Self-adjoint extensions of the Laplace–Beltrami operator and unitaries at the boundary *

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Abstract

We construct in this article a class of closed semi-bounded quadratic forms on the space of square integrable functions over a smooth Riemannian manifold with smooth compact boundary. Each of these quadratic forms specifies a semi-bounded self-adjoint extension of the Laplace–Beltrami operator. These quadratic forms are based on the Lagrange boundary form on the manifold and a family of domains parametrized by a suitable class of unitary operators on the boundary that will be called admissible. The corresponding quadratic forms are semi-bounded below and closable. Finally, the representing operators correspond to semi-bounded self-adjoint extensions of the Laplace–Beltrami operator. This family of extensions is compared with results existing in Boundary conditions the literature and various examples and applications are dis-cussed.

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Contents

1. Introduction

In this article we construct a family of closed quadratic forms corresponding to a class of self-adjoint extensions of the Laplace–Beltrami operator on a smooth Riemannian manifold with smooth boundary. It is well known that in a smooth manifold Ω with no boundary the minimal closed extension of the Laplace–Beltrami operator $\Delta_{\min}$ is essentially self-adjoint. However, if the manifold has a non-empty boundary $\partial\Omega$, then $\Delta_{\min}$ defines a closed and symmetric but *not self-adjoint* operator. Such situation is common in the study of quantum systems, where some heuristic arguments suggest an expression for the Hamiltonian which is only symmetric. The Laplace–Beltrami operator discussed here can be associated with free quantum systems on the manifold. The description of such systems is not complete until a self-adjoint extension of the Laplace–Beltrami operator has been determined, i.e., a Hamiltonian operator H. Only in this case a unitary evolution of the system is given, because of the one-to-one correspondence between densely defined self-adjoint operators and strongly continuous one-parameter groups of unitary operators $U_t = \exp itH$ provided by Stone's theorem. Therefore the specification of the self-adjoint extension is not just a mathematical artifact, but an essential step in the description of the quantum mechanical system (see, e.g., Chapter X in [40] for further results and motivation).

The collection of all self-adjoint extensions of a densely defined closed symmetric operator T on a complex separable Hilbert space $\mathcal{H}$ was described by von Neumann in terms of the isometries between the deficiency spaces $\mathcal{N}_\pm = \ker(T^\dagger \mp iI)$ of the operator T (see, e.g., [44,40,45]). Unfortunately, beyond the one-dimensional case, the use of von Neumann's theorem to describe the self-adjoint extensions of the Laplace–Beltrami operator is unfeasible. In fact, the computation of deficiency indices requires the knowledge of the adjoint operator which is a difficult problem in itself (see [6] and references therein). Moreover, in von Neumann's classical result the use of important geometrical and physical data becomes rather indirect and for these reasons the theory of extensions has been developed in many different ways and is still today an active research area. The use of the Hermitian quadratic forms to address the extension problem has been one of the most useful approaches since the pioneering work by Friedrichs, Kato, Lax and Milgram (cf., [15,27,41]). If T is a symmetric and semi-bounded operator on the domain $\mathcal{D}(T)$, then the semi-bounded quadratic form

$$Q(\Phi) = \langle \Phi, T\Phi \rangle, \quad \Phi \in \mathcal{D}(T) \subset \mathcal{H}, \tag{1.1}$$

is closable and its closure is represented by a self-adjoint extension of T with the same lower bound (see, e.g., [29,40,45]). Moreover, the domain of the closure of the quadratic form satisfies a natural minimality condition. Theorem 2.4 provides the characterization of closed semi-bounded quadratic forms as those that can be represented by self-adjoint and semi-bounded operators as in (1.1) (cf., [27,41,40]). In the particular instance of the Laplace–Beltrami operator some of these closed extensions on $\mathcal{H} = L^2(\Omega)$ are well known. The simplest examples are the quadratic forms associated with the Dirichlet and Neumann self-adjoint extensions of the Laplacian: Consider the positive and closed quadratic form

$$Q(\Phi) = \|\mathrm{d}\Phi\|^2 \tag{1.2}$$

with domain $\mathcal{D}_D = \mathcal{H}^1_0(\Omega)$ in the Dirichlet case and domain $\mathcal{D}_N = \mathcal{H}^1(\Omega)$ for the Neumann extension (see for instance [13] and references therein). Also equivariant and Robin-type Laplacians can be naturally described in terms of closed and semi-bounded quadratic forms (see, e.g., [19,21,30,32]). In this context the subtle relation between quadratic forms and representing operators manifests through the fact that the form domain $\mathcal{D}(Q)$ always contains the operator domain $\mathcal{D}(T)$ of the representing operator. Therefore it is often possible to compare different form domains while the domains of the representing operators remain unrelated. This fact allows, e.g., to develop spectral bracketing techniques in very different mathematical and physical situations using the language of quadratic forms [33,34].

In spite of the vast literature devoted to the subject, the determination of the self-adjoint or, more generally, sectorial extension of the operator and their spectral properties is still an active field of research (see [3,27] and references therein). Another example where the correct extension of a symmetric operator has been recently analyzed is the case of the so-called Berry's paradox when dealing with a class of Robin boundary conditions with a singular Dirichlet point [11,10,35]. Hence the study of such quadratic forms is instrumental not only for the construction of a complete quantum system but for the analysis of the spectrum of the corresponding self-adjoint Hamiltonian operators [26]. Quadratic forms also provide a natural frame for the analysis of the question of how does the process of selecting self-adjoint extensions of symmetric operators intertwine with the notion of quantum symmetry (see Section 4 in [24]).

The role of boundaries has been highlighted in the case of the study of self-adjoint extensions of formally self-adjoint differential operators leading to the complete classification of boundary conditions by Grubb [17] and to the theory of boundary triples (see, e.g., [12] and references therein and [5] for the generalization to quasi-boundary triples; see also Chapter 2 in [38] for the description of boundary triples for quantum graphs and [39] for the theory of boundary pairs in the context of quadratic forms).

In a similar but slightly different direction focused on the physics of boundary dynamics it was argued in [4] that self-adjoint extensions of the Bochner Laplacian are in one-to-one correspondence with unitary operators on a Hilbert space of boundary data, the trace of the function and its normal derivative at the boundary. Such characterization was shown to be particularly useful as it provides an explicit and easily workable description of the domain of the corresponding self-adjoint extension by means of the condition, called in what follows boundary equation:

$$\varphi - i\dot{\varphi} = U(\varphi + i\dot{\varphi}), \tag{1.3}$$

where $\varphi, \dot{\varphi}$ denote the trace at the boundary of a function Φ, i.e., $\varphi = \Phi|_{\partial\Omega}$ and its outward normal derivative $\dot{\varphi} = \mathrm{d}\Phi(\nu)$, and U is a unitary operator on the Hilbert space at the boundary $L^2(\partial\Omega)$. The analysis of such self-adjoint extensions by means of the corresponding quadratic forms leads (after integration by parts on smooth functions) to the study of the quadratic form:

$$Q(\Phi) = \|\mathrm{d}\Phi\|^2 - \langle \varphi, \dot{\varphi} \rangle. \tag{1.4}$$

Such quadratic form can be considered as a singular perturbation of the standard Dirichlet quadratic form (1.2). Note that Koshmanenko's theorems [29] on closable singular perturbations of quadratic forms cannot be directly applied to domains described by the boundary equation (1.3) in general. Thus, in order to characterize the domains of the self-adjoint extensions of the Laplace–Beltrami operator determined by (1.3) a different approach is needed.

In this article we present a self-contained analysis of the quadratic form (1.4) on domains satisfying Eq. (1.3). Their closability is proved under appropriate conditions on the unitary operator U defining the extension. Actually it is shown that if U has gap, i.e., if the eigenvalue -1 is isolated in its spectrum, and its partial Cayley transform is bounded in the Sobolev norm $1/2$, the singularly perturbed Dirichlet quadratic form (1.4) with domain determined by condition (1.3) is closable and semi-bounded below. These results are obtained after a careful analysis of the domain defined by the boundary equation (1.3), the structure of the radial Laplace operator defined on a collar neighborhood of the boundary, and a judiciously use of Neumann's extension of the given quadratic form on the bulk of the manifold. As particular case these results include that all the Robin boundary conditions of the form $\dot{\varphi} = g\varphi$, $g \in \mathcal{C}(\partial\Omega)$, lead to lower semi-bounded extensions of the Laplace–Beltrami operator. Our method also allows to classify this class of self-adjoint extensions labeled by admissible unitaries according to their invariance properties with respect to a symmetry group, in particular, with respect to a group action on the manifold (see Sections 6 and 7 in [24] for a detailed analysis and concrete examples).

The article is organized as follows. Section 2 is devoted to establish basic definitions and results on quadratic forms and some technicalities on the Laplace–Beltrami operator and Sobolev spaces in smooth manifolds with boundary. In Section 3 we introduce the class of quadratic forms whose closability and semi-boundedness will be established. We will also specify the domains of the self-adjoint extensions in terms of a class of maximal isotropic subspaces (cf., Theorem 3.6 and Proposition 3.7). The class of admissible unitary operators U leading to closable and semi-bounded quadratic forms is introduced at the end of this section paving the way to Section 4, where the main theorems proving the closability and semi-boundedness of the quadratic forms defined are discussed. Section 4.3, is devoted to establish the connections of the approach taken here with other known approaches to describe extensions of symmetric operators, like the theory of quasi-boundary triples or the work of G. Grubb on elliptic even-order systems. Finally, in Section 5 various families of examples with admissible unitaries at the boundary are obtained by using several choices of values of the boundary data. For instance combining Dirichlet, Neumann and diverse identifications of subdomains of the boundary.

2. Preliminaries: Quadratic forms and the Laplace–Beltrami operator

In this section we fix our notation and recall first some standard results of the theory of unbounded operators and quadratic forms that will be useful later on. Standard references are, e.g., [13, Section 4.4], [27, Chapter VI], [41, Section VIII.6] or [42, Chapters 10 and 13]. Then we will also introduce standard material on Riemannian manifolds with boundary, the Laplace–Beltrami operator and the associated Sobolev spaces. Some basic references for this part are, e.g., [1,2,13,31,36].

2.1. Quadratic forms and operators

Definition 2.1. Let $\mathcal{D}$ be a dense subspace of the Hilbert space $\mathcal{H}$ and denote by $Q : \mathcal{D} \times \mathcal{D} \to \mathbb{C}$ a sesquilinear form (anti-linear in the first entry and linear in the second entry). The quadratic form associated with Q with domain $\mathcal{D}$ is its evaluation on the diagonal, i.e., $Q(\Phi) := Q(\Phi, \Phi)$, $\Phi \in \mathcal{D}$. We say that the sesquilinear form is **Hermitian** if

$$Q(\Phi, \Psi) = \overline{Q(\Psi, \Phi)}, \quad \Phi, \Psi \in \mathcal{D}.$$

The quadratic form is **semi-bounded** if there is an $a \geq 0$ such that

$$Q(\Phi) \geq -a\|\Phi\|^2, \quad \Phi \in \mathcal{D}.$$

The smallest possible value a satisfying the preceding inequality is called the **lower bound** for the quadratic form Q. In particular, if $Q(\Phi) \geq 0$ for all $\Phi \in \mathcal{D}$ we say Q is **positive**.

Note that if Q is semi-bounded with lower bound a, then $Q_a(\Phi) := Q(\Phi) + a\|\Phi\|^2$, $\Phi \in \mathcal{D}$, is positive on the same domain. We need to recall also the notions of closable and closed quadratic forms as well as the fundamental representation theorems that relate closed semi-bounded quadratic forms with self-adjoint semi-bounded operators.

Definition 2.2. Let Q be a semi-bounded quadratic form with lower bound $a \geq 0$ and dense domain $\mathcal{D} \subset \mathcal{H}$. The quadratic form Q is **closed** if $\mathcal{D}$ is closed with respect to the norm

$$|||\Phi|||_Q := \sqrt{Q(\Phi) + (1+a)\|\Phi\|^2}, \quad \Phi \in \mathcal{D}.$$

If Q is closed and $\mathcal{D}_0 \subset \mathcal{D}$ is dense with respect to the norm $|||\cdot|||_Q$, then $\mathcal{D}_0$ is called a **form core** for Q. Conversely, the closed quadratic form Q with domain $\mathcal{D}$ is called an **extension** of the quadratic form Q with domain $\mathcal{D}_0$. A quadratic form is said to be **closable** if it has a closed extension.

Remark 2.3.

i) The norm $|||\cdot|||_Q$ is induced by the following inner product on the domain:

$$\langle \Phi, \Psi \rangle_Q := Q(\Phi, \Psi) + (1+a)\langle \Phi, \Psi \rangle, \quad \Phi, \Psi \in \mathcal{D}.$$

ii) The quadratic form Q is closable iff whenever a sequence $\{\Phi_n\}_n \subset \mathcal{D}$ satisfies $\|\Phi_n\| \to 0$ and $Q(\Phi_n - \Phi_m) \to 0$, as $n, m \to \infty$, then $Q(\Phi_n) \to 0$.

iii) In general, it is always possible to close $\mathcal{D} \subset \mathcal{H}$ with respect to the norm $|||\cdot|||_Q$. The quadratic form is closable iff this closure is a subspace of $\mathcal{H}$.

The following relation between quadratic forms and self-adjoint operators goes back to the pioneering work in the 1950s by Friedrichs, Kato, Lax and Milgram, and others (see comments to Section VIII.6 in [41]).

Theorem 2.4 *(Representation theorem). Let Q be a Hermitian, closed, semi-bounded quadratic form defined on the dense domain $\mathcal{D} \subset \mathcal{H}$. Then there exists a unique, self-adjoint, semi-bounded operator T with domain $\mathcal{D}(T)$ and the same lower bound such that:*

i) $\Psi \in \mathcal{D}(T)$ *iff* $\Psi \in \mathcal{D}$ *and there exists* $\chi \in \mathcal{H}$ *such that*

$$Q(\Phi, \Psi) = \langle \Phi, \chi \rangle, \quad \forall \Phi \in \mathcal{D}.$$

In this case we write $T\Psi = \chi$ *and* $Q(\Phi, \Psi) = \langle \Phi, T\Psi \rangle$ *for any* $\Phi \in \mathcal{D}$, $\Psi \in \mathcal{D}(T)$.

ii) $\mathcal{D}(T)$ *is a core for* Q.

One of the most common uses of the representation theorem is to obtain self-adjoint extensions of symmetric, semi-bounded operators. Given a semi-bounded, closed and symmetric operator T one can consider the associated quadratic form

$$Q_T(\Phi, \Psi) = \langle \Phi, T\Psi \rangle, \quad \Phi, \Psi \in \mathcal{D}(T).$$

These quadratic forms are always closable, cf., [40, Theorem X.23], and therefore their closure is associated with a unique self-adjoint operator. Even if the symmetric operator has infinite possible self-adjoint extensions, the representation theorem allows to select a particular one. This extension is called the Friedrichs extension. The approach that we shall take in this article is close to this method.

2.2. Scales of Hilbert spaces

Later on we will need the theory of scales of Hilbert spaces, also known as theory of rigged Hilbert spaces. In the following paragraph we state the main results (see, e.g., [9,29] for proofs and more results).

Let $\mathcal{H}$ be a Hilbert space with scalar product $\langle \cdot,\cdot \rangle$ and induced norm $\| \cdot \|$. Let $\mathcal{H}_+$ be a dense linear subspace of $\mathcal{H}$ which is a complete Hilbert space with respect to another scalar product that will be denoted by $\langle \cdot,\cdot \rangle_+$. The corresponding norm is $\| \cdot \|_+$ and we assume that

$$\|\Phi\| \leq \|\Phi\|_+, \quad \Phi \in \mathcal{H}_+. \tag{2.1}$$

Any vector $\Phi \in \mathcal{H}$ generates a continuous linear functional $L_\Phi : \mathcal{H}_+ \to \mathbb{C}$ as follows. For $\Psi \in \mathcal{H}_+$ define

$$L_\Phi(\Psi) = \langle \Phi, \Psi \rangle. \tag{2.2}$$

Continuity follows by the Cauchy–Schwarz inequality and Eq. (2.1):

$$L_\Phi(\Psi) \leq \|\Phi\| \cdot \|\Psi\| \leq \|\Phi\| \cdot \|\Psi\|_+, \quad \forall \Phi \in \mathcal{H},\ \forall \Psi \in \mathcal{H}_+. \tag{2.3}$$

Since L_Φ represents a continuous linear functional on $\mathcal{H}_+$ it can be represented, according to Riesz theorem, using the scalar product in $\mathcal{H}_+$. Namely, there exists a vector $\xi \in \mathcal{H}_+$ such that

$$\forall \Psi \in \mathcal{H}_+, \quad L_\Phi(\Psi) = \langle \Phi, \Psi \rangle = \langle \xi, \Psi \rangle_+, \tag{2.4}$$

and the norm of the functional coincides with the norm in $\mathcal{H}_+$ of the element ξ, i.e.,

$$\|L_\Phi\| = \sup_{\Psi \in \mathcal{H}_+} \frac{|L_\Phi(\Psi)|}{\|\Psi\|_+} = \|\xi\|_+.$$

One can use the above equalities to define an operator

$$\begin{aligned} \hat{I} &: \mathcal{H} \to \mathcal{H}_+, \\ \hat{I}\Phi &= \xi. \end{aligned} \tag{2.5}$$

This operator is clearly injective since $\mathcal{H}_+$ is a dense subset of $\mathcal{H}$ and therefore it can be used to define a new scalar product on $\mathcal{H}$

$$\langle \cdot, \cdot \rangle_- := \langle \hat{I} \cdot, \hat{I} \cdot \rangle_+. \tag{2.6}$$

The completion of $\mathcal{H}$ with respect to this scalar product defines a new Hilbert space, $\mathcal{H}_-$, and the corresponding norm will be denoted accordingly by $\| \cdot \|_-$. It is clear that $\mathcal{H}_+ \subset \mathcal{H} \subset \mathcal{H}_-$ with dense inclusions. Since $\|\xi\|_+ = \|\hat{I}\Phi\|_+ = \|\Phi\|_-$, the operator $\hat{I}$ can be extended by continuity to an isometric bijection.

Definition 2.5. The Hilbert spaces $\mathcal{H}_+$, $\mathcal{H}$ and $\mathcal{H}_-$ introduced above define a **scale of Hilbert spaces**. The extension by continuity of the operator $\hat{I}$ is called the **canonical isometric bijection**. It is denoted by:

$$I : \mathcal{H}_- \to \mathcal{H}_+. \tag{2.7}$$

Proposition 2.6. *The scalar product in $\mathcal{H}$ can be extended continuously to a pairing*

$$(\cdot, \cdot) : \mathcal{H}_- \times \mathcal{H}_+ \to \mathbb{C}. \tag{2.8}$$

Proof. Let $\Phi \in \mathcal{H}$ and $\Psi \in \mathcal{H}_+$. Using the Cauchy–Schwarz inequality we have the following

$$\big|\langle \Phi, \Psi \rangle\big| = \big|\langle I\Phi, \Psi \rangle_+\big| \leq \|I\Phi\|_+ \|\Psi\|_+ = \|\Phi\|_- \|\Psi\|_+. \qquad \square \tag{2.9}$$

2.3. Laplace–Beltrami operator on Riemannian manifolds and Sobolev spaces

Our aim is to describe a class of closable quadratic forms related to the self-adjoint extensions of the Laplace–Beltrami operator defined on a Riemannian manifold. We shall start with the definition of such manifold and of the different spaces of functions that will appear throughout the rest of this article. We will restrict to smooth manifolds with smooth, compact boundary. These situation is interesting enough and covers a wide variety of examples, as we shall discuss in Section 3 and Section 4. We refer to [16] for an analysis of the Laplace–Beltrami operator in the context of Lipschitz manifolds. In this more general setting also the language of quadratic forms is very convenient.

Let $(\Omega, \partial\Omega, \eta)$ be a smooth, orientable, Riemannian manifold with metric η and smooth, compact, boundary $\partial\Omega$. We will denote as $\mathcal{C}^\infty(\Omega)$ the space of smooth functions of the Riemannian manifold Ω and by $\mathcal{C}^\infty_c(\Omega)$ the space of smooth functions with compact support in the interior of Ω. The Riemannian volume form is written as $\mathrm{d}\mu_\eta$.

Definition 2.7. The **Laplace–Beltrami Operator** associated with the Riemannian manifold $(\Omega, \partial\Omega, \eta)$ is the second order differential operator $\Delta_\eta : \mathcal{C}^\infty(\Omega) \to \mathcal{C}^\infty(\Omega)$ given in local coordinates by

$$\Delta_\eta \Phi = \sum_{i,j} \frac{1}{\sqrt{|\eta|}} \frac{\partial}{\partial x^i} \sqrt{|\eta|} \eta^{ij} \frac{\partial \Phi}{\partial x^j}.$$

Let $(\tilde{\Omega}, \tilde{\eta})$ be a smooth, orientable, boundaryless, Riemannian manifold with metric $\tilde{\eta}$. The Laplace–Beltrami operator $-\Delta_{\tilde{\eta}}$ associated with the Riemannian manifold $(\tilde{\Omega}, \tilde{\eta})$ defines a positive, essentially self-adjoint, second order differential operator, cf. [1]. One can use it to define the following norms.

Definition 2.8. The **Sobolev norm of order** k in the boundaryless Riemannian manifold $(\tilde{\Omega}, \tilde{\eta})$ is defined by

$$\|\Phi\|_k^2 := \int_{\tilde{\Omega}} \overline{\Phi} (I - \Delta_{\tilde{\eta}})^k \Phi \mathrm{d}\mu_{\tilde{\eta}}.$$

The closure of the smooth functions with respect to this norm $\mathcal{H}^k(\tilde{\Omega}) := \overline{\mathcal{C}^\infty(\tilde{\Omega})}^{\|\cdot\|_k}$ is the **Sobolev space of order** k of the Riemannian manifold $(\tilde{\Omega}, \tilde{\eta})$. The scalar products associated with these norms are written as $\langle \cdot, \cdot \rangle_k$. In the case $k = 0$ we will denote the $\mathcal{H}^0(\tilde{\Omega})$ scalar product simply by $\langle \Phi, \Psi \rangle = \int_{\tilde{\Omega}} \overline{\Phi} \Psi \mathrm{d}\mu_{\tilde{\eta}}$.

Note that Definition 2.8 holds only for Riemannian manifolds without boundary. The construction of the Sobolev spaces of functions over a manifold $(\Omega, \partial\Omega, \eta)$ cannot be done directly like in the definition above because the Laplace–Beltrami operator does not define in general a self-adjoint operator. However, it is possible to construct it as a quotient of the Sobolev space of functions over a Riemannian manifold $(\tilde{\Omega}, \tilde{\eta})$ without boundary, cf. [43, Section 4.4].

Definition 2.9. Let $(\Omega, \partial\Omega, \eta)$ be a Riemannian manifold and let $(\tilde{\Omega}, \tilde{\eta})$ be any Riemannian manifold without boundary such that $\mathring{\Omega}$, i.e., the interior of Ω, is an open submanifold of $\tilde{\Omega}$. The **Sobolev space of order k** of the Riemannian manifold $(\Omega, \partial\Omega, \eta)$ is the quotient

$$\mathcal{H}^k(\Omega) := \mathcal{H}^k(\tilde{\Omega})/\{\Phi \in \tilde{\Omega} \mid \Phi|_{\Omega} = 0\}.$$

The norm is denoted again as $\|\cdot\|_k$. When there is ambiguity about the manifold, the subindex shall denote the full space, i.e.,

$$\|\cdot\|_k = \|\cdot\|_{\mathcal{H}^k(\Omega)}.$$

It can be shown that the Sobolev spaces $\mathcal{H}^k(\Omega)$ do not depend on the particular choice of $\tilde{\Omega}$. There are many equivalent ways to define the Sobolev norms. In particular we shall need the following characterization.

Proposition 2.10. *The Sobolev norm of order* 1, $\|\cdot\|_1$, *is equivalent to the norm*

$$\sqrt{\|\mathrm{d}\cdot\|^2_{\Lambda^1} + \|\cdot\|^2},$$

where d *stands for the exterior differential acting on functions, cf. [1], and* $\|\mathrm{d}\cdot\|_{\Lambda^1}$ *is the induced norm from the natural scalar product among* 1*-forms* $\alpha \in \Lambda^1(\Omega)$.

Proof. It is enough to show it for a boundaryless Riemannian manifold $(\tilde{\Omega}, \tilde{\eta})$. The Laplace–Beltrami operator can be expressed in terms of the exterior differential and its formal adjoint,

$$-\Delta_{\tilde{\eta}} = \mathrm{d}^\dagger \mathrm{d},$$

where the formal adjoint is defined to be the unique differential operator $\mathrm{d}^\dagger : \Lambda^1(\tilde{\Omega}) \to \mathcal{C}^\infty(\tilde{\Omega})$ that verifies

$$\langle \alpha, \mathrm{d}\Phi \rangle_{\Lambda^1} = \left\langle \mathrm{d}^\dagger \alpha, \Phi \right\rangle, \quad \alpha \in \Lambda^1(\tilde{\Omega}),\ \Phi \in \mathcal{C}^\infty(\tilde{\Omega}).$$

Let $\Phi \in \mathcal{C}^\infty(\tilde{\Omega})$. Then we have that

$$\begin{aligned} \|\Phi\|_1^2 &= \int_{\tilde{\Omega}} \bar{\Phi}(I - \Delta_{\tilde{\eta}})\Phi \mathrm{d}\mu_{\tilde{\eta}} \\ &= \int_{\tilde{\Omega}} \bar{\Phi}\Phi \mathrm{d}\mu_{\tilde{\eta}} + \int_{\tilde{\Omega}} \bar{\Phi}\mathrm{d}^\dagger \mathrm{d}\Phi \mathrm{d}\mu_{\tilde{\eta}} \\ &= \|\Phi\|^2 + \langle \mathrm{d}\Phi, \mathrm{d}\Phi \rangle_{\Lambda^1} = \|\Phi\|^2 + \|\mathrm{d}\Phi\|^2_{\Lambda^1}. \qquad \square \end{aligned}$$

The subindex Λ^1 will be omitted when it is clear from the context which are the scalar products considered.

The boundary $\partial\Omega$ of the Riemannian manifold $(\Omega, \partial\Omega, \eta)$ has itself the structure of a Riemannian manifold without boundary $(\partial\Omega, \partial\eta)$. The Riemannian metric induced at the boundary is just the pull-back of the Riemannian metric $\partial\eta = i^\star\eta$, where $i : \partial\Omega \to \Omega$

is the inclusion map. The spaces of smooth functions over the two manifolds verify that $\mathcal{C}^\infty(\Omega)|_{\partial\Omega} \simeq \mathcal{C}^\infty(\partial\Omega)$.

There is an important relation between the Sobolev spaces defined over the manifolds Ω and $\partial\Omega$. This is the well-known Lions trace theorem (cf. [2, Theorem 7.39], [31, Theorem 8.3]):

Theorem 2.11 *(Lions trace theorem). Let $\Phi \in \mathcal{C}^\infty(\Omega)$ and let $\gamma : \mathcal{C}^\infty(\Omega) \to \mathcal{C}^\infty(\partial\Omega)$ be the trace map $\gamma(\Phi) = \Phi|_{\partial\Omega}$. There is a unique continuous extension of the trace map such that*

i) $\gamma : \mathcal{H}^k(\Omega) \to \mathcal{H}^{k-1/2}(\partial\Omega)$, $k > 1/2$.
ii) *The map is surjective.*

Finally we introduce for later use some particular operators associated with the Laplacian. Consider the symmetric operator on smooth functions with support away from the boundary $\Delta_0 := \Delta_\eta|_{\mathcal{C}_c^\infty(\Omega)}$. Then we have the following extensions of it.

Definition 2.12.

i) The **minimal closed extension** $\Delta_{\min}$ is defined to be the closure of Δ_0. Its domain is $\mathcal{D}(\Delta_{\min}) = \mathcal{H}_0^2 := \overline{\mathcal{C}_c^\infty(\Omega)}^{\|\cdot\|_2}$.
ii) The **maximal closed extension** $\Delta_{\max}$ is the closed operator defined in the domain $\mathcal{D}(\Delta_{\max}) = \{\Phi \in \mathcal{H}^0(\Omega) | \Delta_\eta\Phi \in \mathcal{H}^0(\Omega)\}$.

Equivalently, one can define $\Delta_{\max}$ as the adjoint of $\Delta_{\min}$.

The trace map defined in Theorem 2.11 can be extended continuously to $\mathcal{D}(\Delta_{\max})$, see for instance [14,17,31]:

Theorem 2.13 *(Weak trace theorem for the Laplacian). The Sobolev space $\mathcal{H}^k(\Omega)$, with $k \geq 2$, is dense in $\mathcal{D}(\Delta_{\max})$ and there is a unique continuous extension of the trace map γ such that*

$$\gamma : \mathcal{D}(\Delta_{\max}) \to H^{-1/2}(\partial\Omega).$$

Moreover, $\ker\gamma = H_0^2(\Omega)$.

3. A class of closable quadratic forms on a Riemannian manifold

We begin presenting a canonical sesquilinear form that, on smooth functions over Ω, is associated with the Laplace–Beltrami operator. Motivated by this quadratic form we will address questions like hermiticity, closability and semi-boundedness on suitable domains.

Integrating once by parts the expression $\langle\Phi, -\Delta_\eta\Psi\rangle$ we obtain, on smooth functions, the following sesquilinear form $Q : \mathcal{C}^\infty(\Omega) \times \mathcal{C}^\infty(\Omega) \to \mathbb{C}$,

$$Q(\Phi, \Psi) = \langle \mathrm{d}\Phi, \mathrm{d}\Psi \rangle_{\Lambda^1} - \langle \varphi, \dot{\psi} \rangle_{\partial\Omega}. \tag{3.1}$$

From now on the restrictions to the boundary are going to be denoted with the corresponding small size Greek letters, $\varphi := \gamma(\Phi)$. The doted small size Greek letters denote the restriction to the boundary of the normal derivatives, $\dot{\varphi} := \gamma(\mathrm{d}\Phi(\nu))$, where $\nu \in \mathfrak{X}(\Omega)$ is any vector field such that $\mathrm{i}_\nu \mathrm{d}\mu_\eta = \mathrm{d}\mu_{\partial\eta}$. Notice that in the expression above $\mathrm{d}\Phi \in \Lambda^1(\Omega)$ is a 1-form on Ω, thus the inner product $\langle \cdot, \cdot \rangle_{\Lambda^1}$ is defined accordingly by using, $\eta^{-1}(\cdot, \cdot)$, the induced Hermitian structure on the cotangent bundle (see, e.g., [36]). We have therefore that

$$\langle \mathrm{d}\Phi, \mathrm{d}\Psi \rangle_{\Lambda^1} = \int_\Omega \eta^{-1}(\mathrm{d}\bar{\Phi}, \mathrm{d}\Psi) \mathrm{d}\mu_\eta.$$

In the second term at the right-hand side of (3.1) $\langle \cdot, \cdot \rangle_{\partial\Omega}$ stands for the induced scalar product at the boundary given explicitly by

$$\langle \varphi, \psi \rangle_{\partial\Omega} = \int_{\partial\Omega} \bar{\varphi} \psi \mathrm{d}\mu_{\partial\eta}, \tag{3.2}$$

where $\mathrm{d}\mu_{\partial\eta}$ is the Riemannian volume defined by the restricted Riemannian metric $\partial\eta$. The subscript Λ^1 will be dropped from now on as along as there is no risk of confusion.

In general, the sesquilinear form Q defined above is not Hermitian. To study subspaces where Q is Hermitian it is convenient to isolate the part of Q related to the boundary data $(\varphi, \dot{\varphi})$.

Definition 3.1. Let $\Phi, \Psi \in \mathcal{C}^\infty(\Omega)$ and denote by $(\varphi, \dot{\varphi})$, $(\psi, \dot{\psi})$ the corresponding boundary data. The **Lagrange boundary form** is defined as:

$$\Sigma(\Phi, \Psi) = \Sigma\big((\varphi, \dot{\varphi}), (\psi, \dot{\psi})\big) := \langle \varphi, \dot{\psi} \rangle_{\partial\Omega} - \langle \dot{\varphi}, \psi \rangle_{\partial\Omega}. \tag{3.3}$$

Any dense subspace $\mathcal{D} \subset \mathcal{H}^0(\Omega)$ is said to be **isotropic with respect to** Σ if $\Sigma(\Phi, \Psi) = 0$ $\forall \Phi, \Psi \in \mathcal{D}$.

Proposition 3.2. *The sesquilinear form Q defined in Eq. (3.1) on a dense subspace $\mathcal{D} \subset \mathcal{H}^0$ is Hermitian iff $\mathcal{D}$ is isotropic with respect to Σ.*

Proof. The sesquilinear form $Q : \mathcal{D} \times \mathcal{D} \to \mathbb{C}$ is Hermitian if $Q(\Phi, \Psi) = \overline{Q(\Psi, \Phi)}$ for all $\Phi, \Psi \in \mathcal{D}$. By definition of Q this is equivalent to $\Sigma(\Phi, \Psi) = 0$, for all $\Phi, \Psi \in \mathcal{D}$, hence $\mathcal{D}$ is isotropic with respect to Σ. The reverse implication is obvious. □

3.1. Isotropic subspaces

The analysis of maximally isotropic subspaces can be handled more easily using the underlying Hilbert space structure of the Lagrange boundary form and not considering for the moment any regularity questions. The expression (3.3) can be understood as a sesquilinear form on the boundary Hilbert space $\mathcal{H}_b := \mathcal{H}^0(\partial\Omega) \times \mathcal{H}^0(\partial\Omega)$,

$$\Sigma(\Psi, \Phi) = \langle \varphi, \dot{\psi} \rangle_{\partial\Omega} - \langle \dot{\varphi}, \psi \rangle_{\partial\Omega}.$$

We will therefore focus now on the study of the sesquilinear form on the Hilbert space $\mathcal{H}_b$ and, while there is no risk of confusion, we will denote the scalar product in $\mathcal{H}^0(\partial\Omega)$ simply as $\langle\cdot,\cdot\rangle$,

$$\Sigma\big((\varphi_1, \varphi_2), (\psi_1, \psi_2)\big) := \langle \varphi_1, \psi_2 \rangle - \langle \varphi_2, \psi_1 \rangle, \quad (\varphi_1, \varphi_2), (\psi_1, \psi_2) \in \mathcal{H}_b.$$

Formally, Σ is a sesquilinear symplectic form by which we mean that it satisfies the following conditions:

i) Σ is conjugate linear in the first argument and linear in the second.
ii) $\Sigma((\varphi_1, \varphi_2), (\psi_1, \psi_2)) = -\overline{\Sigma((\psi_1, \psi_2), (\varphi_1, \varphi_2))}$, $(\varphi_1, \varphi_2), (\psi_1, \psi_2) \in \mathcal{H}_b$.
iii) Σ is nondegenerate, i.e., $\Sigma((\varphi_1, \varphi_2), (\psi_1, \psi_2)) = 0$ for all $(\psi_1, \psi_2) \in \mathcal{H}_b$ implies $(\varphi_1, \varphi_2) = (0, 0)$.

The analysis of the isotropic subspaces of such sesquilinear forms is by no means new and their characterization is well known [12,28]. However, in order to keep this article self-contained, we provide in the following paragraphs independent proofs of the main results that we will need.

First we write the sesquilinear symplectic form Σ in diagonal form. This is done introducing the unitary Cayley transformation $\mathcal{C} : \mathcal{H}_b \to \mathcal{H}_b$,

$$\mathcal{C}(\varphi_1, \varphi_2) := \frac{1}{\sqrt{2}}(\varphi_1 + \mathbf{i}\varphi_2, \varphi_1 - \mathbf{i}\varphi_2), \quad (\varphi_1, \varphi_2) \in \mathcal{H}_b.$$

Putting

$$\Sigma_c\big((\varphi_+, \varphi_-), (\psi_+, \psi_-)\big) := -\mathbf{i}\big(\langle \varphi_+, \psi_+ \rangle - \langle \varphi_-, \psi_- \rangle\big), \quad (\varphi_+, \varphi_-), (\psi_+, \psi_-) \in \mathcal{H}_b,$$

the relation between Σ and Σ_c is given by

$$\Sigma\big((\varphi_1, \varphi_2), (\psi_1, \psi_2)\big) = \Sigma_c\big(\mathcal{C}(\varphi_1, \varphi_2), \mathcal{C}(\psi_1, \psi_2)\big), \quad (\varphi_1, \varphi_2), (\psi_1, \psi_2) \in \mathcal{H}_b. \tag{3.4}$$

Definition 3.3. Consider a subspace $\mathcal{W} \subset \mathcal{H}_b$ and define the **Σ-orthogonal subspace** by

$$\mathcal{W}^{\perp_\Sigma} := \big\{(\varphi_1, \varphi_2) \in \mathcal{H}_b \bigm| \Sigma\big((\varphi_1, \varphi_2), (\psi_1, \psi_2)\big) = 0,\ \forall (\psi_1, \psi_2) \in \mathcal{W}\big\}.$$

A subspace $\mathcal{W} \subset \mathcal{H}_b$ is **Σ-isotropic** [resp. **maximally Σ-isotropic**] if $\mathcal{W} \subset \mathcal{W}^{\perp_\Sigma}$ [resp. $\mathcal{W} = \mathcal{W}^{\perp_\Sigma}$].

We begin enumerating some direct consequences of the preceding definitions:

Lemma 3.4. *Let $\mathcal{W} \subset \mathcal{H}_b$ and put $\mathcal{W}_c := \mathcal{C}(\mathcal{W})$.*

i) *$\mathcal{W}$ is Σ-isotropic [resp. maximally Σ-isotropic] iff $\mathcal{W}_c$ is Σ_c-isotropic [resp. maximally Σ_c-isotropic].*
ii) *If $(\varphi_1, \varphi_2) \in \mathcal{W} \subset \mathcal{W}^{\perp_\Sigma}$, then $\langle \varphi_1, \varphi_2 \rangle = \overline{\langle \varphi_1, \varphi_2 \rangle}$. If $(\varphi_+, \varphi_-) \in \mathcal{W}_c \subset \mathcal{W}_c^{\perp_{\Sigma_c}}$, then $\|\varphi_+\| = \|\varphi_-\|$.*

Proof. Part (i) follows directly from Eq. (3.4) and the fact that $\mathcal{C}$ is a unitary transformation. To prove (ii) note that if (φ_1, φ_2) is in an isotropic subspace $\mathcal{W}$, then

$$\Sigma\big((\varphi_1, \varphi_2), (\varphi_1, \varphi_2)\big) = \langle \varphi_1, \varphi_2 \rangle - \langle \varphi_2, \varphi_1 \rangle = 0.$$

One argues similarly in the other case. □

Proposition 3.5. *Let $\mathcal{W}_\pm \subset \mathcal{H}^0(\partial\Omega)$ be closed subspaces and put $\mathcal{W}_c := \mathcal{W}_+ \times \mathcal{W}_- \subset \mathcal{H}_b$.*

i) *The subspace $\mathcal{W}_c$ is Σ_c-isotropic iff there exists a partial isometry $V : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ with initial space $\mathcal{W}_+$ and final space $\mathcal{W}_-$, i.e., $V^*V(\mathcal{H}^0(\partial\Omega)) = \mathcal{W}_+$ and $VV^*(\mathcal{H}^0(\partial\Omega)) = \mathcal{W}_-$ and*

$$\mathcal{W}_c = \big\{(\varphi_+, V\varphi_+) \bigm| \varphi_+ \in \mathcal{W}_+\big\} = \operatorname{gra} V.$$

ii) *The subspace $\mathcal{W}_c$ is maximally Σ_c-isotropic iff there exists a unitary $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ such that*

$$\mathcal{W}_c = \big\{(\varphi_+, U\varphi_+) \bigm| \varphi_+ \in \mathcal{H}^0(\partial\Omega)\big\} = \operatorname{gra} U. \tag{3.5}$$

Proof. (i) For any $(\varphi_+, \varphi_-) \in \mathcal{W}_c$ we define the mapping $V : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ by $V(\varphi_+) := \varphi_-$, $\varphi_+ \in \mathcal{W}_+$ and $V(\varphi) = 0$, $\varphi \in \mathcal{W}_+^\perp$. Since $\mathcal{W}_c \subset \mathcal{W}_c^{\perp_{\Sigma_c}}$ we have from part (ii) of Lemma 3.4 that V is a well-defined linear map and a partial isometry. The reverse implication is immediate: For any $(\varphi_+, V\varphi_+) \in \mathcal{W}_c$ we have

$$\Sigma_c\big((\varphi_+, V\varphi_+), (\psi_+, V\psi_+)\big) = -\mathbf{i}\big(\langle \varphi_+, \psi_+ \rangle - \langle V\varphi_+, V\psi_+ \rangle\big) = 0, \quad \psi_+ \in \mathcal{H}^0(\partial\Omega),$$

hence, $\mathcal{W}_c = \{(\varphi_+, V\varphi_+) \mid \varphi_+ \in \mathcal{W}_+\} = \operatorname{gra} V$ is Σ_c-isotropic.

(ii) Suppose that $\mathcal{W}_c = \mathcal{W}_c^{\perp_{\Sigma_c}}$. By the previous item we have $\mathcal{W}_c = \{(\varphi_+, U\varphi_+) \mid \varphi_+ \in \mathcal{W}_+\}$ for some partial isometry $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$. Consider the following decompositions $\mathcal{H}^0(\partial\Omega) = \mathcal{W}_+ \oplus \mathcal{W}_+^\perp = (U\mathcal{W}_+) \oplus (U\mathcal{W}_+)^\perp$ and note that any $(\varphi_+^\perp, \varphi_-^\perp) \in \mathcal{W}_+^\perp \times (U\mathcal{W}_+)^\perp$ satisfies $(\varphi_+^\perp, \varphi_-^\perp) \in \mathcal{W}_c^{\perp_{\Sigma_c}}$. Since $\mathcal{W}_c = \mathcal{W}_c^{\perp_{\Sigma_c}}$ we must have $\varphi_+^\perp = \varphi_-^\perp = 0$, or, equivalently, $\mathcal{W}_+ = \mathcal{H}^0(\partial\Omega) = U\mathcal{W}_+$, hence $\ker U = \ker U^* = \{0\}$ and U is a unitary map.

To prove the reverse implication consider $\mathcal{W}_c = \{(\varphi_+, U\varphi_+) \mid \varphi_+ \in \mathcal{H}^0(\partial\Omega)\}$ with U unitary and choose $(\psi_+, \psi_-) \in \mathcal{W}_c^{\perp_{\Sigma_c}}$. Then for any $\varphi_+ \in \mathcal{H}^0(\partial\Omega)$ we have

$$
\begin{aligned}
0 &= \Sigma_c\big((\varphi_+, U\varphi_+), (\psi_+, \psi_-)\big) = -\mathbf{i}\big(\langle \varphi_+, \psi_+\rangle - \langle U\varphi_+, \psi_-\rangle\big) \\
&= -\mathbf{i}\big(\langle \varphi_+, (\psi_+ - U^*\psi_-)\rangle\big).
\end{aligned}
$$

This shows that $\psi_- = U\psi_+$ and hence $(\psi_+, \psi_-) \in \mathcal{W}_c$, therefore $\mathcal{W}_c$ is maximally Σ_c-isotropic. □

The previous analysis allows to characterize finally the Σ-isotropic subspaces of the boundary Hilbert space $\mathcal{H}_b$.

Theorem 3.6. *A closed subspace $\mathcal{W} \subset \mathcal{H}_b$ is maximally Σ-isotropic iff there exists a unitary $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ such that*

$$
\mathcal{W} = \big\{\big((\mathbb{I} + U)\varphi, -\mathbf{i}(\mathbb{I} - U)\varphi\big) \bigm| \varphi \in \mathcal{H}^0(\partial\Omega)\big)\big\}.
$$

Proof. By Lemma 3.4(i) and Proposition 3.5(ii) we have that $\mathcal{W}$ is maximally Σ-isotropic iff $\mathcal{W} = \mathcal{C}^{-1}\mathcal{W}_c$, where $\mathcal{W}_c$ is given by Eq. (3.5). □

Proposition 3.7. *Let $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ be a unitary operator and consider the maximally isotropic subspace $\mathcal{W}$ given in Theorem 3.6. Then $\mathcal{W}$ can be rewritten as*

$$
\mathcal{W} = \big\{(\varphi_1, \varphi_2) \in \mathcal{H}_b \bigm| \varphi_1 - \mathbf{i}\varphi_2 = U(\varphi_1 + \mathbf{i}\varphi_2)\big\}. \tag{3.6}
$$

Proof. Let $\mathcal{W}$ be given as in Theorem 3.6 and let $\mathcal{W}'$ be a subspace defined as in Eq. (3.6). Put $\varphi_1 := (\mathbb{I}+U)\varphi$ and $\varphi_2 := -\mathbf{i}(\mathbb{I}-U)\varphi$. Then it is straightforward to verify that (φ_1, φ_2) satisfy the relation defining Eq. (3.6) and therefore $\mathcal{W} \subset \mathcal{W}'$.

Consider a subspace $\mathcal{W}'$ defined as in Eq. (3.6) and let $(\varphi_1, \varphi_2) \in \mathcal{W}'$. Then the following relation holds

$$
(1 - U)\varphi_1 - \mathbf{i}(1 + U)\varphi_2 = 0. \tag{3.7}
$$

Now consider that $(\varphi_1, \varphi_2) \in \mathcal{W}^\perp$. Then for all $\varphi \in \mathcal{H}^0(\partial\Omega)$

$$
\begin{aligned}
0 &= \big\langle \varphi_1, (1 + U)\varphi\big\rangle + \big\langle \varphi_2, -\mathbf{i}(1 - U)\varphi\big\rangle \\
&= \big\langle \big(1 + U^*\big)\varphi_1 + \mathbf{i}\big(1 - U^*\big)\varphi_2, \varphi\big\rangle
\end{aligned}
$$

and therefore

$$
\big(1 + U^*\big)\varphi_1 + \mathbf{i}\big(1 - U^*\big)\varphi_2 = 0. \tag{3.8}
$$

Now we can arrange Eqs. (3.7) and (3.8)

$$M\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix} := \begin{pmatrix}1-U & -\mathbf{i}(1+U)\\ 1+U^* & \mathbf{i}(1-U^*)\end{pmatrix}\begin{pmatrix}\varphi_1\\ \varphi_2\end{pmatrix} = 0, \tag{3.9}$$

where now $M : \mathcal{H}_b \to \mathcal{H}_b$. But clearly M is a unitary operator so that Eq. (3.9) implies that $(\varphi_1, \varphi_2) = 0$ and therefore $\mathcal{W} \oplus \mathcal{W}'^{\perp} = (\mathcal{W}^{\perp} \bigcap \mathcal{W}')^{\perp} = \mathcal{H}_b$. This condition together with $\mathcal{W} \subset \mathcal{W}'$ implies $\mathcal{W} = \mathcal{W}'$ because $\mathcal{W}$ is a closed subspace, as it is easy to verify. □

3.2. Admissible unitaries and closable quadratic forms

In this subsection we will restrict to a family of unitaries $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ that will allow us to describe a wide class of quadratic forms whose Friedrichs' extensions are associated with self-adjoint extensions of the Laplace–Beltrami operator.

Definition 3.8. Let $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ be unitary and denote by $\sigma(U)$ its spectrum. We say that the unitary U on the boundary **has gap at** -1 if one of the following conditions holds:

i) $\mathbb{I} + U$ is invertible.
ii) $-1 \in \sigma(U)$ and -1 is not an accumulation point of $\sigma(U)$.

Definition 3.9. Let U be a unitary operator acting on $\mathcal{H}^0(\partial\Omega)$ with gap at -1. Let E_λ be the spectral resolution of the identity associated with the unitary U, i.e.,

$$U = \int_{[0,2\pi]} e^{\mathbf{i}\lambda} \mathrm{d}E_\lambda.$$

The **invertibility boundary space** W is defined by $W = \operatorname{Ran} E^{\perp}_{\{\pi\}}$. The orthogonal projection onto W is denoted by P.

Definition 3.10. Let U be a unitary operator acting on $\mathcal{H}^0(\partial\Omega)$ with gap at -1. The **partial Cayley transform** $A_U : \mathcal{H}^0(\partial\Omega) \to W$ is the operator

$$A_U := \mathbf{i}P(U - \mathbb{I})(U + \mathbb{I})^{-1}.$$

Proposition 3.11. *The partial Cayley transform is a bounded, self-adjoint operator on* $\mathcal{H}^0(\partial\Omega)$.

Proof. First notice that the operators P, U and A_U commute. That A_U is bounded is a direct consequence of the Definition 3.8, because the operator $P(\mathbb{I} + U)$ is under these assumptions an invertible bounded operator on the boundary space W. To show that A_U is self-adjoint consider the spectral resolution of the identity of the operator U. Since U has gap at -1, either $\{e^{\mathbf{i}\pi}\} \notin \sigma(U)$ or there exists a neighborhood V of $\{e^{\mathbf{i}\pi}\}$ such that it does not contain any element of the spectrum $\sigma(U)$ besides $\{e^{\mathbf{i}\pi}\}$. Pick $\delta \in V \cap S^1$.

Then one can express the operator A_U using the spectral resolution of the identity of the operator U as

$$A_U = \int_{-\pi+\delta}^{\pi-\delta} \mathbf{i}\frac{e^{\mathbf{i}\lambda} - 1}{e^{\mathbf{i}\lambda} + 1}\mathrm{d}E_\lambda = \int_{-\pi+\delta}^{\pi-\delta} -\tan\frac{\lambda}{2}\mathrm{d}E_\lambda.$$

Since $\lambda \in [-\pi+\delta, \pi-\delta]$, then $\tan\frac{\lambda}{2} \in \mathbb{R}$. Therefore the spectrum of A_U is a subset of the real line, necessary and sufficient condition for a closed, symmetric operator to be self-adjoint. □

We can now introduce the class of closable quadratic forms that was announced at the beginning of this section.

Definition 3.12. Let U be a unitary with gap at -1, A_U the corresponding partial Cayley transform and γ the trace map considered in Theorem 2.11. The Hermitian quadratic form associated with the unitary U is defined by

$$Q_U(\Phi, \Psi) = \langle \mathrm{d}\Phi, \mathrm{d}\Psi \rangle - \big\langle \gamma(\Phi), A_U\gamma(\Phi) \big\rangle_{\partial\Omega}$$

on the domain

$$\mathcal{D}_U = \big\{ \Phi \in \mathcal{H}^1(\Omega) \;\big|\; P^\perp\gamma(\Phi) = 0 \big\}.$$

Proposition 3.13. *The quadratic form Q_U is bounded by the Sobolev norm of order* 1*,*

$$Q_U(\Phi, \Psi) \leq K\|\Phi\|_1\|\Psi\|_1.$$

Proof. That the first summand of Q_U is bounded by the $\mathcal{H}^1(\Omega)$ norm is direct consequence of the Cauchy–Schwarz inequality and Proposition 2.10.

For the second term we have that

$$\begin{aligned} \big|\big\langle \gamma(\Phi), A_U\gamma(\Psi) \big\rangle_{\partial\Omega}\big| &\leq \|A_U\| \cdot \big\|\gamma(\Phi)\big\|_0 \|\gamma(\Psi)\|_0 \\ &\leq C\|A_U\| \cdot \big\|\gamma(\Phi)\big\|_{\frac{1}{2}} \|\gamma(\Psi)\|_{\frac{1}{2}} \\ &\leq C'\|A_U\| \cdot \|\Phi\|_1\|\Psi\|_1, \end{aligned}$$

where we have used Theorem 2.11 in the last inequality. □

Finally, we need an additional condition of admissibility on the unitaries on the boundary that will be needed to prove the closability of Q_U.

Definition 3.14. Let U be a unitary with gap at -1. The unitary is said to be **admissible** if the partial Cayley transform $A_U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ is continuous with respect to the Sobolev norm of order 1/2, i.e.,

$$\|A\varphi\|_{\mathcal{H}^{1/2}(\partial\Omega)} \leq K\|\varphi\|_{\mathcal{H}^{1/2}(\partial\Omega)}.$$

Example 3.15. Consider a manifold with boundary given by the unit circle, i.e., $\partial\Omega = S^1$, and define the unitary $(U_\beta\varphi)(z) := e^{i\beta(z)}\varphi(z)$, $\varphi \in L^2(S^1)$. If $\beta \in L^2(S^1)$ and $\operatorname{ran}\beta \subset \{\pi\} \cup [0, \pi - \delta] \cup [\pi + \delta, 2\pi)$, for some $\delta > 0$, then U_β has gap at -1. If, in addition, $\beta \in C^\infty(S^1)$, then U_β is admissible.

4. Closable and semi-bounded quadratic forms

This section addresses the questions of semi-boundedness and closability of the quadratic form Q_U defined on its domain $\mathcal{D}_U$ (cf. Definition 3.12).

4.1. Functions and operators on collar neighborhoods

We will need first some technical results that refer to the functions and operators in a collar neighborhood close to the compact boundary $\partial\Omega$ and that we will denote by Ξ. Recall the conventions at the beginning of Section 3: If $\Phi \in \mathcal{H}^1(\Omega)$, then $\varphi = \gamma(\Phi)$ denotes its restriction to $\partial\Omega$ and for Φ smooth, $\dot{\varphi}$ is the restriction to the boundary of the normal derivative.

Lemma 4.1. *Let $\Phi \in \mathcal{H}^1(\Omega)$ and $f \in \mathcal{H}^{1/2}(\partial\Omega)$. Then, for every $\epsilon > 0$ there exists $\tilde{\Phi} \in \mathcal{C}^\infty(\Omega)$ such that $\|\Phi - \tilde{\Phi}\|_1 < \epsilon$, $\|\varphi - \tilde{\varphi}\|_{\mathcal{H}^{1/2}(\partial\Omega)} < \epsilon$ and $\|f - \dot{\tilde{\varphi}}\|_{\mathcal{H}^{1/2}(\partial\Omega)} < \epsilon$.*

Proof. The first two inequalities are standard (cf., Theorem 2.11). Moreover, it is enough to consider $\Phi \in \mathcal{C}^\infty(\Omega)$ with $\mathrm{d}\Phi(\nu) \equiv 0$, where $\nu \in \mathfrak{X}(\Omega)$ is the normal vector field, on a collar neighborhood Ξ of $\partial\Omega$ (see [23, Chapter 4] for details on such neighborhoods). According to the proof of [13, Theorem 7.2.1] this is a dense subset of $\mathcal{H}^1(\Omega)$. The compactness assumption on the boundary $\partial\Omega$ ensures that the collar neighborhood has a minimal width δ. Without loss of generality we can consider that the collar neighborhood Ξ has Gaussian coordinates $\mathbf{x} = (r, \boldsymbol{\theta})$, being $\frac{\partial}{\partial r}$ the normal vector field pointing outwards. In particular, we have that $\Xi \simeq [-\delta, 0] \times \partial\Omega$ and $\partial\Omega \simeq \{0\} \times \partial\Omega$. Moreover, it is enough to restrict to $f \in \mathcal{H}^1(\partial\Omega)$, because $\mathcal{H}^1(\partial\Omega)$ is dense in $\mathcal{H}^{1/2}(\partial\Omega)$.

Consider a smooth function $g \in \mathcal{C}^\infty(\mathbb{R})$ with the following properties:

- $g(0) = 1$ and $g'(0) = -1$.
- $g(s) \equiv 0$, $s \in [2, \infty)$.
- $|g(s)| \leq 1$ and $|g'(s)| \leq 1$.

Define now the rescaled functions $g_n(r) := \frac{1}{n}g(-nr)$. Let $\{f_n(\boldsymbol{\theta})\}_n \subset \mathcal{C}^\infty(\partial\Omega)$ be any sequence such that $\|f_n - f\|_{\mathcal{H}^1(\partial\Omega)} \to 0$. Now consider the smooth functions

$$\tilde{\Phi}_n(\mathbf{x}) := \Phi(\mathbf{x}) + g_n(r)f_n(\boldsymbol{\theta}). \tag{4.1}$$

Clearly we have that $\dot{\tilde{\varphi}}_n(\boldsymbol{\theta}) \equiv f_n(\boldsymbol{\theta})$ and therefore $\|\dot{\tilde{\varphi}}_n - f\|_{\mathcal{H}^1(\partial\Omega)} \to 0$ as needed. Now we are going to show that $\tilde{\Phi}_n \xrightarrow{\mathcal{H}^1} \Phi$. According to Proposition 2.10 it is enough to show that the functions and all their first derivatives converge in the $\mathcal{H}^0(\Omega)$ norm.

$$\begin{aligned}
\big\|\tilde{\Phi}_n(\mathbf{x}) - \Phi(\mathbf{x})\big\|_{\mathcal{H}^0(\Omega)} &= \big\|g_n(r)f_n(\boldsymbol{\theta})\big\|_{\mathcal{H}^0(\Omega)} \\
&\leq M\big\|g_n(r)\big\|_{\mathcal{H}^0(-\frac{2}{n},0)}\|f_n\|_{\mathcal{H}^0(\partial\Omega)} \\
&\leq M\frac{\sqrt{2}}{n^{3/2}}\|f_n\|_{\mathcal{H}^0(\partial\Omega)}; &\text{(4.2a)}\\
\left\|\frac{\partial}{\partial r}\tilde{\Phi}_n(\mathbf{x}) - \frac{\partial}{\partial r}\Phi(\mathbf{x})\right\|_{\mathcal{H}^0(\Omega)} &= \left\|\frac{\partial}{\partial r}g_n(r)f_n(\theta)\right\|_{\mathcal{H}^0(\Omega)} \\
&\leq M\|\frac{\partial}{\partial r}g_n(r)\|_{\mathcal{H}^0(-\frac{2}{n},0)}\|f_n\|_{\mathcal{H}^0(\partial\Omega)} \\
&\leq M\frac{\sqrt{2}}{n^{1/2}}\|f_n\|_{\mathcal{H}^0(\partial\Omega)}; &\text{(4.2b)}\\
\left\|\frac{\partial}{\partial\theta}\tilde{\Phi}_n(\mathbf{x}) - \frac{\partial}{\partial\theta}\Phi(\mathbf{x})\right\|_{\mathcal{H}^0(\Omega)} &= \left\|g_n(r)\frac{\partial}{\partial\theta}f_n(\boldsymbol{\theta})\right\|_{\mathcal{H}^0(\Omega)} \\
&\leq M\big\|g_n(r)\big\|_{\mathcal{H}^0(-\frac{2}{n},0)}\left\|\frac{\partial}{\partial\theta}f_n(\boldsymbol{\theta})\right\|_{\mathcal{H}^0(\partial\Omega)} \\
&\leq \frac{\sqrt{2}}{n^{3/2}}M'\|f_n\|_{\mathcal{H}^1(\partial\Omega)}. &\text{(4.2c)}
\end{aligned}$$

The constant M depends only on the Riemannian metric. The constant M' in the last inequality comes from the fact that $\|\partial_\theta f_n\|_{\mathcal{H}^0(\partial\Omega)} \leq \tilde{M}\|f_n\|_{\mathcal{H}^1(\partial\Omega)}$. Since $\{f_n(\boldsymbol{\theta})\}$ is a convergent sequence in $\mathcal{H}^1(\partial\Omega)$ the norms appearing at the right-hand sides are bounded. □

Lemma 4.2. *Let $\Phi \in \mathcal{H}^1(\Omega)$ and $c \in \mathbb{R}$. Then for every $\epsilon > 0$ there exists a $\tilde{\Phi} \in \mathcal{C}^\infty(\Omega)$ with $\dot{\tilde{\varphi}} = c\tilde{\varphi}$ such that $\|\Phi - \tilde{\Phi}\|_1 < \epsilon$.*

Proof. As in the proof of the preceding lemma it is enough to approximate any smooth function Φ with vanishing normal derivative in a collar neighborhood.

Consider a smooth function $g \in \mathcal{C}^\infty(\mathbb{R})$ with the following properties:

- $g(0) = 0$ and $g'(0) = -1$.
- $g(s) \equiv 0$, $s \in [2, \infty)$.
- $|g(s)| \leq 1$ and $|g'(s)| \leq 1$.

Notice the difference in the definition of this function with the one in the previous lemma. Define the rescaled functions $g_n(r) := \frac{1}{n}g(-nr)$. Pick now a sequence of smooth functions

$$\tilde{\Phi}_n(\mathbf{x}) := \Phi(\mathbf{x}) + c\Phi(0,\boldsymbol{\theta})g_n(r),$$

This family of functions clearly verifies the boundary condition $\dot{\tilde{\varphi}} = c\tilde{\varphi}$. The inequalities (4.2) now read

$$\begin{aligned}
\big\|\tilde{\Phi}_n(\mathbf{x}) - \Phi(\mathbf{x})\big\|_{\mathcal{H}^0(\Omega)} &= \big\|cg_n(r)\Phi(0,\boldsymbol{\theta})\big\|_{\mathcal{H}^0(\Omega)} \\
&\leq cM\big\|g_n(r)\big\|_{\mathcal{H}^0(-\frac{2}{n},0)}\big\|\Phi(0,\boldsymbol{\theta})\big\|_{\mathcal{H}^0(\partial\Omega)} \\
&\leq cM\frac{\sqrt{2}}{n^{3/2}}\big\|\Phi(0,\boldsymbol{\theta})\big\|_{\mathcal{H}^0(\partial\Omega)}; \qquad (4.3a)
\end{aligned}$$

$$\begin{aligned}
\left\|\frac{\partial}{\partial r}\tilde{\Phi}_n(\mathbf{x}) - \frac{\partial}{\partial r}\Phi(\mathbf{x})\right\|_{\mathcal{H}^0(\Omega)} &= \left\|c\frac{\partial}{\partial r}g_n(r)\Phi(0,\boldsymbol{\theta})\right\|_{\mathcal{H}^0(\Omega)} \\
&\leq cM\left\|\frac{\partial}{\partial r}g_n(r)\right\|_{\mathcal{H}^0(-\frac{2}{n},0)}\big\|\Phi(0,\boldsymbol{\theta})\big\|_{\mathcal{H}^0(\partial\Omega)} \\
&\leq cM\frac{\sqrt{2}}{n^{1/2}}\big\|\Phi(0,\boldsymbol{\theta})\big\|_{\mathcal{H}^0(\partial\Omega)}; \qquad (4.3b)
\end{aligned}$$

$$\begin{aligned}
\left\|\frac{\partial}{\partial \theta}\tilde{\Phi}_n(\mathbf{x}) - \frac{\partial}{\partial \theta}\Phi(\mathbf{x})\right\|_{\mathcal{H}^0(\Omega)} &= \left\|cg_n(r)\frac{\partial}{\partial \theta}\Phi(0,\boldsymbol{\theta})\right\|_{\mathcal{H}^0(\Omega)} \\
&\leq cM\big\|g_n(r)\big\|_{\mathcal{H}^0(-\frac{2}{n},0)}\left\|\frac{\partial}{\partial \theta}\Phi(0,\boldsymbol{\theta})\right\|_{\mathcal{H}^0(\partial\Omega)} \\
&\leq cM\frac{\sqrt{2}}{n^{3/2}}\left\|\frac{\partial}{\partial \theta}\Phi(0,\boldsymbol{\theta})\right\|_{\mathcal{H}^1(\partial\Omega)}. \qquad (4.3c)
\end{aligned}$$

As in the previous lemma the constant M depends only on the Riemannian metric. □

Corollary 4.3. *Let $\{\Phi_n\}_n \subset \mathcal{H}^1(\Omega)$ and A_U be the partial Cayley transform of an admissible unitary U. Then there exists a sequence of smooth functions $\{\tilde{\Phi}_n\} \subset \mathcal{C}^\infty(\Omega)$ such that $\|\Phi_n - \tilde{\Phi}_n\|_{\mathcal{H}^1(\Omega)} < \frac{1}{n}$, $\|\varphi_n - \tilde{\varphi}_n\|_{\mathcal{H}^{1/2}(\partial\Omega)} < \frac{1}{n}$, and $\|\dot{\tilde{\varphi}}_n - A_U\tilde{\varphi}_n\|_{\mathcal{H}^{1/2}(\partial\Omega)} < \frac{1}{n}$.*

Proof. For Φ_{n_0}, $n_0 \in \mathbb{N}$, take the approximating smooth function $\tilde{\Phi}_{n_0}$ as in Lemma 4.1 with

$$f := A_U\varphi_{n_0} \in \mathcal{H}^{1/2}(\partial\Omega)$$

(note that since U is admissible we have indeed that $f \in \mathcal{H}^{1/2}(\partial\Omega)$, cf. Definition 3.14). Choose also $\epsilon > 0$ such that

$$\epsilon \leq \frac{1}{(1 + \|A_U\|_{\mathcal{H}^{1/2}(\partial\Omega)})n_0}$$

and note that this implies $\epsilon \leq \frac{1}{n_0}$. Then the first two inequalities follow directly from Lemma 4.1. Moreover, we also have

$$\begin{aligned}\|\dot{\tilde{\varphi}}_{n_0} - A_U\tilde{\varphi}_{n_0}\|_{\mathcal{H}^{1/2}(\partial\Omega)} &\leq \|\dot{\tilde{\varphi}}_{n_0} - A_U\varphi_{n_0}\|_{\mathcal{H}^{1/2}(\partial\Omega)} + \|A_U\varphi_{n_0} - A_U\tilde{\varphi}_{n_0}\|_{\mathcal{H}^{1/2}(\partial\Omega)} \\ &\leq \epsilon + \|A_U\|_{\mathcal{H}^{1/2}(\partial\Omega)}\|\varphi_{n_0} - \tilde{\varphi}_{n_0}\|_{\mathcal{H}^{1/2}(\partial\Omega)} \\ &\leq \big(1 + \|A_U\|_{\mathcal{H}^{1/2}(\partial\Omega)}\big)\epsilon \leq \frac{1}{n_0},\end{aligned}$$

which concludes the proof. □

For the analysis of the semi-boundedness and closability of the quadratic form $(Q_U, \mathcal{D}_U)$ defined in the previous section we need to analyze first the following one-dimensional problem in an interval. The operator is defined with Neumann conditions on one end of the interval and Robin-type conditions on the other end.

Definition 4.4. Consider the interval $I = [0, 2\pi]$ and a real constant $c \in \mathbb{R}$. Define the second order differential operator

$$R_c : \mathcal{D}(R_c) \to \mathcal{H}^0\big([0, 2\pi]\big) \quad \text{by } R_c = -\frac{\mathrm{d}^2}{\mathrm{d}r^2}$$

on the domain

$$\mathcal{D}(R_c) := \left\{\Phi \in \mathcal{C}^\infty(I) \;\middle|\; \frac{\partial\Phi}{\partial r}\bigg|_{r=0} = 0 \text{ and } \frac{\partial\Phi}{\partial r}\bigg|_{r=2\pi} = c\Phi|_{r=2\pi}\right\} \subset \mathcal{H}^0\big([0, 2\pi]\big).$$

Proposition 4.5. *The symmetric operator R_c of Definition 4.4 is essentially self-adjoint with discrete spectrum and semi-bounded below with lower bound Λ_0.*

Proof. It is well known that this operator together with this boundary conditions defines an essentially self-adjoint operator (see, e.g., [4,12,17,20]). We show next that its spectrum is semi-bounded below. Its closure is a self-adjoint extension of the Laplace operator defined on $\mathcal{H}_0^2[0, 2\pi]$. The latter operator has finite dimensional deficiency indices and its Dirichlet extension is known to have empty essential spectrum. According to [45, Theorem 8.18] all the self-adjoint extensions of a closed, symmetric operator with finite deficiency indices have the same essential spectrum and therefore the spectrum of R_c is discrete.

Consider now the following spectral problem:

$$R_c\Phi = \Lambda\Phi, \qquad \frac{\partial\Phi}{\partial r}\bigg|_{r=0} = 0, \qquad \frac{\partial\Phi}{\partial r}\bigg|_{r=2\pi} = c\Phi|_{r=2\pi}, \tag{4.4}$$

with c a real constant. On general solutions $\Phi(r) = Ae^{\mathbf{i}\lambda r} + Be^{-\mathbf{i}\lambda r}$ we impose the boundary conditions. For nonzero solutions we obtain the following relation

$$-(\mathbf{i}\lambda + c)e^{-\mathbf{i}2\pi\lambda} + (\mathbf{i}\lambda - c)e^{\mathbf{i}2\pi\lambda} = 0, \tag{4.5}$$

where $\Lambda = \lambda^2 \in \mathbb{R}$. The equation is symmetric under the interchange $\lambda \to -\lambda$. It is therefore enough to consider either $\lambda \geq 0$ or $\lambda = \mathbf{i}\mu$ with $\mu > 0$. These two choices correspond to the positive and negative eigenvalues, respectively. The imaginary part of Eq. (4.5) vanishes identically. If $\lambda \geq 0$ its real part takes the form

$$\tan 2\pi\lambda = -\frac{c}{\lambda},$$

which leads to infinite solutions for each $c \in \mathbb{R}$ and therefore there are infinite positive eigenvalues. If $\lambda = \mathbf{i}\mu$ we obtain from Eq. (4.5)

$$e^{-4\pi\mu} = \frac{\mu - c}{\mu + c}, \tag{4.6}$$

which has either no solution for $c < 0$, the trivial solution $\mu = 0$ for $c = 0$ and exactly one negative solution for $c > 0$. So the operator R_c is positive for $c \leq 0$ and semi-bounded below for $c > 0$. We denote the lowest possible eigenvalue by Λ_0. □

Definition 4.6. Consider the interval $I = [0, 2\pi]$ and let $\{\Gamma_i(\boldsymbol{\theta})\} \subset \mathcal{H}^0(\partial\Omega)$ be an orthonormal basis. Consider the following operator $\mathfrak{R}_c$ on the tensor product $\mathcal{H}^0(I) \otimes \mathcal{H}^0(\partial\Omega) \simeq \mathcal{H}^0(I \times \partial\Omega)$ given by

$$\mathfrak{R}_c : \mathcal{D}(\mathfrak{R}_c) \to \mathcal{H}^0(I) \otimes \mathcal{H}^0(\partial\Omega) \quad \text{where } \mathfrak{R}_c := R_c \otimes \mathbb{I},$$

on its natural domain

$$\mathcal{D}(\mathfrak{R}_c) = \left\{ \Phi \in \mathcal{H}^0(I) \otimes \mathcal{H}^0(\partial\Omega) \;\middle|\; \Phi = \sum_{i=1}^{n} \Phi_i(r)\Gamma_i(\boldsymbol{\theta}),\ n \in \mathbb{N},\ \Phi_i \in \mathcal{D}(R) \right\}.$$

Proposition 4.7. *The operator $\mathfrak{R}_c$ is essentially self-adjoint, semi-bounded below and has the same lower bound Λ_0 as the operator R_c of Proposition 4.5.*

Proof. Let $\Psi \in \ker(\mathfrak{R}_c^\dagger \mp \mathbf{i})$ and consider its decomposition in terms of the orthonormal basis $\{\Gamma_i(\theta)\} \subset \mathcal{H}^0(\partial\Omega)$ such that $\Psi = \sum_{i=1}^{\infty} \Psi(r)_i \Gamma_i(\boldsymbol{\theta})$. We have that $\langle \Psi, (\mathfrak{R}_c \pm \mathbf{i})\Phi\rangle = 0$ $\forall \Phi \in \mathcal{D}(\mathfrak{R}_c)$. In particular for any $\Phi = \Phi_{i_0}\Gamma_{i_0} \in \mathcal{D}(\mathfrak{R}_c)$. Then

$$\begin{aligned} 0 = \left\langle \Psi, (\mathfrak{R}_c \pm \mathbf{i})\Phi_{i_0}\Gamma_{i_0} \right\rangle &= \sum_{i=1}^{\infty} \left\langle \Psi_i, (R_c \pm \mathbf{i})\Phi_{i_0} \right\rangle_{\mathcal{H}^0(I)} \langle \Gamma_i, \Gamma_{i_0} \rangle_{\mathcal{H}^0(\partial\Omega)} \\ &= \left\langle \Psi_{i_0}, (R_c \pm \mathbf{i})\Phi_{i_0} \right\rangle_{\mathcal{H}^0(I)}, \quad \forall \Phi_{i_0} \in \mathcal{D}(R_c). \end{aligned}$$

This implies that $\Psi_{i_0} = 0$ because, by Proposition 4.5, R_c is essentially self-adjoint. Therefore $\Psi = 0$ and $\mathfrak{R}_c$ is essentially self-adjoint.

Finally we show the semi-boundedness condition. Using the orthonormality of the basis $\{\Gamma_i(\boldsymbol{\theta})\}$ and for any $\Phi \in \mathcal{D}(\mathfrak{R}_c)$ we have that

$$\begin{aligned}\langle \Phi, \mathfrak{R}_c \Phi \rangle_{\mathcal{H}^0(I\times\partial\Omega)} &= \sum_{i=1}^{n} \langle \Phi_i, R_c \Phi_i \rangle_{\mathcal{H}^0(I)} \geq \Lambda_0 \sum_{i=1}^{n} \langle \Phi_i, \Phi_i \rangle_{\mathcal{H}^0(I)} \\ &= \Lambda_0 \langle \Phi, \Phi \rangle_{\mathcal{H}^0(I\times\partial\Omega)}. \qquad \square\end{aligned}$$

4.2. Quadratic forms and extensions of the minimal Laplacian

We begin associating quadratic forms with some of the operators on a collar neighborhood of the precedent subsection.

Lemma 4.8. *Denote by Q_c the closed quadratic form represented by the closure of $\mathfrak{R}_c$. Then its domain $\mathcal{D}(Q_c)$ contains the Sobolev space of order 1. For any $\Phi \in \mathcal{H}^1(I\times\partial\Omega) \subset \mathcal{D}(Q_c)$ we have the expression*

$$Q_c(\Phi) = \int_{\partial\Omega} \left[\int_I \frac{\partial \bar{\Phi}}{\partial r} \frac{\partial \Phi}{\partial r} \mathrm{d}r - c\big|\gamma(\Phi)\big|^2 \right] \mathrm{d}\mu_{\partial\eta}.$$

Proof. Let $\Phi \in \mathcal{D}(\mathfrak{R}_c)$. Then we have, recalling the boundary conditions specified in the domain $\mathcal{D}(R_c)$ that

$$\begin{aligned} Q_c(\Phi) = \langle \Phi, \mathfrak{R}_c \Phi \rangle_{\mathcal{H}^0(I\times\partial\Omega)} &= \sum_i \langle \Phi_i, R_c \Phi_i \rangle_{\mathcal{H}^0(I)} \\ &= \sum_i \left\langle \frac{\partial \Phi_i}{\partial r}, \frac{\partial \Phi_i}{\partial r} \right\rangle_{\mathcal{H}^0(I)} - c\bar{\Phi}_i(0)\Phi_i(0) \\ &= \int_{\partial\Omega} \left[\int_I \frac{\partial \bar{\Phi}}{\partial r} \frac{\partial \Phi}{\partial r} \mathrm{d}r - c|\varphi|^2 \right] \mathrm{d}\mu_{\partial\eta}. \end{aligned} \tag{4.7}$$

Now it is easy to check that the graph norm of this quadratic form is dominated by the Sobolev norm of order 1, $\mathcal{H}^1(I \times \partial\Omega)$:

$$\begin{aligned} \|\Phi\|_{Q_c}^2 &= \big(1 + |\Lambda_0|\big) \|\Phi\|_{\mathcal{H}^0(I\times\partial\Omega)}^2 + Q_c(\Phi) \\ &\leq \big(1 + |\Lambda_0|\big) \|\Phi\|_{\mathcal{H}^0(I\times\partial\Omega)}^2 + \int_{\partial\Omega} \int_I \frac{\partial \bar{\Phi}}{\partial r} \frac{\partial \Phi}{\partial r} \mathrm{d}r \mathrm{d}\mu_{\partial\eta} + c\|\varphi\|_{\mathcal{H}^0(\partial\Omega)}^2 \\ &\leq \big(1 + |\Lambda_0|\big) \|\Phi\|_{\mathcal{H}^0(I\times\partial\Omega)}^2 + C\|\Phi\|_{\mathcal{H}^1(I\times\partial\Omega)}^2 \\ &\leq C' \|\Phi\|_{\mathcal{H}^1(I\times\partial\Omega)}^2, \end{aligned}$$

where in the second step we have used again the equivalence appearing in Proposition 2.10 and Theorem 2.11. The above inequality shows that $\overline{\mathcal{D}(\mathfrak{R}_c)}^{\|\cdot\|_1} \subset \mathcal{D}(Q_c)$.

Moreover, Lemma 4.2 states that $\mathcal{D}(\mathfrak{R}_c)$ is dense in $\mathcal{H}^1(I \times \partial\Omega)$. Hence the expression Eq. (4.7) holds also on $\mathcal{H}^1(I \times \partial\Omega)$. □

Theorem 4.9. *Let $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ be a unitary operator with gap at -1. Then the quadratic form Q_U of Definition 3.12 is semi-bounded from below.*

Proof. Let $(\Omega, \partial\Omega, \eta)$ be a Riemannian manifold with smooth, compact boundary. One can always select a collar neighborhood Ξ of the boundary with coordinates $(r, \boldsymbol{\theta})$ such that $\Xi \simeq [-L, 0] \times \partial\Omega$ and where

$$\eta(r, \boldsymbol{\theta}) = \begin{bmatrix} 1 & 0 \\ 0 & g(r, \boldsymbol{\theta}) \end{bmatrix}.$$

The normal vector field to the boundary is going to be $\frac{\partial}{\partial r}$. With this choice, the induced Riemannian metric at the boundary becomes $\partial\eta(\boldsymbol{\theta}) \equiv g(0, \boldsymbol{\theta})$. The thickness L of the collar neighborhood Ξ can be also selected such that there exists $\delta \ll 1$ that verifies

$$(1-\delta)\sqrt{|g(0,\boldsymbol{\theta})|} \leq \sqrt{|g(r,\boldsymbol{\theta})|} \leq (1+\delta)\sqrt{|g(0,\boldsymbol{\theta})|}. \tag{4.8}$$

The quadratic form Q_U can be adapted to this splitting. Let $\Phi \in \mathcal{D}_U \subset \mathcal{H}^1(\Omega)$. Obviously $\Phi|_\Xi \in \mathcal{H}^1(\Xi) \simeq \mathcal{H}^1(I \times \partial\Omega)$. In what follows, to simplify the notation and since there is no risk of confusion, the symbol Φ will stand for both $\Phi \in \mathcal{H}^1(\Omega)$ and $\Phi|_\Xi \in \mathcal{H}^1(\Xi)$.

$$Q_U(\Phi) = \int_\Omega \eta^{-1}(\mathrm{d}\bar{\Phi}, \mathrm{d}\Phi)\mathrm{d}\mu_\eta - \int_{\partial\Omega} \bar{\varphi} A_U \varphi \mathrm{d}\mu_{\partial\eta} \tag{4.9a}$$

$$= \int_\Xi \eta^{-1}(\mathrm{d}\bar{\Phi}, \mathrm{d}\Phi)\mathrm{d}\mu_\eta + \int_{\Omega\setminus\Xi} \eta^{-1}(\mathrm{d}\bar{\Phi}, \mathrm{d}\Phi)\mathrm{d}\mu_\eta - \int_{\partial\Omega} \bar{\varphi} A_U \varphi \mathrm{d}\mu_{\partial\eta} \tag{4.9b}$$

$$\geq \int_\Xi \eta^{-1}(\mathrm{d}\bar{\Phi}, \mathrm{d}\Phi)\mathrm{d}\mu_\eta - \int_{\partial\Omega} \bar{\varphi} A_U \varphi \mathrm{d}\mu_{\partial\eta} \tag{4.9c}$$

$$= \int_{\partial\Omega}\int_I \left[\frac{\partial\bar{\Phi}}{\partial r}\frac{\partial\Phi}{\partial r} + g^{-1}(\mathrm{d}_{\boldsymbol{\theta}}\Phi, \mathrm{d}_{\boldsymbol{\theta}}\Phi)\right]\sqrt{|g(r,\boldsymbol{\theta})|}\mathrm{d}r \wedge \mathrm{d}\boldsymbol{\theta} - \int_{\partial\Omega} \bar{\varphi} A_U \varphi \mathrm{d}\mu_{\partial\eta} \tag{4.9d}$$

$$\geq \int_{\partial\Omega}\int_I \frac{\partial\bar{\Phi}}{\partial r}\frac{\partial\Phi}{\partial r}\sqrt{|g(r,\boldsymbol{\theta})|}\mathrm{d}r \wedge \mathrm{d}\boldsymbol{\theta} - \int_{\partial\Omega} \bar{\varphi} A_U \varphi \mathrm{d}\mu_{\partial\eta} \tag{4.9e}$$

$$\geq (1-\delta)\int_{\partial\Omega}\int_I \frac{\partial\bar{\Phi}}{\partial r}\frac{\partial\Phi}{\partial r}\sqrt{|g(0,\boldsymbol{\theta})|}\mathrm{d}r \wedge \mathrm{d}\boldsymbol{\theta} - \int_{\partial\Omega} \bar{\varphi} A_U \varphi \sqrt{|g(0,\boldsymbol{\theta})|}\mathrm{d}\boldsymbol{\theta} \tag{4.9f}$$

$$\geq (1-\delta)\int_{\partial\Omega}\left[\int_I \frac{\partial\bar{\Phi}}{\partial r}\frac{\partial\Phi}{\partial r}\mathrm{d}r - \frac{\|A_U\|}{(1-\delta)}|\varphi|^2\right]\sqrt{|g(0,\boldsymbol{\theta})|}\mathrm{d}\boldsymbol{\theta} \tag{4.9g}$$

$$\geq -|\Lambda_0|(1-\delta)\|\Phi\|^2_{\mathcal{H}^0(I\times\partial\Omega)} \geq -|\Lambda_0|\left(\frac{1-\delta}{1+\delta}\right)\|\Phi\|^2_{\mathcal{H}^0(\Xi)} \tag{4.9h}$$

$$\geq -|\Lambda_0|\left(\frac{1-\delta}{1+\delta}\right)\|\Phi\|^2_{\mathcal{H}^0(\Omega)}.$$

In the step leading to (4.9c) we have used the fact that the second term is positive. In the step leading to (4.9e) we have used that the second term in the first integrand is positive. Then (4.9f) follows using the bounds (4.8). The last chain of inequalities follows by Proposition 4.7 and Lemma 4.8, taking $c = \|A_U\|/(1-\delta)$. Notice that the semi-bound of Proposition 4.7 is always negative in this case because $c = \|A_U\|/(1-\delta) > 0$. In Definition 4.4 the interval I was taken of length 2π whereas in this case it has length L. This affects only in a constant factor that can be absorbed in the constant c by means of a linear transformation of the manifold $T : [0, 2\pi] \to I$. $\square$

Theorem 4.10. *Let $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ be an admissible, unitary operator. Then the quadratic form Q_U of Definition 3.12 is closable.*

Proof. According to Remark 2.3 a quadratic form is closable iff for any $\Phi \in \overline{\mathcal{D}_U}^{\|\cdot\|_{Q_U}}$ such that the corresponding Cauchy sequence $\{\Phi_n\}$ verifies $\|\Phi_n\| \to 0$ then $Q(\Phi) = 0$. Let $\Phi \in \overline{\mathcal{D}_U}^{\|\cdot\|_{Q_U}}$.

(a) Let us show that there exist $\{\tilde{\Phi}_n\} \in \mathcal{C}^\infty(\Omega)$ such that

$$\|\Phi - \tilde{\Phi}_n\|_{Q_U} \to 0,$$
$$\|\dot{\tilde{\varphi}}_n - A_U\tilde{\varphi}_n\|_{\mathcal{H}^{1/2}(\partial\Omega)} \to 0.$$

There exists $\{\Phi_n\} \in \mathcal{D}_U \subset \mathcal{H}^1(\Omega)$ such that $\|\Phi - \Phi_n\|_{Q_U} \to 0$. For the sequence $\{\Phi_n\}$ take $\{\tilde{\Phi}_n\} \in \mathcal{C}^\infty(\Omega)$ as in Corollary 4.3. Then we have that

$$\begin{aligned}\|\Phi - \tilde{\Phi}_n\|_{Q_U} &\leq \|\Phi - \Phi_n\|_{Q_U} + \|\Phi_n - \tilde{\Phi}_n\|_{Q_U}\\ &\leq \|\Phi - \Phi_n\|_{Q_U} + K\|\Phi_n - \tilde{\Phi}_n\|_1,\end{aligned}$$

where we have used Proposition 3.13.

(b) Let us assume that $\|\Phi_n\| \to 0$. This implies that $\|\tilde{\Phi}_n\| \to 0$. For every $\Psi \in \mathcal{H}^2_0 = \mathcal{D}(\Delta_{\min})$ we have that

$$|\langle\Delta_{\min}\Psi, \tilde{\Phi}_n\rangle| \leq \|\Delta_{\min}\Psi\|\|\tilde{\Phi}_n\| \to 0.$$

Hence $\lim \tilde{\Phi}_n \in \mathcal{D}(\Delta^\dagger_{\min}) = \mathcal{D}(\Delta_{\max})$. According to Theorem 2.13 the traces of such functions exist and are elements of $\mathcal{H}^{-1/2}(\partial\Omega)$, i.e., $\tilde{\varphi}_n \xrightarrow{\mathcal{H}^{-1/2}(\partial\Omega)} \tilde{\varphi}$.

(c) Finally we have that

$$
\begin{aligned}
Q_U(\Phi) &= \lim_{m\to\infty}\lim_{n\to\infty}\left[\langle \mathrm{d}\tilde{\Phi}_n, \mathrm{d}\tilde{\Phi}_m\rangle - \langle \tilde{\varphi}_n, A_U\tilde{\varphi}_m\rangle_{\partial\Omega}\right] \\
&= \lim_{m\to\infty}\lim_{n\to\infty}\left[\langle \tilde{\Phi}_n, -\Delta_\eta\tilde{\Phi}_m\rangle + \langle \tilde{\varphi}_n, \dot{\tilde{\varphi}}_m\rangle_{\partial\Omega} - \langle \tilde{\varphi}_n, A_U\tilde{\varphi}_m\rangle_{\partial\Omega}\right] \\
&= \lim_{m\to\infty}(\tilde{\varphi}, \dot{\tilde{\varphi}}_m - A_U\tilde{\varphi}_m)_{\partial\Omega} = 0.
\end{aligned}
$$

Notice that in the last step we have used the continuous extension given in Proposition 2.6 of the scalar product of the boundary $\langle\cdot,\cdot\rangle_{\partial\Omega}$ to the pairing $(\cdot,\cdot)_{\partial\Omega} : \mathcal{H}^{-1/2}(\partial\Omega) \times \mathcal{H}^{1/2}(\partial\Omega) \to \mathbb{C}$ associated with the scale of Hilbert spaces $\mathcal{H}^{1/2}(\partial\Omega) \subset \mathcal{H}^0(\partial\Omega) \subset \mathcal{H}^{-1/2}(\partial\Omega)$. □

Theorem 4.9 and Theorem 4.10 ensure that Theorem 2.4 applies and that the closure of the quadratic form Q_U for an admissible unitary U is representable by means of a unique self-adjoint operator T, with domain $\mathcal{D}(T) \subset \mathcal{D}(\overline{Q}_U) := \overline{\mathcal{D}_U}^{\|\cdot\|_{Q_U}}$, i.e.,

$$
\overline{Q}_U(\Psi, \Phi) = \langle \Psi, T\Phi\rangle, \quad \Psi \in \mathcal{D}(\overline{Q}_U),\ \Phi \in \mathcal{D}(T).
$$

Admissibility of U is a sufficient but not necessary condition to ensure the closability of the corresponding quadratic form Q_U. In Example 5.5 we prove a slightly weaker condition adapted to a particular decomposition of the boundary.

The following theorem establishes the relation between this operator T and the Laplace–Beltrami operator.

Theorem 4.11. *Let T be the self-adjoint operator with domain $\mathcal{D}(T)$ representing the closed quadratic form $\overline{Q}_U$ with domain $\mathcal{D}(\overline{Q}_U)$. The operator T is a self-adjoint extension of the closed symmetric operator $-\Delta_{\min}$.*

Proof. By Theorem 2.4 we have that $\Phi \in \mathcal{D}(T)$ iff $\Phi \in \mathcal{D}(\overline{Q}_U)$ and there exists $\chi \in \mathcal{H}^0(\Omega)$ such that

$$
Q_U(\Psi, \Phi) = \langle \Psi, \chi\rangle, \quad \forall \Psi \in \mathcal{D}(\overline{Q}_U).
$$

Let $\Phi \in \mathcal{H}_0^2(\Omega) \subset \mathcal{D}_U$ and $\Psi \in \mathcal{D}_U$. Then

$$
\begin{aligned}
Q_U(\Psi, \Phi) &= \langle \mathrm{d}\Psi, \mathrm{d}\Phi\rangle - \langle \psi, A_U\varphi\rangle_{\partial\Omega} \\
&= \langle \Psi, -\Delta_{\min}\Phi\rangle + \langle \psi, \dot{\varphi}\rangle_{\partial\Omega} - \langle \psi, A_U\varphi\rangle_{\partial\Omega} \\
&= \langle \Psi, -\Delta_{\min}\Phi\rangle.
\end{aligned}
$$

Since $\mathcal{D}_U$ is a core for $\overline{Q}_U$ and $\mathcal{D}(\overline{Q}_U) \subset \mathcal{H}^0(\Omega)$ the above equality holds also for every $\Psi \in \mathcal{D}(\overline{Q}_U)$. Therefore $\mathcal{D}(\Delta_{\min}) = \mathcal{H}_0^2(\Omega) \subset \mathcal{D}(T)$ and moreover $T|_{\mathcal{D}(\Delta_{\min})} = -\Delta_{\min}$. □

4.3. Relations to existing approaches

The analysis and classification of classes of self-adjoint extensions of second order elliptic differential operators on n-dimensional manifolds Ω is incomparably more involved and rich in the case $n \geq 2$, than in the case of one-dimensional ordinary differential operators of Sturm–Liouville type. One of the reasons is that the associated boundary Hilbert space $L^2(\partial\Omega)$ is a separable infinite dimensional Hilbert space if $n \geq 2$, while in the one-dimensional case it is just isomorphic to $\mathbb{C}^k$, $k \in \mathbb{N}$. Moreover, the deficiency indices of the corresponding closed symmetric differential operators are typically infinite if $n \geq 2$. As mentioned in the introduction, the complexity of the classification of self-adjoint extensions in the former case has opened the possibility of many different approaches [17,19,5,8,39]. In this subsection we will briefly explain some relations to existing results and techniques.

(i) The notion of quasi-boundary triple was introduced in [5] as a generalization of the notion of (ordinary) boundary triples and was applied to second order elliptic differential operators on bounded domains of $\mathbb{R}^n$, $n \geq 2$ (see also [8], [38, Section 3.4] and references cited therein). We refer to the introduction of [8] for a motivation of these structures through Sturm–Liouville like operators and to [26] for a one-dimensional motivation of the analysis done in this article.
The analysis of quasi-boundary triples is based on the analysis of unbounded operators and, therefore, the corresponding domains require the use of functions with more regularity than in the quadratic form approach used in this article. In the context of second order elliptic operators $\mathcal{L}$ on Ω consider a minimal, closed, symmetric and densely defined operator S. A quasi-boundary triple for the maximal operator S^* is given by $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$, where $\mathcal{G} = L^2(\partial\Omega)$ is the boundary Hilbert space, $\Gamma_0 : H^s_{\mathcal{L}}(\Omega) \to L^2(\partial\Omega)$ is the restriction from the space $H^s_{\mathcal{L}}(\Omega)$, $s \in [\frac{3}{2}, 2]$ (which contains the Sobolev space $H^2(\Omega)$) to the boundary $\partial\Omega$ and $\Gamma_1 : H^s_{\mathcal{L}}(\Omega) \to L^2(\partial\Omega)$ is (up to a sign) the normal derivative restricted to the boundary (see, e.g., [8, Section 1.4] for details). In this context the Neumann extension of the operator is obtained as a restriction of the differential operator with domain $H^s_{\mathcal{L}}(\Omega)$ to $\ker \Gamma_1$ (cf., [8, Proposition 4.19]). A class of self-adjoint extensions of the minimal operator are parametrized by a self-adjoint operator Θ on the boundary Hilbert space $L^2(\partial\Omega)$ satisfying certain conditions (see Theorem 1.21 in [8] for details). Roughly speaking, on the domain of the extensions labeled by Θ we have $\Theta\Gamma_0 = \Gamma_1$. In the case that the scale $s = 2$ it is required, among other things, that Θ preserves the fractional Sobolev space $\mathcal{H}^{1/2}(\partial\Omega)$ similarly as in the admissibility condition of the partial Cayley transform in Definition 3.14 above. (We refer to [5, Section 4] and [7] for the more general situation where the parameter Θ is a linear, self-adjoint relation on the boundary Hilbert space and for use of Weyl functions in this context). Note also that, in contrast with ordinary boundary triples, in the context of quasi-boundary triples there is not a bijective correspondence between the self-adjoint extensions of

S labeled by Θ and the self-adjoint parameters Θ. In this sense, the quasi-boundary triple approach specifies a class of so-called Krein–von Neumann-type extensions (see, e.g., Proposition 4.5 in [5]).

In contrast with the quasi-boundary triple approach, we study the extension purely from a quadratic form point of view. This allows in general larger domains (i.e., domains containing less regular functions) and the classification of extensions is done through the analysis of the (non locally compact) group of unitaries $\mathcal{U}(L^2(\partial\Omega))$ on the boundary Hilbert space. In particular, we recover the Dirichlet extension through the selection of the unitary $U = -\mathbb{I}$ which trivially satisfies admissibility and the spectral gap condition at -1. In this sense, our approach is closer to the boundary pair approach introduced by Post in [39] (see [39, Section 7.4], where a positive quadratic form without a boundary term is considered). Moreover, our approach selects Friedrichs-type self-adjoint extensions of the corresponding minimal operator.

(ii) The pioneering work of Grubb [17,18] gives a complete characterization of the closed extensions of an even order elliptic differential operator in terms of boundary conditions. These boundary conditions are expressed in terms of pseudo-differential operators acting on spaces of functions at the boundary. More concretely these spaces are orthogonal sums of Sobolev spaces of fractional order, $\mathcal{H}^s(\partial\Omega)$, where s can take negative values, cf. [17, Theorem 2.2] and [22, Theorem 3.1]. There are given sufficient and necessary conditions on the pseudo-differential operators at the boundary to define closed symmetric and self-adjoint extensions of the given elliptic operator. The necessity of the boundary operators to be pseudo-differential operators acting on the Sobolev spaces at the boundary shows up in our context in the sufficient condition that the unitary operator $U : L^2(\partial\Omega) \to L^2(\partial\Omega)$ is admissible, i.e., that A_U is a bounded operator in $\mathcal{H}^1(\partial\Omega)$.

A necessary condition for the lower semi-boundedness of even order elliptic boundary problems can already be found in [18, Theorem 4.3]. A characterization of sufficient and necessary conditions for the lower semi-boundedness is given in [20, Theorem 2.12]. In particular the boundary operator needs to be semi-bounded in a Sobolev space of negative order. The gap condition in our approach ensures that the operator A_U is bounded in $L^2(\partial\Omega)$ and this is a sufficient condition to prove the semi-boundedness of the quadratic form. It is clear from the proof of Theorem 4.9 that it is enough that the operator A_U is semi-bounded in $L^2(\partial\Omega)$ and thus our sufficient condition for the semi-boundedness is weaker.

Our approach to the boundary problem aims to preserve the local structure of the space of boundary data although loosing some generality with respect to the works by Grubb. The simpler form of the boundary conditions presented in this article allows to relax the regularity condition imposed in Definition 3.14, as will be shown in Example 5.5, and treat discontinuities in smooth subsets of codimension one. Therefore generalizing the results appearing in [21].

5. Examples

In this section we introduce some examples that show that the characterization of the quadratic forms of Section 3 and Section 4 include a large class of possible self-adjoint extensions of the Laplace–Beltrami operator. This section also illustrates the simplicity in the description of extensions using admissible unitaries at the boundary.

For the purpose of this section it is enough to consider that the boundary admits a covering with sets of non-empty interior, that are disjoint up to subsets of codimension one and such that they are diffeomorphic to a reference set Γ_0. The following construction ensures that such a covering does always exist.

As the boundary manifold $\partial\Omega$ is an $(n-1)$-dimensional, smooth manifold, there always exist an $(n-1)$-simplicial complex $\mathcal{K}$ and a smooth diffeomorphism $f : \mathcal{K} \to \partial\Omega$ such that $f(\mathcal{K}) = \partial\Omega$, cf., [46,47]. Any simplex in the complex is diffeomorphic to a reference polyhedron $\Gamma_0 \subset \mathbb{R}^{n-1}$. The simplicial complex $\mathcal{K}$ defines therefore a triangulation of the boundary $\partial\Omega = \bigcup_{i=1}^{N}\Gamma_i$, where $\Gamma_i := f(A_i)$, $A_i \in \mathcal{K}$. For each element of the triangulation Γ_i there exists a diffeomorphism $g_i : \Gamma_0 \to \Gamma_i$. Consider a reference Hilbert space $\mathcal{H}^0(\Gamma_0, \mathrm{d}\mu_0)$, where $\mathrm{d}\mu_0$ is a fixed smooth volume element. Each diffeomorphism g_i defines a unitary transformation as follows:

Definition 5.1. Let $|J_i|$ be the Jacobian determinant of the transformation of coordinates given by the diffeomorphism $g_i : \Gamma_0 \to \Gamma_i$. Let $\mu_i \in \mathcal{C}^\infty(\partial\Omega)$ be the proportionality factor $g_i^\star \mathrm{d}\mu_{\partial\eta} = \mu_i \mathrm{d}\mu_0$, where $g_i^\star$ stands for the pull-back of the diffeomorphism. The unitary transformation $T_i : \mathcal{H}^0(\Gamma_i, \mathrm{d}\mu_{\partial\eta}) \to \mathcal{H}^0(\Gamma_0, \mathrm{d}\mu_0)$ is defined by

$$T_i\Phi := \sqrt{|J_i|\mu_i}(\Phi \circ g_i). \tag{5.1}$$

We show that the transformation above is unitary. First note that T is invertible. It remains to show that T is an isometry:

$$\begin{aligned}\langle\Phi,\Psi\rangle_{\Gamma_i} &= \int_{\Gamma_i} \bar{\Phi}\Psi \mathrm{d}\mu_{\partial\eta} \\ &= \int_{\Gamma_0} (\overline{\Phi\circ g_i})(\Psi\circ g_i)|J_i| g_i^\star \mathrm{d}\mu_{\partial\eta} \\ &= \int_{\Gamma_0} (\overline{\Phi\circ g_i})(\Psi\circ g_i)|J_i|\mu_i \mathrm{d}\mu_0 = \langle T_i\Phi, T_i\Psi\rangle_{\Gamma_0}.\end{aligned}$$

Example 5.2. Consider that the compact boundary of the Riemannian manifold $(\Omega, \partial\Omega, \eta)$ admits a triangulation of two elements, i.e., $\partial\Omega = \Gamma_1 \cup \Gamma_2$. (Note that Γ_1 and Γ_2 need not be disjoint sets.) The Hilbert space of the boundary satisfies $\mathcal{H}^0(\partial\Omega) = \mathcal{H}(\Gamma_1 \cup \Gamma_2) \simeq \mathcal{H}^0(\Gamma_1) \oplus \mathcal{H}^0(\Gamma_2)$. The isomorphism is given explicitly by the characteristic functions χ_i of the submanifolds Γ_i, $i = 1, 2$. Modulo a null measure set we have that

$$\Phi = \chi_1\Phi + \chi_2\Phi.$$

We shall define unitary operators $U = \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ that are adapted to the block structure induced by the latter direct sum:

$$U = \begin{bmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{bmatrix},$$

where $U_{ij} : \mathcal{H}^0(\Gamma_j) \to \mathcal{H}^0(\Gamma_i)$. Hence consider the following unitary operator

$$U = \begin{bmatrix} 0 & T_1^* T_2 \\ T_2^* T_1 & 0 \end{bmatrix}, \tag{5.2}$$

where the unitaries T_i are defined as in Definition 5.1. Clearly, $U^2 = \mathbb{I}$, and therefore the spectrum of U is $\sigma(U) = \{-1, 1\}$ with the corresponding orthogonal projectors given by

$$P^\perp = \frac{1}{2}(\mathbb{I} - U),$$
$$P = \frac{1}{2}(\mathbb{I} + U).$$

The partial Cayley transform A_U is in this case the null operator, since $P(\mathbb{I} - U) = 0$. The unitary operator is therefore admissible and the corresponding quadratic form will be closable. The domain of the corresponding quadratic form Q_U is given by all the functions $\Phi \in \mathcal{H}^1(\Omega)$ such that $P^\perp\gamma(\Phi) = 0$, which in this case becomes

$$P^\perp\gamma(\Phi) = \frac{1}{2}\begin{bmatrix} \mathbb{I}_1 & -T_1^* T_2 \\ -T_2^* T_1 & \mathbb{I}_2 \end{bmatrix}\begin{bmatrix} \chi_1\gamma(\Phi) \\ \chi_2\gamma(\Phi) \end{bmatrix} = \begin{bmatrix} \chi_1\gamma(\Phi) - T_1^* T_2\chi_2\gamma(\Phi) \\ -T_2^* T_1\chi_1\gamma(\Phi) + \chi_2\gamma(\Phi) \end{bmatrix} = 0. \tag{5.3}$$

We can rewrite the last condition as

$$T_1\big(\chi_1\gamma(\Phi)\big) = T_2\big(\chi_2\gamma(\Phi)\big). \tag{5.4}$$

More concretely, this boundary conditions describe generalized periodic boundary conditions identifying the two triangulation elements of the boundary with each other. The unitary transformations T_i are necessary to make the triangulation elements congruent. In particular, if (Γ_1, η_1) and (Γ_2, η_2) are isomorphic as Riemannian manifolds then one can recover the standard periodic boundary conditions.

Example 5.3. Consider the same situation as in the previous example but with the unitary operator replaced by

$$U = \begin{bmatrix} 0 & T_1^* e^{i\alpha} T_2 \\ T_2^* e^{-i\alpha} T_1 & 0 \end{bmatrix}, \quad \alpha \in \mathcal{C}^\infty(\Gamma_0). \tag{5.5}$$

In this case we have also that $U^2 = \mathbb{I}$ and the calculations of the previous example can be applied step by step. More concretely, $P^\perp = (I - U)/2$ and the partial Cayley transform also vanishes. The boundary condition becomes in this case

$$T_1\big(\chi_1\gamma(\Phi)\big) = e^{i\alpha}T_2\big(\chi_2\gamma(\Phi)\big). \tag{5.6}$$

This boundary conditions can be called generalized, quasiperiodic boundary conditions. For simple geometries and constant function α these are the boundary conditions that define the periodic Bloch functions.

The condition $\alpha \in \mathcal{C}^\infty(\Gamma_0)$ in the example above can be relaxed. First we will show that the isometries T_i do preserve the regularity of the function.

Proposition 5.4. *Let T_i be a unitary transformation as given by Definition 5.1. Let $\Phi \in \mathcal{H}^k(\Gamma_i)$, $k \geq 0$. Then $T_i\Phi \in \mathcal{H}^k(\Gamma_0)$.*

Proof. It is well known, cf. [2, Theorem 3.41] or [13, Lemma 7.1.4], that the pull-back of a function under a smooth diffeomorphism $g : \Omega_1 \to \Omega_2$ preserves the regularity of the function, i.e., $g^\star\Phi \in \mathcal{H}^k(\Omega_1)$ if $\Phi \in \mathcal{H}^k(\Omega_2)$, $k \geq 0$. It is therefore enough to prove that multiplication by a smooth positive function also preserves the regularity. According to Definition 2.9 it is enough to prove it for a smooth, compact, boundaryless Riemannian manifold $(\tilde{\Omega}, \tilde{\eta})$ and to consider that $\Phi \in \mathcal{C}^\infty(\tilde{\Omega})$, since this set is dense in $\mathcal{H}^k(\tilde{\Omega})$. Let $f \in \mathcal{C}^\infty(\tilde{\Omega})$.

$$\begin{aligned}
\int_{\tilde{\Omega}} \overline{f\Phi}(I - \Delta_{\tilde{\eta}})^k(f\Phi)\mathrm{d}\mu_{\tilde{\eta}} &\leq \sup_{\tilde{\Omega}}|f| \int_{\tilde{\Omega}} \overline{\Phi}(I - \Delta_{\tilde{\eta}})^k(f\Phi)\mathrm{d}\mu_{\tilde{\eta}} \\
&\leq \sup_{\tilde{\Omega}}|f| \int_{\tilde{\Omega}} \overline{(I - \Delta_{\tilde{\eta}})^k\Phi} f\Phi\mathrm{d}\mu_{\tilde{\eta}} \\
&\leq \Big(\sup_{\tilde{\Omega}}|f|\Big)^2 \int_{\tilde{\Omega}} \overline{(I - \Delta_{\tilde{\eta}})^k\Phi}\Phi\mathrm{d}\mu_{\tilde{\eta}} < \infty.
\end{aligned}$$

We have used Definition 2.8 directly and the fact that the operator $(I - \Delta_{\tilde{\eta}})^k$ is essentially self-adjoint over the smooth functions. □

According to Proposition 5.4 we have that $T_i(\chi_i\gamma(\Phi)) \in \mathcal{H}^{1/2}(\Gamma_0)$, $i = 1, 2$. Therefore, to get nontrivial solutions for the expression (5.6), the function $\alpha : \Gamma_0 \to [0, 2\pi]$ can be chosen such that $e^{i\alpha}T_2(\chi_2\gamma) \in \mathcal{H}^{1/2}(\Gamma_0)$. Since $\mathcal{C}^0(\Gamma_0)$ is a dense subset in $\mathcal{H}^{1/2}(\Gamma_0)$, and point-wise multiplication is a continuous operation for continuous functions it is enough to consider $\alpha \in \mathcal{C}^0(\Gamma_0)$.

Example 5.5. Consider that the boundary of the Riemannian manifold $(\Omega, \partial\Omega, \eta)$ admits a triangulation of two elements like in the Example 5.2. So we have that $\partial\Omega = \Gamma_1 \cup \Gamma_2$.

Consider the following unitary operator $U : \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ adapted to the block structure defined by this triangulation

$$U = \begin{bmatrix} e^{\mathrm{i}\beta_1}\mathbb{I}_1 & 0 \\ 0 & e^{\mathrm{i}\beta_2}\mathbb{I}_2 \end{bmatrix}, \tag{5.7}$$

where $\mathcal{C}^0(\Gamma_i) \ni \beta_i : \Gamma_i \to [-\pi+\delta, \pi-\delta]$ with $\delta > 0$. The latter condition guaranties that the unitary matrix has gap at -1. Since the unitary is diagonal in the block structure, it is clear that $P^{\perp} = 0$. The domain of the quadratic form Q_U is given in this case by all the functions $\Phi \in \mathcal{H}^1(\Omega)$. The partial Cayley transform is in this case the operator $A_U = \mathcal{H}^0(\partial\Omega) \to \mathcal{H}^0(\partial\Omega)$ defined by

$$A_U = \begin{bmatrix} -\tan\frac{\beta_1}{2} & 0 \\ 0 & -\tan\frac{\beta_2}{2} \end{bmatrix}. \tag{5.8}$$

A matrix like the one above will lead to self-adjoint extensions of the Laplace–Beltrami operator that verify generalized Robin-type boundary conditions $\chi_i\dot{\varphi} = -\tan\frac{\beta_i}{2}\chi_i\varphi$. Notice that this example allows discontinuities in the Robin parameter between each piece of the triangulation.

The partial Cayley transform does not satisfy the admissibility condition in this case. Nevertheless, we will show that the quadratic form above is indeed closable.

Given a triangulation of the boundary $\partial\Omega = \bigcup_{i=1}^{N}\Gamma_i$ we can consider the Hilbert space that results of the direct sum of the corresponding Sobolev spaces. We will denote it as

$$\bigoplus \mathcal{H}^k := \bigoplus_{i=1}^{N} \mathcal{H}^k(\Gamma_i). \tag{5.9}$$

For simplicity we will denote, using the preceding notation, the norms of these Hilbert spaces by

$$\|\varphi\|^2_{\bigoplus \mathcal{H}^k} := \sum_{i=1}^{N} \|\varphi|_{\Gamma_i}\|^2_{\mathcal{H}^k(\Gamma_i)}. \tag{5.10}$$

Now we can give the following generalizations of Lemma 4.1 and Corollary 4.3, respectively. The main difference is that we allow more general normal derivatives. In particular they may be discontinuous at intersections of the different neighboring elements of the triangulation.

Lemma 5.6 *(Lemma 4.1*). Let $\Phi \in \mathcal{H}^1(\Omega)$, $f \in \bigoplus \mathcal{H}^{1/2}$. Then, for every $\epsilon > 0$ there exists $\tilde{\Phi} \in \mathcal{C}^\infty(\Omega)$ such that $\|\Phi - \tilde{\Phi}\|_1 < \epsilon$, $\|\varphi - \tilde{\varphi}\|_{\mathcal{H}^{1/2}(\partial\Omega)} < \epsilon$ and $\|f - \dot{\tilde{\varphi}}\|_{\bigoplus \mathcal{H}^{1/2}} < \epsilon$.*

Proof. The proof of this lemma follows exactly the one for the Lemma 4.1. It is enough to notice that the space $\mathcal{H}^1(\partial\Omega)$ is dense in $\bigoplus \mathcal{H}^{1/2}$. □

Corollary 5.7 *(Corollary 4.3*). Let $\{\Phi_n\} \subset \mathcal{H}^1(\Omega)$ and let A_U be the partial Cayley transform of a unitary operator with gap at -1 such that $\|A_U\gamma(\Phi)\|_{\bigoplus \mathcal{H}^{1/2}} \leq K\|\gamma(\Phi)\|_{\bigoplus \mathcal{H}^{1/2}}$. Then there exists a sequence of smooth functions $\{\tilde{\Phi}_n\} \in \mathcal{C}^\infty(\Omega)$ such that $\|\Phi_n - \tilde{\Phi}_n\|_{\mathcal{H}^1(\Omega)} < \frac{1}{n}$, $\|\varphi_n - \tilde{\varphi}_n\|_{\mathcal{H}^{1/2}(\partial\Omega)} < \frac{1}{n}$, and $\|\dot{\tilde{\varphi}}_n - A_U\tilde{\varphi}_n\|_{\bigoplus \mathcal{H}^{1/2}} < \frac{1}{n}$.*

Proof. The proof is the same as for Corollary 4.3 but now we take $\tilde{\Phi}_{n_0}$ as in Lemma 5.6 with $f = A_U\varphi_{n_0} \in \bigoplus \mathcal{H}^{1/2}$. □

Now we can show that the quadratic forms Q_U defined for unitary operators of the form appearing in Example 5.5 are closable. We show first that the partial Cayley transform of Eq. (5.8) verifies the conditions of the Corollary 5.7 above. We have that

$$\begin{aligned}
\|A_U\varphi\|^2_{\bigoplus \mathcal{H}^{1/2}} &= \|A_U\chi_1\varphi\|^2_{\mathcal{H}^{1/2}(\Gamma_1)} + \|A_U\chi_2\varphi\|^2_{\mathcal{H}^{1/2}(\Gamma_2)} \\
&= \left\|\tan\frac{\beta_1}{2}\chi_1\varphi\right\|^2_{\mathcal{H}^{1/2}(\Gamma_1)} + \left\|\tan\frac{\beta_2}{2}\chi_2\varphi\right\|^2_{\mathcal{H}^{1/2}(\Gamma_2)} \\
&\leq K\left[\|\chi_1\varphi\|^2_{\mathcal{H}^{1/2}(\Gamma_1)} + \|\chi_2\varphi\|^2_{\mathcal{H}^{1/2}(\Gamma_2)}\right] = K\|\varphi\|^2_{\bigoplus \mathcal{H}^{1/2}}.
\end{aligned}$$

The last inequality follows from the discussion after Example 5.3 because the functions $\beta_i : \Gamma_i \to [-\pi + \delta, \pi - \delta]$ are continuous. Take the sequence $\{\Phi_n\} \in \mathcal{D}_U$ as in the proof of Theorem 4.10 and accordingly take $\{\tilde{\Phi}_n\} \in \mathcal{C}^\infty(\Omega)$ as in Corollary 5.7. Then we have that

$$\begin{aligned}
\left|Q(\Phi)\right| &= \lim_{m\to\infty}\lim_{n\to\infty}\left|\langle \mathrm{d}\tilde{\Phi}_n, \mathrm{d}\tilde{\Phi}_m\rangle - \langle\tilde{\varphi}_n, A\tilde{\varphi}_m\rangle_{\partial\Omega}\right| \\
&\leq \lim_{m\to\infty}\lim_{n\to\infty}\left[\left|\langle\tilde{\Phi}_n, -\Delta_\eta\tilde{\Phi}_m\rangle\right| + \left|\langle\tilde{\varphi}_n, \dot{\tilde{\varphi}}_m - A_U\tilde{\varphi}_m\rangle_{\partial\Omega}\right|\right] \\
&= \lim_{m\to\infty}\lim_{n\to\infty}\left[\left|\langle\tilde{\Phi}_n, -\Delta_\eta\tilde{\Phi}_m\rangle\right| + \left|\sum_{i=1}^N\langle\tilde{\varphi}_n, \dot{\tilde{\varphi}}_m - A_U\tilde{\varphi}_m\rangle_{\Gamma_i}\right|\right] \\
&\leq \lim_{m\to\infty}\lim_{n\to\infty}\sum_{i=1}^N\left|\langle\tilde{\varphi}_n, \dot{\tilde{\varphi}}_m - A_U\tilde{\varphi}_m\rangle_{\Gamma_i}\right| \\
&\leq \lim_{m\to\infty}\lim_{n\to\infty}\sum_{i=1}^N\|\chi_i\tilde{\varphi}_n\|_{\mathcal{H}^{-1/2}(\Gamma_i)}\|\chi_i\dot{\tilde{\varphi}}_m - \chi_iA_U\tilde{\varphi}_m\|_{\mathcal{H}^{1/2}(\Gamma_i)} \\
&\leq \lim_{m\to\infty}\lim_{n\to\infty}\|\tilde{\varphi}_n\|_{\mathcal{H}^{-1/2}(\partial\Omega)}\sum_{i=1}^N\|\chi_i\dot{\tilde{\varphi}}_m - \chi_iA_U\tilde{\varphi}_m\|_{\mathcal{H}^{1/2}(\Gamma_i)} = 0.
\end{aligned}$$

We have used Definition 2.9 and the structure of the scales of Hilbert spaces $\mathcal{H}^{1/2}(\Gamma_i) \subset \mathcal{H}^0(\Gamma_i) \subset \mathcal{H}^{-1/2}(\Gamma_i)$. Hence, the unitary operators of Example 5.5 are closable. In particular, this class of closable quadratic forms defines generalized Robin-type boundary conditions $\dot{\varphi} = -\tan\frac{\beta}{2}\varphi$ where β is allowed to be a piecewise continuous function with discontinuities at the vertices of the triangulation.

Example 5.8. Consider a unitary operator at the boundary of the form

$$U = \begin{bmatrix} -\mathbb{I}_1 & 0 \\ 0 & e^{\mathrm{i}\beta_2}\mathbb{I}_2 \end{bmatrix}, \tag{5.11}$$

with $\beta_2 : \Gamma_2 \to [-\pi+\delta, \pi-\delta]$ continuous. Again we need the condition $\delta > 0$ in order to guaranty that the unitary matrix U has gap at -1. In this case it is clear that

$$P^{\perp} = \begin{bmatrix} \mathbb{I}_1 & 0 \\ 0 & 0 \end{bmatrix},$$

and that the partial Cayley transform becomes

$$A_U = \begin{bmatrix} 0 \\ -\tan\frac{\beta_2}{2} \end{bmatrix}.$$

This partial Cayley transform verifies the weaker admissibility condition of the previous example and therefore defines a closable quadratic form too. This one defines a boundary condition of the mixed type where

$$\chi_1\varphi = 0, \quad \chi_2\dot{\varphi} = -\tan\frac{\beta_2}{2}\chi_2\varphi.$$

In particular when $\beta_2 \equiv 0$ this mixed-type boundary condition defines the boundary conditions of the so-called *Zaremba problem* with

$$\chi_1\varphi = 0, \qquad \chi_2\dot{\varphi} = 0.$$

Example 5.9. Let $(\Omega, \partial\Omega, \eta)$ be a smooth, Riemannian manifold with compact boundary. Suppose that the boundary manifold admits a triangulation $\partial\Omega = \bigcup_{i=1}^{N}\Gamma_i$. Any unitary matrix that has block-wise the structure of any of the above examples, i.e., Eqs. (5.2), (5.5), (5.7) or (5.11) leads to a closable, semi-bounded quadratic form Q_U.

6. Outlook

In the present article we give a procedure to select a large class of self-adjoint extensions of the Laplace–Beltrami operator. These were introduced by using directly a family of associated quadratic forms labeled by suitable unitaries acting on the Hilbert space of the boundary. It has been proved a sufficient condition for the Laplace–Beltrami operator to be semi-bounded from below in smooth manifolds, not necessarily compact, with compact boundary. This is not the first characterization of such situation which was addressed recently in [22]. However, as explained in Section 4.3, the condition introduced here is weaker.

The particular form of the boundary conditions introduced here and the semi-boundedness makes this approach suitable for numerical purposes and there are already one and higher dimensional algorithms approximating the spectrum of such problems, cf. [25,26]. Moreover, since the proof introduced in this article is related with the geometrical character of the Laplace–Beltrami operator one can easily detect what assumptions are essential for the proof and which ones are susceptible to be weakened. For instance, the existence of the collar neighborhood and the bounds of Eq. (4.8) are crucial but the assumption on the compactness of the boundary is there to guaranty that these are satisfied. Hence the results of this article can be taken as a step forward towards the generalization to manifolds with non-compact boundary. The conjecture stated in [22, Remark 4.7] that the lower bound for second order elliptic operators is of order c^2, where c is the lower bound for the boundary operator, holds for the quadratic forms considered here and the proportionality factor depends only on the Riemannian metric. Just notice that Λ_0 in Eq. (4.9h) is the lowest eigenvalue of the one dimensional problem of Proposition 4.5 and Eq. (4.6) establishes that $\Lambda_0 \sim c^2$ for large c.

An advantage of using the representation theorem to obtain self-adjoint extensions is that it regularizes automatically the domains. For instance, the Zaremba problem, where Dirichlet and Neumann boundary conditions are imposed on disjoint subsets of the boundary is known to be irregular at the points where the two boundary conditions meet (see, e.g., [39, Section 7.7] for an introduction to this problem). This type of boundary conditions can be treated with the present approach using the splitting of the boundary explained in Section 5 and in fact is a particular case of Example 5.8 when $\beta_2 \equiv 0$.

There are important extensions of the Laplace–Beltrami operator that can not be treated with this approach. In particular the Krein–von Neumann extension of the Laplace–Beltrami operator defined by considering as the self-adjoint operator A_U the Dirichlet–von Neumann map $\Lambda_o : \mathcal{H}^{1/2}(\partial\Omega) \to \mathcal{H}^{-1/2}(\partial\Omega)$ does not verify the admissibility condition. Moreover, even though the boundary term associated with this case is bounded in $\mathcal{H}^{1/2}(\partial\Omega)$, i.e.,

$$\left|\langle \varphi, \Lambda_o \varphi\rangle\right| \leq C\|\varphi\|^2_{\mathcal{H}^{1/2}(\partial\Omega)},$$

this is not enough to proof semi-boundedness with our approach where a bound in $L^2(\partial\Omega)$ is needed.

An interesting problem where the approach taken here does not hold is the problem considered in [11] where a particular class of Robin boundary conditions is introduced. In particular these conditions fail to satisfy the gap condition. It is already known, cf. [35, 10], that in order to select a self-adjoint extension in this case one needs to fix an extra phase at the so-called *Dirichlet Singularity*. This suggests the following generalization of the approach presented here. Consider the splitting of the boundary introduced in Section 5 and impose that the functions in the domain acquire a local phase shift across the boundaries of the subsets of the boundary. This could lead to a characterization of a wider class of self-adjoint extensions and could also include the situation where the manifold has non-convex corners, cf. [37]. Eventually this procedure could also be applied to the situation with the Dirichlet Singularity.

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