Boundary systems and (skew-)self-adjoint operators on infinite metric graphs

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Abstract

We generalize the notion of Lagrangian subspaces to self-orthogonal subspaces with respect to a (skew-)symmetric form, thus characterizing (skew-)self-adjoint and unitary operators by means of self-orthogonal subspaces. By orthogonality preserving mappings, these characterizations can be transferred to abstract boundary value spaces of (skew-)symmetric operators. Introducing the notion of boundary systems we then present a unified treatment of different versions of boundary triples and related concepts treated in the literature. The application of the abstract results yields a description of all (skew-)self-adjoint realizations of Laplace and first derivative operators on graphs.

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Introduction

The problem of obtaining (skew-)self-adjoint extensions of (skew-)symmetric operators is a standard task in operator theory and applications. The classical description, given by von Neumann, is by finding unitary maps between deficiency spaces. A seemingly different established description is to find all Lagrangian subspaces with respect to the corresponding boundary form; see e.g. [2–4, 6, 8, 9]. This method has been formalized in the language of boundary triples. For the case of (skew-)symmetric operators a procedure has been described in [19], using the notion of SWIPs (systems with integration by parts).

It is one of the purposes of our paper to present a unified treatment of the methods mentioned above. This is achieved by introducing the notion of ‘boundary systems’, a generalized version of boundary triples. The generalization consists in allowing more flexibility for the quantities occurring in the setup.

Self-adjoint Laplace operators on metric graphs arise by choosing appropriate boundary conditions at the vertices. The first treatment of this topic was given in [12], characterizing self-adjointness of Laplacians on finite star graphs by Lagrangian subspaces with respect to a standard form. Kuchment [13] gave another description of the boundary conditions leading to semi-bounded self-adjoint Laplacians on graphs with finite vertex degree. The question whether all self-adjoint realizations of the Laplacian on a metric graph can be obtained by choosing self-adjoint operators in the space of boundary values arose in the thesis [16] of one of the authors. With the help of our methods we answer this question for graphs with a positive lower bound for the edge lengths in Theorem 3.2. This is essentially the description of Laplacians on graphs in the form treated by Kuchment [13]. We stress that we can deal with infinite metric graphs with infinite vertex degree which have been studied recently [15,16]. Since we also do not assume semi-boundedness of the corresponding operator, the form approach may not be applicable.

In Section 1 we introduce the abstract context, and we describe the relation of self-orthogonal subspaces to (skew-)self-adjoint or unitary operators.

In Section 2 we introduce boundary systems, and we present the abstract results how (skew-)self-adjointness of extensions of (skew-)symmetric operators can be described by self-orthogonal subspaces in the ‘boundary space’. We mention that in the hypotheses of a boundary system there is no a priori requirement concerning the deficiency indices of the operator to be extended.

In Section 3 we apply the abstract theory to Laplace operators and the first derivative operator on metric graphs. On a metric graph, the Laplace operator is self-adjoint if and only if all the boundary values of a function in the domain are related to all boundary values of the derivative of the function via some self-adjoint operator acting in a subspace of all possible boundary values. In two examples we present the application of our result to infinite graphs, one of them with infinite vertex degree. For the derivative operator, we have that the respective operator is skew-self-adjoint if and only if the relation between the boundary values at the end points of the edges and the boundary values at the starting points of the edges is unitary.

1 Sesquilinear forms and self-orthogonal subspaces

We start with basic observations concerning a version of 'orthogonality'. Let X be a set, and let $R \subseteq X \times X$ be an 'orthogonality relation'. For $U \subseteq X$ we define the *R-orthogonal complement*

$$U^{\perp_R} := \big\{x \in X;\, (x,y) \in R \ (y \in U)\big\}$$

of U, and U will be called *R-self-orthogonal* if $U^{\perp_R} = U$.

1.1 Theorem. *Let X_1, X_2 be sets, and let $R_j \subseteq X_j \times X_j$ $(j \in \{1,2\})$. Let $F\colon X_1 \to X_2$ be surjective, and assume that*

$$R_1 = (F \times F)^{-1}(R_2).$$

Then a set $U \subseteq X_1$ is R_1-self-orthogonal if and only if there exists an R_2-self-orthogonal set $V \subseteq X_2$ such that $U = F^{-1}(V)$.

Proof. Taking into account the surjectivity of F, one easily obtains that

$$F^{-1}(V)^{\perp_{R_1}} = F^{-1}(V^{\perp_{R_2}})$$

for all $V \subseteq X_2$. Also, one obtains that

$$U^{\perp_{R_1}} = F^{-1}(F(U))^{\perp_{R_1}} \,\big(= F^{-1}(F(U)^{\perp_{R_2}})\big)$$

for all $U \subseteq X_1$.

From these observations the assertions of the theorem are immediate. □

We now introduce (skew-)symmetric forms and self-orthogonal subspaces. All vector spaces will be vector spaces over $\mathbb{K}$, where $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$.

Definition. Let X be a vector space, and let $\omega\colon X \times X \to \mathbb{K}$ be sesquilinear. We use the relation

$$R := \big\{(x,y) \in X \times X;\, \omega(x,y) = 0\big\}$$

in order to define 'orthogonality' in X, and we thus write

$$U^{\perp_\omega} := U^{\perp_R} = \big\{x \in X;\, \omega(x,y) = 0 \ (y \in U)\big\},$$

for $U \subseteq X$. We will use the terminology *ω-self-orthogonal* to mean orthogonality with respect to the above relation R.

The form ω is called *symmetric*, if

$$\omega(x,y) = \overline{\omega(y,x)} \quad (x,y \in X),$$

and *skew-symmetric* (or *symplectic*), if

$$\omega(x,y) = -\overline{\omega(y,x)} \quad (x,y \in X).$$

In the case of skew-symmetric forms, self-orthogonal subspaces are also called *Lagrangian*. Note that there are different definitions of Lagrangian subspaces in the literature; see e.g. [7, 9, 11].

The following result is a reformulation of Theorem 1.1 for the present context.

1.2 Corollary. *Let X_1, X_2 be vector spaces, and let ω_j be a sesquilinear form on X_j ($j \in \{1,2\}$). Let $F\colon X_1 \to X_2$ be linear and surjective, and such that*

$$\omega_1(x,y) = \omega_2(F(x),F(y)) \quad (x,y \in X_1).$$

Then a subspace $U \subseteq X_1$ is ω_1-self-orthogonal if and only if there exists an ω_2-self-orthogonal subspace $V \subseteq X_2$ such that $U = F^{-1}(V)$.

1.3 Remark. In the context of the preceeding corollary, one should think of X_1 as a (big) space of functions, of X_2 as the (small) space of boundary values, and of the mapping F as the evaluation of the boundary values of the functions in X_1.

Definition. Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces.

(a) A subspace $M \subseteq \mathcal{H}_1 \oplus \mathcal{H}_2$ is called a *linear relation*. For a linear relation $M \subseteq \mathcal{H}_1 \oplus \mathcal{H}_2$ we define the *inverse relation* $M^{-1} \subseteq \mathcal{H}_2 \oplus \mathcal{H}_1$ by

$$M^{-1} := \big\{(y,x) \in \mathcal{H}_2 \oplus \mathcal{H}_1;\, (x,y) \in M\big\},$$

the *orthogonal relation* of M by

$$M^{\perp} := \big\{(x,y) \in \mathcal{H}_1 \oplus \mathcal{H}_2;\, ((x,y) \,|\, (u,v))_{\mathcal{H}_1 \oplus \mathcal{H}_2} = 0 \ ((u,v) \in M)\big\},$$

and the *adjoint relation* $M^* \subseteq \mathcal{H}_2 \oplus \mathcal{H}_1$ by

$$M^* := \big\{(y,x) \in \mathcal{H}_2 \oplus \mathcal{H}_1;\, (y \,|\, v)_{\mathcal{H}_2} = (x \,|\, u)_{\mathcal{H}_1} \ ((u,v) \in M)\big\}.$$

(b) If $\mathcal{H}_1 = \mathcal{H}_2$ and $M \subseteq M^*$, then M is called *symmetric*, and if $M = M^*$, then M is called *self-adjoint*.

(c) Denote $S := \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. If $\mathcal{H}_1 = \mathcal{H}_2$ and $M \subseteq SM^*$, then M is called *skew-symmetric*, and if $M = SM^*$, then M is called *skew-self-adjoint*.

(d) If $M^* = M^{-1}$, then M is called *unitary*. In fact, unitary relations are graphs of unitary operators; see Proposition 1.8 below.

1.4 Remark. Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces, $M \subseteq \mathcal{H}_1 \oplus \mathcal{H}_2$ a linear relation. Then

$$M^* = (SM^\perp)^{-1} = ((SM)^\perp)^{-1} = ((SM)^{-1})^\perp = (SM^{-1})^\perp = S(M^{-1})^\perp.$$

1.5 Examples. (a) Let $\mathcal{H}$ be a Hilbert space. The *standard skew-symmetric* (or *symplectic*) *form* on $\mathcal{H} \oplus \mathcal{H}$ is defined as $\omega\colon (\mathcal{H} \oplus \mathcal{H}) \times (\mathcal{H} \oplus \mathcal{H}) \to \mathbb{K}$,

$$\omega((x,y),(u,v)) = \left(\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \,\middle|\, \begin{pmatrix} u \\ v \end{pmatrix} \right)_{\mathcal{H}\oplus\mathcal{H}} = (x \,|\, v)_{\mathcal{H}} - (y \,|\, u)_{\mathcal{H}}.$$

Let $M \subseteq \mathcal{H} \oplus \mathcal{H}$ be a linear relation. Then

$$M^{\perp_\omega} = ((SM)^{-1})^\perp = M^*. \tag{1.1}$$

Hence, Lagrangian subspaces with respect to the standard skew-symmetric form are exactly the self-adjoint linear relations.

(b) Let $\mathcal{H}$ be a Hilbert space. We define the *standard symmetric form* on $\mathcal{H} \oplus \mathcal{H}$ by $\omega\colon (\mathcal{H} \oplus \mathcal{H}) \times (\mathcal{H} \oplus \mathcal{H}) \to \mathbb{K}$,

$$\omega((x,y),(u,v)) = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \,\middle|\, \begin{pmatrix} u \\ v \end{pmatrix} \right)_{\mathcal{H}\oplus\mathcal{H}} = (x \,|\, v)_{\mathcal{H}} + (y \,|\, u)_{\mathcal{H}}.$$

Let $M \subseteq \mathcal{H} \oplus \mathcal{H}$ be a linear relation. Then

$$M^{\perp_\omega} = (M^{-1})^\perp = SM^*. \tag{1.2}$$

Hence, self-orthogonal subspaces with respect to the standard symmetric form are exactly the skew-self-adjoint linear relations.

(c) Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces. We define the *standard unitary form* on $\mathcal{H}_1 \oplus \mathcal{H}_2$ by $\omega\colon (\mathcal{H}_1 \oplus \mathcal{H}_2) \times (\mathcal{H}_1 \oplus \mathcal{H}_2) \to \mathbb{K}$,

$$\omega((x,y),(u,v)) = \left(\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} \,\middle|\, \begin{pmatrix} u \\ v \end{pmatrix} \right)_{\mathcal{H}_1\oplus\mathcal{H}_2} = (x \,|\, u)_{\mathcal{H}_1} - (y \,|\, v)_{\mathcal{H}_2}.$$

Let $M \subseteq \mathcal{H}_1 \oplus \mathcal{H}_2$ be a linear relation. Then

$$M^{\perp_\omega} = (SM)^\perp = (M^*)^{-1}. \tag{1.3}$$

Hence, the self-orthogonal subspaces with respect to the standard unitary form are exactly the unitary relations.

We now describe the self-orthogonal subspaces we are dealing with in the applications.

1.6 Proposition (cf. [1; Theorem 5.3])**.** *Let $\mathcal{H}$ be a Hilbert space. Then a linear relation $U \subseteq \mathcal{H} \oplus \mathcal{H}$ is self-adjoint (i.e., Lagrangian in $\mathcal{H} \oplus \mathcal{H}$ with respect to the standard skew-symmetric form) if and only if there exist a closed linear subspace $X \subseteq \mathcal{H}$ and a self-adjoint operator L in X, such that $U = G(L) \oplus (\{0\} \oplus X^\perp)$, where $G(L) = \big\{(x, Lx) \in X \oplus X;\ x \in D(L)\big\}$ denotes the graph of L.*

Proof. We only give a short outline of the ideas. For a more detailed proof we refer to [1; Section 5].

If X and L are as indicated, then the space $G(L)$ is Lagrangian in $X \oplus X$ and clearly, $\{0\} \oplus X^\perp$ is a Lagrangian subspace of $X^\perp \oplus X^\perp$. It is not difficult to show that this implies that $U = G(L) \oplus (\{0\} \oplus X^\perp)$ is Lagrangian.

Assume that U is Lagrangian, and let $\mathcal{H}_\infty := \big\{y \in \mathcal{H};\ (0, y) \in U\big\}$, $X := \mathcal{H}_\infty^\perp$. Then one shows that $U \cap (X \oplus X)$ is the graph of an operator L, and that then U is of the described form. □

1.7 Remarks. (a) It follows that a self-adjoint linear relation $U \subseteq \mathcal{H} \oplus \mathcal{H}$ is the graph of an operator if and only if its domain $P_1 U$ (P_1 the projection onto the first component) is dense in $\mathcal{H}$.

(b) A result analogous to Proposition 1.6 holds for self-orthogonal subspaces with respect to the standard symmetric form. Then L will be a skew-self-adjoint operator.

1.8 Proposition. *Let $\mathcal{H}_1, \mathcal{H}_2$ be Hilbert spaces, $U \subseteq \mathcal{H}_1 \oplus \mathcal{H}_2$ a subspace. Then U is the graph of a unitary operator L if and only if $U = U^{\perp_\omega}$, where ω is the standard unitary form on $\mathcal{H}_1 \oplus \mathcal{H}_2$.*

Proof. Let $U = U^{\perp_\omega}$. Then

$$0 = \omega((x, y), (x, y)) = (\|x\|^2_{\mathcal{H}_1} - \|y\|^2_{\mathcal{H}_2}) \quad ((x, y) \in U), \tag{1.4}$$

and this implies that U is the graph of a (closed) isometric operator L. Let $u \in D(L)^{\perp}$. Then $(u,0) \in U^{\perp_\omega} = U$, and (1.4) implies that $u = 0$, i.e., $D(L)$ is dense. Similarly one obtains that the range of L is dense. This implies that L is unitary.

Let $L\colon \mathcal{H}_1 \to \mathcal{H}_2$ be unitary. Then $G(L)^* = G(L^*) = G(L^{-1}) = G(L)^{-1}$ and therefore $G(L)^{\perp_\omega} = G(L)$. □

The following correspondence between skew-self-adjoint relations and unitary operators will establish the link between our setup and one of the versions of boundary triples; cf. Remark 2.6. We define the unitary mapping C in $\mathcal{H} \oplus \mathcal{H}$, given by the matrix $C := \frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 1 & 1 \\ -1 & 1 \end{smallmatrix} \right)$. Let ω_{s} be the standard symmetric form and ω_{u} the standard unitary form on $\mathcal{H} \oplus \mathcal{H}$. One checks that then

$$\omega_{\mathrm{s}}((x,y),(u,v)) = \omega_{\mathrm{u}}(C(x,y), C(u,v)) \qquad ((x,y),(u,v) \in \mathcal{H} \oplus \mathcal{H}).$$

1.9 Proposition. *Let C be as above. Then a linear relation $U \subseteq \mathcal{H} \oplus \mathcal{H}$ is skew-self-adjoint if and only if CU is the graph of a unitary operator.*

Proof. Theorem 1.2(b) implies that the ω_{s}-self-orthogonality of U is equivalent to the ω_{u}-self-orthogonality of CU. Applying Remark 1.7(b) and Proposition 1.8 one obtains the assertion. □

1.10 Remarks. (a) If A is a skew-self-adjoint operator in $\mathcal{H}$, then C applied to the graph of A yields the graph of the Cayley transform $(A-I)(A+I)^{-1}$ of A.

(b) The statement corresponding to Proposition 1.9, for self-adjoint operators instead of skew-self-adjoint operators requires a complex Hilbert space. In this form, the result is contained in [1; Theorem 4.6]. The mapping inducing the equivalence is then defined by the matrix $C := \frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 1 & -\mathrm{i} \\ -1 & -\mathrm{i} \end{smallmatrix} \right)$, for the Cayley transform $(A - \mathrm{i})(A + \mathrm{i})^{-1}$ of a self-adjoint operator A.

2 Boundary systems

Let $\mathcal{H}$ be a Hilbert space, H_0 a symmetric or skew-symmetric operator in $\mathcal{H}$.

Definition. A *boundary system* $(\Omega, \mathcal{G}_1, \mathcal{G}_2, F, \omega)$ for H_0 consists of a sesquilinear form Ω on $G(H_0^*)$, two Hilbert spaces $\mathcal{G}_1, \mathcal{G}_2$, a linear and surjective mapping $F\colon G(H_0^*) \to \mathcal{G}_1 \oplus \mathcal{G}_2$ and a sesquilinear form ω on $\mathcal{G}_1 \oplus \mathcal{G}_2$, such that

$$\Omega((x, H_0^*x),(y, H_0^*y)) = \omega(F(x, H_0^*x), F(y, H_0^*y)) \quad (x, y \in D(H_0^*)).$$

For a boundary system let $F_j\colon D(H_0^*) \to \mathcal{G}_j$ ($j \in \{1,2\}$) such that $F(x, H_0^*x) = (F_1(x), F_2(x))$ for all $x \in D(H_0^*)$.

2.1 Remarks. (a) If $\mathcal{G}_1 = \mathcal{G}_2 = \mathcal{G}$ and both Ω and ω are the standard skew-symmetric forms (on the corresponding spaces), then $(\Omega, \mathcal{G}, \mathcal{G}, F, \omega)$ corresponds to the version of a *boundary triple* as treated in [2,3]. The usual notation is $(\mathcal{G}, \Gamma_1, \Gamma_2)$, where $\Gamma_1, \Gamma_2\colon D(H_0^*) \to \mathcal{G}$ are such that $(\Gamma_1, \Gamma_2)\colon D(H_0^*) \to \mathcal{G} \oplus \mathcal{G}$ is surjective. Note that here $\Gamma_j = F_j$ ($j \in \{1,2\}$).

(b) If Ω is the standard skew-symmetric form on $G(H_0^*)$, then Γ, given by $\Gamma(x,y) := \Omega((x, H_0^*x),(y, H_0^*y))$ ($x, y \in D(H_0^*)$) is also called the *boundary form* of H_0; cf. [5; Def. 7.1.1].

(c) The notion of *systems with integration by parts (SWIPs)*, defined in [19; Definition 3.4] deals with a skew-symmetric operator H_0. Then SWIPs correspond to the case that Ω and ω are the standard skew-symmetric forms on $\mathcal{H} \oplus \mathcal{H}$ and $\mathcal{G} \oplus \mathcal{G}$, respectively, with $\mathcal{G} = \mathcal{G}_1 = \mathcal{G}_2$. Additionally, $F\colon G(H_0^*) \to \mathcal{G} \oplus \mathcal{G}$ is assumed to be continuous (with respect to the graph norm of H_0^*), to vanish on $G(H_0)$, and to be bijective on $G(H_0)^\perp \cap G(H_0^*)$.

The following theorem is a version of the well-established result how self-adjoint extensions of symmetric operators can be obtained using boundary triples; see [2, 3, 5] and references therein. In our context the domains of the self-adjoint extensions are characterized by means of self-adjoint relations in the space of boundary values.

2.2 Theorem. *Let H_0 be a symmetric operator, and let $(\Omega, \mathcal{G}, \mathcal{G}, F, \omega)$ be a boundary system for H_0, where Ω, ω are the standard skew-symmetric forms. Then an operator $H \subseteq H_0^*$ is self-adjoint if and only if there exist a closed subspace $X \subseteq \mathcal{G}$ and a self-adjoint operator L in X such that*

$$D(H) = \bigl\{x \in D(H_0^*);\, F_1(x) \in D(L),\, LF_1(x) = QF_2(x)\bigr\},$$

where $Q\colon \mathcal{G} \to X$ is the orthogonal projection.

In the proof we will need the following auxiliary result:

2.3 Lemma. *Let H_0 be a symmetric operator, and let Ω be the standard skew-symmetric form on $\mathcal{H} \oplus \mathcal{H}$ and $\check{\Omega}$ its restriction to $G(H_0^*)$. Then an operator $H \subseteq H_0^*$ is self-adjoint if and only if its graph is a Lagrangian subspace of $G(H_0^*)$ with respect to $\check{\Omega}$.*

Proof. Necessity is trivial. In order to show sufficiency let $U \subseteq G(H_0^*)$ be Lagrangian in $G(H_0^*)$. Then $U^{\perp_\Omega} \supseteq G(H_0^*)^{\perp_\Omega} = (G(H_0)^{\perp_\Omega})^{\perp_\Omega} \supseteq G(H_0)$, and therefore $U = U^{\perp_{\check{\Omega}}} = U^{\perp_\Omega} \cap G(H_0^*) \supseteq G(H_0)$. This implies that $U^{\perp_\Omega} \subseteq G(H_0^*)$, and finally that $U^{\perp_\Omega} = U^{\perp_\Omega} \cap G(H_0^*) = U^{\perp_{\check{\Omega}}} = U$. □

Proof of Theorem 2.2. By Lemma 2.3, H is self-adjoint if and only if $G(H)$ is Ω-self-orthogonal in $G(H_0^*)$. By Corollary 1.2, this is equivalent to the existence of an ω-self-orthogonal subspace $V \subseteq \mathcal{G} \times \mathcal{G}$ such that $G(H) = F^{-1}(V)$. The description of V in Proposition 1.6 then yields the description of H as a restriction of H_0^*. □

2.4 Remark. The corresponding statement for skew-symmetric and skew-self-adjoint operators is shown in the same way.

Boundary systems as in the previous theorem make use of standard skew-symmetric forms in the (big) Hilbert space $\mathcal{H}$ as well as in the (small) Hilbert space $\mathcal{G}$, thus characterizing self-adjoint restrictions of H_0^* by means of Lagrangian subspaces in $\mathcal{G} \oplus \mathcal{G}$. In the following statement we describe the application of boundary systems to the characterization of skew-self-adjoint extensions of skew-symmetric operators by unitary operators in the 'boundary space'.

2.5 Theorem. *Let H_0 be a skew-symmetric operator, and let $(\Omega, \mathcal{G}_1, \mathcal{G}_2, F, \omega)$ be a boundary system for H_0, where Ω is the standard symmetric form and ω is the standard unitary form. Then the operator $H \subseteq H_0^*$ is skew-self-adjoint if and only if there exists a unitary operator L from $\mathcal{G}_1$ to $\mathcal{G}_2$ such that*

$$D(H) = \{x \in D(H_0^*);\, LF_1(x) = F_2(x)\}.$$

Proof. By Remark 1.7(b), skew-self-adjoint operators correspond to self-orthogonal subspaces with respect to the standard symmetric form. By Corollary 1.2, F establishes a correspondence between these subspaces and self-orthogonal subspaces with respect to the standard unitary form. According to Proposition 1.8 these subspaces are just the graphs of unitary operators. □

2.6 Remarks. (a) Assuming that $\mathcal{H}$ is a complex Hilbert space, that H_0 is symmetric, and letting Ω be the standard skew-symmetric form multiplied by the imaginary unit, the (otherwise unchanged) setup of Theorem 2.5 yields the version of boundary triples as treated in [5, 8]. (We note that the hypothesis in [5; Section 7.1.1] that ρ_1, ρ_2 have dense range should be replaced by the requirement that $\rho_1 \times \rho_2$ is surjective.) The equivalence of the two versions of boundary triples is clear from Proposition 1.9.

(b) We mention that in our setup there is no need for the a priori requirement of equality of deficiency indices.

3 Application to quantum graphs

We now apply the results of Section 2 to Laplacians and first derivative operators on metric graphs. In order to do so we first introduce the relevant notions. The following description of (directed multi-) graphs is an extension of the notation presented in [10].

Let $\Gamma = (V, E, a, b, \gamma_0, \gamma_1)$ be a metric graph. This means that V is the set of *vertices* (or *nodes*) of Γ and E the set of *edges*. Furthermore let $a, b\colon E \to [-\infty, \infty]$, and assume that $a_e < b_e$ and that the interval $(a_e, b_e) \subseteq \mathbb{R}$ corresponds to the edge e ($e \in E$). Denote $E_{\mathrm{l}} := \{e \in E;\ a_e > -\infty\}$ and $E_{\mathrm{r}} := \{e \in E;\ b_e < \infty\}$. Let $\gamma_0\colon E_{\mathrm{l}} \to V$, $\gamma_1\colon E_{\mathrm{r}} \to V$ associate with each edge $e \in E_{\mathrm{l}}$ or $e \in E_{\mathrm{r}}$, respectively, a "starting vertex" $\gamma_0(e)$ or an "end vertex" $\gamma_1(e)$, respectively. Note that we do not assume finiteness (or countability) of V and E.

Assume that there is a positive lower bound for the lengths of the edges, i.e.,

$$l := \inf_{e \in E} (b_e - a_e) > 0. \tag{3.1}$$

The self-adjoint operators we treat will act in the Hilbert space

$$\mathcal{H}_\Gamma := \bigoplus_{e \in E} L_2(a_e, b_e).$$

3.1 Remark. By Sobolev's lemma there exists a continuous linear operator $\psi\colon W_2^1(0, l) \to \mathbb{K}^2,\ f \mapsto (f(0), f(l))$ from the first order Sobolev space to the space of boundary values of an interval. (In fact, one can compute that $\|\psi\| = \bigl(\frac{\cosh l + 1}{\sinh l}\bigr)^{1/2}$.)

Let $E' := (E_{\mathrm{l}} \times \{0\}) \cup (E_{\mathrm{r}} \times \{1\})$. The set E' encodes all finite boundary points of all edges. Note that (3.1) and Remark 3.1 give rise to continuous linear mappings $\mathrm{tr}, \mathrm{str}\colon \bigoplus_{e \in E} W_2^1(a_e, b_e) \to \ell_2(E')$, the *trace* and *signed* *trace*, respectively, defined by

$$(\operatorname{tr} f)(e,j) := \begin{cases} f_e(a_e) & (e \in E_{\mathrm{l}}, j = 0), \\ f_e(b_e) & (e \in E_{\mathrm{r}}, j = 1), \end{cases}$$
$$(\operatorname{str} f)(e,j) := \begin{cases} f_e(a_e) & (e \in E_{\mathrm{l}}, j = 0), \\ -f_e(b_e) & (e \in E_{\mathrm{r}}, j = 1). \end{cases}$$

The trace mappings defined above will be used in the study of the Laplacian on the graph. For the case of the derivative operator we need the mappings $\operatorname{tr}_{\mathrm{l}} \colon \bigoplus_{e\in E} W_2^1(a_e,b_e) \to \ell_2(E_{\mathrm{l}})$ and $\operatorname{tr}_{\mathrm{r}} \colon \bigoplus_{e\in E} W_2^1(a_e,b_e) \to \ell_2(E_{\mathrm{r}})$, defined by

$$(\operatorname{tr}_{\mathrm{l}} f)(e) := f_e(a_e) \quad (e \in E_{\mathrm{l}}), \qquad (\operatorname{tr}_{\mathrm{r}} f)(e) := f_e(b_e) \quad (e \in E_{\mathrm{r}}).$$

3.1 The Laplace operator

As a first application of the considerations in the previous sections we now treat the Laplacian in $\mathcal{H}_\Gamma$. Define the maximal operator $\hat{H}$ in $\mathcal{H}_\Gamma$,

$$D(\hat{H}) := \bigoplus_{e\in E} W_2^2(a_e,b_e),$$
$$\hat{H}f := (-f_e'')_{e\in E}.$$

The operator $\hat{H}$ is the adjoint of the minimal operator defined as the closure of the restriction of $\hat{H}$ to $\left(\prod_{e\in E} C_c^\infty(a_e,b_e)\right) \cap D(\hat{H})$.

For $f \in \bigoplus_{e\in E} W_2^1(a_e,b_e)$ abbreviate $(f_e')_{e\in E}$ by f'. Define $F \colon G(\hat{H}) \to \ell_2(E') \oplus \ell_2(E')$ by

$$F(f, \hat{H}f) := (\operatorname{tr} f, \operatorname{str} f').$$

Then F is linear. Using (3.1) one obtains that F is continuous and surjective. To show surjectivity, let $\eta \in C^\infty(0,l)$, with support $\operatorname{spt}\eta \subseteq (0,l/2)$, $\eta = 1$ in a neighbourhood of 0. For prescribed boundary values $\alpha,\beta \in \mathbb{K}$ for the function and its derivative define $f(\xi) := (\alpha + \beta\xi)\eta(\xi)$ $(\xi \in (0,l))$. Then there exists a constant $c \geqslant 0$ (independent of α,β) such that $\|f\|_2^2 + \|f''\|_2^2 \leqslant c(|\alpha|^2 + |\beta|^2)$. As a consequence one obtains that for each $(\alpha,\beta) \in \ell_2(E') \oplus \ell_2(E')$ there exists $f \in D(\hat{H})$ such that $F(f,\hat{H}f) = (\alpha,\beta)$. (See also [15, 16].)

For $f, g \in D(\hat{H})$, integration by parts yields

$$
\begin{aligned}
&(f \,|\, \hat{H} g) - (\hat{H} f \,|\, g) \\
&= \sum_{e \in E_{\mathrm{l}} \cap E_{\mathrm{r}}} \big(f_e \overline{(-g_e')}\big)\Big|_{a_e}^{b_e} + \sum_{e \in E_{\mathrm{l}} \setminus E_{\mathrm{r}}} f_e(a_e) \overline{g_e'(a_e)} - \sum_{e \in E_{\mathrm{r}} \setminus E_{\mathrm{l}}} f_e(b_e) \overline{g_e'(b_e)} \\
&\qquad - \sum_{e \in E_{\mathrm{l}} \cap E_{\mathrm{r}}} \big(-f_e' \overline{g_e}\big)\Big|_{a_e}^{b_e} - \sum_{e \in E_{\mathrm{l}} \setminus E_{\mathrm{r}}} f_e'(a_e) \overline{g_e(a_e)} + \sum_{e \in E_{\mathrm{r}} \setminus E_{\mathrm{l}}} f_e'(b_e) \overline{g_e(b_e)} \\
&= (\operatorname{tr} f \,|\, \operatorname{str} g') - (\operatorname{str} f' \,|\, \operatorname{tr} g) = \left(\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} F(f, \hat{H} f) \,\middle|\, F(g, \hat{H} g) \right).
\end{aligned}
$$

Defining Ω and ω to be the standard skew-symmetric form on $G(\hat{H})$ and $\ell_2(E') \oplus \ell_2(E')$, respectively, we obtain

$$
\Omega((f, \hat{H} f), (g, \hat{H} g)) = \omega(F(f, \hat{H} f), F(g, \hat{H} g)) \quad (f, g \in D(\hat{H})).
$$

3.2 Theorem. *An operator $H \subseteq \hat{H}$ is self-adjoint if and only if there exist a closed subspace $X \subseteq \ell_2(E')$ and a self-adjoint operator L in X such that*

$$
D(H) = \big\{ f \in D(\hat{H});\ \operatorname{tr} f \in D(L),\ L \operatorname{tr} f = Q \operatorname{str} f' \big\},
$$

where $Q \colon \ell_2(E') \to X$ is the orthogonal projection.

Proof. The previous discussion shows that $(\Omega, \ell_2(E'), \ell_2(E'), F, \omega)$ is a boundary system. Therefore the assertion follows from Theorem 2.2. □

3.3 Remarks. (a) We note that the boundary conditions leading to self-adjoint Laplacians can be described in different ways. We refer to [14; Theorem 5] for an account of these descriptions. However, as already mentioned in the Introduction, in the present general case the obtained self-adjoint operator may fail to be semibounded, and therefore the form method may not be available.

(b) In the known cases where the operator H in Theorem 3.2 can be constructed by the form method, the space X and the (bounded) operator L take a special role in the definition of the form: The space X restricts the domain of the form, whereas L occurs in a term of the form itself; cf. [10, 13].

3.4 Examples. (a) Let $V := \mathbb{Z}$ and $E := \mathbb{Z}$. We set $a(n) := n$, $b(n) := n+1$ and $\gamma_0(n) := n$, $\gamma_1(n) := n+1$ for all $n \in \mathbb{Z}$. Then $\Gamma = (V, E, a, b, \gamma_0, \gamma_1)$ is the metric graph $\mathbb{Z}$ with nearest neighbour edges. For $n \in \mathbb{Z}$ let $X_n := \operatorname{lin}\{(1,1)\}$ and $X := \bigoplus_{n\in\mathbb{Z}} X_n$. Define L in X by

$$D(L) := \bigl\{(x_n)_{n\in\mathbb{Z}} \in X;\, (nx_n)_{n\in\mathbb{Z}} \in X\bigr\}, \quad L(x_n) := (nx_n).$$

Then L is self-adjoint but not bounded from below. By Theorem 3.2 the opeator $H \subseteq \hat{H}$ with

$$D(H) = \bigl\{f \in D(\hat{H});\ \operatorname{tr} f \in D(L),\, L \operatorname{tr} f = Q \operatorname{str} f'\bigr\}$$

is self-adjoint. It is easy to see that $f \in D(\hat{H})$ is in $D(H)$ if and only if

$$f_n(n) = f_{n-1}(n), \quad -f_n'(n) + f_{n-1}'(n) = 2nf_n(n) \quad (n \in \mathbb{Z}).$$

So, we have encoded δ-type boundary conditions (see e.g. [13; Section 3.2.1]) at n with coupling parameter $2n$, for all $n \in \mathbb{Z}$. Note that since L is unbounded, also H is not bounded from below and the form method cannot be applied to define H.

(b) Let $V := \mathbb{N}_0$ and $E := \mathbb{N}$. We set $a(n) := 0$, $b(n) := n$, $\gamma_0(n) := 0$, $\gamma_1(n) := n$ for all $n \in \mathbb{N}$. Then $\Gamma = (V, E, a, b, \gamma_0, \gamma_1)$ is a metric graph, and $0 \in V$ is a vertex with infinite degree. Let $X_0 := \ell_2(\mathbb{N})$ and for $n \in \mathbb{N}$ set $X_n := \{0\}$. Let $X := \bigoplus_{n\in\mathbb{N}_0} X_n$. Let L_0 be a self-adjoint operator in $\ell_2(\mathbb{N})$ which is not bounded from below. We set

$$D(L) := \bigl\{(x_n)_{n\in\mathbb{N}_0} \in X;\, x_0 \in D(L_0)\bigr\}, \quad L(x_n) := (L_0x_0, 0, \ldots).$$

Then L is self-adjoint in X and not bounded from below. By Theorem 3.2, $H \subseteq \hat{H}$ defined by X and L is self-adjoint, and also not bounded from below. Thus, the form method to define H is not applicable.

3.2 The first derivative operator

As another application, we describe boundary conditions for the derivative operator that lead to skew-self-adjoint operators. We define the maximal operator $\hat{H}$ on $\mathcal{H}_\Gamma$,

$$D(\hat{H}) := \bigoplus_{e\in E} W_2^1(a_e, b_e),$$
$$\hat{H}f := (f_e')_{e\in E}.$$

The operator $\hat{H}$ is the negative adjoint of the minimal one defined as the closure of the restriction of $\hat{H}$ to $\big(\prod_{e\in E} C_c^\infty(a_e,b_e)\big) \cap D(\hat{H})$.

Let $F\colon G(\hat{H}) \to \ell_2(E_\mathrm{r}) \oplus \ell_2(E_\mathrm{l})$,

$$F(f,\hat{H}f) := (\mathrm{tr}_\mathrm{r}\, f, \mathrm{tr}_\mathrm{l}\, f).$$

Then F is linear, surjective and continuous (for surjectivity construct piecewise affine functions). For $f,g \in D(\hat{H})$, integration by parts yields

$$\begin{aligned}(f\,|\,\hat{H}g) + (\hat{H}f\,|\,g) &= \sum_{e\in E_\mathrm{r}} f_e(b_e)\overline{g_e(b_e)} - \sum_{e\in E_\mathrm{l}} f_e(a_e)\overline{g_e(a_e)} \\ &= \omega(F(f,\hat{H}f), F(g,\hat{H}g)),\end{aligned}$$

where ω is the standard unitary form on $\ell_2(E_\mathrm{r}) \oplus \ell_2(E_\mathrm{l})$; cf. Example 1.5(c). As a consequence, denoting by Ω the standard symmetric form on $G(\hat{H})$, we obtain

$$\Omega((f,\hat{H}f),(g,\hat{H}g)) = \omega(F(f,\hat{H}f), F(g,\hat{H}g)) \quad (f,g \in D(\hat{H})).$$

3.5 Theorem. *An operator $H \subseteq \hat{H}$ is skew-self-adjoint if and only if there exists a unitary operator L from $\ell_2(E_\mathrm{r})$ to $\ell_2(E_\mathrm{l})$ such that*

$$D(H) = \{f \in D(\hat{H});\, L\,\mathrm{tr}_\mathrm{r}\, f = \mathrm{tr}_\mathrm{l}\, f\}.$$

Proof. The previous discussion shows that $(\Omega, \ell_2(E_\mathrm{r}), \ell_2(E_\mathrm{l}), F, \omega)$ is a boundary system. Therefore the assertions follow from Theorem 2.5. □

3.6 Remarks. (a) Theorem 3.5 precisely characterizes when there exist skew-self-adjoint restrictions of $\hat{H}$. Namely, the spaces $\ell_2(E_\mathrm{r})$ and $\ell_2(E_\mathrm{l})$ have to be unitarily equivalent, i.e., E_r and E_l have the same cardinality.

(b) An operator H is skew-self-adjoint if and only if it is the generator of a C_0-group of unitary operators. Therefore, Theorem 3.5 describes precisely the unitary groups in $\mathcal{H}_\Gamma$ yielding solutions for the Cauchy problem for the transport equation

$$u'(t) = Hu(t) \quad (t \in \mathbb{R})$$

on Γ.

(c) Let $\mathbb{K} = \mathbb{C}$. The Dirac operator in $\mathcal{H}_\Gamma$ is defined to be a self-adjoint restriction of $-i\hat{H}$. Since H is skew-self-adjoint if and only if $-iH$ is self-adjoint we obtain that a Dirac operator $-iH$ is self-adjoint if and only if

$$D(-iH) = \{f \in D(\hat{H}); L\,\mathrm{tr}_\mathrm{r}\, f = \mathrm{tr}_\mathrm{l}\, f\}$$

for some unitary L from $\ell_2(E_\mathrm{r})$ to $\ell_2(E_\mathrm{l})$.

In both of the situations of operators on graphs, i.e., the Laplacian and the first order derivative, the given structure of the graphs, encoded in the two maps γ_0 and γ_1, did not occur in the description of the boundary conditions. In other words, we replaced the graph by a so-called *rose* (cf. [14; Section 4.3]), possibly with infinitely many edges. If one wants to consider only 'local boundary conditions', i.e., boundary conditions respecting the adjacency relations, one will obtain the relations and operators describing the boundary conditions in block form; cf. [18; Section 5] (for the case of singular diffusion on finite graphs) and [16; Chapter 1]. In the case of the self-adjoint Laplacian, each of the blocks would be a self-adjoint relation, whereas in the case of the skew-self-adjoint derivative operator, each of the blocks would be unitary.

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