) is the (strong) operator associated with \( L_2 \), see (2.26)

For \( \mathcal{J}^1 = \text{dom} \Lambda(z) \) we use the equality
\[
L_2(\varphi, \psi) - L(\varphi, \psi) = -(z + 1)(S(z)\varphi, S\psi).
\]
for \( \varphi, \psi \in \mathcal{J}^{1/2} \) (see (2.24b)). The inclusion \( \subseteq \) follows from
\[
\|\Lambda(z)\varphi\| = \sup_{\psi \in \mathcal{J}^{1/2}} \frac{L_2(\varphi, \psi)}{\|\psi\|_{\mathcal{J}}} \leq \|\Lambda\varphi\| + \|S\|_{0 \to 0} \|S\|_{1/2 \to 0} \|\Lambda^{1/2}\varphi\|,
\]
as \( \varphi \in \mathcal{J} \) implies \( \varphi \in \text{dom} \Lambda(z) \). For the inclusion \( \supseteq \) we argue similarly. The boundedness of \( \Lambda \) as operator \( \mathcal{J}^1 \to \mathcal{J} \) follows also from (3.10).

(v)–(vi) can be deduced similarly as in [MNP10, Sec. 2].
Note that if the boundary pair is not elliptically regular then \( I_z \) and \( \Lambda(z) \) are not necessarily closed forms and operators, respectively. We need the closeness for the spectral characterisation e.g. in Theorem 4.18 (i) (in order to apply Proposition 4.8).

Recall that we denote by \( B(z): \mathcal{H} \rightarrow \mathcal{G} \) the adjoint of \( \overline{S}(\overline{z}): \mathcal{G} \rightarrow \mathcal{H} \), i.e., the restriction of \( S(\overline{z})^* : \mathcal{H}^{-1} \rightarrow \mathcal{G}^{-1/2} \) to \( \mathcal{H} \) for an elliptically regular boundary pair. The proof of the following is straightforward from Proposition 2.19 and Theorem 2.23:

**Proposition 3.11.** Assume that \((\Gamma, \mathcal{G})\) is an elliptically regular boundary pair, and that \( z, w \notin \sigma(H^D) \), then the following assertions are true:

1. We have \( B(z) - B(w) = (z - w)B(w)R_D(z) : \mathcal{H} \rightarrow \mathcal{G} \) and the operator is bounded.
2. The map \( z \rightarrow B(z) \) is holomorphic and the derivatives \( B^{(k)}(z) = k!B(z)R_D(z)^k : \mathcal{H} \rightarrow \mathcal{G} \) are bounded.
3. We have \( \Lambda(z) - \Lambda(w) = -(z - w)\overline{S}(\overline{z})^*\overline{S}(w) = -(z - w)B(z)B(w)^* : \mathcal{G} \rightarrow \mathcal{G} \) and the operator is bounded.
4. The derivatives of \( \Lambda(z) \) are bounded, i.e.,
   \[
   \Lambda^{(k)}(z) = -k!\overline{S}(\overline{z})R_D(z)^k\overline{S}(z) = -(k!B(z)R_D(z)^k B(\overline{z})^* : \mathcal{H} \rightarrow \mathcal{G};
   \]
   in particular, \( \Lambda'(z) = -\overline{S}(\overline{z})^*\overline{S}(z) = -B(z)B(\overline{z})^* \).
5. The imaginary part \( \text{Im} \Lambda(z) = -(\text{Im} z)\overline{S}(\overline{z})^*\overline{S}(z) = -(\text{Im} z)B(\overline{z})B(\overline{z})^* \) is bounded and non-positive for \( \text{Im} z \geq 0 \).

### 3.2 Uniformly positive boundary pairs

We have a sort of “inverse” notion of elliptic regularity, namely, that the norm of the Dirichlet solution operator is bounded from below:

**Definition 3.12.** We say that the boundary pair \((\Gamma, \mathcal{G})\) is (uniformly) positive, if there is a constant \( c > 0 \) such that

\[
\| S\varphi \|_\mathcal{H} \geq c \| \varphi \|_\mathcal{G}
\]

for all \( \varphi \in \mathcal{G}^{1/2} \).

**Remark 3.13.** Not all boundary pairs are uniformly positive: a counterexample is given by the manifold model of Section 7.4.

For the positivity of a boundary pair, we have the following equivalent characterisations:

**Theorem 3.14.** Let \((\Gamma, \mathcal{G})\) be a boundary pair and let \( S(z) \) be the corresponding weak Dirichlet solution operator. Then the following conditions are equivalent:

1. The boundary pair is uniformly positive.
2. For some (any) \( z \in \mathbb{C} \setminus \sigma(H^D) \), there exists \( c(z) > 0 \) such that
   \[
   \| S(z)\varphi \|_\mathcal{H} \geq c(z) \| \varphi \|_\mathcal{G}
   \]
   for all \( \varphi \in \mathcal{G}^{1/2} \).
3. For some (any) \( z \in \mathbb{C} \setminus \sigma(H^D) \), the operator \( \Gamma: \mathcal{N}^1(z) \rightarrow \mathcal{G}^{1/2} \) extends to a bounded operator \( \overline{\Gamma}: \mathcal{N}^0(z) \rightarrow \mathcal{G} \), where \( \mathcal{N}^0(z) := \overline{\mathcal{N}^1(z)}^\mathcal{H} \) denotes the closure of the solution space in the \( \mathcal{H} \)-norm.
4. For some (any) \( z \in \mathbb{C} \setminus \sigma(H^D) \), there exists \( c(z) > 0 \) such that the adjoint fulfils
   \[
   \| S(\overline{z})^*f \|_\mathcal{G} \geq c(z) \| f \|_\mathcal{H}
   \]
   for all \( f \in \mathcal{H} \).
5. The quadratic form \( q_z \) given by \( q_z(\varphi) := \| S(z)\varphi \|_\mathcal{G}^2 \) is uniformly positive for some (any) \( z \in \mathbb{C} \setminus \sigma(H^D) \) and closable. We denote the operator associated with the closure of \( q_z \) by \( Q(z) \).
6. The negative imaginary part \( -\text{Im} I_z := -\frac{1}{\overline{z}}(I_z - I_z^*) \) is uniformly positive for some (any) \( z \in \mathbb{C} \) with \( \text{Im} z > 0 \).
vii. The form-valued function $z \mapsto -I_z$ is a uniformly positive Herglotz function.

viii. We have $0 \not\in \sigma(\Lambda(z))$ for some (any) $z \in \mathbb{C} \setminus \mathbb{R}$.

ix. The negative derivative $-\Lambda_z$ is a uniformly positive form for some (any) $\lambda \in \mathbb{R} \setminus \sigma(H_D)$.

Proof. The proof is very much the same as the one of Theorem 3.5. For example for (ii) $\Rightarrow$ (v) we have

$$c(z)^2\|\varphi\|^2 \leq \|S(z)\varphi\|^2 = q_z(\varphi) \leq \|S(\varphi)\|^2 \leq C(\varphi) < 1/2.$$

In particular, the form $q_z$ is uniformly positive and the closure $\mathcal{G}_z$ of $\mathcal{G}^{1/2}$ with respect to the norm $\sqrt{q_z(\cdot)}$ lies in between $\mathcal{G}$ and $\mathcal{G}^{1/2}$. In particular, the form $q_z$ is closable.

\section{4 Krein’s resolvent formula and spectral relations}

In this section we present some of our main results: a Krein-type resolvent formula (Theorem 4.4) and spectral relations between the Neumann operator and the family of Dirichlet-to-Neumann operators (Theorems 4.9 and 4.18).

\subsection{4.1 Krein's resolvent formula for boundary pairs}

We first need some technical preparation. Denote by $\pi_z : \mathcal{H}^1 \rightarrow \mathcal{H}^1, D$ the canonical map associating with $f = w + h \in \mathcal{H}^1 = \mathcal{H}^{1,D} + \mathcal{N}(z)$ the component $w \in \mathcal{H}^{1,D}$ (see (2.16a)) and $\pi_z$ its dual. We denote by $\tilde{H}, \tilde{H}^D$ and $\tilde{\Lambda}(z)$ the operators $H, H^D$ and $\Lambda(z)$ extended to $\mathcal{H}^1 \rightarrow \mathcal{H}^{-1}, \mathcal{H}^{1,D} \rightarrow \mathcal{H}^{-1,D}, \mathcal{G} \rightarrow \mathcal{G}^{-1}$, respectively. The natural inclusion $\iota = \iota_{1,D} : \mathcal{H}^{1,D} \hookrightarrow \mathcal{H}$ is an isometry and induces a surjective operator $\iota^* : \mathcal{H}^{-1} \rightarrow \mathcal{H}^{1,D}$.

Note that $\iota^* f : \mathcal{H}^{1,D} \rightarrow \mathbb{C}$ is defined by $(\iota^* f)(g) = \tilde{f}(fg)$ for $f \in \mathcal{H}^{-1}$ and $g \in \mathcal{H}^{1,D}$. If $f \in \mathcal{H}$ is embedded in $\mathcal{H}^{-1}$ via $\tilde{f} = \langle f, \cdot \rangle$, then

$$\iota^* f(g) = \langle f, \iota g \rangle = \langle f, g \rangle = \tilde{f}(g), \quad (4.1)$$

i.e., $\iota^*$ restricted to $\mathcal{H}$ can be considered as the identity on $\mathcal{H}$.

We have now the following relation between the operators $\tilde{H}$ and $\tilde{H}^D$ and their resolvents extended to the scale of Hilbert spaces.

\textbf{Lemma 4.2.} Let $z \in \mathbb{C} \setminus (\sigma(H^D) \cup \sigma(H))$, then we have the following identities:

i. $\iota^* (\tilde{H} - z)\iota = \tilde{H}^D - z : \mathcal{H}^{1,D} \rightarrow \mathcal{H}^{-1,D}$,

ii. $\iota^* (\tilde{H} - z) = (\tilde{H}^D - z)\pi_z : \mathcal{H}^1 \rightarrow \mathcal{H}^{-1,D}$,

iii. $\mathcal{R}(\tilde{H} - z)\pi_z = \pi_z \mathcal{R}(z) : \mathcal{H}^1 \rightarrow \mathcal{H}^{-1,D}$,

iv. $\pi_z = \iota^* \mathcal{R}(z) : \mathcal{H}^1 \rightarrow \mathcal{H}^{1,D}$ is the projection onto $\mathcal{H}^{1,D}$ with kernel $\mathcal{N}^1(z)$, Moreover, the complementary projection is given by $\text{id} - \pi_z = \mathcal{P}(z)(= S(z)\Gamma)$. 

v. $\mathcal{P}(z)\mathcal{R}(z) = \mathcal{R}(z)\mathcal{P}(z)^* : \mathcal{H}^{-1} \rightarrow \mathcal{H}^1$.

Proof. (i) The first assertion follows immediately from

$$(\iota^* (\tilde{H} - z)\iota f, g)_{-1,1} = (\tilde{H}^D - z)\iota f, g)_{-1,1} = (\iota^* (\tilde{H} - z)\iota f, g)_{-1,1}$$

for $f, g \in \mathcal{H}^{1,D}$.

(ii) Let $f \in \mathcal{H}^{1,D}$ and $g \in \mathcal{H}^1$. Then $g = w + h = \pi_z g$ according to the decomposition (2.16a) and

$$(\iota^* (\tilde{H} - z) g, f)_{-1,1} = (h - z\iota)(g, f) = (h - z\iota)(w, f) = ((\tilde{H}^D - z)\pi_z g, f)_{-1,1},$$

since $(h - z\iota)(h, f) = 0$ for $f \in \mathcal{H}^{1,D}$.

(iii) follows by multiplying with the resolvents.

For (iv), note that $(\text{id} - \pi_z) g = h = \mathcal{P}(z) g$ (cf. Proposition 2.15 (ii) and Theorem 2.21 (i)). The remaining assertions of (iv) and (v) follow from (ii) and an easy calculation.

We have another representation of the Dirichlet solution operator:

\footnote{\text{We denote by $\Pi(\cdot)$ the operator associated with the closure of the non-positive form $\Pi(\varphi) = -\Pi(z)\varphi$ on $\mathcal{H}^1$. Note that $\Pi(z)$ is closable. Such functions $-\Pi(\cdot)$ are called \textit{uniformly strict Neumann or Herglotz functions} in [DHMD06, p. 5354].}}
4.2 Spectral relations for the Dirichlet-to-Neumann operator

Proposition 4.3. Let \( z \in \mathbb{C} \setminus \sigma(H^D) \) and \( g \in \mathcal{G}^1 \), then \( h := g - \hat{R}^D(z) = (\tilde{H} - z)g \) depends only on \( \varphi := \Gamma g \) and not on \( g \in \mathcal{G}^1 \) itself. Moreover, \( h \in \mathcal{M}^1(z) \). Therefore, the Dirichlet solution operator can be expressed as

\[
S(z) = (\text{id}_{\mathcal{G}^1} - i\hat{R}^D(z)) \sigma(\tilde{H} - z)S : \mathcal{G}^{1/2} \rightarrow \mathcal{H}^1.
\]

Proof. We have

\[
(h - z1)(h, f) = (h - z1)(g, f) - \langle \tilde{H} - z, \hat{R}^D(z) \tilde{H} - zg, f \rangle_{1,-1} = 0
\]

for all \( f \in \mathcal{G}^{1,D} \) using Lemma 4.2 (ii). In particular, we have shown that \( h \in \mathcal{M}^1(z) \). If follows from the uniqueness of the Dirichlet problem that \( h = S(z)\varphi \) depends only on \( \varphi \). \( \square \)

We have now prepared all ingredients in order to prove one of the main theorems for boundary pairs, a weak version of the so-called Krein’s resolvent formula. This formula allows us to detect the Neumann spectrum as the “zeros” (Theorems 4.9 and 4.18) of the Dirichlet-to-Neumann operator.

Theorem 4.4. Assume that \((\Gamma, \mathcal{G})\) is a boundary pair associated with the quadratic form \( h \) and that \( z \in \mathbb{C} \setminus (\sigma(H^D) \cup \sigma(H)) \), then

\[
\hat{R}(z) - i\hat{R}^D(z) = P(z)\hat{R}(z) = S(z)\tilde{\Lambda}(z)^{-1}S(\tilde{\sigma})^* : \mathcal{H}^{-1} \rightarrow \mathcal{H}^1.
\]

(4.5)

Proof. We have

\[
\hat{R}(z) - i\hat{R}^D(z) = (id - \pi_z)\hat{R}(z) = P(z)\hat{R}(z) = P(z)^2\hat{R}(z) = P(z)\hat{R}(z)P(\tilde{\sigma})^* = S(z)\Gamma \hat{R}(z)\Gamma^* S(\tilde{\sigma})^*
\]

using Lemma 4.2. Finally, in Theorem 2.29 we showed that

\[
\Gamma \hat{R}(z)\Gamma^* = \tilde{\Lambda}(z)^{-1}
\]

as an operator \( \mathcal{G}^{-1/2} \rightarrow \mathcal{G}^{1/2} \), and the resolvent formula follows. \( \square \)

Corollary 4.6. Assume that \((\Gamma, \mathcal{G})\) is a boundary pair associated with the quadratic form \( h \) and that \( z \in \mathbb{C} \setminus (\sigma(H^D) \cup \sigma(H)) \), then

\[
R(z) - R^D(z) = S(z)\tilde{\Lambda}(z)^{-1}S(\tilde{\sigma})^* : \mathcal{H}^{-1/2} \rightarrow \mathcal{G}^{-1/2} \rightarrow \mathcal{G}^{1/2} \rightarrow \mathcal{H}.
\]

(4.7a)

If in addition, the boundary pair is elliptically regular, then the operator on the RHS can be considered as sequence of bounded operators

\[
R(z) - R^D(z) = \mathcal{S}(z)\tilde{\Lambda}(z)^{-1}\mathcal{S}(\tilde{\sigma})^* : \mathcal{H}^{-1/2} \rightarrow \mathcal{G}^{-1/2} \rightarrow \mathcal{G}^{1/2} \rightarrow \mathcal{H},
\]

(4.7b)

i.e., these operators do not leave the original Hilbert spaces \( \mathcal{G} \) and \( \mathcal{H} \).

4.2 Spectral relations for the Dirichlet-to-Neumann operator

The following is a useful criterion for the spectrum of an operator in terms of its associated (sesquilinear) form.

Assume that \( \mathcal{H}^1 \subset \mathcal{H} \) is a Hilbert space such that the embedding \( \iota : \mathcal{H}^1 \rightarrow \mathcal{H} \) is bounded and \( \mathcal{H}^1 \) is dense in \( \mathcal{H} \). Denote by \( \mathcal{H}^{-1} \) the dual of \( \mathcal{H}^1 \) with respect to the pairing given by the inner product in \( \mathcal{H} \), i.e., the space of antilinear and bounded functionals \( u : \mathcal{H}^1 \rightarrow \mathbb{C} \). We embed \( \mathcal{H} \rightarrow \mathcal{H} \) of bounded functionals \( u \). Let \( \mathcal{H} \times \mathcal{H}^1 \rightarrow \mathcal{H} \) be a bounded sesquilinear form, and denote by \( \hat{T} : \mathcal{H}^{-1} \rightarrow \mathcal{H}^{-1} \) the weak operator associated with the form \( t \), i.e., \( \langle \hat{T}\varphi, \psi \rangle = t(\varphi, \psi) \). Denote by \( T \) (the strong) operator associated with \( t \), defined by

\[
\text{dom} T := \{ f \in \mathcal{H}^1 \mid \exists g \in \mathcal{H} \forall u \in \mathcal{H}^1 : t(f, u) = (g, u) \}, \quad T f := g
\]

(\( T f \) is well-defined since \( \mathcal{H}^1 \) is dense in \( \mathcal{H} \)). Clearly, \( \text{dom} T = \{ f \in \mathcal{H}^1 : \hat{T} f \in \mathcal{H} \} \) and \( \hat{T} f = T f \) if \( f \in \text{dom} T \).

If \( t \) is bounded from below (i.e., there exists \( \lambda_0 \in \mathbb{R} \) such that \( t(f) \geq \lambda_0 \|f\|^2_{\mathcal{H}^1} \) for all \( f \in \mathcal{H}^1 \)) and a closed form (i.e., the norm given by \( \|f\|^2_{\mathcal{H}^1} := (t + (1 - \lambda_0)1)(f) \) is equivalent with the norm on the Hilbert space \( \mathcal{H}^1 \)), then \( T \) is the operator associated with \( t \) and in particular self-adjoint and bounded from below.

Proposition 4.8. Assume that \( t \) is closed and bounded from below, then \( \lambda \in \sigma(T) \) iff there exists \( \{f_n\}_n \subset \mathcal{H}^1, \|f_n\|_{\mathcal{H}^{-1}} = 1 \) (or \( \geq 1 \)), such that

\[
\|\hat{T}(\lambda) f_n \|_{\mathcal{H}^{-1}} = \sup_{g \in \mathcal{H}^1} \frac{|t(\lambda - 1) (f_n, g)|}{\|g\|_{\mathcal{H}^1}} \rightarrow 0.
\]

We call the sequence \( \{f_n\}_n \) a weak spectral approaching sequence.

20
Proof. Without loss of generality, we can assume that \( t \geq 0 \) (otherwise consider the form \( t - \lambda \varpi \geq 0 \)) and that \( \|f\|^{2}_{\mathcal{H}^1} = \|f\|^{2}_{\mathcal{H}^1} + t(f) = \|(T + 1)\frac{1}{2}f\|^{2} \) (and therefore \( \|f\|^{2}_{\mathcal{H}^{-1}} = \|(T + 1)^{-\frac{1}{2}}f\|^{2} \) if \( f \in \mathcal{H} \). We use the characterisation that \( \lambda \in \sigma(T) \) iff there exists \( \{f_n\} \subset \text{dom} T \), \( \|f\| = 1 \) (or \( \geq 1 \)), such that \( \|(T - \lambda)f_n\| \to 0 \). Moreover, we have the equality

\[
\|(T - \lambda)f\| = \sup_{g \in \mathcal{H}} \frac{|\langle((T - \lambda)f, g\rangle|}{\|g\|_{\mathcal{H}}}
\]

where \( f = (T + 1)^{\frac{1}{2}} \tilde{f} \in \mathcal{H}^1 \) (and \( \tilde{f} \in \text{dom} T \)) and \( g = (T + 1)^{-\frac{1}{2}} \tilde{g} \in \mathcal{H}^1 \). Moreover, we used the fact that \( (T + 1)^{\pm 1} \) commutes with \( T - \lambda \) for the last equality. Note additionally that \( \tilde{f} \in \mathcal{H} \) so now follows with \( f_n = (T + 1)^{\frac{1}{2}} \tilde{f}_n \).

We can now prove some important consequences of Krein’s resolvent formula, namely the following spectral relation:

**Theorem 4.9.** Assume that \((\Gamma, \mathcal{F})\) is a boundary pair associated with the quadratic form \( \vartheta \) and let \( \lambda \in \mathbb{C} \setminus \sigma(H^D) \). Then the following assertions are true:

1. The Dirichlet solution operator \( S(\lambda) \) is a topological isomorphism from \( \ker \Lambda(\lambda) \) onto \( \ker(H - \lambda) \) with inverse \( \Gamma \), i.e.,

\[
\ker(H - \lambda) = S(\lambda)\ker(\Lambda(\lambda)).
\]

In particular, we have the spectral relation

\[
\lambda \in \sigma_p(H) \Leftrightarrow 0 \in \sigma_p(\Lambda(\lambda)).
\]

for the point spectrum (the set of eigenvalues). Moreover, the multiplicity of an eigenspace is preserved.

2. Assume that \( R: \mathcal{H} \to \mathcal{H} \) and \( \Gamma: \mathcal{H}^1 \to \mathcal{F} \) are compact operators, then the spectra of \( H \), \( H^D \) and \( \Lambda(\lambda) \) are purely discrete. Moreover, the spectral relation (4.10b) is true for the discrete (hence the entire) spectrum, i.e., (4.10b) holds with \( \sigma_p(\cdot) \) replaced by \( \sigma(\cdot) \) (the entire spectrum).

3. Assume that \( \lambda \) is isolated in \( \sigma(H) \), then

\[
\|\Lambda(z)^{-1}\|_{\mathcal{F} \to \mathcal{F}} \leq \frac{C_{\lambda}}{|z - \lambda|}
\]

for all \( z \neq \lambda \) in some neighbourhood of \( \lambda \), where \( C_{\lambda} > 0 \) is a constant depending only on \( \|\Gamma\|_{1 \to 0} \), \( \lambda \) and \( \sigma(H) \).

**Proof.** (i) Let \( \varphi \in \ker \Lambda(\lambda) \) and \( h := S(\lambda)\varphi \), then

\[
(h - \lambda \varpi)(\varphi, \Gamma g) = 0.
\]

for \( g \in \mathcal{H}^1 \) by the definition of \( t_\lambda \) in (2.24a), hence \( h \in \text{dom} H \) and \( (H - \lambda)h = 0 \).

On the other hand, if \( h \in \ker(\tilde{\Gamma} - \lambda) \) then it is easily seen that \( h \in \mathcal{A}^1(\lambda) \). Set \( \varphi := \Gamma h \), then \( h = S(\lambda)\varphi \) and a similar calculation as above shows that \( \varphi \in \text{dom} \Lambda(\lambda) \) and \( \Lambda(\lambda)\varphi = 0 \).

The spectral equivalence (4.10b) for the point spectrum is obvious from (4.10a), as well as the preserved multiplicity.

(ii) It follows from Theorem 2.35 that the spectrum of \( \Lambda(\lambda) \) is discrete (see also Proposition 5.2 (vi) for the discreteness of \( \sigma(H^D) \)). The spectral relation is then a consequence of part (i).

(iii) If \( \lambda \) is isolated in \( \sigma(H) \), then there exists \( r_1 > 0 \) such that, for all \( z \in \mathbb{C} \) with \( 0 < |z - \lambda| \leq r_1 \), the resolvent \( \tilde{R}(z) \) has a first order pole at \( \lambda \), i.e.,

\[
R(z) = \frac{1}{\lambda - z} \Gamma(\lambda)(\varpi) + R_\lambda(z),
\]

where \( R_\lambda(H) \) is the resolvent of \( H|_{\text{ker}(H - \lambda)^{1}} \). By Theorem 2.29, we have

\[
\Lambda(z)^{-1} = \Gamma \tilde{R}(z) \Gamma^* = \frac{1}{\lambda - z} \Gamma \Gamma(\lambda)(\varpi) \Gamma^* + \Gamma \tilde{R}_\lambda(z) \Gamma^*
\]
as operator in $\mathcal{G}$. In particular, $\Lambda(z)^{-1}$ has a first order pole at $z = \lambda$ and

\[
\| (\lambda - z)\Lambda(z)^{-1} \| \leq \| \Gamma \|^2_{1,0} \left( 1 + |\lambda - z| \sup_{\lambda' \in \mathcal{G}(\lambda)} \frac{|\lambda' + 1|}{|z - \lambda'|} \right) =: C_\lambda(z)
\]

Note that $C_\lambda(z) < \infty$ since $\lambda$ is isolated in $\sigma(H)$ and since the supremum equals the constant $C^D(z, -1)$ defined in (2.20a) with the operator $H^D$ replaced by $H|_{\ker(H - \lambda)}$. Since $z \mapsto C_\lambda(z)$ is continuous, $C_\lambda := \sup C_\lambda(\{ z \in \mathbb{C} | |z - \lambda| \leq r_1 \}) < \infty$. \hfill \qed

Before proving further spectral relations for elliptically regular boundary pairs, we need some results on operator pencils on $\mathcal{G}$, which we define here in the form we need it (see e.g. [Tr00, EL04] and references therein):

**Definition 4.12.** Let $D \subset \mathbb{C}$ be open with $\overline{D} = D$. We say that $T(\cdot) = \{ T(z) \}_{z \in D}$ is a holomorphic self-adjoint operator pencil if $T(z)^* = T(\overline{z})$ and $z \mapsto T(z) - T(z_0)$ is holomorphic with values in the set of bounded operators on $\mathcal{G}$ for some $z_0 \in D$.

The spectrum of $T(\cdot)$ is given by

\[
\sigma(T(\cdot)) := \{ z \in \mathbb{C} | T(z) \text{ is not invertible} \}.
\]

We say that $\lambda$ is an eigenvalue of $T(\cdot)$ (shortly $\lambda \in \sigma_p(T(\cdot))$) if $T(\lambda)$ is not injective.

Fix $\lambda \in D \cap \mathbb{R}$. It follows that

\[
T(z) = A_0 - (z - \lambda)A_1 - (z - \lambda)^2A_2(z),
\]

where $A_0 = T(\lambda)$ is self-adjoint (and possibly unbounded), where $A_1 = -T'(\lambda)$ is self-adjoint and bounded and where $z \mapsto A_2(z)$ is holomorphic with values in the bounded operators on $\mathcal{G}$. Then it is obvious that $\lambda \in \sigma_p(A_0)$ iff $\lambda \in \sigma_p(A_0)$, but it is not clear whether $\lambda \in \sigma(T(\cdot))$ iff $\lambda \in \sigma_p(A_0)$ or whether $\lambda$ is isolated in $\sigma(T(\cdot))$ iff $\lambda$ is isolated in $\sigma(A_0)$.

For the latter assertion, we need more assumptions:

**Proposition 4.13.** Assume that $T(\cdot)$ is a holomorphic self-adjoint operator pencil on $D$ and that $\lambda \in D \cap \mathbb{R}$.

i. Assume that the operator pencil has the form $T(z) := A_0 - (z - \lambda)A_1$, where $A_1$ is (bounded and) uniformly positive (i.e., there are $0 < c \leq C < \infty$ such that $c\| \varphi \|^2 \leq \langle A_1 \varphi, \varphi \rangle \leq C\| \varphi \|^2$).

Then

\[
\lambda \text{ is isolated in } \sigma(T(\cdot)) \Leftrightarrow 0 \text{ is isolated in } \sigma(A_0).
\]

ii. Assume now that $A_1 := -T'(\lambda)$ is (bounded and) uniformly positive. Then the following assertions are equivalent:

a) $\lambda$ is isolated in $\sigma(T(\cdot))$ and

\[
T(z)^{-1} = \frac{1}{z - \lambda} T_\lambda(z) + \hat{T}_\lambda(z),
\]

where $T_\lambda(\cdot)$ and $\hat{T}_\lambda(\cdot)$ are holomorphic (bounded) operator functions near $z = \lambda$;

b) $0$ is isolated in $\sigma(A_0)$.

**Proof.** Without loss of generality, we can assume that $\lambda = 0$; otherwise, consider $\tilde{T}(z) := T(z + \lambda)$.

(i) Note first that $\ker T(0) = \ker A_0$, hence $0 \in \sigma_p(T(\cdot))$ iff $0 \in \sigma_p(A_0)$. Moreover, we have

\[
T(z) = A_0 - zA_1 = A_1^{1/2}(A_1^{-1/2}A_0A_1^{-1/2} - z)A_1^{1/2}.
\]

Now, $T(z)$ is invertible iff $A_1^{-1/2}A_0A_1^{-1/2} - z$ is invertible, and $0$ is isolated in $\sigma(A_1^{-1/2}A_0A_1^{-1/2})$ iff $0$ is isolated in $\sigma(A_0)$ (see e.g. [BGP08, Lem 3.1]).

(ii) $\Rightarrow (iii)$: We have

\[
S(z) := T(z)^{-1}(A_0 - zA_1) = T(z)^{-1}(T(z) + z^2A_2(z)) = id_{\mathcal{G}} + z^2T(z)^{-1}A_2(z).
\]

Using (4.14) we have

\[
z^2T(z)^{-1}A_2(z) = (zT_0(z) + z^2\hat{T}_0(z))A_2(z)
\]

and this operator family is bounded near $z = 0$ (including $z = 0$). In particular, if $|z|$ is small enough, then $S(z)$ is invertible, hence $A_0 - zA_1 = T(z)S(z)$ is invertible, too. Therefore, we have shown that $0$ is isolated in the spectrum of the operator pencil $z \mapsto A_0 - zA_1$. Using (i), it follows that $0 \in \sigma(A_0)$ is isolated.
Theorem 4.18. Assume that \( \sigma(A_0) \) be isolated then 0 is isolated in the spectrum of \( z \mapsto A_0 - zA_1 \), again by (i). Using (4.15) we have
\[
(A_0 - zA_1)^{-1} = A_1^{-1/2}(B - z)^{-1}A_1^{-1/2} = A_1^{-1/2}\left(-\frac{1}{z}1_{\emptyset}(B) + B_0^{-1}\right)A_1^{-1/2}
\]
where \( B := A_1^{-1/2}A_0A_1^{-1/2} \) and where \( B_0 \) is the restriction of \( B \) onto \( \ker B^{-1} \). In particular, we have a representation of the inverse as in (4.14), and we can then argue similarly as in (iii) \( \Rightarrow \) (iib).

\[ \square \]

Remark 4.16.

i. The non-trivial assertion in Proposition 4.13 is the fact that \( \lambda \) and 0 are isolated in the spectra, i.e., that \( T(z) \) and \( A_0 - z \) are invertible for all \( z \neq \lambda \) near \( \lambda \).

ii. In our application, the operator pencil will be \( \Lambda(\cdot) \). If we assume that the boundary pair is elliptically regular, then \( \Lambda(\cdot) \) is a holomorphic self-adjoint operator pencil on \( D = \mathbb{C} \setminus \sigma(H^D) \) as in Definition 4.12 since \( \Lambda(z)^* = \Lambda(\overline{z}) \) (Theorem 3.8 (iv)) and
\[
\Lambda(z) = \Lambda(\lambda) - (z - \lambda)S(\lambda)^*S(z) = \Lambda(\lambda) - (z - \lambda)S(\lambda)^*S(\lambda) + (z - \lambda)R^D(z)S(\lambda)
\]
\[
\Lambda(z) = \Lambda(\lambda) - (z - \lambda)Q(\lambda) - (z - \lambda)^2A_{2,\lambda}(z), \quad A_{2,\lambda}(z) := S(\lambda)^*R^D(z)S(\lambda)
\]
by Theorem 2.21 and Proposition 3.11, where \( A_0 = \Lambda(\lambda) \) and \( A_1 = Q(\lambda) \). Moreover, \( z \rightarrow A_{2,\lambda}(z) \) is holomorphic and \( \|A_{2,\lambda}(z)\| \leq \|S(\lambda)\|^2/d(z, \sigma(H^D)) \). In particular, \( \Lambda(z) - \Lambda(\lambda) \) is a bounded operator.

The boundedness of \( A_1 \) means that the boundary pair is elliptically regular and the uniform positivity of \( A_1 \) means that the boundary pair is uniformly positive.

iii. We would like to weaken the assumptions on \( A_1 \), but the counterexample given in Example 4.17 shows that this is not always possible (e.g., assuming that \( A_1 \) is bounded and injective, but not uniformly positive).

This means that it is not enough for the application of Proposition 4.13 that the boundary pair is elliptically regular, but not uniformly positive (as one of our main examples, a Laplacian on a manifold with smooth boundary, is). Nevertheless, we are not aware of a boundary pair such that for \( A_0 = \Lambda(\lambda) \) and \( A_1 = Q(\lambda) \), the assertion of Proposition 4.13 is false for a bounded, injective, but not uniformly positive \( A_1 \).

The author is indebted to Michael Strauss for the following example:

Example 4.17. We give here a counterexample for \( \subset \subset \) in Proposition 4.13 (i) violating the uniform positivity of \( A_1 \). Let \( T(z) := A_0 - zA_1 \) with \( A_0 = A_0^* \) and \( A_1 = A_1^* \geq 0 \) specified below:

Let \( \varphi \) be an isolated eigenvalue of \( A_0 \) of infinite multiplicity in the essential spectrum of \( A_0 \). Denote by \( \langle \varphi_n \rangle \) an orthonormal basis of the eigenspace ker \( A_0 \). Set
\[
A_1 := 1_{\mathbb{R}\setminus\emptyset}(A_0) + \sum_n \frac{1}{n} \langle \varphi_n, \cdot \rangle \varphi_n
\]
then \( A_1 \) is bounded, non-negative and injective (but not uniformly positive). Moreover, \( T(z)\varphi_n = -(z/n)\varphi_n \), hence \( -z/n \in \sigma(T(\cdot)) \) and \( \|T(z)\varphi_n\| \rightarrow 0 \) showing that \( T(z) \) does not have a bounded inverse for any \( z \in \mathbb{C} \). In particular, \( 0 \in \sigma(T(\cdot)) \), but \( 0 \) is not isolated.

If we assume elliptic regularity for the boundary pair then we can conclude the following spectral relations:

Theorem 4.18. Assume that \( (\Gamma, \mathcal{G}) \) is an elliptically regular boundary pair associated with the quadratic form \( h \) and let \( \lambda \in \mathbb{C} \setminus \sigma(H^D) \). Then the following assertions are true:

i. The spectral relation
\[
\lambda \in \sigma(H) \iff 0 \in \sigma(\Lambda(\lambda)).
\]

holds for the entire spectrum.

ii. Assume that \( \Gamma : \mathcal{H}^1 \rightarrow \mathcal{G} \) is a compact operator (see Theorem 2.35 for equivalent characterisations) then \( \sigma_{\text{ess}}(H) = \sigma_{\text{ess}}(H^D) \), and \( \sigma(H) \setminus \sigma(H^D) \) consists of discrete eigenvalues of \( H \), only. In particular, if \( \lambda \notin \sigma(H^D) \), then the relation (4.19a) is true for the discrete spectrum, i.e., with \( \sigma(\cdot) \) replaced by \( \sigma_{\text{disc}}(\cdot) \).
iii. An eigenvalue $\lambda$ is isolated in the spectrum of $H$ iff $\lambda$ is isolated in the spectrum of the operator pencil $\Lambda(\cdot)$, i.e.,
\[
\lambda \text{ is isolated in } \sigma(H) \iff \lambda \text{ is isolated in } \sigma(\Lambda(\cdot)).
\]

If one of the conditions is fulfilled, then the estimate (4.10c) holds.

iv. Assume additionally, that the boundary pair is uniformly positive, then
\[
\lambda \text{ is isolated in } \sigma(H) \iff 0 \text{ is isolated in } \sigma(\Lambda(\lambda))
\]
(i.e., isolated in the spectrum of the individual operator $\Lambda(\lambda)$). In particular, the spectral relation (4.19a) is also true for the discrete and essential spectrum, i.e., with $\sigma(\cdot)$ replaced by $\sigma_{\text{disc}}(\cdot)$ resp. $\sigma_{\text{ess}}(\cdot)$.

Proof. (i) “$\Rightarrow$”: Note first that the elliptic regularity of the boundary pair implies that the quadratic form $I_1$ is bounded from below and closed with domain $\mathcal{D}^{1/2}$ (Theorem 3.8), hence we can apply Proposition 4.8 here.

Let $\lambda \in \sigma(H)$, let $\{f_n\}_n$ be a weak spectral approaching sequence, and set $\varphi_n := \Gamma f_n$. We have to show that $\|\Lambda(\lambda)\varphi_n\|_{-1/2} \to 0$ as $n \to \infty$ and that $\|\varphi_n\|_{-1/2} \geq 1$. Now
\[
\|\Lambda(\lambda)\varphi_n\|_{-1/2} = \|S(\lambda)^*\Gamma^*\Lambda(\lambda)\Gamma f_n\|_{-1/2} = \|S(\lambda)^*(H - \lambda)f_n\|_{-1/2} \leq \|S(\lambda)\|_{1/2 \to 1}\|(H - \lambda)f_n\|_{-1} \to 0
\]
using $\Gamma^*\Lambda(\lambda)\Gamma = (H - \lambda)P(\lambda) = P(\lambda)^*(H - \lambda)$ and $P(\lambda)S(\lambda) = S(\lambda)$ by Lemma 4.2. Moreover,
\[
\|\varphi_n\|_{-1/2} = \langle \Lambda \varphi_n, \varphi_n \rangle_{-1/2} = \langle \Gamma^*\Lambda \Gamma f_n, f_n \rangle_{-1,1} = \langle R f_n, f_n \rangle_{-1,1} = \|f_n\|_{-1}^2
\]
using (2.30).

“(⇐”): We argue by contraposition. Assume that $\lambda \notin \sigma(H)$, then $\Lambda(\lambda)^{-1} = \Gamma R(\lambda)\Gamma^*$ exists and is bounded as operator $\mathcal{D} \to \mathcal{D}$ by Theorem 2.29 (iv). In particular, $\Lambda(\lambda)$ has a bounded inverse, hence $0 \notin \sigma(\Lambda(\lambda))$.

(ii) By Theorem 2.35, $\Lambda^{-1}$ is compact, and by (4.7b) and the elliptic regularity, it follows that the resolvent difference $R - R^D$ is compact, too. In particular, the essential spectra agree. The spectral relation follows from Theorem 4.9 (i), since the spectrum now consists of eigenvalues of finite multiplicity only.

(iii) That $\lambda$ is an eigenvalue of $\sigma(H)$ iff ker $\Lambda(\lambda)$ is nontrivial follows already by Theorem 4.9 (i).

“(⇒”): If $\lambda$ is isolated in $\sigma(H)$, then $\Lambda(\lambda)^{-1}$ exists and is bounded by Theorem 2.29 (iv) for $z \in \mathbb{C} \setminus \sigma(H^D)$ with $0 < |z - \lambda|$ small enough, i.e., $\lambda$ is isolated in $\sigma(\Lambda(\cdot))$.

“⇐” Using Krein's resolvent formula (4.7b), we conclude that $R(z)$ is defined for $z$ with $0 < |z - \lambda|$ small enough, and also has a pole at $z = \lambda$, hence $\lambda \in \sigma(H)$ is isolated.

(iv) is a consequence of (iii) and Proposition 4.13 (ii). For the representation (4.14) we refer to (4.11). \hfill $\square$

Remark 4.20.

i. Note that the spectral characterisations of Theorems 4.9 and 4.18 are void if $\sigma(H) = \sigma(H^D) = [0, \infty)$ as in the example of a non-compact cylindrical manifold in Section 7.5. In this case, the Dirichlet-to-Neumann operator is not defined for $\lambda \in [0, \infty)$.

ii. The elliptic regularity condition for the spectral equivalence (i) is needed for the implication “$\Rightarrow$” in order to assure that the form $I_1$ is semi-bounded and closed on $\mathcal{D}^{1/2}$, and that $\Lambda(\lambda)$ is the associated operator, see Theorem 3.8. For the opposite implication it is enough to assume that $\Lambda(\lambda)$ is closed.

We give a counterexample for this spectral equivalence (a boundary pair which is not elliptically regular) in Example 7.10, where $0 \in \sigma(H)$ but $0 \notin \sigma(\Lambda(0))$.

iii. Without the elliptic regularity assumption, the conclusion of Theorem 4.18 (ii) is generally false: From Krein's resolvent formula (4.7a) the compactness of $\Lambda^{-1}$ does not in general imply that $R - R^D$ is compact: In Example 7.9 we have a non-elliptically regular boundary pair for which $R^D$ is compact, but $R$ is not, even though $\Lambda^{-1}$ can be compact.

iv. The implication “$0 \in \sigma(\Lambda(\lambda))$ isolated $\Rightarrow \lambda \in \sigma(H)$ isolated” in Theorem 4.18 (iv) is generally false: if e.g. the boundary pair is only uniformly positive, but not elliptically regular. In Example 7.11 we give an example where $0 \in \sigma(\Lambda(0))$ is isolated, while $0 \in \sigma(H) = [0, \infty)$ is not.
v. For bounded and uniformly positive boundary pairs (hence for ordinary boundary triples, see Theorem 6.11),
there is also a characterisation for the absolutely and singular continuous spectrum (see [BGP08]) if the
Dirichlet-to-Neumann operator has the special form
\[ \Lambda(z) = \frac{\bar{\Delta} - m(z)}{n(z)}, \]
where \( \bar{\Delta} \) is a bounded, self-adjoint operator on \( G \)
and where \( m, n \) are functions holomorphic on \( \mathbb{C} \setminus \sigma(H^D) \).
We believe that this assertion remains true for elliptically regular and uniformly positive boundary pairs, but
where \( \bar{\Delta} \) may be unbounded. We hope to come back to the analysis of the absolutely continuous spectrum in
a forthcoming publication.

5 Boundary pairs constructed from other boundary pairs

In this section, we give classes of of boundary pairs constructed from others like Robin-type perturbations (where
we change the quadratic form with which the boundary pair is associated), coupled boundary pairs or the bounded
modification of an unbounded boundary pair (where we change the boundary space).

5.1 Robin boundary conditions

We start explaining how to use our concept of boundary pairs also for more general “boundary conditions” than
Dirichlet or Neumann. The basic idea is to change the underlying quadratic form \( h \), but leave the boundary pair
\( (\Gamma, G) \) as it is. For simplicity, we consider only constants \( a \) and no operators on \( G \), here.

Let \( (\Gamma, G) \) be a boundary pair associated with a quadratic form \( h \). For \( a \geq 0 \), we define
\[ h_a(f) := h(f) + a\|\Gamma f\|^2_G. \tag{5.1} \]
Since
\[ (h + 1)(f) \leq (h_a + 1)(f) \leq (1 + a\|\Gamma\|^2)(h + 1)(f), \]
the norms associated with \( h \) and \( h_a \) (see (2.2)) are equivalent, and \( h_a \) is also a closed quadratic form. We will now
derive the objects arising from the boundary pair associated with \( h_a \), denoted with a subscript \( \cdot_a \):

Proposition 5.2.

i. The Dirichlet operator is unchanged, i.e., \( \mathcal{H}^1_D = \mathcal{H}^1_D = \text{ker } \Gamma \) and \( H^D = H^D_a \).

ii. The Neumann operator \( H_a \) has domain
\[ \text{dom } H_a = \{ f \in \mathcal{W} \mid \Gamma f + a\Gamma f = 0 \} \]
(see Section 6.1 for the notation).

iii. The range of the boundary map is unchanged, as well as the Dirichlet solution operator; i.e., \( \mathcal{G}^1/2 = \mathcal{G}^1/2 = \text{ran } \Gamma \) and \( S_a(z) = S(z) \).

iv. The Dirichlet-to-Neumann form \( \mathcal{L}_{\gamma,a} \) for the boundary pair associated with \( h_a \) is given by
\[ \mathcal{L}_{\gamma,a}(\varphi) = \mathcal{L}_{\gamma}(\varphi) + a\|\varphi\|^2_G \quad \text{or, in operator form,} \quad \bar{\Lambda}_a(z) = \bar{\Lambda}(z) + a. \]

v. The boundary pair associated with \( h_a \) is elliptically regular/uniformly positive iff the boundary pair associated
with \( h \) is.

vi. We have \( R \geq R_a \geq R^D \). In particular, if \( R: \mathcal{H} \longrightarrow \mathcal{H} \) is compact, then \( R_a: \mathcal{H} \longrightarrow \mathcal{H} \) and \( R^D: \mathcal{H} \longrightarrow \mathcal{H} \)
are also compact, and the eigenvalues fulfil
\[ \lambda_k(H) \leq \lambda_k(H_a) \leq \lambda_k(H^D) \]
(labelled in increasing order respecting their multiplicity).
Proof. We only indicate some of the arguments here: For the domain inclusion “$\subset$” of (ii) note that $f \in \text{dom } H_a$ implies that there is $h \in \mathcal{H}$ such that

$$b(f, g) + a(f, \Gamma g) = (h, g)$$

for all $g \in \mathcal{H}$. If we assume $g \in \text{dom } H_{\min} = \text{dom } H^D \cap \text{dom } H$ in the last equation, then the boundary term vanishes and $b(f, g) = \langle f, Hg \rangle$, hence $f \in \text{dom } H_{\max}$ and $H_{\max} f = h$. Moreover, the defining equation for $\mathcal{H}_{\max}$ in (6.5) is fulfilled (again, for $g \in \mathcal{H}^1$, the boundary term vanishes). Finally, comparing the above formula with Green’s formula (6.7), we see that $\hat{\Gamma} f = -a\Gamma f$, and hence $\hat{\Gamma} f \in \mathcal{G}$. Therefore, we have shown that $f \in \mathcal{H}$ (see (6.6)).

(vi) For the last assertion note that (0 ≤) implies that there is $\lambda > 0$ such that $\lambda \in \sigma(H)$. If we assume $\lambda /\in \sigma(H^D)$, then there exists $a_0 > 0$ such that $\lambda \not\in \sigma(H_a)$ for all $a \geq a_0$. Therefore, $R \geq R_a \geq R^D(\geq 0)$, i.e., $R_a$ and $R^D$ are also compact.

The following proposition is useful when proving statements for $\lambda$ inside the Neumann spectrum $H$ saying that one can always find an $a > 0$ such that $\lambda$ is not in the spectrum of $H_a$, even if $\lambda \in \sigma(H)$, provided all spectra are purely discrete.

**Proposition 5.3.** Let $(\Gamma, \mathcal{G})$ be a boundary pair and $\lambda \in [0, \infty)$. Assume in addition that $R$ is compact. If $\lambda /\in \sigma(H^D)$ then there exists $a_0 > 0$ such that $\lambda /\in \sigma(H_a)$ for all $a \geq a_0$.

Proof. The operator

$$\Lambda^{1/2} \Gamma R^{1/2} : \mathcal{H} \xrightarrow{\Gamma} \mathcal{G}$$

is bounded and $R^{1/2}$ is compact as operator in $\mathcal{H}$, since $R$ is compact. In particular, $\Lambda^{1/2} \Gamma R = \Lambda^{1/2} \Gamma R^{1/2} R^{1/2} : \mathcal{H} \rightarrow \mathcal{G}$ is compact. By [BBAB11, Thm. 2.6], we have $\|R_a - R^D\| \rightarrow 0$ as $a \rightarrow \infty$, i.e., $H_a$ converges in norm resolvent sense to $H^D$. This implies in particular, that if $\lambda /\in \sigma(H^D)$, then there exists $a_0 > 0$ such that $\lambda /\in \sigma(H_a)$ for all $a \geq a_0$ (see e.g. [RS80, Thm VIII.23]).

### 5.2 Coupled boundary pairs

Assume that $(\Gamma_i, \mathcal{G}_i)$ is a boundary pair associated with $h_i$ (dom $h_i = \mathcal{H}^1_i$) in the Hilbert space $\mathcal{H}_i$ for $i = 1, 2$. Note that the boundary space is the same for both boundary pairs. We assume additionally that

$$\mathcal{G}^{1/2} := \text{ran } \Gamma_1 \cap \text{ran } \Gamma_2 \text{ is dense in } \mathcal{G}.$$  \hfill (5.4)

We set $\mathcal{H} := \mathcal{H}_1 \oplus \mathcal{H}_2$ and $\mathcal{H}^{1, \text{dec}} := \mathcal{H}^1_1 \oplus \mathcal{H}^1_2$. It follows easily from the boundedness of $\Gamma_i : \mathcal{H}_i \rightarrow \mathcal{G}_i$ that

$$\mathcal{H}^1 := \{ f \in \mathcal{H}^{1, \text{dec}} \mid \Gamma_1 f_1 = \Gamma_2 f_2 \}$$

is a closed subspace of $\mathcal{H}^{1, \text{dec}}$, and $h := (h_1 \oplus h_2)|_{\mathcal{H}^1}$ is a non-negative, closed form in $\mathcal{H}$ with associated operator $H$. We call $h$ the coupled form obtained from $h_1$ and $h_2$.

Set

$$\Gamma : \mathcal{H}^1 \rightarrow \mathcal{G}, \quad \Gamma f := \Gamma_1 f_1 = \Gamma_2 f_2.$$  \hfill (5.5)

**Proposition 5.6.** Assume that $(\Gamma_i, \mathcal{G}_i)$ are boundary pairs for $i = 1, 2$ such that (5.4) holds. Then the following assertions are true:

**i.** The pair $(\Gamma, \mathcal{G})$ is a boundary pair associated with the coupled quadratic form $h$, called the (Neumann-)coupled boundary pair.

**ii.** The Dirichlet operator associated with the coupled boundary pair is decoupled, i.e., $H^D = H^D_1 \oplus H^D_2$, while the Neumann operator (the operator associated with $h$) is (in general) coupled. Moreover, the (weak) Dirichlet solution operator and the Dirichlet-to-Neumann operator of the coupled boundary pair are given by

$$S(z) \varphi = S_1(z) \varphi \oplus S_2(z) \varphi \quad \text{and} \quad \Lambda(z) \varphi = \Lambda_1(z) \varphi + \Lambda_2(z) \varphi$$

for $\varphi \in \mathcal{G}^{1/2} = \text{ran } \Gamma$, where $z \in \mathbb{C} \setminus \sigma(H^D) = \mathbb{C} \setminus (\sigma(H^D_1) \cup \sigma(H^D_2))$.

**iii.** We have

$$\|\varphi\|_{\mathcal{G}^{1/2}}^2 := \|S \varphi\|_{\mathcal{G}^1}^2 = \|S_1 \varphi\|_{\mathcal{G}^1_1}^2 + \|S_2 \varphi\|_{\mathcal{G}^1_2}^2 \geq \|\varphi\|_{\mathcal{G}^{1/2}}^2,$$

i.e., the embedding $\mathcal{G}^{1/2} \hookrightarrow \mathcal{G}^{1/2} = \text{ran } \Gamma$ is bounded for $i = 1, 2$. If in addition $\text{ran } \Gamma_1 = \text{ran } \Gamma_2$, then the embedding is surjective, and the norms on $\mathcal{G}^{1/2}$, $\mathcal{G}^{1/2}_1$ and $\mathcal{G}^{1/2}_2$ are mutually equivalent.
iv. If the boundary pairs \((\Gamma_1, \mathcal{G})\) are elliptically regular (uniformly positive), then the coupled boundary pair \((\Gamma, \mathcal{G})\) is elliptically regular (uniformly positive).

v. Krein’s resolvent formula in this context reads as

\[
\tilde{R}(z) = i_1 \tilde{R}_1^D(z) u_1^* + i_2 \tilde{R}_2^D(z) u_2^* + S(z) \Lambda(z)^{-1} S(\tilde{z})^* : \mathcal{H}^{-1} \longrightarrow \mathcal{H}^1
\]  

(with \(\tilde{R}_1^D(z) = (\tilde{R}_1^D - z)^{-1} : \mathcal{H}_1^{-1, D} \longrightarrow \mathcal{H}_1^{1, D}\) and \(i_1 : \mathcal{H}_1^{1, D} \rightarrow \mathcal{H}_1^1\), i.e., the resolvent of the coupled operator can be expressed by operators of the individual boundary pairs only, namely, the direct sum of the Dirichlet resolvents and a coupling term.

Proof. (i) The boundedness of \(\Gamma\) is obvious, as well as the density of

\[
\mathcal{H}^{1, D} := \text{ker} \Gamma = \text{ker} \Gamma_1 \oplus \text{ker} \Gamma_2 = \mathcal{H}_1^{1, D} \oplus \mathcal{H}_2^{1, D}.
\]

Moreover, \(\text{ran} \Gamma = \mathcal{G}^{1/2}\) is dense in \(\mathcal{G}\) by assumption (5.4).

(ii) That \(H^D\) is decoupled is obvious, as well as the formula for the coupled Dirichlet solution operator. The corresponding Neumann operator is (in general) coupled (i.e., not a direct sum of the individual Neumann operators). For the coupled Dirichlet-to-Neumann operator, note that

\[
(\Lambda(z) \varphi, \psi) = (h - z1)(S(z), g) = (h_1 - z1)(S_1(z), g_1) + (h_2 - z1)(S_2(z), g_2) = (\tilde{\Lambda}_1(z) \varphi, \psi) + (\tilde{\Lambda}_2(z) \varphi, \psi)
\]

for \(\varphi \in \mathcal{G}^{1/2}\) and any \(g = g_1 \oplus g_2 \in \mathcal{H}^1\) with \(\Gamma g = \psi\) (see (2.24a) and Definition 2.25).

(iii) The equivalence of the norms follows from the open mapping theorem (a bounded bijective operator has also a bounded inverse).

(iv) The last assertion is also obvious, using Definitions 3.1 and 3.12. We have e.g.

\[
\|S_{\varphi}\|_{\mathcal{G}}^2 = \|S_{\varphi}\|_{\mathcal{H}^1}^2 + \|S_{\varphi}\|_{\mathcal{H}^2}^2 \leq (C_1 + C_2)\|\varphi\|_{\mathcal{G}}^2
\]

if \(C_1, C_2\) are the constants in the estimate of Definition 3.1 for the individual boundary pairs. \(\square\)

In many applications, the RHS of Krein’s resolvent formula (5.7) in the coupled case can be calculated explicitly, hence we have a formula for the resolvent of the coupled operator (see Remark 7.19 for an example).

There is another way of coupling two boundary pairs: Let \(h_{\text{dec}} = h_1 \oplus h_2\). As boundary operator, we define here

\[
\tilde{\Gamma} := \Gamma_1 f_1 - \Gamma_2 f_2.
\]

It is again easily seen that \((\tilde{\Gamma}, \mathcal{G})\) is a boundary pair associated with \(h_{\text{dec}}\). Then the associated Neumann operator is \(\tilde{H} = H_1 \oplus H_2\), hence decoupled. Moreover, \(\text{ker} \Gamma\) equals \(\mathcal{H}^1\) defined in (5.5), and the Dirichlet operator \(\tilde{H}^D\) associated with this boundary pair is the coupled operator. We call this boundary pair the Dirichlet-coupled boundary pair, since the Dirichlet operator is coupled here.

It is now straightforward to calculate the associated Dirichlet solution operators and the Neumann-to-Dirichlet operator of the coupled boundary pair as

\[
\tilde{S}_{\varphi} = S_1 (\tilde{\Lambda}_1 + \tilde{\Lambda}_2)^{-1} \tilde{\Lambda}_2 \varphi \oplus S_2 (\tilde{\Lambda}_1 + \tilde{\Lambda}_2)^{-1} \tilde{\Lambda}_1 \varphi \quad \text{and} \quad \tilde{\Lambda}(z)^{-1} \varphi = \tilde{\Lambda}_1(z)^{-1} \varphi + \tilde{\Lambda}_2(z)^{-1} \varphi
\]

for \(\varphi \in \mathcal{G}^{1/2}\).

### 5.3 Direct sum of boundary pairs

Another way of obtaining a new boundary pair from two boundary pairs \((\Gamma_i, \mathcal{G}_i)\) associated with \(h_i\) on \(\mathcal{H}_i\) \((i = 1, 2)\) is by taking the direct sum of all objects, i.e., \(\mathcal{H} := \mathcal{H}_1 \oplus \mathcal{H}_2\), \(\mathcal{G} := \mathcal{G}_1 \oplus \mathcal{G}_2\), \(\Gamma := \Gamma_1 \oplus \Gamma_2\) etc. We call this boundary pair the direct sum of the boundary pairs \((\Gamma_1, \mathcal{G}_1)\) and \((\Gamma_2, \mathcal{G}_2)\). The corresponding derived objects and the properties of the direct sum can easily be derived; e.g. \(\Lambda(z) = \Lambda_1(z) \oplus \Lambda_2(z)\) and its spectrum is the union of the spectra of \(\Lambda_i(z)\). Note that the direct sum is different from the coupled pairs defined in Section 5.2.
5.4 Making a boundary pair bounded

Let us finally define a bounded boundary pair \((\tilde{\Gamma}, \tilde{\mathcal{H}})\) constructed from an unbounded boundary pair \((\Gamma, \mathcal{H})\) associated with \(\mathfrak{h}\) as follows: We set
\[
\tilde{\mathcal{H}} := \mathcal{H}^{1/2} \quad \text{and} \quad \tilde{\Gamma} : \mathcal{H}^1 \to \tilde{\mathcal{H}},
\]
where \(\tilde{\mathcal{H}}\) is endowed with the norm \(\|\varphi\|_{\tilde{\mathcal{H}}} = \|\varphi\|_{\mathcal{H}^{1/2}} = \|S\varphi\|_{\mathcal{H}^1},\) i.e., we just change the range space of \(\Gamma,\) and obviously, \(\text{ran} \tilde{\Gamma} = \tilde{\mathcal{H}},\) i.e., \((\tilde{\Gamma}, \tilde{\mathcal{H}})\) is a bounded boundary pair. For the new boundary pair, called the bounded modification of \((\Gamma, \mathcal{H})\), we have \(\|\tilde{\Gamma}\|_{1 \to 0} = 1.\) Moreover its weak Dirichlet solution operator and Dirichlet-to-Neumann operator are given as follows:

**Proposition 5.9.** Assume that \((\Gamma, \mathcal{H})\) is an unbounded boundary pair associated with a quadratic form \(\mathfrak{h}.\) Denote by \((\tilde{\Gamma}, \tilde{\mathcal{H}})\) its bounded modification, given by \(\tilde{\mathcal{H}} = \mathcal{H}^{1/2}, \tilde{\Gamma} : \mathcal{H}^1 \to \tilde{\mathcal{H}}, \tilde{\Gamma} f = \Gamma f,\) where the objects without tilde refer to \((\Gamma, \mathcal{H})\) and the tilded objects refer to \((\tilde{\Gamma}, \tilde{\mathcal{H}}).\) Then the following assertions are true:

i. The Neumann and Dirichlet operators remain unchanged, i.e., \(\tilde{H}^D = H^D\) and \(\tilde{H} = H.\)

ii. We have
\[
\tilde{\mathcal{S}}(z) : \tilde{\mathcal{H}} \to \mathcal{H}^1, \quad \tilde{\mathcal{S}}(z) \varphi = S(z) \varphi, \quad \tilde{\Lambda} = \lambda_{\mathcal{H}} \quad \text{and} \quad \tilde{\Lambda}(z) : \tilde{\mathcal{H}} \to \tilde{\mathcal{H}} \text{ are bounded operators, the norm of the latter is bounded by } L(z) \text{ (cf. (2.24c)).}
\]

iii. The boundary pair \((\tilde{\Gamma}, \tilde{\mathcal{H}})\) is bounded and in particular elliptically regular. Moreover \(\tilde{\mathcal{S}}(z) : \tilde{\mathcal{H}} \to \mathcal{H}^1\) and \(\tilde{\Lambda}(z) : \tilde{\mathcal{H}} \to \tilde{\mathcal{H}}\) are bounded operators, the norm of the latter is bounded by \(L(z)\) (cf. (2.24c)).

iv. If \((\Gamma, \mathcal{H})\) is not uniformly positive, then \((\tilde{\Gamma}, \tilde{\mathcal{H}})\) is not either.

**Remark 5.10.** Note that although we could only work with bounded boundary pairs, there is not always an associated ordinary boundary triple (for this we need that the new boundary pair is uniformly positive, see Theorem 6.11 (vi)). The bounded modification of an unbounded boundary pair is obviously elliptically regular (because it is bounded), but not necessarily uniformly positive (see Example 7.20).

Moreover, the unbounded boundary pair is in many examples more “natural” like in the manifold example in Section 7.4 since the modified boundary pair involves the Dirichlet-to-Neumann operator in the norm of the new boundary space.

6 Relation to boundary triples and other concepts

In this section, we relate our concept of encoding boundary value problems with other concepts such as boundary triples.

6.1 Relation to boundary triples

We start with associating a boundary triple with a boundary pair; a related approach can be found in [Ar99]. Let \((\Gamma, \mathcal{H})\) be a boundary pair associated with a quadratic form \(\mathfrak{h}.\) Denote by \(H^{\min} = H \cap H^D\) the minimal operator, i.e., \(H^{\min} f = H f = H^D f\) for \(f \in \text{dom } H^{\min} = \text{dom } H \cap \text{dom } H^D.\)

**Assumption 6.1.** We assume in this section that \(H^{\min}\) is densely defined, i.e., that \(\text{dom } H^{\min} = \text{dom } H^D \cap \text{dom } H\) is dense in \(\mathcal{H}.\)

It is not clear to us whether the above density condition already follows from the general assumptions on a boundary pair, namely that \(\ker \Gamma\) is dense in \(\mathcal{H}.\) But this assumption excludes large boundary spaces, i.e., boundary pairs where \(\ker \Gamma = \mathcal{H}^{1,D}\) is not dense in \(\mathcal{H}.\) Nevertheless, some results remain true in this case, see the example in Section 7.8.

Under Assumption 6.1, we can uniquely define the maximal operator as \(H^{\max} := (H^{\min})^+.\) We set \(\mathcal{W}^{\max} := \text{dom } H^{\max}\) with norm given by \(\|f\|^2_{\mathcal{W}^{\max}} = \|H^{\max} f\|^2 + \|f\|^2.\) Since \(H^{\max}\) is closed, \(\mathcal{W}^{\max}\) is a Hilbert space.

We have the following simple fact (recall that \(\mathcal{A}^0(z) = \mathcal{A}^1(z)\) denotes the closure of the weak solution space in the \(\mathcal{H}\)-norm):

**Proposition 6.2.**

i. For \(z \in \mathbb{C} \setminus \sigma(H^D),\) we have \(\text{dom } H^{\max} = \ker (H^{\max} - z)^+ \cap \text{dom } H^D.\)
ii. For $z \in \mathbb{C} \setminus \sigma(H)$, we have $\text{dom} H^{\max} = \ker(H^{\max} - z) + \text{dom} H$.

iii. If $z \in \mathbb{C} \setminus \sigma(H^D)$ then $\mathcal{N}^0(z) = \ker(H^{\max} - z)$. In particular, $\mathcal{N}^1(z) \subset \ker(H^{\max} - z)$.

Proof. (i) If $f \in \text{dom} H^{\max}$, then we have
\[
 f = (f - R^D(z)(H^{\max} - z)f) + R^D(z)(H^{\max} - z)f
\]
and the first summand is in $\ker(H^{\max} - z)$, while the second is in $\text{dom} H^D$. If $f \in \ker(H^{\max} - z) \cap \text{dom} H^D$, then actually, $(H^D - z)f = 0$, and since $z \notin \sigma(H^D)$, we have $f = 0$. The argument for the Neumann operator in (ii) is similar.

(iii) "⊂": Let $h_n \to h$ in $\mathcal{H}$ with $h_n \in \mathcal{N}^1(z)$. It is easy to see that $\mathcal{N}^1(z) \subset \text{dom} H^{\max}$ and that $H^{\max}h_n = zh_n$. Since $\ker(H^{\max} - z)$ is a closed subspace of $\mathcal{H}$, we conclude $h \in \ker(H^{\max} - z)$.

"⊃": Let now $h \in \ker(H^{\max} - z)$. Note first that $\mathcal{W}^{\max} \cap \mathcal{H}^1$ is dense in $\mathcal{W}^{\max}$ (endowed with its graph norm), since
\[
\text{dom} H^D + \text{dom} H \subset \mathcal{H}^1 \cap \mathcal{W}^{\max}
\]
and since $\text{dom} H^D + \text{dom} H$ is dense in $\mathcal{W}^{\max}$. The latter follows by considering the graphs graph $H^D = \{ (f, H^D f) \mid f \in \text{dom} H^D \}$ and graph $H$ of the operators, and the fact that the closure of graph $H^D + \text{graph} H$ in $\mathcal{H} \oplus \mathcal{H}$ equals graph $H^{\max}$.

By the density, there exists a sequence $(g_n)_n$ such that $g_n \in \mathcal{H}^1$ and $g_n \to h$ in $\mathcal{W}^{\max}$. Set now $h_n := S(z)G_n$, then
\[
 g_n - h_n = R^D(z)(H^{\max} - z)g_n \to H^{\max}h - zh = 0
\]
by Proposition 4.3 and the fact that $g_n \in \text{dom} H^{\max}$ (for the first equality) and $g_n \to h$ in $\mathcal{W}^{\max}$ (for the convergence). In particular, $h_n = (h_n - g_n) + g_n \to h$ in $\mathcal{H}$ and $h_n \in \mathcal{N}^1(z)$, hence $h \in \mathcal{N}^0(z)$.

Let us now shortly review different concepts of boundary triples. For a more detailed discussion we refer to [BL10] and the references therein:

**Definition 6.3.** Let $H^{\min}$ be a closed, densely defined and symmetric operator in $\mathcal{H}$ and set $H^{\max} = (H^{\min})^*$. 

i. A triple $(\Gamma_0, \Gamma_1, \mathcal{G})$ is a *quasi-boundary triple* associated with $H^{\max}$ (see [BL07, Def. 2.1] or [BL10, Def. 3.1]) if there is a subspace $\mathcal{W}$ of $\text{dom} H^{\max}$, dense in $\mathcal{H}$, such that

a) “joint dense range”: $(\Gamma_0, \Gamma_1) : \mathcal{W} \to \mathcal{G} \oplus \mathcal{G}$ has dense range, where $(\Gamma_0, \Gamma_1)f := (\Gamma_0f, \Gamma_1f)$.

b) “self-adjointness”: $H_0 := H^{\max}|_{\ker \Gamma_0}$ is self-adjoint.

c) Green’s identity
\[
\langle H^{\max}f, g \rangle_{\mathcal{H}} - \langle f, H^{\max}g \rangle_{\mathcal{H}} = (\Gamma_0 f, \Gamma_1 g)_{\mathcal{G}} - (\Gamma_0 f, \Gamma_0 g)_{\mathcal{G}}
\]
(6.4)

holds for $f, g \in \mathcal{W}$.

ii. The triple $(\Gamma_0, \Gamma_1, \mathcal{G})$ is (here) called an *ordinary boundary triple* associated with $H^{\max}$ if it fulfils Green’s identity (6.4), if $\mathcal{W} = \text{dom} H^{\max}$ and if the joint dense range condition (ia) is replaced by “surjective joint range”, i.e., $(\Gamma_0, \Gamma_1)(\mathcal{W}) = \mathcal{G} \oplus \mathcal{G}$.

iii. The triple $(\Gamma_0, \Gamma_1, \mathcal{G})$ is called a *generalised boundary triple* associated with $H^{\max}$ (in the sense of [DM95, Def. 6.1]) if it fulfils Green’s identity (6.4) and if the joint dense range condition (ia) is replaced by the surjectivity of $\Gamma_0$, i.e., by $\Gamma_0(\mathcal{W}) = \mathcal{G}$.

A generalised boundary triple is a quasi-boundary triple [BL07, Cor. 3.7] (see also [DM95, Lem. 6.1]). The following material will be discussed in more detail in a forthcoming publication [P12b]. Set
\[
\mathcal{W}^{\max}_0 := \{ u \in \mathcal{W}^{\max} \cap \mathcal{H}^1 \mid \forall v \in \mathcal{H}^{1,D} : b(u, v) = \langle H^{\max}u, v \rangle \}
\]
with norm given by $\|u\|_{\mathcal{W}^{\max}_0} := \|u\|^2 + b(u) + \|H^{\max}u\|^2$. It is easy to see that $\mathcal{W}^{\max}_0$ is a Hilbert space.

Moreover, we can define a bounded operator $\Gamma' : \mathcal{W}^{\max}_0 \to \mathcal{G}^{1/2}$ (bounded by 1) such that
\[
\langle \Gamma' u, \varphi \rangle_{-1/2,1/2} = b(u, v) - \langle H^{\max}u, v \rangle
\]
for all $u \in \mathcal{W}^{\max}_0$ and $v \in \mathcal{H}^1$ such that $\Gamma v = \varphi$. Note that the right hand side only depends on $\varphi$ and not on $v$, which follows from the defining formula in $\mathcal{W}^{\max}_0$. 

29
6.1 Relation to boundary triples

We set now
\[ \mathcal{W} := \{ u \in \mathcal{W}_0^{1,\text{max}} \mid \Gamma' u \in \mathcal{G} \} \]
with norm \[ \|u\|_{\mathcal{W}}^2 := \|u\|^2 + h(u) + \|H^{\text{max}} u\|^2 + \|\Gamma' f\|^2_{\mathcal{G}} \] (6.6)
and \( \Gamma' u := \hat{\Gamma}' u \) for \( u \in \mathcal{W} \). We call \((\Gamma_{\mathcal{W}}, \Gamma', \mathcal{G})\) the maximal boundary triple associated with the boundary pair \((\Gamma, \mathcal{G})\). Note that we have the following Green’s formula
\[ h(f, g) = (H^{\text{max}} f, g) + (\Gamma' f, \Gamma g)_\mathcal{G} \] (6.7)
for \( f \in \mathcal{W} \) and \( g \in \mathcal{H}^1 \).

Let us now justify the names “Dirichlet-to-Neumann” and “Neumann-to-Dirichlet” operator:

**Proposition 6.8.** Let \( z \in \mathbb{C} \setminus \sigma(H^{\text{Dirichlet}}) \). If \( h = S(z) \varphi \in \mathcal{W} \), then \( \varphi \) is in the domain of the associated Dirichlet-to-Neumann operator, i.e., \( \varphi \in \text{dom} \Lambda(z) \) (see (2.26)), and we have
\[ \Lambda(z) \varphi = \Gamma h \]
i.e., the Dirichlet-to-Neumann operator associates to a boundary value \( \varphi \) the “normal derivative” \( \Gamma h \) of the solution of the Dirichlet problem \( h = S(z) \varphi \).

If, additionally, \( z \notin \sigma(H) \) then \( \varphi \in \text{dom} \Lambda(z)^{-1} \psi = \Gamma h \) with \( \psi = \Gamma h \), i.e., \( \varphi \in \text{dom} \Lambda(z)^{-1} \) associates to the Neumann data \( \psi \) the Dirichlet data of \( h \).

**Proof.** The proof follows immediately from Green’s formula (6.7) (since \( h \in \mathcal{W} \)), namely
\[ I_z(\varphi, \psi) = (h - z) (S(z) \varphi, g) = ((H^{\text{max}} - z) h, g) + (\Gamma h, \Gamma g)_\mathcal{G} = (\Gamma h, \psi)_\mathcal{G} \]
where \( g \in \mathcal{H}^1 \) with \( \Gamma g = \psi \). Note that \( (H^{\text{max}} - z) h = 0 \) since \( h \in \mathcal{A}^{1,\text{Dirichlet}}(z) \subseteq \ker(H^{\text{max}} - z) \) by Proposition 6.2 (iii). The assertion on \( \Lambda(z)^{-1} \) follows easily from the bijectivity of \( \Lambda(z) \) (see Theorem 2.29). \( \square \)

We have the following result relating our concept of boundary pairs to quasi-boundary triples:

**Theorem 6.9.**

i. Let \((\Gamma, \mathcal{G})\) be a boundary pair, then the following assertions are equivalent:
   a) \((\Gamma, \mathcal{G})\) is elliptically regular;
   b) \( \hat{\Gamma}' u \in \mathcal{G} \) for all \( u \in \text{dom} H^{\text{Dirichlet}} \);
   c) \((\Gamma_{\mathcal{W}}, \Gamma', \mathcal{G})\) is a quasi-boundary triple associated with \( H^{\text{max}} \);

ii. If the boundary pair is bounded then \((\Gamma_{\mathcal{W}}, \Gamma', \mathcal{G})\) is a generalised boundary triple associated with \( H^{\text{max}} \).

**Proof.** (ia) \( \Rightarrow \) (ib) From Green’s formula (6.7) we have
\[ (\hat{\Gamma}' u, \varphi) = h(u, S\varphi) - (H^{\text{Dirichlet}} u, S\varphi) = (h + 1)(u, S\varphi) - (H^{\text{Dirichlet}} + 1) u, S\varphi) \]
The first term vanishes since \( u \in \text{dom} H^{\text{Dirichlet}} \subset \mathcal{A}^{1,\text{Dirichlet}} \) is orthogonal to \( S\varphi \) in \( \mathcal{H}^1 \). In particular, we have
\[ \langle S\varphi, v \rangle = \langle \varphi, -\Gamma' R^D v \rangle \] (6.10)
for all \( v \in \mathcal{H} \) and \( \varphi \in \mathcal{G}^{1/2} \). By elliptic regularity, \( \varphi \rightarrow \langle S\varphi, v \rangle \) extends to a bounded functional on \( \mathcal{G} \), hence \( \Gamma' u \in \mathcal{G} \) for all \( u \in R^D v \in \text{dom} H^{\text{Dirichlet}} \).

(ib) \( \Rightarrow \) (ia) From (6.10) and the assumption we see that \( S^* v \) is defined for all \( v \in \mathcal{H} \). Since \( S^* \) is closed, it is bounded by the closed graph theorem, hence the boundary pair is elliptically regular.

(ia) \( \Rightarrow \) (ic) We check the conditions in Definition 6.3. The “joint dense range” condition will be shown in [P12b], as well as the fact that for elliptically regular boundary pairs, we have \( \text{dom} H^{\text{Dirichlet}} \subset \mathcal{W} \) and the self-adjointness of \( H_0 \) follows. Green’s identity (6.4) is easily seen. (ic) \( \Rightarrow \) (ia) follows from [BL07, Cor. 2.6 (i)].

(ii) We will give a proof of this fact in a forthcoming publication [P12b]. \( \square \)

To summarise: Our concept of boundary pairs is more general in the sense that the associated boundary triple is a quasi-boundary triple only if the boundary pair is elliptically regular. On the other hand, our concepts is only suitable for non-negative operators \( H \) and \( H^{\text{Dirichlet}} \) (although there is a natural extension to sectorial operators).

The relation to an ordinary boundary triple is as follows. Again, the proof of the following result will be given in [P12b] (parts of the proof are given in [BL07, Cor. 3.2]):
Theorem 6.11. Let $(\Gamma, \mathcal{G})$ be a boundary pair. Then the following conditions are equivalent:

i. There is a corresponding ordinary boundary triple $(\Gamma|_{\mathcal{W}}, \Gamma', \mathcal{G})$ (the maximal boundary triple associated with $(\Gamma, \mathcal{G})$);

ii. $\mathcal{W}^{\text{max}} \subset \mathcal{W}^{1,\text{max}}_0$, i.e., $\text{dom } H^{\text{max}} \subset \mathcal{H}^1$ and $b(f, g) = \langle H^{\text{max}}f, g \rangle$ for all $f \in \text{dom } H^{\text{max}}$ and $g \in \mathcal{H}^{1,\text{D}}$.

iii. $\text{dom } H^{\text{max}} = \text{dom } H + \text{dom } H^{\text{D}}$.

iv. $\ker(H^{\text{max}} - z) \subset N^1(z)$ for some (any) $z \in \mathbb{C} \setminus \sigma(H^{\text{D}})$.

v. $N^0(z) = N^1(z)$ (or $N^0(z) \subset N^1(z)$) for some (any) $z \in \mathbb{C} \setminus \sigma(H^{\text{D}})$.

vi. The boundary pair is bounded and uniformly positive.

In particular, if one of the conditions is fulfilled, then the boundary pair is bounded, and the norms on $\mathcal{W}^{\text{max}}$ and $\mathcal{W}^{1,\text{max}}_0$ are equivalent, i.e., there is a constant $C > 0$ such that $b(f) \leq C(\|f\|^2 + \|H^{\text{max}}f\|^2)$.

Proof. The equivalence of (i), (ii) and (iii) will be shown in [P12b]. Basically, we use that the associated boundary triple is a quasi-boundary triple iff the boundary pair is elliptic (Theorem 6.9 (i)) and the characterisation [BL07, Cor. 3.2] for quasi-boundary triples to be ordinary.

(iii) $\Rightarrow$ (iv): By assumption, we have $\ker(H^{\text{max}} - z) \subset \text{dom } H + \text{dom } H^{\text{D}} \subset \mathcal{H}^1$, and $N^0(z) = \ker(H^{\text{max}} - z)$ by Proposition 6.2 (iii), hence $N^0(z) \subset \ker(H^{\text{max}} - z) \subset \mathcal{H}^1 \cap N^0(z) = N^1(z)$.

(iv) $\Rightarrow$ (iii): By Proposition 6.2 (i), $H^{\text{max}} = \ker(H^{\text{max}} - z) + \text{dom } H^{\text{D}}$. Moreover $\ker(H^{\text{max}} - z) \subset N^1(z) \subset \mathcal{H}^1$, and it is easily seen that $\ker(H^{\text{max}} - z) \cap \mathcal{H}^1 \subset \text{dom } H$.

(iv) $\Leftrightarrow$ (v) is obvious using the characterisation $N^0(z) = \ker(H^{\text{max}} - z)$ from Proposition 6.2 (iii).

(i) $\Rightarrow$ (vi): An ordinary boundary triple induces a bounded and uniformly positive boundary pair (see e.g. [BGP08, (1.22c) in Prp. 1.2]) for the uniform positivity). (vi) $\Rightarrow$ (v): For a boundary pair, $S(z)$ is a topological isomorphism from $\mathcal{G}^{1/2}$ onto $N^1(z)$ with inverse $\Gamma: N^1(z) \to \mathcal{G}^{1/2}$. If, additionally, the boundary pair is elliptically regular and uniformly positive, then its extension $\bar{S}(z)$ is a topological isomorphism from $\mathcal{G}$ onto $N^0(z)$ with inverse $\bar{\Gamma}: N^0(z) \to \mathcal{G}$. For bounded boundary pairs, we have in addition that $\mathcal{G} = \mathcal{G}^{1/2}$ (with equivalent norms), hence $N^0(z) = N^1(z)$.

Corollary 6.12. If the boundary space $\mathcal{G}$ of a boundary pair is finite-dimensional, then the boundary pair is bounded and uniformly positive, hence there is a corresponding ordinary boundary triple.

Proof. We check condition (vi): A boundary pair with $\dim \mathcal{G} < \infty$ is necessarily bounded. Moreover, $S$ is injective on $\mathcal{G}^{1/2} = \mathcal{G}$, and since $\mathcal{G}$ is finite-dimensional, we also have $\|S \varphi\| \geq c\|\varphi\|$ for some $c > 0$. In particular, the boundary pair is uniformly positive.

Remark 6.13. In [LS83], Lyantse and Storozh also used the notation “boundary pair”, but in a slightly different context: They considered two closed operators $L$ and $L_0$ in a Hilbert space $\mathcal{H}$ such that $L_0$ is a restriction of $L$. The domain $\mathcal{G}_L$ of $L$ is endowed with its graph norm $\|u\|_{\mathcal{G}_L} := \|u\|^2 + \|Lu\|^2$. They call $(\mathcal{G}, \Gamma)$ a boundary pair if

i. $\Gamma: \mathcal{G}_L \to \mathcal{G}$ is bounded,

ii. $\ker \Gamma = \text{dom } L_0$ and

iii. $\text{ran } \Gamma = \mathcal{G}$.

They call an operator $\Pi: \mathcal{G} \to \mathcal{G}_L$ a lifting operator associated with $(\mathcal{G}, L)$ if $\Pi$ is bounded, injective, $\text{ran } \Pi \cap \text{dom } L_0 = \{0\}$ and $\text{ran } \Pi \cap \mathcal{G}_L = \mathcal{G}$.

Starting with a boundary pair $(\Gamma, \mathcal{G})$ associated with a quadratic form $\mathcal{H} \geq 0$, we can construct a boundary pair in the sense of Lyantse and Storozh as follows: Let $L_0 := H^{\text{D}}$ be the Dirichlet operator, and $L = H^{\text{max}} = (H^{\text{D}} \cap H)^*$ be the maximal operator. If we assume now, that there is an associated ordinary boundary triple (see Theorem 6.11 for equivalent conditions) then one can actually show that $\Gamma$ is bounded (see e.g. [BGP08, Prp. 1.9]), that $\ker \Gamma = \text{dom } H^{\text{D}}$ and that $\Gamma$ is surjective. Moreover, a Dirichlet solution operator $S(z)$ is then a lifting operator in the sense of Lyantse and Storozh.

To summarise, boundary pairs in the sense of Lyantse and Storozh are related to ordinary boundary triples and operators, while our notation is related to quadratic forms and more general boundary triples.
6.2 Relation to extension theory

The theory of boundary triples is also closely related with the theory of self-adjoint extensions of a given symmetric operator $H^{\min}$. Let us explain how extension theory is related to the concept of boundary pairs. For a detailed reference list, we refer to the introduction.

Let $H^{\min}$ be a closed, symmetric and densely defined operator in a Hilbert space $\mathcal{H}$ and set $H^{\max} := (H^{\min})^*$. We are here only interested in operators bounded from below, hence we assume that $H^{\min} \geq \lambda_0$ for some $\lambda_0 > 0$, i.e., $\langle H^{\min} u, u \rangle \geq \lambda_0 \|u\|^2$ for all $u \in \text{dom} H^{\min}$. For such an operator $H^{\min}$ we define a closed quadratic form $h^D$ as the closure of $h^D(u) := \langle H^{\min} u, u \rangle$, $u \in \text{dom} H^{\min}$. The operator $H^D$ associated with $h^D$ is called the Friedrichs or hard extension of a symmetric operator $H^{\min}$ (clearly, $H^{\min} \subset H^D \subset H^{\max}$). All quadratic form domains in the sequel are endowed with their natural norm as in (2.2).

If we assume that $0 \notin \sigma(H^D)$, then we can choose $\lambda_0 = \inf \sigma(H^D) > 0$, since
\[
\langle H^{\min} u, u \rangle \geq h^D(u) \geq \lambda_0 \|u\|^2
\]
for $u \in \text{dom} H^{\min}$.

There is another self-adjoint extension, the Krein or soft extension, defined as the operator associated with the non-negative and closed quadratic form $h^K$ given by
\[
\text{dom } h^K := \text{dom } h^D + \ker H^{\max}, \quad h^K(u) := h^D(u^D),
\]
where $u^D$ is the projection of $u \in \text{dom } h^K$ onto $\text{dom } h^D$ along $\ker H^{\max}$. The associated operator $H^K$ acts on $\text{dom } H^K = \text{dom } H^{\min} + \ker H^{\max}$ (a result of Krein, see [Kr47, Thm. 14]). Grubb described in [Gr70, Sec. 1] (see also [Kr47], [Bi56], [DM95, Ch. 4] and [Ar96, Ar99, Ar12]) all self-adjoint and non-negative extensions $H$ of $H^{\min}$, i.e., all self-adjoint operators $H \geq 0$ with $H^{\min} \subset H \subset H^{\max}$. Such operators naturally arise from their associated quadratic forms $h$. A special case of her main result of the abstract theory is as follows (cf. [Gr70, Thm. 1.1 and Cor. 1.3]):

**Proposition 6.14.** Let $H^{\min} \geq \lambda_0$ ($\lambda_0 > 0$) be a closed and uniformly positive operator in a Hilbert space $\mathcal{H}$, let $H^{\max} = (H^{\min})^*$ and denote by $h^D$ the closed form associated with $H^{\min}$ as above. Moreover assume that $H \geq 0$ is a self-adjoint operator in $\mathcal{H}$ with associated quadratic form $h$. Then the following conditions are equivalent:

i. $H$ is an extension of $H^{\min}$ ($H^{\min} \subset H$);

ii. there exists a closed, non-negative quadratic form $t$ defined on $\text{dom } t \subset \ker H^{\max}$ such that
\[
\text{dom } h = \text{dom } h^D + \text{dom } t \ni u = u^D + u_t, \quad h(u) = h^D(u^D) + t(u_t).
\]

iii. The following three conditions hold:
   a) $\text{dom } h^D \subset \text{dom } h \subset \text{dom } h^D + \ker H^{\max}$;
   b) $h^D \subset h$ (i.e., $h(u) = h^D(u)$ for $u \in \text{dom } h^D$);
   c) $h^K(u) \leq h(u)$ for all $u \in \text{dom } h$.

Actually, there is a bijection between the set of self-adjoint extensions $H \geq 0$ and the set of (not necessarily densely defined!) closed and non-negative quadratic forms $t$ in $\ker H^{\max}$ (see [Gr70, Sec. 1]). Note that the Krein (or soft) extension $H^K$ corresponds to the form $t = 0$ with $\text{dom } t = \ker H^{\max}$.

The relation with boundary pairs is as follows: Given a closed, non-negative and densely defined operator $H^{\min}$, the operator $H^D$ (the Friedrichs extension) is defined as well as $H^{\max} := (H^{\min})^*$. Assume that $H$ is a self-adjoint and non-negative extension of $H^{\min}$. Denote by $\mathcal{H}$ the corresponding quadratic form, and by $t$ the associated quadratic form in $\ker H^{\max}$ as above.

We set $\mathcal{H}^1 := \text{dom } h$ and denote by $\mathcal{G}$ the closure of $\text{dom } t$ in $\mathcal{H}$. Let $\Gamma: \mathcal{H}^1 \rightarrow \mathcal{G}$ be the projection of $u \in \mathcal{H}^1 = \text{dom } h^D + \text{dom } t$ onto $\text{dom } t$ along $\text{dom } h^D$. We have the following result:

**Theorem 6.15.** Assume that $0 \notin \sigma(H^D)$. Let $t$ be the quadratic form obtained from $h$ as in Proposition 6.14.

i. The pair $(\Gamma, \mathcal{G})$ is a boundary pair associated with the quadratic form $h$. Moreover, $(\Gamma, \mathcal{G})$ is bounded if $t$ (or $T$) is.

ii. The Dirichlet operator $H^D$ is the Friedrichs extension of $H^{\min} \geq 0$; the Neumann operator is $H$.

iii. The Dirichlet solution operator is given by $S(z)\varphi = U(z,0)\varphi = \varphi + z(H^D)^{-1}\varphi$ for $\varphi \in \mathcal{G}^{1/2} = \text{dom } t \subset \mathcal{G} \subset \mathcal{H}$. 


iv. The boundary pair \((\Gamma, \mathcal{G})\) is elliptically regular and uniformly positive.

v. The Dirichlet-to-Neumann operator is \(\Lambda(z) = T - zU(z,0)\); in particular, for \(z = 0\), we have \(\Lambda(0) = T\), where \(T\) is the operator associated with \(t\) on \(\mathcal{G} \subset \mathcal{H}\).

**Proof.** (i) Since the projection is bounded on \(\mathcal{H}^1\) and since \(\mathcal{H}^1\) is continuously embedded in \(\mathcal{H}\), \(\Gamma\) is bounded. Moreover, \(\ker \Gamma = \text{dom} \tilde{h}^D\) is dense in \(\mathcal{H}\), since \(H^{\text{min}}\) is densely defined. In addition, \(\mathcal{G}^{1/2} = \text{ran} \Gamma = \text{dom} t\) is dense in \(\mathcal{G}\) by definition. Finally, \(\Gamma\) is surjective if \(\text{dom} t = \mathcal{G}\), i.e., if \(t\) is defined everywhere on \(\mathcal{G}\) and hence bounded. (ii) is clear; as well as (iii) (note that \(L_0(\varphi) = b(S(0)\varphi) = t(\varphi)\); the latter implies that \(\Lambda(0) = T\).

It may happen that \(\mathcal{G} = \{0\}\) (if we choose \(H = H^D\)). If we want that \(H^{\text{min}} = H^D \cap H\), then we have to assume that \(H^D\) and \(H\) are disjoint, i.e., that

\[
H^{\text{min}} \subset H, \quad (H^{\text{min}} \subset H^D) \quad \text{and} \quad \text{dom} H^{\text{min}} = \text{dom} H \cap \text{dom} H^D. \tag{6.16}
\]

**Remark 6.17.** For the boundary pair \((\Gamma, \mathcal{G})\) associated with \(h^R\) constructed in Theorem 6.15 we have \(H = H^R\), \(\text{ran} \Gamma = \mathcal{G}\) (the boundary pair is bounded), \(t = 0\), \(\Lambda(0) = 0\) and \(\Lambda(z) = -zU(z,0)\).

A bounded boundary pair \((\Gamma, \mathcal{G})\) associated with \(h^R\) is actually called boundary pair by Arlinskii (see [Ar96, Ar99, Ar12]). Arlinskii [Ar99] also associates a boundary triple with such a boundary pair.

On the other hand, starting with a boundary pair \((\Gamma, \mathcal{G})\) associated with a non-negative and closed quadratic form \(h\) we have the following result:

**Theorem 6.18.** Assume that \((\Gamma, \mathcal{G})\) is a boundary pair associated with a quadratic form \(h\), such that \(0\) is not in the spectrum of the associated Dirichlet operator \(H^D\).

i. Denote by \(t\) the form as given in Proposition 6.14 related with \(h\), then the Dirichlet-to-Neumann form of the boundary pair at the spectral point \(0\) is given by \(L_0(\varphi) = t(S(0)\varphi)\).

ii. Let \(\tilde{H}\) be a self-adjoint and non-negative extension of \(H^{\text{min}} = H^D \cap H\) and denote by \(\tilde{h}\) its associated quadratic form. Assume that \(\text{dom} \tilde{h}^D\) and \(\text{dom} \tilde{h}\) are topologically isomorphic, i.e., that there exists \(\tau \geq 1\) such that \(\text{dom} \tilde{h} = \text{dom} \tilde{h}\) and

\[
\tau^{-1}(\tilde{h}(u) + \|u\|^2) \leq \tilde{h}(u) + \|u\|^2 \leq \tau(h(u) + \|u\|^2)
\]

for all \(u \in \text{dom} \tilde{h}\). Then \((\Gamma, \mathcal{G})\) is also a boundary pair associated with \(\tilde{h}\) with Dirichlet operator \(H^D\) and Neumann operator \(\tilde{H}\). Moreover, there exists a quadratic form \(p\) in \(\mathcal{G}\) with \(\text{dom} p = \mathcal{G}^{1/2}\) such that

\[
\tilde{h}(u) = h(u) + p(\Gamma u). \tag{6.19}
\]

**Proof.** (i) By Proposition 6.14, we have

\[
h(u) = h^D(u^D) + t(u),
\]

and hence \(L_0(\varphi) = h(S(0)\varphi) = t(S(0)\varphi)\).

(ii) Denote by \(t\) and \(\tilde{t}\) the forms related to the self-adjoint extensions \(H\) and \(\tilde{H}\) as in Proposition 6.14. Then we have

\[
\tilde{h}(u) - h(u) = \tilde{t}(S(0)\Gamma u) - t(S(0)\Gamma u) =: p(\Gamma u),
\]

where \(S(0)\Gamma u\) is the projection of \(u \in \mathcal{H}^1\) onto \(H^{1,D}\) along \(H^D\). Note that \(p\) is well-defined, since the difference in the middle expression depends only on \(\Gamma u\). Since \(\mathcal{H}^1 := \text{dom} \tilde{h}^D\), the intrinsic norms are by assumption topologically isomorphic, \(\Gamma\) is also bounded as map \(\mathcal{H}^1 \to \mathcal{G}\). Moreover, \(\tilde{h}\) and \(h\) agree with \(h^D\) on \(\ker \Gamma\), hence the Dirichlet operator for both boundary pairs is \(H^D\).

**Remark 6.20.**

i. The form \(\tilde{h}\) associated with the self-adjoint and non-negative extension of \(H^{\text{min}}\) can be seen as a Robin-type perturbation of \(h\), i.e., \(h(u) = \tilde{h}(u) + p(\Gamma u)\). One can express the Dirichlet-to-Neumann operator of the boundary pair \((\Gamma, \mathcal{G})\) associated with \(h\) in terms of the boundary pair \((\Gamma, \mathcal{G})\) associated with \(h\) as in Section 5.1. We will treat this in a forthcoming publication.
ii. If $\tilde{H} = H^K$ then $\text{dom } \mathfrak{h} \subseteq \text{dom } \tilde{\mathfrak{h}}$ since $\mathfrak{h}(u) = h^K(u) = \mathfrak{h}(u) - l_0(\Gamma \varphi) \leq \mathfrak{h}(u)$ (i.e., $p = l_0$), but there is no lower estimate on $h^K$ in terms of $\mathfrak{h}$ and $\Gamma^1 : \mathcal{H}^1 \rightarrow \mathcal{G}$ is not bounded. Nevertheless, one can see that (with the notation of Section 6.1)

$$\text{dom } H^K = \{ u \in H^{1,\text{max}}_0 | \Gamma' u = \tilde{\Lambda}(0) \Gamma u \}$$

where the latter equality holds in $\mathcal{G}^{-1/2}$. In particular, $H^{\text{max}} = \ker H^K$, $0 \in \sigma(H^K)$, and $0 \in \sigma_{\text{ess}}(H^K)$ iff $\dim \mathcal{G} = \infty$.

iii. If $0 \in \sigma(H^D)$ we can shift all operators by 1, i.e., work with the form $\mathfrak{h} + 1$ etc. In this case $t$ is a form acting in $\mathcal{A}^0 = \mathcal{A}^0(-1) \subset \ker(H^{\text{max}} + 1)$ and $\tilde{H} = H^K$ is no longer non-negative, since $-1$ is an eigenvalue with eigenspace $\ker(H^{\text{max}} + 1)$.

iv. Note that not all self-adjoint extensions of a closed operator $H^{\text{min}} \geq 0$ are covered in the above Robin-type way (see (6.19)). If e.g. $\text{dom } \mathfrak{h} \subseteq \text{dom } \tilde{\mathfrak{h}}$ (as for the Krein form $\mathfrak{h} = h^K$) then we cannot express $\mathfrak{h}$ as a Robin-type perturbation of $\mathfrak{h}$ as in the previous theorem. We may allow less restrictive conditions on $\text{dom } \mathfrak{h}$ and $\text{dom } \tilde{\mathfrak{h}}$, leading to more general Robin-type perturbations (with possibly different boundary space $\mathcal{G}$). We will again treat such questions in a forthcoming publication.

To summarise: We can associate an elliptically regular and uniformly positive boundary pair to a non-negative closed symmetric operator and a non-negative self-adjoint extension (Theorem 6.15). For a boundary pair associated with a form $\mathfrak{h}$, we can express certain other non-negative self-adjoint realisations as Robin-type perturbations of the original boundary pair (Theorem 6.18).

### 6.3 Relation to generalised elliptic forms and associated operators

There is a related concept to boundary pairs, namely the concept of $J$-ellipticity introduced by Arendt and ter Elst in [AtE08]. We explain the ideas here briefly and refer to [AtE08] for more details and a more abstract version: Let $\mathcal{V}$ and $\mathcal{G}$ be two Hilbert spaces, and $J : \mathcal{V} \rightarrow \mathcal{G}$ a bounded operator with dense range. Moreover, let $a : \mathcal{V} \times \mathcal{V} \rightarrow \mathbb{C}$ be a bounded sesquilinear form.

**Definition 6.21.** We say that $a$ is $J$-elliptic if there exist $\alpha > 0$ and $\omega \in \mathbb{R}$ such that

$$\text{Re } a(u) + \omega \|Ju\|_{\mathcal{G}}^2 \geq \alpha \|u\|_{\mathcal{V}}^2 \quad (6.22)$$

holds for all $u \in \mathcal{V}$.

To such a $J$-elliptic form, we can associate an operator $A$ on $\mathcal{G}$ by setting $\varphi \in \text{dom } A$ and $A\varphi = \psi$ iff there exists $u \in \mathcal{V}$ such that $Ju = \varphi$ and

$$a(u,v) = \langle \psi,Jv \rangle_{\mathcal{G}}$$

for all $v \in \mathcal{V}$. We say that $A$ is the operator associated with $(\mathcal{V},J,a)$.

In the case where $a$ is a sectorial form with domain $\mathcal{V}$ in the Hilbert space $\mathcal{G}$, we let $J$ be the embedding $\mathcal{V} \hookrightarrow \mathcal{G}$, i.e., $Ju = u$ for $u \in \mathcal{V}$. Then the operator associated with $(\mathcal{V},J,a)$ is just the operator associated with the sectorial form $a$ in the sense of Kato (see [Kat66, Thm. VI.2.1]).

Assume now that $(\Gamma, \mathcal{G})$ is a boundary pair associated with a non-negative self-adjoint form $\mathfrak{h}$ with domain $\mathcal{H}^1$ in a Hilbert space $\mathcal{H}$. In this case, we set $\mathcal{V} := \mathcal{H}^1$ (with its intrinsic norm $\|u\|_{\mathcal{V}}^2 := \mathfrak{h}(u) + \|u\|_{\mathcal{H}^1}^2$) and $J := \Gamma$.

We have the following relations to our notation:

**Proposition 6.23.** Assume that $(\Gamma, \mathcal{G})$ is a boundary pair associated with $\mathfrak{h}$ and let $z \in \mathbb{C}$.

i. If $\text{Re } z < 0$, then $\mathfrak{h} - z \mathcal{I}$ is $\Gamma$-elliptic (with $\alpha = \min \{1,-\text{Re } z\}$ and $\omega = 0$).

ii. Assume that $(\Gamma, \mathcal{G})$ is elliptically regular. If $0 \leq \text{Re } z < \min \{1,\inf \sigma(H^D)\}/2$, then $\mathfrak{h} - z \mathcal{I}$ is $\Gamma$-elliptic. In particular, $\mathfrak{h}$ is elliptic, provided $0 \notin \sigma(H^D)$.

In both cases, the operator associated with $(\mathcal{H}^1, \Gamma, \mathfrak{h} - z \mathcal{I})$ is the Dirichlet-to-Neumann operator, i.e., the operator associated with $I_z$ (see (2.26)). In the latter case, we have $\text{dom } \Lambda(z) = \mathcal{G}^1$.

**Proof.** (i) It is easily seen that

$$\mathfrak{h}(u) - (\text{Re } z)\|u\|^2 \geq \alpha(\mathfrak{h}(u) + \|u\|^2) = \|u\|_{\mathcal{H}^1}^2$$

with $\alpha$ as given above.
we necessarily have $\alpha < 1$. Since $0 \notin \sigma(H^D)$ we have the decomposition $u = f + h \in \mathcal{H}^{1,D} + \mathcal{A}^1(0)$, and therefore

$$h(u) \geq \frac{1}{1 - \alpha}(\Re z + \alpha\|u\|^2_{\mathcal{H}^1}) - \frac{\omega}{1 - \alpha}\|\Gamma u\|^2_{\mathcal{H}^2}$$

provided $\alpha < 1$. Since $0 \notin \sigma(H^D)$ we have the decomposition $u = f + h \in \mathcal{H}^{1,D} + \mathcal{A}^1(0)$, and therefore

$$h(u) = h(f) + h(h) \geq \lambda^D\|f\|^2 + L_0(\Gamma h) - \gamma\|\Gamma h\|^2_{\mathcal{H}^2}$$

$$= \lambda^D\|f\|^2 + (\beta + 1)(h) - \gamma\|\Gamma h\|^2_{\mathcal{H}^2} \geq \lambda^D\|f\|^2 + \|h\|^2 - \gamma\|\Gamma u\|^2_{\mathcal{H}^2}$$

by Theorem 2.23 and the elliptic regularity of the boundary pair (second inequality) for some $\gamma > 0$, where $\lambda^D := \inf\sigma(H^D) > 0$. Now $\|u\|^2 = \|f + h\|^2 \leq 2(\|f\|^2 + \|h\|^2)$, and therefore we have

$$h(u) \geq \beta\|u\|^2 - \gamma\|\Gamma u\|^2_{\mathcal{H}^2}$$

with $\beta = \min\{\lambda^D, 1\}/2$. A simple calculation shows that

$$\alpha = \frac{\beta - \Re z}{1 + \beta} \quad \text{and} \quad \omega = \frac{\gamma(1 + \Re z)}{1 + \beta}$$

are the constants ensuring the $\Gamma$-ellipticity of $\mathcal{H} - z\mathcal{I}$. Note that $0 < \alpha < 1$ and $\omega > 0$. That $\Lambda(z)$ is the operator associated with $\mathcal{H}^1, \Gamma, \mathcal{H} - z\mathcal{I}$ follows from (2.27). The domain of the associated operator is $\mathcal{G}^1$ by Theorem 3.8 (iv).

**Proposition 6.24.** Assume that $\mathcal{H} \geq 0$ is $\Gamma$-elliptic and assume that $\mathcal{V} = \mathcal{H}^1$ with its intrinsic norm. Then the constant $\alpha$ in the definition of $\Gamma$-ellipticity fulfills $0 < \alpha < 1$ and we have

$$\inf\sigma(H^D) \geq \frac{\alpha}{1 - \alpha}.$$

**Proof.** Note that for $u \in \mathcal{H}^{1,D}$, the $\Gamma$-ellipticity is equivalent with $\alpha\|u\|^2 \leq (1 - \alpha)h(u)$. Since $\alpha > 0$ and $h \geq 0$, we necessarily have $\alpha < 1$. Moreover, the above equation is equivalent with

$$\frac{\alpha}{1 - \alpha}\|u\|^2 \leq h(u)$$

for all $u \in \mathcal{H}^{1,D}$. The spectral lower bound on $H^D$ now follows from the variational characterisation of the infimum of the spectrum. \hfill \Box

**Remark 6.25.** Note that the notion of $\Gamma$-ellipticity does not refer to the Hilbert space $\mathcal{H}$, in which the quadratic form $\mathcal{H}$ is defined. Only the domain $\mathcal{V}$ of $\mathcal{H}$ is fixed. Therefore, we cannot expect that the notions of ellipticity and elliptic regularity are equivalent (recall the notion “elliptically regular’’ for a boundary pair refers to the norm on $\mathcal{H}$) as the following example shows:

**Example 6.26.** In Example 7.8 in Section 7.3 we construct a boundary pair which is unbounded and not elliptically regular (choose $\beta > 0$, then $\ell = \sum_n \ell_n < \infty$).

On the other hand, $\mathcal{H}$ is $\Gamma$-elliptic since $\mathcal{H} \geq \pi^2/(4\ell^2)$ (the lowest eigenvalue of the “Neumann” operator is actually the lowest eigenvalue of the Laplacian with Neumann condition at $0$ and Dirichlet condition at $\ell$). In this case, it is easily seen that (6.22) is fulfilled with $\alpha = \min\{1, \pi^2/(4\ell^2)\}/2 > 0$ and $\omega = 0$.

7 Examples

Basically all our examples (except the trivial ones of the next subsection) are of the form $\mathcal{H} = L_2(X, \mu)$ and $\mathcal{G} := L_2(Y, \nu)$ where $(X, \mu)$ and $(Y, \nu)$ are measure spaces and $Y \subset X$, as explained in Example 2.4.

7.1 Trivial examples

Two very trivial example are given as follows: Let $\mathcal{H}$ be a non-negative quadratic form with domain $\mathcal{H}^1$ in $\mathcal{H}$.

For the first example, set $\mathcal{G} := \mathcal{H}$ and $\Gamma f := f$, then it is readily seen that $(\Gamma, \mathcal{G})$ is a boundary pair with large boundary space (since $\mathcal{H}$ is densely defined). In this case, $\mathcal{H}^{1,D} = \ker \Gamma = \{0\}$. The Neumann operator is the operator associated with $\mathcal{H}$ and the Dirichlet operator associated with $(\Gamma, \mathcal{G})$ is $H^D = 0$ on $\{0\}$. By convention,
we set \( \sigma(H^D) := \emptyset \) and \( R^D(z) := 0 \). The Dirichlet solution operator is \( S = \text{id}_{\mathcal{H}^1} \), and the weak solution space is \( \mathcal{N}^1(z) = \mathcal{H}^1 = \mathcal{F}^{1/2} \). Moreover, the Dirichlet-to-Neumann form and operator are given by \( L_z = \mathfrak{h} - z \mathfrak{a} \) and \( \Lambda(z) = H - z \). The boundary pair is unbounded iff \( \mathfrak{h} \) is unbounded. Moreover, the boundary pair is elliptically regular and uniformly positive, since \( ||S\varphi||_{\mathcal{H}^1} = ||\varphi||_{\mathcal{H}^0} \). Krein’s resolvent formula is trivial here since \( R^D(z) = 0 \).

The bounded modification \( (\tilde{\Gamma}, \tilde{\mathcal{G}}) \) (see Proposition 5.9) of the unbounded boundary pair \( (\Gamma, \mathcal{G}) \) fulfills \( \tilde{\mathcal{G}} = \mathcal{H}^1 \) and \( \tilde{\Lambda}(z) = (H + 1)(H - z)^{-1} \).

For the second example, set \( \mathcal{G} = \{0\} \) and \( \Gamma = 0 \), then \( H^D = H \) and \( \Lambda(z) = 0 \).

### 7.2 Examples with finite-dimensional boundary space

We treat here a simple example where \( X = I \) is a compact interval and \( Y = \partial I \) consists of two points only. The corresponding boundary space is two-dimensional and the boundary pair is automatically associated with an ordinary boundary triple (see Corollary 6.12).

More precisely, let \( I = [0, \ell] \) for some \( \ell \in (0, \infty) \) and set \( \mathcal{H} := L_2(I) \), \( \mathcal{H}^1 := H^1(I) \), \( \mathfrak{h}(f) := \|f\|^2_{L_2(I)} \). As boundary operator, we choose \( \Gamma f = (f(0), f(\ell)) \). As quadratic form, we choose \( \mathfrak{h}(f) = \|f\|^2_{L_2(I)} \). The boundary pair is unbounded iff \( \mathfrak{h} \) is unbounded. Moreover, the Neumann and Dirichlet operators are the usual Neumann and Dirichlet Laplacians on \([0, \ell]\), and the Dirichlet solution operator is given by

\[
S(z)\varphi = \varphi_0 \frac{\sin(\sqrt{\ell}(\ell - s))}{\sin(\sqrt{\ell}))} + \varphi_1 \frac{\sin(\sqrt{\ell}s)}{\sin(\sqrt{\ell}))} \tag{7.1}
\]

for \( z \notin \sigma(H^D) = \{ k^2\pi^2/\ell^2 \mid k = 1, 2, \ldots \} \), where \( \varphi = (\varphi_0, \varphi_1) \in \mathbb{C}^2 \) and where the complex square root is suitably chosen. If \( z = 0 \), we use the continuous extension of the above expressions. The Dirichlet-to-Neumann operator is represented by the matrix

\[
\Lambda(z) = \frac{\sqrt{\ell}}{\sin(\sqrt{\ell}))} \begin{pmatrix} \cos(\sqrt{\ell}) & -1 \\ -1 & \cos(\sqrt{\ell}) \end{pmatrix} \tag{7.2}
\]

with eigenvalues \( -\sqrt{\ell}\tan(\sqrt{\ell}/2) \) and \( \sqrt{\ell}\cot(\sqrt{\ell}/2) \). For \( z = -\kappa^2 < 0 \) \( (\kappa > 0) \), the former \( (\kappa\tanh(\kappa\ell/2)) \) is smaller than the latter \( (\kappa\coth(\kappa\ell/2)) \). The corresponding eigenvectors are \((1, 1)\) and \((-1, 1)\). The eigenvalues of \( \Lambda(0) \) are \( 0 \) and \( \ell/2 \). The matrix \( Q(z) = S(z)^*S(z) \) has the same eigenvectors and the eigenvalues for \( z = 0 \) are given by \( \ell/2 \) and \( \ell/6 \). It follows that \( \|G\|^2_{L_2(I)} = (\inf_{\lambda(\lambda)}\Lambda(\lambda)\Lambda(\lambda)^{-1}) = (\tan(\ell/2))^{-1} = \coth(\ell/2) \) \( (\kappa = 1; \text{see Proposition 2.8 (ii))}. \)

We call \( (\Gamma, \mathcal{G}) \) the boundary pair associated with \( I = [0, \ell] \) and \( \partial I = \{0, \ell\} \).

### 7.3 Examples with Jacobi operators

We present here a boundary pair which mainly serves as a “zoo” of examples in which \( X = [0, \ell] \) and \( Y = \partial I \) is a countable subset of \( X \) accumulating only at \( \ell \in (0, \infty) \). It will turn out that the associated Dirichlet-to-Neumann operator (for certain values of \( z \)) is actually a Jacobi operator in \( L_2(\mathbb{N}) \) acting as

\[
(J\varphi)_n = a_{n-1}\varphi_{n-1} + b_n\varphi_n + a_n\varphi_{n+1}, \quad n = 1, 2, \ldots, \tag{7.3}
\]

and \( \varphi_0 = 0 \). Here, \( a_n, b_n \) are suitable real-valued sequences. We call \( J \) the Jacobi operator associated with \( (a_n)_n \) and \( (b_n)_n \).

Note that if \( a_n < 0 \) and \( b_n = -(a_n + a_{n-1}) \), then we can interpret \( J \) as a discrete weighted Laplacian with corresponding form

\[
\langle J\varphi, \varphi \rangle = \sum_{n=1}^{\infty} (-a_n)||\varphi_{n+1} - \varphi_n||^2,
\]

i.e., we can consider \( -a_n \) as a weight of the edge from vertex \( n \) to \( n + 1 \) of the half-line graph \( \mathbb{N} \). If \( q_n := b_n + a_n + a_{n-1} \neq 0 \) then we can interpret \( (q_n)_n \) as a discrete potential, and \( J \) is a discrete Schrödinger operator with this potential.

Recently, boundary triple methods have also been used by [KM10] for the spectral analysis of Jacobi type operators.

Let \( I := [0, \ell] \) for some \( \ell \in (0, \infty) \) and set \( \mathcal{H} := L_2(I) \). As quadratic form, we choose \( \mathfrak{h}(f) = \|f\|^2_{L_2(I)} \) with domain

\[
\mathcal{H}^1 := \{ f \in H^1(I) \mid f(0) = 0 \}.
\]

The associated Neumann operator \( H \) is the Laplacian with Dirichlet condition at \( 0 \) and Neumann condition at \( \ell \) (if \( \ell < \infty \)). Its spectrum is purely discrete and given by \( \{ (k + 1/2)^2/\ell^2 \mid k = 0, 1, \ldots \} \) if \( \ell < \infty \), and purely absolutely continuous and given by \( \sigma(H) = [0, \infty) \) if \( \ell = \infty \).

36
As boundary $Y$, we choose a sequence of points $(x_n)_n$ such that $x_0 = 0$, $\ell_n := x_{n+1} - x_n > 0$ and $\lim_{n \to \infty} x_n = \ell$. We set $I_n := [x_n, x_{n+1}]$. As boundary space and operator we set $\mathcal{G} := \ell_2(\mathbb{N})$ and $(\Gamma f)_n := g_n^{1/2} f(x_n)$, respectively, where $(g_n)_n$ is a sequence of positive numbers. To simplify some estimates, we assume that there are constants $\ell_+ = 0, \infty$ such that
\[
\ell_n \leq \ell_+ \quad \text{and} \quad 0 < \frac{g_n}{g_{n+1}} < \ell_+
\]
for all $n \in \mathbb{N}$. The latter condition allows us to replace $g_{n+1}$ by $g_n$ in estimates.

**Proposition 7.5.** Assume that $\tau_+ := \sup_n g_n/\ell_n < \infty$, then the following assertions are true:

i. The operator $\Gamma : \mathcal{G} \to \mathcal{G}$ is bounded; moreover, $(\Gamma, \mathcal{G})$ is a boundary pair associated with $\mathfrak{h}$.

ii. The associated Dirichlet operator is given by $H^D = \bigoplus_n \Delta_n^D$ and in particular decoupled. Its spectrum is given by
\[
\sigma(H^D) = \{(k\pi/\ell_n)^2 | k = 1, 2, \ldots, n = 0, 1, \ldots \}
\]
and we can omit the closure if $\ell_n \to 0$.

iii. The Dirichlet-to-Neumann operator $\Lambda(z)$ at $z = 0$ is a Jacobi operator associated with
\[
a_n = a_n(0) = -\frac{1}{\ell_n} \cdot \frac{1}{(g_n g_{n+1})^{1/2}} \quad \text{and} \quad b_n = b_n(0) = \left(\frac{1}{\ell_{n-1}} + \frac{1}{\ell_n}\right) \cdot \frac{1}{g_n}.
\]

iv. The boundary pair is bounded iff $\inf_n \ell_n g_n > 0$. In particular, if the boundary pair is bounded, then $\ell_- := \inf_n \ell_n > 0$ and $\ell = \sum_n \ell_n = \infty$.

v. The boundary pair is uniformly positive.

vi. The boundary pair is elliptically regular iff $\tau_- := \inf_n g_n/\ell_n > 0$.

vii. The boundary pair is elliptically regular and unbounded iff $(\ell_n)$ and $(g_n)_n$ are of same order ($0 < \tau_- \leq g_n/\ell_n \leq \tau_+ < \infty$) and $\inf_n \ell_n = 0$.

**Proof.** (i) Let us denote the objects of the boundary pair associated with $I_n$ and $\{x_n, x_{n+1}\}$ using the subscript $(\cdot)_{I_n}$. We have
\[
\|\Gamma f\|^2 = \sum_{n=1}^{\infty} g_n |f(x_n)|^2 \leq \sum_{n=1}^{\infty} g_n \coth(\ell_n/2) \|f\|^2_{H^1(I_n)} \leq C \|f\|^2_{H^1(I)}
\]
for some constant $C > 0$ using the optimal bound $|f(x_n)|^2 \leq \coth(\ell_n/2) \|f\|^2_{H^1(I_n)}$ from the two-dimensional boundary pair $(\Gamma_{I_n}, C^2)$ in Section 7.2. Moreover, it is easily seen that $\ker \Gamma = \bigoplus_n H^1(I_n)$ is dense in $L_2(I)$ as well as ran $\Gamma$ is dense in $L_2(\mathbb{N})$ (the sequences with finite support are obviously in ran $\Gamma$).

(ii) The form of the associated Dirichlet operator is clear. Note that the set $\{(k\pi/\ell_n)^2 | k = 1, 2, \ldots, n = 0, 1, \ldots \} \cap [0, \lambda]$ is finite for any $\lambda > 0$ if $\ell_n \to 0$, hence we can omit the closure in this case.

(iii) The Dirichlet solution operator is given as follows: Let $h = S(z) \varphi$ for $\varphi \in \mathcal{G}^{1/2}$. Then $h_n := h|_{I_n} = S_{I_n}(z) \Phi_n$, where $\Phi_n = (\tilde{\varphi}_n, \tilde{\varphi}_{n+1})$ and $\tilde{\varphi}_n = g_n^{-1/2} \varphi_n$. Moreover, the Dirichlet-to-Neumann operator is given by
\[
\langle \Lambda(z) \varphi, \varphi \rangle_{L^2(\mathbb{N})} = (h - z I)(S(z) \varphi, S \varphi) = \sum_{n=0}^{\infty} (h_n - z) (S_{I_n}(z) \Phi_n, S_{I_n} \Phi_n)
\]
\[
= \sum_{n=0}^{\infty} \langle \Lambda_n(z) \Phi, \Phi_n \rangle_{\mathbb{C}^2}
\]
\[
= \sum_{n=1}^{\infty} (a_n(z) \varphi_n + b_n(z) \varphi_n + a_n(z) \varphi_{n+1}) \tilde{\varphi}_n
\]
for suitable $\varphi \in \mathcal{G}^{1/2}$, where
\[
a_n(z) = -\frac{1}{\sin(\sqrt{\ell_n})} \cdot \frac{1}{(g_n g_{n+1})^{1/2}} \quad \text{and} \quad b_n(z) = \sqrt{z} \left(\cot(\sqrt{\ell_n}) + \cot(\sqrt{\ell_{n+1}})\right) \cdot \frac{1}{g_n}.
\]

10Here, $\Delta^D_n$ denotes the Dirichlet operator on the interval $I_n$. Note that we use the sign convention $\Delta^D_n f = -f''$, see also Footnote 11.
The formula for $z = 0$ follows by taking $z \to 0$.

(iv) The boundary pair is bounded iff $\Lambda(0)$ is bounded (see Theorem 2.11 (iii) and the footnote); and the Jacobi operator $\Lambda(0)$ is bounded iff $(a_n(0))_n$ and $(b_n(0))_n$ are bounded sequences. Moreover, we have

$$|a_n(0)| \leq \frac{1}{\ell_n \ell_n} \text{ and } |b_n(0)| \leq \frac{1}{\ell_n \ell_n} + \frac{\varrho_+}{\ell_n-1 \ell_n-1},$$

using again (7.4), and a similar lower bound on $|a_n(0)|$ and $|b_n(0)|$. In particular, these sequences are bounded iff $\inf_n (\ell_n \ell_n) > 0$. Since $\ell_n \ell_n \geq \tau_n + \ell_n^2$ by the assumption on $q_n/\ell_n$, $\inf_n \ell_n = 0$ implies that $\inf_n (\ell_n \ell_n) = 0$.

(v) The uniform positivity is seen by

$$\|S(0)\varphi\|_{L^2(I)}^2 = \sum_{n=0}^{\infty} \|S\ell_n(0)\Phi_n\|_{L^2(\mathbb{R})}^2 = \sum_{n=0}^{\infty} |Q\ell_n(0)\Phi_n, \Phi_n|_{L^2} \geq \sum_{n=0}^{\infty} \ell_n^2 |\Phi_n|_{L^2}^2 \geq \frac{1 + \varrho}{6 \tau} \|\varphi\|_{L^2(\mathbb{R})}^2,$$

using again the results of Section 7.2, (7.4) and the assumption on $q_n/\ell_n$.

(vi) Similarly, if $\tau_n > 0$, then $\|S(0)\varphi\|^2$ is bounded from above by $(1 + \varrho)/(2\tau)|\varphi|^2$, hence the boundary pair is elliptic. On the other hand, if $\tau_n = 0$, then let $\varphi^k \in L^2(\mathbb{N})$ with $\varphi_n^k = \delta_{kn}$. In particular, $\|S(0)\varphi^k\|^2 \geq \tau_k/(6\varrho_k)$ and this expression is not bounded in $k$, hence $S(0)$ has no bounded extension as operator $L^2(\mathbb{N}) \to L^2(I)$.

(vii) is a consequence of (iv) and (vi).

The Dirichlet-to-Neumann operator is also a Jacobi operator (with sequence $(a_n)$ being entirely negative or positive) for $z < 0$, but we have chosen the spectral point $z = 0$ because then the dependence on $\ell_n$ is rather simple.

**Example 7.7** (Example of an unbounded, uniformly positive and elliptically regular boundary pair). Let $\ell_n$ and $\varrho_n$ of the same order ($0 < \tau_n \leq \varrho_n/\ell_n \leq \tau_n + \infty$) and $\inf_n \ell_n = 0$, then the boundary pair is unbounded and elliptically regular (and of course uniformly positive), see Proposition 7.5 (v) and (vii).

This example shows that the spectral characterisation in Theorem 4.9 (iii) can be actually used in a slightly wider class than ordinary boundary triples (see also Theorem 6.11 (vi)).

The Neumann operator in this case has purely discrete spectrum iff $\sum_n \ell_n < \infty$.

**Example 7.8** (Example of a boundary pair not elliptically regular, but uniformly positive). Choose $(\ell_n)$ and $(\varrho_n)$ such that $\sup_n \varrho_n/\ell_n < \infty$, but $\inf_n \varrho_n/\ell_n = 0$, then the boundary pair is not elliptic (in particular not bounded). For example, if $\varrho_n = q^n$ ($0 < q < 1$) or $\varrho_n = n^{-\gamma}$ and $\ell_n = n^{-\beta}$, $\gamma > \beta > 0$, then the boundary pair is not elliptic.

Let us now choose $(\ell_n)$ and $(\varrho_n)$ such that the corresponding Jacobi coefficients have the form $a_n = a_n(0) = -n^\alpha$ and $b_n = b_n(0) = -(a_n + a_{n-1})$, i.e., the corresponding Jacobi operator $J(0) = \Lambda(0)$ is a pure (discrete) Laplacian. We use the ansatz $\ell_n = n^{-\beta} \ell_n^{-1}$ and $\varrho_n = n^{-\gamma} \ell_n^{-1}$ with $\alpha = \beta + \gamma > 0$. It can then be shown that the sequences $(\ell_n)$ and $(\varrho_n)$ defined above actually converge to 1 as $n \to \infty$.

This ansatz allows us to use known results on the spectrum of this special Jacobi operator (see e.g. [Sa08, Thm 1.1] and references therein; as well as [JN01] for the case $\alpha = 1$ and the general ideas of the spectral analysis). The spectrum of $J$ is purely discrete if $\alpha > 2$, and absolutely continuous if $0 < \alpha < 2$. If $\alpha = 2$ then $\sigma(J) = [0, \infty)$ and if $\alpha < 2$ then $\sigma(J) = [1/4, \infty)$. In the latter case $(\alpha = 2)$, the spectrum is purely absolutely continuous.

**Example 7.9.** If we choose $\beta$ and $\gamma$ such that $\gamma \geq \beta$, $\beta \geq 1$ and $\alpha = \beta + \gamma > 2$ then the Dirichlet-to-Neumann operator $\Lambda(0) = \Lambda(0)$ has purely discrete spectrum. By the monotonicity (Theorem 2.23 (vi)), $0 \leq \alpha \leq 1 = \lambda_1$, and this inequality remains true for the closure of the form $I_0$ (see the remark in the next example and [Dav95, Sec. 4.4] for an order on quadratic forms). In particular, the associated non-negative operators fulfill $0 \leq \Lambda(0) \leq \Lambda = \Lambda(-1)$, hence $\Lambda(0)-1 \geq \Lambda^{-1} \geq 0$, and $\Lambda^{-1}$ is also compact, while for $\beta = 1$ $H$ has purely absolutely continuous spectrum, and $H$ has purely discrete spectrum.

If $\beta = 1$ and $\gamma = 1$, then $\alpha = 2$ and the Dirichlet-to-Neumann operator $\Lambda(0)$ has purely absolutely continuous spectrum $[1/4, \infty)$. In both cases, the Neumann operator $H$ has purely absolutely continuous spectrum $[0, \infty)$ since $\sum_n \ell_n = \infty$, while the Dirichlet operator $H^D$ has purely discrete spectrum. The boundary pair is elliptic iff $\gamma = \beta$.

**Example 7.10** (Example violating the spectral relation Theorem 4.18 (i)). Choose $0 < \beta < 1$ and $\gamma = 2 - \beta > 0$. Then $\alpha = 2$, and $\sigma(\Lambda(0)) = [1/4, \infty)$, but the spectrum of the Neumann operator is $[0, \infty)$. In particular, the implication $0 \in \sigma(H) = \sigma(\Lambda(0))$ is not true. Since $\beta < \gamma$, the boundary pair is not elliptic.

What is actually happening here is that the norm on $\mathbb{R}^{1/2}$ given by the form $L_1$ associated with $\Lambda(-1)$ actually corresponds to a discrete Schrödinger operator with potential $q_n = b_n(-1) + a_n(-1) + a_{n-1}(-1)$ (given in (7.6) with $z = -1$). It can be seen that this potential is unbounded and there is no upper estimate of the quadratic form
corresponding to this Schrödinger operator in terms of the squared norm generated by the (pure) Laplacian form \( b_0 \). In particular, taking the closure of the form \( b_0 \), originally defined on \( \mathcal{H}^{1/2} \) only, we obtain a Hilbert space \( \mathcal{H}_0^{1/2} \) strictly larger than \( \mathcal{H}^{1/2} \) (we have \( \mathcal{H}^{1/2} \not\subset \mathcal{H}_0^{1/2} \subset \mathcal{H} \).

**Example 7.11** (Example violating the spectral relation Theorem 4.18 (iv)). We can actually modify Example 7.10 such that the implication \( \emptyset \in \sigma_{\text{disc}}(\Delta(0)) \Rightarrow 0 \in \sigma_{\text{disc}}(\Delta) \) is false: Take the direct sum \((\Gamma, \mathcal{G})\) (see Section 5.3) of the boundary pair of the previous example (denoted now \((\Gamma_1, \mathcal{G}_1)\)) and any boundary pair \((\Gamma_2, \mathcal{G}_2)\) such that 0 is a simple and isolated eigenvalue in \( \sigma(\Lambda(0)) \) and \( \sigma(H_2) \) (e.g., the boundary pair on \([0, 1]\) as in Section 7.2). Then 0 is a discrete eigenvalue of \( \sigma(\Lambda(0)) = \sigma(\Lambda_1(0)) \cup \sigma(\Lambda_2(0)) \), but 0 is not isolated in \( \sigma(H) = \sigma(H_1) \cup \sigma(H_2) = [0, \infty) \).

### 7.4 Laplacian on a manifold with Lipschitz boundary

We consider now a compact \( d \)-dimensional Riemannian manifold \((X, g)\) with Lipschitz boundary \( Y = \partial X \) (i.e., a neighbourhood of \( \partial X \) in \( X \) can be covered by \( \text{bi-Lipschitz} \) continuous charts with model space \( \mathbb{R}^d := [0, \infty) \times \mathbb{R}^{d-1} \), the charts on \( X \setminus \partial X \) are assumed to be smooth). We set \( \mathcal{H} := L_2(\partial X, \sigma) \). For more details on elliptic boundary value problems on Lipschitz domains we refer e.g. to [JK95, GM09, AM08] and references therein.

Some of our results extend to the case when \( X \) is non-compact but \( \partial X \) is compact, e.g. products (see Remark 7.19 and Section 7.5) or warped products \( X = [0, \infty) \times Y \) with metric \( g = ds^2 + r(s)^2 h \), where \((Y, h)\) is a compact Riemannian manifold. We come back to this situation in a forthcoming publication.

Denote by \( C^\infty(X) \) the space of functions, which are smooth on the interior \( X := X \setminus \partial X \) such that all derivatives extend continuously onto \( X \).

We set \( \mathcal{H} := L_2(X, g) \) (with the natural measure induced by the metric \( g \)). Moreover, \( \mathcal{H}^1 := H^1(X, g) \) denotes the completion of \( C^\infty(X) \) with respect to the norm given by \( \|u\|_{H^1(X, g)} := \|u\|_{L_2(X, g)}^2 + \|\nabla u\|_{L_2(X, g)}^2 \), where \( \nabla \) denotes the exterior derivative of \( u \). We consider the form \( h \) given by \( h(u) := \|\nabla u\|_{L_2(X, g)}^2, \quad u \in \mathcal{H}^1 \).

For a Riemannian manifold with Lipschitz boundary \( \partial X \), it can be shown that \( \partial X \) has a natural measure \( \nu \), the \((d-1)\)-dimensional Hausdorff measure. For smooth functions \( u \) we set \( \Gamma u := u|_{\partial X} \). This Sobolev trace map \( \Gamma \) extends to a bounded operator \( \mathcal{H}^1(X, g) \rightarrow L_2(\partial X, \nu) \) (see e.g. [AM08, AE11] and references therein).

**Theorem 7.12.** The boundary pair \((\Gamma, \mathcal{G})\) associated with the form \( \mathcal{G} \) is unbounded, elliptically regular and not uniformly positive. The Dirichlet and Neumann operators \( H^D \) and \( H \) are the usual Dirichlet and Neumann Laplacians on \( X \), respectively. Moreover, the Dirichlet-to-Neumann operator \( \Lambda(z) \) has the usual interpretation, i.e., \( \psi = \Lambda(z) \varphi \) iff \( \psi \) is the normal derivative of the solution of the Dirichlet problem \( (\Delta^{\max} - z)h = 0 \) and \( h|_{\partial X} = \varphi \) (provided \( \varphi \) is smooth enough).

**Proof.** We already noted that \( \Gamma \) is bounded. Moreover, smooth functions with support away from \( \partial X \) are in \( \ker \Gamma := H^1(X, g) \), and also dense in \( \mathcal{H} = L_2(X, g) \), hence \( \ker \Gamma \) is dense in \( \mathcal{H} \). Moreover, \( \Gamma(C^\infty(X)) \) is dense in \( L_2(\partial X, \nu) \). In particular, \((\Gamma, \mathcal{G})\) is a boundary pair. It is also well-known, that the range of the Sobolev trace map \( \Gamma \) is not surjective, hence the boundary pair is unbounded.

In order to show the elliptic regularity, we use the fact that dom \( H^D \) (the domain of the Dirichlet Laplacian) is included in \( H^1_\Delta(X, g) \), where
\[
H^r_\Delta(X, g) := \left\{ u \in H^r(X, g) \mid \Delta^r u \in L_2(X, g) \right\}
\]
for \( r \geq 0 \). This fact was proven in Thm. B in [JK95]. In particular, \( \partial_\alpha u|_{\partial X} \in L_2(\partial X, \nu) \). The abstract Green’s formula (6.7) is actually the usual one, hence \( H^{r+1}_\Delta u = \partial_\alpha u|_{\partial X} \in \mathcal{G} \). By Theorem 6.9 (i), the boundary pair \((\Gamma, \mathcal{G})\) is elliptically regular.

If the boundary pair was uniformly positive, then \( \Gamma : \mathcal{A}^0 \rightarrow \mathcal{G}^{1/2} \) would extend to a bounded operator \( \widetilde{\Gamma} : \mathcal{A}^0 \rightarrow \mathcal{G} \) by Theorem 3.14 (iii). In particular, \( \widetilde{\Gamma} h |_{L_2(\partial X, \nu)} \) for all \( h \in \mathcal{A}^0 = \ker(\Delta^{\max} + 1) \) which is known not to be true.\(^{12}\) Here, \( H^{\max} = \Delta^{\max} \) is the Laplacian in the distributional sense (with domain \( H^1_\Delta(X, g) \)). \( \square \)

**Definition 7.13.** We call \((\Gamma, \mathcal{G})\) the boundary pair associated with the manifold \((X, g)\) and boundary \( \partial X \).

**Remark 7.14.** The notion “elliptically regular” for a boundary pair has another motivation from this manifold example: The boundary triple \((\Gamma, \Gamma', \mathcal{W})\) associated with the boundary pair \((\Gamma, \mathcal{G})\) (see Section 6.1) is called elliptically regular if dom \( H^D \subset \mathcal{W} \) and dom \( H \subset \mathcal{W} \); and a boundary triple is elliptic if the corresponding boundary pair is. Here, \( \mathcal{W} \) is a space on which \( \Gamma' \) is defined and bounded \((\Gamma' : \mathcal{W} \rightarrow \mathcal{G})\) and on which Green’s formula

11 In our convention, (self-adjoint) Laplacians are non-negative operators, e.g. in the Euclidean case we have \( \Delta u = -\sum_j \partial_{x_j} u \).
12 Actually, at least if \( \partial X \) is smooth, then \( \Gamma : \mathcal{A}^0 \rightarrow \mathcal{G}^{1/2} \Rightarrow H^{-1/2}(\partial X) \) is bounded.

39
holds (see (6.7)). If we assume (for simplicity) that \( \partial X \) is smooth then we can choose \( W = H^2(X) \). The condition \( \text{dom} \, H^D \subset W \) is then equivalent to an “elliptic regularity estimate”
\[
\|u\|_{H^2(X)} \leq C(\|\Delta_X^D u\|_{L^2(X)} + \|\Delta_\partial^D u\|_{L^2(X)})
\]
(7.15)
for all \( u \in \text{dom} \Delta_X^D \cap H^2(X) \) and similarly for the Neumann operator \( H = \Delta_X^N \). We will treat boundary triples associated with quadratic forms in a forthcoming publication [P12b] (see also [P12a]).

Krein’s resolvent formula now is valid for the Neumann and Dirichlet Laplacian, i.e.,
\[
(\Delta_X^N - z)^{-1} - (\Delta_X^D - z)^{-1} = \Sigma(z)\Lambda(z)^{-1}\Sigma(\partial)^*, \tag{7.16}
\]
Moreover, the (extension of the) solution operator \( \Sigma(z) : L_2(\partial X, \nu) \rightarrow L_2(X, g) \) is usually called Poisson operator in this context. In addition, we have the characterisation of the spectrum
\[
\lambda \in \sigma(\Delta^N) \iff 0 \in \sigma(\Lambda(\lambda)) \tag{7.17}
\]
provided \( \lambda \not\in \sigma(\Delta^D) \). Since the spectrum of \( \Delta^N \) is purely discrete, and since \( \Gamma : H^1(X, g) \rightarrow L_2(\partial X, \nu) \) is a compact operator, the spectra of \( \Delta^D \) and \( \Lambda(\lambda) \) are purely discrete, too (see Proposition 5.2 (vi) and Theorem 2.35). Moreover, the multiplicities of the eigenvalues are preserved (Theorem 4.9).

**Remark 7.18.** If the boundary is smooth then \( \mathcal{G}^k = H^k(\partial X) \). This follows from the fact that \( \mathcal{G}^k = \text{dom} \, \Lambda^k \), and that \( \Lambda \) is a pseudo-differential operator of order 1 (see e.g. [LM68]). We do not characterise the spaces \( \mathcal{G}^k \) in the case of non-smooth boundaries here, but refer to [GM09, Lem. 2.3] (the statement that \( \Gamma \) is bounded as operator in [JK95] is a periodic sawtooth region with period 2, not necessarily have a tangential derivative and hence are not necessarily in \( H^1(\partial X) \)). The domain constructed in [JK95] is a periodic sawtooth region with period 2\( \varepsilon \) and with slopes alternating between 1 and \(-1\), and can even be chosen to have a C^1-boundary.

Let us illustrate how coupling of boundary pairs can be used in the manifold case

**Remark 7.19.** A prominent example of a coupled boundary pair (see Section 5.2) we have in mind is a smooth manifold \( X = X_1 \cup X_2 \) without boundary such that \( Y = X_1 \cap X_2 \) is a smooth submanifold of co-dimension 1, \( X_1 \) is a compact manifold with boundary \( Y \) and \( X_2 = I \times Y \) is a warped product over an interval \( I \), i.e., a manifold with metric \( g = ds^2 + r(s)^2 h \) (\( r : I \rightarrow (0, \infty), h \) a metric on \( Y \)). For a warped product, we have explicit formulas for the solution and the Dirichlet-to-Neumann operators (in terms of solutions of some ODEs related with \( r \)). As boundary pairs we now choose \( (\Gamma, \mathcal{G}) \) associated with the quadratic forms \( h_i(u) = \|du\|^2_{X_i}, u \in \mathcal{H}^1_i = H^1(X_i) \), where \( \mathcal{G} = L_2(Y) \) and \( \Gamma_i u = u|_{Y} \). The coupled form and operator (i.e., the Neumann operator) is now the form and Laplacian on the entire manifold \( X \). Moreover, for the boundary pairs \( (\Gamma, \mathcal{G}) \) on the compact part of the manifold one can derive explicit formulas for the Dirichlet solution operators and Dirichlet-to-Neumann maps, as well as for the (possibly non-compact) warped product. Hence we have rather explicit formulas for the resolvent of the entire Laplacian on \( X \) in terms of simpler building blocks. We will come back to these ideas, treating also more complicated coupled structures, in a forthcoming publication.

**Bounded modification of the manifold boundary pair**

**Example 7.20** (A bounded, but not uniformly positive boundary pair). Let us now show that the bounded modification \( (\bar{\Gamma}, \bar{\mathcal{G}}) \) of the above boundary pair \( (\Gamma, \mathcal{G}) \) associated with \((X, g)\) (see Section 5.4) gives rise to some examples: it follows from Proposition 5.9 that \( (\bar{\Gamma}, \bar{\mathcal{G}}) \) is not uniformly positive, although bounded.

**Example 7.21** (Non-compact Dirichlet-to-Neumann operator, but compact Dirichlet and Neumann operator). If we assume (with the notation of the previous example) that the manifold \( X \) is compact, then \( \bar{\Gamma} = R \) and \( \bar{R}^D = R^D \) are compact. But since \( \tilde{\Lambda} = \text{id}_\mathcal{G} \) and since \( \mathcal{G} = H^{1/2}(\partial X) \) is infinite-dimensional, \( \tilde{\Lambda}^{-1} \) is not compact (see also Remark 2.36 (ii)).

**7.5 Laplacian on a non-compact cylindrical manifold**

Let us consider here a simple example in which the space \( X \) is a product manifold \( X = [0, \infty) \times Y \) with corresponding product metric \( g = ds^2 + h \), where \( (Y, h) \) is a non-compact Riemannian manifold without boundary. In this case, we have again \( \mathcal{H} = L_2(X, g), \mathcal{H}^1 = H^1(X, g), b(u) = \|du\|^2 \) and \( \mathcal{G} = L_2(Y, h) \). Identifying a function \( u : X \rightarrow \mathbb{C} \) with the corresponding vector-valued function \( s \mapsto u(s) \) on \([0, \infty)\), we set \( \Gamma u = u(0), u \in \mathcal{H}^1 \). It can be seen similarly as
before that $\Gamma$ is bounded and that $(\Gamma, \mathcal{G})$ is an unbounded, elliptically regular, but not uniformly positive boundary pair.

This example can be seen as a vector-valued version of the interval case in Section 7.2 (except that $I = [0, \infty)$ is non-compact here). Namely, we can write

$$
\mathfrak{h}(u) = \int_I (\|u'(s)\|^2_{L^2(Y,h)} + \|d_Y u(s)\|^2_{L^2(Y,h)}) \, ds,
$$

where $d_Y \varphi$ denotes the exterior derivative on $Y$.

Moreover, all objects can be calculated rather explicitly using separation of variables (denoting the eigenvalues and eigenfunctions of the Laplacian on $Y$ by $\kappa_k \geq 0$ and $\Phi_k$, respectively). For example, we have

$$
S(z)\varphi = \sum_k f_{z,k} \otimes \Phi_k,
$$

where $f_{z,k}(s) = \exp(is\sqrt{z - \kappa_k})$ (the square root is cut along the positive real line). Moreover,

$$
\Lambda(z)\varphi = \sum_k (\varphi, \Phi_k)_{L^2(Y,h)} f_{z,k} \otimes \Phi_k = -i(\sqrt{z - \Delta_{(Y,h)}})\varphi
$$

(see [P12a, Sec. 3.5] for details, e.g., the type of convergence of the sums). In particular, for $z = -1$ we have

$$
\Lambda = \sqrt{\Delta_{Y} + I}.
$$

Similarly, we can treat more general cases like warped products (i.e., $X = I \times Y$ with metric $g = ds^2 + r(s)^2 h$ for some function $r : I \rightarrow (0, \infty)$). We will come back to this point in a forthcoming publication.


\section{7.6 Dirichlet-to-Neumann operator supported on a metric graph}

Let us consider here a case of a Dirichlet-to-Neumann operator defined on a singular space $Y$, where $Y$ is a metric graph embedded in a 2-dimensional Riemannian manifold $(X, g)$, i.e., $Y = \bigcup_{e \in E} Y_e$, and each $Y_e$ is a closed one-dimensional (smooth) submanifold in $X$, called \textit{edge segment}. We assume for simplicity that $X$ is compact, but under suitable uniformity assumptions the results below remain true; e.g. if $(X, g)$ is a covering manifold with compact quotient. We suppress in the following the dependence on the metric $g$.

We call the closure of each connected component of $X \setminus Y$ a \textit{face} of $Y$ in $X$, and label the faces by $(X_f)_{f \in F}$. We assume that each face is compact in $X$, and that the boundary of each face, consisting of the adjacent edges $E_f$, is Lipschitz (if $X$ is non-compact, one needs e.g. that the Lipschitz constants are globally bounded). Let $(\Gamma_f, \mathcal{G}_f)$ be the boundary pair associated with the manifold $X_f$ and boundary $\partial X_f$. Note that each function $\varphi_f \in \mathcal{G} = L^2(\partial X_f)$ decomposes into its components $\varphi_f = (\varphi_{e,f})_{e \in E_f}$ of the adjacent edge segments $Y_e$, i.e., $\varphi_{e,f} \in L^2(Y_e)$.

A global boundary map is now defined on

$$
\mathcal{H}^1 := \left\{ u \in \bigoplus_{f \in F} H^1(X_f) \mid (\Gamma u)_{e,f_1} = (\Gamma u)_{e,f_2} \text{ whenever } X_{f_1} \cap X_{f_2} = Y_e \right\}
$$

by $\Gamma u := u|_Y$ ($u \in \mathcal{H}^1$). This map is well-defined since the boundary values of $u$ from different sides on an edge agree by definition. It is not difficult to see that $\mathcal{H}^1 = H^1(X)$, and that $\Gamma : \mathcal{H}^1 \rightarrow \mathcal{G} := L^2(Y)$ is bounded, since $\Gamma$ is the restriction of the direct sum of the boundary maps $\Gamma_f : H^1(X_f) \rightarrow L^2(\partial X_f)$ to $\mathcal{H}^1$ after suitable identifications.

As quadratic form, we consider $\mathfrak{h}(u) := \|du\|^2$, $u \in \mathcal{H}^1 = H^1(X)$.

\begin{proposition}
The boundary pair $(\Gamma, \mathcal{G})$ is unbounded, elliptically regular and not uniformly positive. The Neumann operator $H$ is the Laplacian on $X$, and the Dirichlet Laplacian is given by the direct sum of the Dirichlet Laplacians on $X_f$, i.e.,

$$
H^D = \bigoplus_{f \in F} \Delta^D_{X_f}
$$

and $H^D$ is in particular decoupled. The Dirichlet-to-Neumann operator $\Lambda(z)$ acts as follows: if $\varphi$ is a (suitably smooth) function on $Y$, then $\psi = \Lambda(z)\varphi$ is given on $Y_e$ as the sum of the normal derivatives of the solutions of the Dirichlet problem on the two adjacent faces of $e$ (i.e., $\psi_e$ is the jump in the derivative when crossing $Y_e$ form one face to the other).

\end{proposition}
Proof. We omit the details here, since we will consider these questions in a forthcoming publication in more detail. We only indicate how to prove the elliptic regularity of the boundary pair: this can be seen by showing that \( \Gamma' u \in L_2(Y) \) if \( u \in \text{dom } H^D \) (Theorem 6.9 (i)). Since \( \Gamma' u \) is a sum of normal derivatives of \( u_f \in \text{dom } \Delta^D_{X_f} \subset H^2(X_f) \), it follows that \( \Gamma' u \in L_2(Y) \).

Remark 7.24. Let \( h_a \) be the Robin-type perturbation of the form \( h \) (i.e., \( h_a(u) := h(u) + a\|\Gamma u\|^2 \) for \( a \geq 0 \), see Section 5.1). Then \( h_a \) is non-negative and closed, and we can consider \( (\Gamma, \mathcal{G}) \) associated with the form \( h_a \). The associated (Neumann) operator \( H_a \) then has a Robin-type boundary condition of the type \( \Gamma' u + a\Gamma u = 0 \), where \( \Gamma' u \) on \( Y \) is the sum of the normal (outwards) derivative of \( a \) on the adjacent faces.

The resolvent difference of \( H_a \) and \( H^D \) (the latter is still decoupled) can be expressed by a Krein-type formula, and \( H_a \) converges to \( H^D \) in norm resolvent sense as \( a \to \infty \). Moreover, the associated Dirichlet-to-Neumann operator of \( (\Gamma, \mathcal{G}) \) associated with \( h_a \) is \( \Lambda_a(z) = \Lambda(z) + a \).

This situation is closely related to a model called \textit{leaky graph} (see the overview article [Exo08]). Note that in the situation of a leaky graph, one has \( X = \mathbb{R}^2 \) and \( a < 0 \) (this needs some modifications of our arguments). Moreover, some faces may be non-compact with finitely many adjacent edges, some of them having infinite length.

In [KK02] (see also the references therein), Kuchment and Kunyansky consider the above-mentioned operator \( H_a \) appearing as the limit operator in the analysis of photonic crystals supported on a hexagonal lattice \( \Gamma \) embedded in \( \mathbb{R}^2 \). As in our approach, they reduce the eigenvalue problem for \( H_a \) to an eigenvalue problem for \( \Lambda(z) \). Then they investigate the nature of the operator \( \Lambda(z) \) on \( Y \), and try find a good candidate of a \textit{differential} operator on \( Y \) being close to the \textit{pseudo-differential} operator \( \Lambda(z) \). This problem is still not yet completely understood and we believe that our method helps to analyse the problem further.

7.7 Laplacian with mixed boundary conditions: the Zaremba problem

Let \((X, g)\) be a compact Riemannian manifold with smooth boundary \( \partial X \). Let \( Y \subset \partial X \) be a compact submanifold of the same dimension as \( \partial X \), with \textit{smooth} boundary in \( \partial X \), and let \( Z := \partial X \setminus Y \). We call the Laplacian on \( X \) with Dirichlet condition on \( Z \) and Neumann condition on \( Y \) the \textit{Zaremba Laplacian}, denoted by \( \Delta^Z_X \) (in particular, \( \Delta^D = \Delta^0_X \) and \( \Delta^N = \Delta^0_Y \)).

The domain of the Zaremba Laplacian is contained in \( H^{1/2-\varepsilon}_X \) for all \( \varepsilon > 0 \), but not contained in \( H^{1/2}_X \) itself. The latter can be seen in the following situation where \( X = [0, \infty) \times \mathbb{R} \) (or some bounded subset containing 0) and \( u(x, y) := \text{Im} \sqrt{x + iy} \) (see [Sha68]); \( u \) fulfills a Dirichlet condition on the positive \( x \)-axis \( Z \) and a Neumann condition on the negative \( x \)-axis \( Y \), and \( \Delta u = 0 \). Moreover, \( \partial_x u \big|_Z \) is not in \( L_2(Y) \), and hence \( u \notin H^{3/2}(X) \). At first sight surprisingly, the Zaremba problem is less regular for smooth boundaries than for certain boundaries with corners (see the discussion in [Gr11, Sec. 4.3])

Let us now compare the Zaremba Laplacian with the Dirichlet Laplacian on \( X \). We will see that we can again treat this problem with our boundary pair method.

Set \( \mathcal{H} := L_2(X) \) (again, we suppress the dependence on the metric \( g \)) and set

\[ \mathcal{H}^1 := H^1_2(X) := \{ u \in H^1(X) \mid u \big|_Z = 0 \}, \quad h(u) := \| du \|^2. \]

As boundary operator we choose \( \Gamma u := u \big|_Y \).

Theorem 7.25. The boundary pair \((\Gamma, \mathcal{G})\) associated with the form \( h \) is unbounded, elliptically regular and not uniformly positive. The Neumann operator \( H \) is the Zaremba Laplacian \( \Delta^Z_X \) on \( X \) with Dirichlet condition on \( Z \) and Neumann condition on \( Y \). Moreover, the Dirichlet operator is the Laplacian \( \Delta^Z_X = \Delta^0_X \) with (pure) Dirichlet condition on \( \partial X \).

The Dirichlet solution operator is given by \( S(\varphi) = S_{(X, \partial X)}(\varphi \bar{\varphi}) \), where \( S_{(X, \partial X)}(\varphi) \) is the Dirichlet solution (Poisson) operator for the boundary pair associated with \( X \) and the entire boundary \( \partial X \), and where \( \bar{\varphi} = \varphi + 0 \) is the extension of \( \varphi \in \mathcal{G}^{1/2} \) by 0 on \( Z \).

Finally, the Zaremba Laplacian and the Dirichlet-to-Neumann operator \( \Lambda(z) \), \( z \notin \sigma(\Delta^D_X) \) have discrete spectrum.

Proof. Clearly, \( \Gamma : \mathcal{H} \to \mathcal{G} := L_2(Y) \) is bounded since \( u \to u \big|_{\partial X} \) is bounded, as well as the restriction map \( L_2(\partial Y) \to L_2(Y) \). Moreover, that \((\Gamma, \mathcal{G})\) is an unbounded boundary pair can be seen similarly as in Section 7.4. We show the elliptic regularity as before using Theorem 6.9 (i): Since \( H^D \) is the pure Dirichlet Laplacian on \( X \) with smooth boundary, we have \( \text{dom } H^D \subset H^2(X) \), and in particular, \( \partial_x u \in H^{1/2}(\partial X) \), hence \( \Gamma' u = \partial_x u \big|_Y \in L_2(Y) \).

The assumption on the Dirichlet solution operator is easily seen by noting that for \( \varphi \in \mathcal{G}^{1/2} \) there exists \( u \in H^2_2(X) \) such that \( \varphi = u \big|_Y \). In particular, the extension by 0 is just \( \bar{\varphi} = u \big|_{\partial X} \), and hence in \( H^{1/2}(\partial X) \).

The Neumann operator (i.e., Neumann Laplacian) has discrete spectrum since \( X \) is compact and \( \partial X \) is Lipschitz. Then also the Dirichlet operator has discrete spectrum. Moreover, \( \Gamma \) is a compact operator, since \( \Gamma u = \Gamma u \big|_Y \), and \( \Gamma : H^1(X) \to L_2(\partial X) \) is compact. In particular, \( \Lambda(z) \) has discrete spectrum (Theorem 2.35).
Krein’s resolvent formula here relates the resolvent of the Zaremba Laplacian with the pure Dirichlet Laplacian
\[(\Delta^N_X - z)^{-1} - (\Delta^D_X - z)^{-1} = S(z)\Lambda(z)^{-1}S(z)^*\] \hspace{1cm} (7.26)
Since the boundary pair is elliptic, the operators on the RHS all act in the Hilbert spaces \(\mathcal{G} = L_2(Y)\) and \(\mathcal{H} = L_2(X)\).

If we use the pure Neumann Laplacian as reference operator (by choosing \(\mathcal{H}^1 := H^1(X)\)) and again, \(\Gamma u = u|_Y\), then the Dirichlet operator \(H^D\) is the Zaremba Laplacian \(\Delta^N_X\), now with Dirichlet condition on \(Y\) and Neumann condition on \(Z\), and the Neumann operator \(H\) is the pure Neumann Laplacian \(\Delta^N_X\).

**Theorem 7.27.** The boundary pair \((\Gamma, \mathcal{G})\) associated with the form \(\mathcal{H}\) corresponding to the pure Neumann Laplacian on \(X\) is unbounded, and not elliptically regular. The Dirichlet operator \(H^D\) is the Zaremba Laplacian \(\Delta^N_X\), now with Dirichlet condition on \(Y\) and Neumann condition on \(Z\). Finally, the Zaremba Laplacian and the Dirichlet-to-Neumann operator \(\Lambda(z)\) (\(z \notin \sigma(\Delta^N_X)\)) have discrete spectrum.

**Proof.** That the boundary pair is not elliptically regular can be seen as follows: As in the example above, where \(X = [0, \infty) \times \mathbb{R}\), one can find functions \(u \in \text{dom} H^D\) (the Zaremba domain) such that \(\Gamma^* u\) is not contained in \(\mathcal{G}\), and hence by Theorem 6.9 (i) the boundary pair is not elliptic.

The Neumann operator has discrete spectrum since \(X\) is compact with smooth boundary. The compactness of \(\Lambda^{-1}\) can be seen as before.

Krein’s resolvent formula in this case still holds, but only in its “weak” form
\[(\Delta^N_X - z)^{-1} - (\Delta^N_Y - z)^{-1} = S(z)\Lambda(z)^{-1}S(z)^*\] \hspace{1cm} (7.28)
since now, the operators on the RHS map as \(\mathcal{H} \to \mathcal{G}^{-1/2} \to \mathcal{G}^{1/2} \to \mathcal{H}\). Similar formulas have also been shown in [Gr11] and [Pa06]. Moreover, since \(R\) and \(\Lambda^{-1}\) are compact, we have the spectral relation
\[\lambda \in \sigma(\Delta^N_X) \Leftrightarrow 0 \in \sigma(\Lambda(\lambda)),\]
if \(\lambda \notin \sigma(\Delta^N_Y)\). In other words, if the spectrum and eigenfunctions of \(\Delta^N_X\) are known, we know the 0-eigenspace of the Dirichlet-to-Neumann operator (cf. Theorem 4.9 (ii)).

**Remark 7.29.** We would like to stress here that the boundary pair of Theorem 7.25 can also be treated with the methods of quasi-boundary triples, according to Theorem 6.9 (i). On the other hand, the boundary pair of Theorem 7.27 does not correspond to a quasi boundary triple, and can hence be treated only by the boundary pair concept.

### 7.8 Example with large boundary space: discrete Laplacians

Let us present here another class of examples; in this case, the boundary space is large, i.e., \(\ker \Gamma\) is no longer dense in \(\mathcal{H}\).

Let \((V, E, \partial)\) be a discrete graph, i.e., \(V\) denotes the set of vertices, \(E\) the set of edges and \(\partial: E \to V \times V\) maps \(e\) onto \((\partial_e, e, \partial_e)\), the initial and terminal vertex of \(e\); fixing therefore also an orientation. Denote by \(E_v\) the set of edges \(e\) adjacent with the vertex \(v \in V\) (i.e., \(e \in E_v\) if \(v = \partial_+ e\) or \(v = \partial_- e\)). If \(e \in E_v\), we denote by \(v_e\) the vertex on the other end of \(e\).

We assume for simplicity here that the graph is finite. Let \(\mu: V \to (0, \infty)\) and \(g: E \to (0, \infty)\) be functions, the vertex and edge weights. Let
\[\mathcal{H} := \ell^2(V, \mu), \quad \|f\|^2_{\ell^2(V, \mu)} := \sum_{v \in V} |f(v)|^2 \mu(v),\]
and set
\[\mathcal{H}(f) := \sum_{e \in E} (f(\partial_+ e) - f(\partial_- e))^2 g(e)\]
with \(\text{dom} \mathcal{H} = \mathcal{H}^1 = \mathcal{H}\). Since this form is bounded, we can omit the subscripts \((\cdot)^1\) indicating the form domain. The Neumann operator \(H\), i.e., the operator associated with \(\mathcal{H}\) acts as
\[(Hf)(v) = \frac{1}{\mu(v)} \sum_{e \in E_v} g(e)(f(v) - f(v_e)).\]
If we choose \(\mu(v) = 1\) and \(g(e) = 1\) then we arrive at the combinatorial Laplacian; if we choose \(\mu(v) = \deg v = |E_v|\) and \(g(e) = 1\), then we arrive at the normalised Laplacian.
We now declare a subset of $V$ as boundary of the graph, i.e., let $\partial V \subset V$ be the set of boundary vertices. The vertices in its complement, $\tilde{V} := V \setminus \partial V$, are called inner vertices. We set

$$\mathcal{G} := \ell_2(\partial V, \mu), \quad \Gamma f := f|_{\partial V}.$$  

Note that $\mathcal{H}^D := \ker \Gamma = \ell_2(\tilde{V}, \mu)$ is not dense in $\mathcal{H} = \ell_2(V, \mu)$. Therefore, $(\Gamma, \mathcal{G})$ is a bounded boundary pair with large boundary space associated with $\mathcal{G}$. The Dirichlet operator acts formally as $H$, but only on $\ell_2(\tilde{V}, \mu)$; if $i : \ell_2(V, \mu) \to \ell_2(\tilde{V}, \mu)$ denotes the natural embedding, and $\pi := i^*$ the corresponding projection, then $H^D = \pi H$. Note that this example corresponds to $X = V, Y = \partial V$ and $\nu = \mu|_{\partial V}$ in the notation of Example 2.4.

Before giving a formula for the Dirichlet solution operator, let us represent the operator $H$ in block structure

$$H = \begin{pmatrix} A & B \\ B^* & D \end{pmatrix}$$

with respect to the splitting $\mathcal{H} = \mathcal{G} \oplus \mathcal{H}^D$, i.e., $\ell_2(V, \mu) = \ell_2(\partial V, \mu) \oplus \ell_2(\tilde{V}, \mu)$. Here, $D = H^D$ is the Dirichlet operator, and $A : \mathcal{G} \to \mathcal{G}, B : \mathcal{H}^D \to \mathcal{G}$. Let $z \notin \sigma(D)$, then $h \in \mathcal{N}(z) := \mathcal{N}^1(z)$ iff $(H-z)h|_{\tilde{V}} = 0$. Denote by $H^{\max} : \mathcal{H} \to \mathcal{H}^D$ the operator $H$ restricted to $\mathcal{H}^D$ (this is actually consistent with $H^{\min} := H^D \cap H$, the minimal operator $H^{\min}$, which acts as $\mathcal{H}^D \to \mathcal{H}$, and $H^{\max} = (H^{\min})^*$. Using the matrix decomposition, we have $H^{\max} f = B^* f_0 + D f_0$, where $f = f_0 + f_0 \in \mathcal{G} \oplus \mathcal{H}^D$.

Moreover,

$$\mathcal{G}(f,g) = \langle H f, g \rangle_{\mathcal{H}} = \langle B^* f_0 + D f_0, g_0 \rangle_{\mathcal{H}^D} + \langle A f_0 + B f_0, g_0 \rangle_{\mathcal{G}},$$

which can be interpreted as Green’s formula (6.7), where the “normal derivative” $\Gamma' : \mathcal{H} \to \mathcal{G}$ is given by $\Gamma' f := A f_0 + B f_0$, i.e.,

$$(\Gamma' f)(v) = \frac{1}{m(v)} \sum_{e \in E, v} g(e)(f(v) - f(v)),$$ 

$v \in \partial V$.

It is now easily seen that the Dirichlet solution operator is given by

$$S(z)\phi = \phi \oplus (- (D-z)^{-1} B^* \phi),$$

(since $(H^{\max}-z)S(z) = 0$ on $\mathcal{H}^D$ and $\Gamma S(z) \phi = \phi$): note that the inverse exists since $z \notin \sigma(D)$. The Dirichlet-to-Neumann operator is defined as

$$\langle \Lambda(z) \phi, \psi \rangle_{\mathcal{G}} = \langle (H-z) S(z) \phi, \psi \rangle_{\mathcal{H}} = \langle (A - z - B(D-z)^{-1}B^*) \phi, \psi \rangle_{\mathcal{H}} + \langle B^* \phi - (D-z)(D-z)^{-1}B^* \phi, g_0 \rangle_{\mathcal{H}^D}$$

where $g \in \mathcal{H}$ is arbitrary with $g|_{\partial V} = \psi$. Since the latter summand vanishes, we obtain for the Dirichlet-to-Neumann operator

$$\Lambda(z) = (A - z - B(D-z)^{-1}B^* : \mathcal{G} \to \mathcal{G}.$$  

Moreover, the interpretation is the same as in the manifold case: We have $\Lambda(z) \phi = \Gamma' S(z) \phi$, i.e., the Dirichlet-to-Neumann operator associates to the boundary data $\phi$ the “normal” derivative of the Dirichlet solution $h = S(z) \phi$.

Note that the Dirichlet-to-Neumann operator can also be understood as the Schur complement of the block operator $H - z$ with respect to the lower left $(\mathcal{H}^D \times \mathcal{H}^D)$-block.

Finally, Krein’s resolvent formula is just a variant of the inversion of the block operator $H - z$, namely,

$$R(z) - \tau^* R^D(z) = \begin{pmatrix} A - z & B \\ B^* & D - z \end{pmatrix}^{-1} - \begin{pmatrix} 0 & 0 \\ 0 & (D-z)^{-1} \end{pmatrix} = \begin{pmatrix} \id_{\mathcal{G}} \\ -(D-z)^{-1}B^* \end{pmatrix} (A - z - B(D-z)^{-1}B^*)^{-1} \begin{pmatrix} \id_{\mathcal{G}} \\ -B(D-z)^{-1} \end{pmatrix} = S(z) \Lambda(z)^{-1} S(z)^* \tau.$$  

If we allow infinite graphs, then we may also have unbounded forms $\mathcal{G}$ (if, e.g., $\mu(v) = 1$, $g(v) = 1$ and $\deg v$ is unbounded on the graph). Such cases and even more general ones (“discrete Dirichlet forms”) are considered in [HKLW11]. We can also use different weights for the boundary space and therefore also have unbounded boundary pairs. We hope to come back to the unbounded case in a forthcoming publication.
References


References


References


