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Self-adjoint extensions and unitary operators on the boundary

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Abstract We establish a bijection between the self-adjoint extensions of the Laplace operator on a bounded regular domain and the unitary operators on the boundary. Each unitary encodes a specific relation between the boundary value of the function and its normal derivative. This bijection sets up a characterization of all physically admissible dynamics of a nonrelativistic quantum particle confined in a cavity. Moreover, this correspondence is discussed also at the level of quadratic forms. Finally, the connection between this parametrization of the extensions and the classical one, in terms of boundary self-adjoint operators on closed subspaces, is shown.

Keywords Quantum boundary conditions · Self-adjoint extensions · Quadratic forms

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1 Introduction

In the last few years, there has been an increasing interest in the physics of quantum systems confined in a bounded spatial region and in the role of quan-

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tum boundary conditions. It has been realized that the presence of boundaries can often catalyze and amplify the quantum behavior of a system. For a review, see, e.g., [2,5,16].

All physical dynamics of closed quantum systems are implemented by strongly continuous one-parameter unitary groups, which by Stone's theorem are in one-to-one correspondence with their generators, which are self-adjoint operators. See, e.g., [28].

The characterization of the self-adjoint extensions of a symmetric operator is given by von Neumann in his theory of self-adjoint extensions, one of the gems of functional analysis [32]. This theory is fully general and completely solves the problem of self-adjoint extensions of every densely defined and closed symmetric operator in an abstract Hilbert space in terms of unitary operators between its deficiency subspaces. See, e.g., [13].

However, for specific classes of operators, e.g., differential operators, it would be desirable to have a more concrete characterization of the set of self-adjoint extensions. A concrete characterization was given by Grubb [19] for symmetric even-order elliptic differential operators in a bounded regular spatial domain. Building on the earlier work of Višik [31], Birman [9], and Lions and Magenes [25], she was able to characterize all the self-adjoint extensions in terms of boundary conditions parametrized by (unbounded) self-adjoint boundary operators $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$ acting on closed (proper) subspaces $\mathcal{X}$ of the boundary Hilbert space. See Theorem 2 for the Laplace operator.

At an intermediate level of abstraction between Grubb's and von Neumann's descriptions lies the theory of boundary triples [10,13], which elaborates on ideas of Calkin [11] and Višik [31], and is valid for every symmetric operator, because it relies on an abstraction of boundary values in function spaces. A related description was discovered in the last years by Posilicano [26,27], who introduced a parametrization in terms of pairs (Π, Θ), where Π is an orthogonal projection in an auxiliary Hilbert space $\mathfrak{h}$ and Θ is a self-adjoint operator in the range of Π. See also [12]. When particularized to differential operators, one recovers Grubb's parametrization, where $\mathfrak{h}$ is essentially the boundary space, Π is the projection onto $\mathcal{X}$, and Θ is L.

Recently, Asorey, Marmo and Ibort [5,6] proposed on physical ground a different parametrization of the self-adjoint extensions of differential operators in terms of *unitary* operators U on the boundary. This description relies more directly on physical intuition, and in the last years it has been applied to several physical systems [3,4,7,8,14,15,17].

The large use of this description in several applications is also due to its great manageability: The parametrization is in terms of a single unitary operator U on the boundary, instead of a pair $(\mathcal{X}, L)$ composed of a closed subspace $\mathcal{X}$ and a self-adjoint operator L, which in general is unbounded and thus also needs a domain specification $D(L)$. Here, all information is encoded in a single simpler object.

Our main objective is to establish a characterization of the self-adjoint extensions of an elliptic differential operator in terms of unitary operators on the boundary. In this paper, we will focus on the paradigmatic model of the Laplacian in a *bounded regular* domain. We will establish, in Theorem 1, a bijection between the set of the self-adjoint extensions of the Laplace operator on a bounded regular domain and the set of boundary unitary operators. Each unitary operator is characteristic of a specific boundary condition that is a relation between the boundary value, $\boldsymbol{\gamma}\psi$, of the function ψ and its normal derivative at the boundary, $\boldsymbol{\nu}\psi$ (in the sense of traces).

The explicit relation, given in Remark 2, reads

$$\boldsymbol{\mu}\psi - i\boldsymbol{\gamma}\psi = U(\boldsymbol{\mu}\psi + i\boldsymbol{\gamma}\psi),$$

and, in fact, it links the boundary value $\boldsymbol{\gamma}\psi$ of the function ψ to the *regular part* $\boldsymbol{\mu}\psi$ of its normal derivative $\boldsymbol{\nu}\psi$, see Definition 1. This is consistent with a different regularity of the boundary values of the function and of its normal derivative: In general, their traces belong to different Sobolev spaces, $H^{-1/2}(\partial\Omega)$ and $H^{-3/2}(\partial\Omega)$, respectively, and cannot be compared. Interestingly enough, the irregular part of the normal derivative plays no role in the boundary conditions; in fact it is not an independent boundary datum and indeed is completely determined by the trace of the function $\boldsymbol{\gamma}\psi$ through the Dirichlet-to-Neumann operator [1,20].

The link between Grubb's parametrization and our parametrization, $(\mathcal{X}, L) \leftrightarrow U$, will be given in Theorem 3. In a few words, the unitary U is adapted to the direct sum $H^{-1/2}(\partial\Omega) = \mathcal{X} \oplus \mathcal{X}^{\perp}$ and reads $U = V \oplus \mathbb{I}$. Here, the unitary component V is essentially the (partial) Caley transform of L and, as such, it does not have 1 as eigenvalue. Therefore, the eigenspace associated with the eigenvalue 1 (the idle subspace) coincides with $\mathcal{X}^{\perp}$. As a matter of fact, at the level of Hilbert spaces, the relevant information is encoded in $\mathcal{X}$. Its orthogonal $\mathcal{X}^{\perp}$, which for this reason is called *idle*, is only necessary to extend V to a unitary operator U on the whole Hilbert space of boundary data.

A final remark is in order. In this paper, for definiteness, we explicitly consider only the case of the Laplace operator in a bounded regular domain of $\mathbb{R}^n$. However, Theorem 3 which establishes the link $(\mathcal{X}, L) \leftrightarrow U$, and the general strategy of encoding boundary conditions in a unitary operator by using an idle subspace and a partial Caley transform, would allow us to generalize our results to a larger class of operators (e.g., Laplace–Beltrami [23], Dirac [6], pseudodifferential operators [19]) and/or settings (e.g., manifolds with boundaries [22]).

Notice that, up to this point, we considered only *regular* domains. Recently, there has been an increasing interest in domains with nonsmooth boundaries, and by now there are general approaches to this circle of ideas, see, for example, [18]. It would be interesting to understand whether a parametrization in terms of unitary boundary operators might also be available in this more general setting.

This article is organized as follows. In Sect. 2, after setting the notation and defining the regularized normal derivative at the boundary, we state our main result, Theorem 1. Then, after recalling Grubb's characterization of self-adjoint extensions, Theorem 2, we establish the connection between the two parametrizations in Theorem 3. Then, we state our result in terms of quadratic forms in Theorem 4, which is a corollary of Theorem 1. Sections 4 and 5 are devoted to the proofs of the theorems. The main properties of the Cayley transform which are used in the proofs are gathered in the final Sect. 6.

2 Notation and main results

We are going to consider complex separable Hilbert spaces. The inner product between two vectors u,v of a Hilbert space $\mathscr{H}$ is denoted by $\langle u|v\rangle_{\mathscr{H}}$. In our convention, it is anti-linear in the first argument and linear in the second one.

Given two Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$, the set of unitary operators from $\mathscr{H}_1$ to $\mathscr{H}_2$ is denoted by $\mathscr{U}(\mathscr{H}_1, \mathscr{H}_2)$, while $\mathscr{U}(\mathscr{H}_1)$ stands for $\mathscr{U}(\mathscr{H}_1, \mathscr{H}_1)$.

Let $\mathscr{H}$ be an Hilbert space and A a densely defined linear operator on $\mathscr{H}$,

$$A : D(A) \subset \mathscr{H} \to \mathscr{H}.$$

We are going to denote by A^* the adjoint operator of A,

$$A^* : D(A^*) \subset \mathscr{H} \to \mathscr{H}.$$

We say that A is *self-adjoint* if $A = A^*$.

Let Ω be a *regular domain* that is an open bounded set of $\mathbb{R}^n$, $n \in \mathbb{N}$, whose boundary $\partial\Omega$ is a $(n-1)$-dimensional infinitely differentiable manifold, with Ω being locally on one side of $\partial\Omega$ [25]. By convention, the normal ν of $\partial\Omega$ is oriented toward the exterior of the regular domain Ω.

Let $H^s(\Omega)$ (resp. $H^s(\partial\Omega)$), $s \in \mathbb{R}$, be the Sobolev space of order s on Ω (resp. on $\partial\Omega$) with the usual norm [21,25]. Furthermore, we set $H_0^s(\Omega)$ the closure of $C_c^\infty(\Omega)$ in $H^s(\Omega)$, where $C_c^\infty(\Omega)$ is the set of C^∞ functions with compact support in Ω.

In what follows, we will need the following family of operators $\{\Lambda_t\}_{t\in\mathbb{R}}$, where for all $t \in \mathbb{R}$ the operator Λ_t is defined as

$$\Lambda_t = (\mathbb{I} - \Delta_{\mathrm{LB}})^{t/2},$$

where $\mathbb{I}$ is the identity operator on $L^2(\partial\Omega)$ and Δ_{LB} is the Laplace–Beltrami operator on $\partial\Omega$. We will set $\Lambda \equiv \Lambda_1$. The family $\{\Lambda_t\}_{t\in\mathbb{R}}$ has the following property: For all $t, s \in \mathbb{R}$

$$\Lambda_t : H^s(\partial\Omega) \to H^{s-t}(\partial\Omega)$$

is positive and unitary. For an explicit construction of $\{\Lambda_t\}_{t\in\mathbb{R}}$, see [25].

We denote by $\langle\cdot,\cdot\rangle_{s,-s}$, with $s \in \mathbb{R}$, the pairing between $H^{-s}(\partial\Omega)$ and its dual $H^s(\partial\Omega)$ induced by the scalar product in $L^2(\partial\Omega)$, i.e.,

$$\langle u, v\rangle_{s,-s} := \langle \Lambda_s u|\Lambda_{-s} v\rangle_{L^2(\partial\Omega)}, \quad \text{for all } u \in H^s(\partial\Omega), \quad v \in H^{-s}(\partial\Omega).$$

Let T^* be the operator that acts as the distributional Laplacian on the maximal domain

$$D(T^*) = \{\psi \in L^2(\Omega) \,|\, \Delta\psi \in L^2(\Omega)\}.$$

We denote by

$$\boldsymbol{\gamma} : D(T^*) \to H^{-1/2}(\partial\Omega), \quad \psi \mapsto \boldsymbol{\gamma}(\psi) = \psi|_{\partial\Omega}$$

the *trace operator* and by

$$\boldsymbol{\nu} : D(T^*) \to H^{-3/2}(\partial\Omega), \quad \psi \mapsto \boldsymbol{\nu}(\psi) = \frac{\partial\psi}{\partial\nu} = (\nabla\psi)|_{\partial\Omega} \cdot \nu$$

the *normal derivative*, and we recall that these operators are continuous with respect to the graph norm of T^* [25].

In the following, we will consider the Laplace operator $T = -\Delta$ on the domain

$$D(T) = \{\psi \in H^2(\Omega) \,|\, \boldsymbol{\gamma}\psi = \boldsymbol{\nu}\psi = 0\} \equiv H_0^2(\Omega) \tag{1}$$

and the Dirichlet Laplacian $T_{\mathrm{D}} = -\Delta$ on

$$D(T_{\mathrm{D}}) = H^2(\Omega) \cap H_0^1(\Omega) = \{\psi \in H^2(\Omega) \,|\, \boldsymbol{\gamma}\psi = 0\}.$$

We recall that T is nothing but the closure in $L^2(\Omega)$ of the symmetric operator given by the Laplacian on functions in $C_c^\infty(\Omega)$. Moreover, T_{D} is a self-adjoint, positive definite operator, $T_{\mathrm{D}} = T_{\mathrm{D}}^* > 0$.

Moreover, T^* is the adjoint operator of the symmetric operator T, and T_{D} is a self-adjoint extension of T, namely

$$T \subset T_{\mathrm{D}} \subset T^*.$$

Our main objective is to characterize all the possible self-adjoint extensions of the symmetric operator T. As the Dirichlet Laplacian, they will all be contained between the minimal Laplacian T and the maximal one T^*. The domain of each self-adjoint extension will be characterized by a specific relation between the values of the functions and those of their normal derivatives at the boundary.

We will need a regularized version of the trace operator for the normal derivative $\boldsymbol{\nu}$.

Definition 1 The *regularized normal derivative* $\boldsymbol{\mu} : D(T^*) \to H^{-1/2}(\partial\Omega)$ is the linear operator whose action is

$$\boldsymbol{\mu}\psi = \Lambda\, \boldsymbol{\nu} \Pi_{\mathrm{D}}\psi,$$

for all $\psi \in D(T^*)$, where $\Pi_{\mathrm{D}} = T_{\mathrm{D}}^{-1} T^*$.

Remark 1 Note that T_{D}^{-1} maps $L^2(\Omega)$ onto $D(T_{\mathrm{D}}) \subset H^2(\Omega)$. By the trace theorem, $\boldsymbol{\nu}(H^2(\Omega)) = H^{1/2}(\partial\Omega)$, whence $\boldsymbol{\mu}\psi \in H^{-1/2}(\partial\Omega)$ is more regular than the normal derivative $\boldsymbol{\nu}\psi \in H^{-3/2}(\partial\Omega)$.

The operator Π_{D} is in fact a (nonorthogonal) projection from $D(T^*)$ onto $D(T_{\mathrm{D}})$, since for all $\psi \in D(T_{\mathrm{D}})$ one gets that $\Pi_{\mathrm{D}}\psi = T_{\mathrm{D}}^{-1} T^*\psi = T_{\mathrm{D}}^{-1} T_{\mathrm{D}}\psi = \psi$. Thus, $\boldsymbol{\mu}\psi$ is the image under Λ of the normal derivative of the component $\psi_{\mathrm{D}} = \Pi_{\mathrm{D}}\psi$ of ψ belonging to the regular subspace $D(T_{\mathrm{D}})$ of $D(T^*)$.

Theorem 1 *The set of all self-adjoint extensions of T is*

$$\left\{T_U : D(T_U) \to L^2(\Omega) \,|\, U \in \mathscr{U}(H^{-1/2}(\partial\Omega))\right\},$$

where for all $U \in \mathscr{U}(H^{-1/2}(\partial\Omega))$

$$D(T_U) = \left\{\psi \in D(T^*) \,|\, i(\mathbb{I} + U)\boldsymbol{\gamma}\psi = (\mathbb{I} - U)\boldsymbol{\mu}\psi\right\}.$$

Remark 2 Note the role played by the regularized normal derivative $\boldsymbol{\mu}\psi$ in the above theorem: The trace $\boldsymbol{\gamma}\psi$ and $\boldsymbol{\mu}\psi$ can be compared because they both belong to the same (boundary) space, namely $H^{-1/2}(\partial\Omega)$. Notice also the equivalent relation

$$\boldsymbol{\mu}\psi - i\boldsymbol{\gamma}\psi = U(\boldsymbol{\mu}\psi + i\boldsymbol{\gamma}\psi)$$

defining the domain of the self-adjoint extension T_U.

Now we want to compare the result in Theorem 1 with the classical characterization of the self-adjoint extensions of T due to Grubb [19,20]. We need some notation: A closed linear subspace $\mathcal{X}$ of $H^{-1/2}(\partial\Omega)$ is denoted by $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$, and $\mathcal{X}^*$ denotes its dual; we say that a densely defined operator $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$ is self-adjoint if

$$\Lambda L : D(L) \subset \mathcal{X} \to \mathcal{X}$$

is self-adjoint, $(\Lambda L)^* = \Lambda L$.

Theorem 2 *[19] The set of all self-adjoint extensions of T is*

$$\Big\{T_{(\mathcal{X},L)} : D\left(T_{(\mathcal{X},L)}\right) \to L^2(\Omega) \,|\, \mathcal{X} \sqsubset H^{-1/2}(\partial\Omega),\ L : D(L) \subset \mathcal{X} \to \mathcal{X}^*, L \textit{ self-adjoint}\Big\},$$

where, for all $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$ *and* $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$, *L self-adjoint,*

$$D\left(T_{(\mathcal{X},L)}\right) = \Big\{\psi \in D(T^*) \,|\, \boldsymbol{\gamma}\psi \in D(L),\ \langle \boldsymbol{\nu}\Pi_{\mathrm{D}}\psi, u\rangle_{\frac{1}{2},-\frac{1}{2}} = \langle L\boldsymbol{\gamma}\psi, u\rangle_{\frac{1}{2},-\frac{1}{2}},\ \forall u \in \mathcal{X}\Big\}.$$

The relation between the two different parametrizations of the self-adjoint extensions of T given in Theorems 1 and 2 is established in the next theorem. First we introduce some notation: If $U : H^{-1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ is a linear operator and $\mathcal{X}$ is a subspace of $H^{-1/2}(\partial\Omega)$, we denote by $U\restriction_{\mathcal{X}}$ the operator

$$U\restriction_{\mathcal{X}} : \mathcal{X} \to U(\mathcal{X}), \qquad u \in \mathcal{X} \mapsto Uu.$$

Theorem 3 *For all $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$ and $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$, with L self-adjoint, it results that*

$$T_{(\mathcal{X},L)} = T_U, \quad \textit{with} \;\; U = \mathscr{C}(\Lambda L) \oplus \mathbb{I}_{\mathcal{X}^\perp} \in \mathscr{U}(H^{-1/2}(\partial\Omega)),$$

where

$$\mathscr{C}(\Lambda L) = (\Lambda L - i\mathbb{I}_{\mathcal{X}})(\Lambda L + i\mathbb{I}_{\mathcal{X}})^{-1}$$

is the Cayley transform of ΛL, and $\mathbb{I}_{\mathcal{X}}, \mathbb{I}_{\mathcal{X}^\perp}$ are the identity operators on $\mathcal{X}$ and on $\mathcal{X}^\perp$, respectively.

Conversely, for all $U \in \mathscr{U}(H^{-1/2}(\partial\Omega))$ it results that

$$T_U = T_{(\mathcal{X},L)}, \;\; \textit{with} \;\; \mathcal{X} = \operatorname{Ran} Q_U \;\; \textit{and} \;\; L = \Lambda^{-1}\mathscr{C}^{-1}\left(U\restriction_{\mathcal{X}}\right),$$

where Q_U is the spectral projection of U on the Borel set $\mathbb{R}\backslash\{1\}$ and

$$\mathscr{C}^{-1}(V) = i\,(\mathbb{I}_{\mathcal{X}} + V)\,(\mathbb{I}_{\mathcal{X}} - V)^{-1}$$

is the inverse Cayley transform of $V \in \mathscr{U}(\mathcal{X})$.

Remark 3 The Cayley transform maps bijectively self-adjoint operators on the Hilbert space $\mathcal{X}$ to unitary operators that do not have 1 as eigenvalue. See Sect. 6. In the second part of the theorem, $V = U\restriction_{\mathcal{X}}$ is the restriction of the unitary U to its spectral subspace $\mathcal{X} = \operatorname{Ran} Q_U$ orthogonal to the (possible) eigenspace belonging to the eigenvalue 1. Therefore, its inverse Cayley transform exists. It is a bounded self-adjoint operator if 1 is a point of the resolvent set of V, i.e., if the (possible) eigenvalue 1 of U is isolated; otherwise, it is an unbounded self-adjoint operator.

3 Quadratic forms

Consider the expectation value of the symmetric operator $T = -\Delta$ at $\psi \in D(T) = H_0^2(\Omega)$:

$$\mathfrak{t}(\psi) = \langle\psi|T\psi\rangle_{L^2(\Omega)} = \|\nabla\psi\|^2_{L^2(\Omega)}. \tag{2}$$

Physically, this represents the kinetic energy of a quantum particle in the vector state ψ (assumed to be normalized). A quadratic form corresponds to a self-adjoint operator—and hence to a physical observable—if and only if it is real and closed [28]. Therefore, the search of the self-adjoint extensions of the symmetric operator T is mirrored in the search of the real and closed quadratic forms that extend the minimal form (2).

As a consequence, Theorem 1 has a counterpart in terms of quadratic forms, through the relation $\mathfrak{t}_U(\psi) = \langle\psi|T_U\psi\rangle$, which must hold for all $\psi \in D(T_U)$.

Theorem 4 *The set of all real closed quadratic forms on $L^2(\Omega)$ that extend $\mathfrak{t}(\psi)$ is*

$$\left\{\mathfrak{t}_U : D(\mathfrak{t}_U) \to \mathbb{R} \,|\, U \in \mathscr{U}(H^{-1/2}(\partial\Omega))\right\},$$

with

$$\mathrm{t}_U(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} + \langle \boldsymbol{\gamma}\psi | K_U \boldsymbol{\gamma}\psi\rangle_{H^{-1/2}(\partial\Omega)}, \qquad \textit{for all } \psi \in D_U,$$

where

$$D_U = D(\mathrm{t}_{\mathrm{D}}) + N(T^*) \cap \boldsymbol{\gamma}^{-1}(D(K_U))$$

is a core of t_U.

Here $\psi_{\mathrm{D}} = \Pi_{\mathrm{D}}\psi \in D(\mathrm{t}_{\mathrm{D}}) = H^1_0(\Omega)$, *the domain of the Dirichlet form, and* K_U *is a self-adjoint operator on the boundary space* $H^{-1/2}(\partial\Omega)$ *defined by*

$$D(K_U) = \mathrm{Ran}(\mathbb{I} - U), \quad K_U(\mathbb{I} - U)g = -i Q_U(\mathbb{I} + U)g, \quad \textit{for all } g \in H^{-1/2}(\partial\Omega),$$

with Q_U *the projection onto the subspace* $\overline{\mathrm{Ran}(\mathbb{I} - U)}$.

Moreover, the domain $D(T_U)$ *of Theorem 1 is a core of* t_U *(in fact it is a subspace of* D_U*), and*

$$\mathrm{t}_U(\psi) = \langle \psi | T_U\psi\rangle_{L^2(\Omega)} \qquad \textit{for all } \psi \in D(T_U).$$

Proof According to assertion 2 of Lemma 1 in Sect. 4, every $\phi \in C^\infty(\overline{\Omega}) \subset D(T^*)$ has a unique decomposition $\phi = \phi_{\mathrm{D}} + \phi_0$, with $\boldsymbol{\gamma}\phi_{\mathrm{D}} = 0$ and $\Delta\phi_0 = 0$. Thus, for any $\phi \in C^\infty(\overline{\Omega})$, we get by the Gauss–Green formula and Definition 1

$$\begin{aligned} \langle \phi | T^*\phi\rangle_{L^2(\Omega)} &= -\int_\Omega \bar{\phi}\Delta\phi_{\mathrm{D}}\mathrm{d}x \\ &= \int_\Omega \nabla\bar{\phi}_0 \cdot \nabla\phi_{\mathrm{D}}\mathrm{d}x + \int_\Omega |\nabla\phi_{\mathrm{D}}|^2\mathrm{d}x - \int_{\partial\Omega} \bar{\phi}\frac{\partial\phi_{\mathrm{D}}}{\partial\nu}\mathrm{d}S \\ &= \|\nabla\phi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle \boldsymbol{\gamma}\phi | \boldsymbol{\mu}\phi\rangle_{H^{-1/2}(\partial\Omega)}, \end{aligned} \tag{3}$$

since

$$\int_\Omega \nabla\bar{\phi}_0 \cdot \nabla\phi_{\mathrm{D}}\mathrm{d}x = -\int_\Omega \Delta\bar{\phi}_0\phi_{\mathrm{D}}\mathrm{d}x + \int_{\partial\Omega} \frac{\partial\bar{\phi}_0}{\partial\nu}\phi_{\mathrm{D}}\mathrm{d}S = 0.$$

By density, formula (3) is valid for all $\phi \in D(T^*)$. Therefore, we can define the following quadratic form

$$\mathrm{t}_*(\psi) = \|\nabla\psi_{\mathrm{D}}\|^2_{L^2(\Omega)} - \langle \boldsymbol{\gamma}\psi | \boldsymbol{\mu}\psi\rangle_{H^{-1/2}(\partial\Omega)}, \tag{4}$$

which on $D(T^*)$ coincides with the expectation value of the operator T^*, namely

$$\mathrm{t}_*(\psi) = \langle \psi | T^*\psi\rangle_{L^2(\Omega)},$$

for all $\psi \in D(T^*)$. However, notice that $D(T_\mathrm{D}) = H^2(\Omega) \cap H_0^1(\Omega)$ is a dense subspace of $D(\mathfrak{t}_\mathrm{D}) = H_0^1(\Omega)$, the domain of the Dirichlet quadratic form,

$$\mathfrak{t}_\mathrm{D}(u) = \|\nabla u\|^2_{L^2(\Omega)}.$$

Therefore, the form (4) can be extended by density to functions

$$\psi \in D(\mathfrak{t}_\mathrm{D}) + N(T^*).$$

[Recall the decomposition of Lemma 1, $D(T^*) = D(T_\mathrm{D}) + N(T^*)$.]

Suppose now that $\psi \in D(T_U) \subset D(T^*)$. Thus,

$$\langle \psi | T_U \psi \rangle_{L^2(\Omega)} = \mathfrak{t}_*(\psi) = \|\nabla \psi_\mathrm{D}\|^2_{L^2(\Omega)} - \langle \boldsymbol{\gamma} \psi | \boldsymbol{\mu} \psi \rangle_{H^{-1/2}(\partial\Omega)},$$

and, by Theorem 1,

$$i(\mathbb{I} + U)\boldsymbol{\gamma}\psi = (\mathbb{I} - U)\boldsymbol{\mu}\psi.$$

Let P_U and Q_U be the spectral projections of U on the Borel sets $\{1\}$ and $\mathbb{R}\backslash\{1\}$, respectively ($P_U$ is zero if 1 is not an eigenvalue of U). Then, the above relation is equivalent to

$$P_U \boldsymbol{\gamma}\psi = 0, \quad i(\mathbb{I} + U)Q_U \boldsymbol{\gamma}\psi = (\mathbb{I} - U)Q_U \boldsymbol{\mu}\psi, \tag{5}$$

which imply that

$$\boldsymbol{\gamma}\psi \in \operatorname{Ran}(\mathbb{I} - U) \subset \operatorname{Ran} Q_U,$$

since $\operatorname{Ran} P_U = \operatorname{Ran}(\mathbb{I} - U)^\perp$. Let us now define the operator K_U with domain

$$D(K_U) = \operatorname{Ran}(\mathbb{I} - U),$$

whose action is

$$K_U(\mathbb{I} - U)g = -iQ_U(\mathbb{I} + U)g = -i(\mathbb{I} + U)Q_U g,$$

for all $g \in H^{-1/2}(\partial\Omega)$. Thus, we get that, for some $g \in H^{-1/2}(\partial\Omega)$,

$$\begin{aligned} i(\mathbb{I} + U)Q_U\boldsymbol{\gamma}\psi &= i(\mathbb{I} + U)Q_U(\mathbb{I} - U)g = (\mathbb{I} - U)iQ_U(\mathbb{I} + U)g \\ &= -(\mathbb{I} - U)K_U(\mathbb{I} - U)g = -(\mathbb{I} - U)K_U Q_U \boldsymbol{\gamma}\psi, \end{aligned}$$

which plugged into (5) gives

$$-(\mathbb{I} - U)Q_U K_U \boldsymbol{\gamma}\psi = (\mathbb{I} - U)Q_U \boldsymbol{\mu}\psi.$$

Since $\mathbb{I} - U$ is injective when restricted to $\operatorname{Ran} Q_U$, we get that

$$K_U \boldsymbol{\gamma}\psi = -Q_U \boldsymbol{\mu}\psi, \tag{6}$$

for all $\boldsymbol{\gamma}\psi \in D(K_U)$. This implies that

$$-\langle \boldsymbol{\gamma}\psi|\boldsymbol{\mu}\psi\rangle_{H^{-1/2}(\partial\Omega)} = \langle \boldsymbol{\gamma}\psi|K_U\boldsymbol{\gamma}\psi\rangle_{H^{-1/2}(\partial\Omega)},$$

for all $\psi \in D(\mathfrak{t}_\mathrm{D}) + N(T^*)$, such that $\boldsymbol{\gamma}\psi \in D(K_U)$.

Thus, we can define the quadratic form

$$\mathfrak{t}_U(\psi) = \|\nabla\psi_\mathrm{D}\|^2_{L^2(\Omega)} + \langle \boldsymbol{\gamma}\psi|K_U\boldsymbol{\gamma}\psi\rangle_{H^{-1/2}(\partial\Omega)},$$

on the domain

$$D_U = D(\mathfrak{t}_\mathrm{D}) + N(T^*) \cap \boldsymbol{\gamma}^{-1}\left(D(K_U)\right).$$

For all $\psi \in D(T_U)$, it coincides with the expectation value of the self-adjoint extension T_U:

$$\mathfrak{t}_U(\psi) = \langle \psi|T_U\psi\rangle_{L^2(\Omega)}.$$

The domain D_U is a core of the quadratic form $\mathfrak{t}_U$ since it contains the domain of its associated self-adjoint operator T_U, namely $D(T_U) \subset D_U$. □

Remark 4 At variance with the domains of their corresponding operators, the domains of the kinetic energy forms are all contained between a minimal domain and a maximal one:

$$D(\mathfrak{t}_{\mathbb{I}}) \subset D(\mathfrak{t}_U) \subset D(\mathfrak{t}_{-\mathbb{I}}).$$

The Dirichlet form $\mathfrak{t}_{\mathbb{I}} = \mathfrak{t}_\mathrm{D}$ has the expression

$$\mathfrak{t}_\mathrm{D}(\psi) = \|\nabla\psi\|^2_{L^2(\Omega)},$$

on the minimal domain $D(\mathfrak{t}_\mathrm{D}) = H^1_0(\Omega)$, while the form $\mathfrak{t}_{-\mathbb{I}}$ has maximal domain $D(\mathfrak{t}_{-\mathbb{I}}) = H^1_0(\Omega) + N(T^*)$ and acts as

$$\mathfrak{t}_{-\mathbb{I}}(\psi) = \|\nabla\psi_\mathrm{D}\|^2_{L^2(\Omega)}.$$

Both forms have no boundary term, since the boundary Hamiltonians are both zero, $K_{\mathbb{I}} = K_{-\mathbb{I}} = 0$, but on the smallest and largest domain, respectively: $D(K_{\mathbb{I}}) = \{0\}$ and $D(K_{-\mathbb{I}}) = H^{-1/2}(\partial\Omega)$. The maximal form $\mathfrak{t}_{-\mathbb{I}}$ corresponds to the Kreĭn-von Neumann extension $T_{-\mathbb{I}}$, whose boundary condition is the vanishing of the regularized normal derivative, $\boldsymbol{\mu}\psi = 0$ [24].

Remark 5 Notice that the boundary Hamiltonian K_U is nothing but the inverse partial Cayley transform of the unitary U on its spectral subspace $\operatorname{Ran} Q_U = \overline{\operatorname{Ran}(\mathbb{I} - U)}$.

(In the above proof, Q_U has been identified as the spectral projection of U on the Borel set $\mathbb{R}\setminus\{1\}$). Explicitly, one gets

$$K_U = \mathscr{C}^{-1}(U\restriction_{\operatorname{Ran} Q_U}).$$

The inverse Cayley transform is well defined since the restriction of U has the eigenvalue 1 stripped out. Notice, however, that if 1 is not an isolated eigenvalue of U, then 1 is not in the resolvent set of $U\restriction_{\operatorname{Ran} Q_U}$, and thus, K_U is an unbounded operator.

4 Proof of Theorem 1

We will first need some properties of the regularized normal derivative $\boldsymbol{\mu}$ and of the projection Π_D.

Lemma 1 *The following properties hold:*

1. *Let $\boldsymbol{\mu}$ be the regularized normal derivative of Definition 1, then*
$$\boldsymbol{\mu} : D(T^*) \to H^{-1/2}(\partial\Omega)$$
is a surjective continuous map with respect to the graph norm of T^*.
2. *The domain of the adjoint $D(T^*)$ is the vector space direct sum of the domain of the Dirichlet Laplacian T_D and the kernel of T^*:*
$$D(T^*) = D(T_\mathrm{D}) + N(T^*), \qquad \psi = \psi_\mathrm{D} + \psi_0,$$
where $\psi \in D(T^*)$, $\psi_\mathrm{D} = \Pi_\mathrm{D}\psi \in D(T_\mathrm{D})$, and $\psi_0 = (\mathbb{I} - \Pi_\mathrm{D})\psi \in N(T^*)$.
3. *The map*
$$\phi \in D(T^*) \mapsto (\boldsymbol{\gamma}\,\phi, \boldsymbol{\mu}\,\phi) \in H^{-1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$$
is surjective.

Proof 1. The map $\boldsymbol{\mu}$ is continuous as a composition of three continuous maps: $\boldsymbol{\mu} = \Lambda\boldsymbol{\nu}\Pi_\mathrm{D}$, with $\Lambda : H^{1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ being unitary,

$$\boldsymbol{\nu} : H^2(\Omega) \to H^{1/2}(\partial\Omega)$$

being continuous by the trace theorem, and

$$\Pi_\mathrm{D} = T_\mathrm{D}^{-1}T^* : D(T^*) \to D(T_\mathrm{D}) = H^2(\Omega) \cap H_0^1(\Omega)$$

being a projection, as pointed out in Remark 1.
Surjectivity follows from the surjectivity of the projection Π_D and from the surjectivity of the map

$$\boldsymbol{\gamma}_1 = (\boldsymbol{\gamma}, \boldsymbol{\nu}) : H^2(\Omega) \to H^{3/2}(\partial\Omega) \times H^{1/2}(\partial\Omega),$$

which implies the surjectivity of its restriction

$$\boldsymbol{\gamma}_1 : H^2(\Omega) \cap \boldsymbol{\gamma}_1^{-1}(\{0\} \times H^{1/2}(\partial\Omega)) \to \{0\} \times H^{1/2}(\partial\Omega)$$

and thus of the map

$$\boldsymbol{\nu} : H^2(\Omega) \cap H_0^1(\Omega) \to H^{1/2}(\partial\Omega).$$

2. For any $\psi \in D(T^*)$, we have $\psi_\mathrm{D} = \Pi_\mathrm{D}\psi \in D(T_\mathrm{D})$ and $\psi_0 = (\mathbb{I} - \Pi_\mathrm{D})\psi \in N(T^*)$. Indeed,

$$T^*\psi_0 = T^*\psi - T^*\Pi_\mathrm{D}\psi = T^*\psi - T^*T_\mathrm{D}^{-1}T^*\psi = T^*\psi - T_\mathrm{D}T_\mathrm{D}^{-1}T^*\psi = 0.$$

3. Since $\Lambda : H^{1/2}(\partial\Omega) \to H^{-1/2}(\partial\Omega)$ is unitary, the surjectivity of the map

$$(\boldsymbol{\gamma}, \boldsymbol{\mu}) : D(T^*) \to H^{-1/2}(\partial\Omega) \times H^{-1/2}(\partial\Omega)$$

is equivalent to the surjectivity of

$$(\boldsymbol{\gamma}, \boldsymbol{\nu}\Pi_\mathrm{D}) : D(T^*) \to H^{-1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega).$$

By the decomposition of point 2 of the lemma, we get that for any $\psi \in D(T^*)$, $\psi = \psi_\mathrm{D} + \psi_0$ with $\boldsymbol{\gamma}\psi_\mathrm{D} = 0$ and $\boldsymbol{\nu}\Pi_\mathrm{D}\psi_0 = \boldsymbol{\nu}\Pi_\mathrm{D}(\mathbb{I} - \Pi_\mathrm{D})\psi = 0$. Therefore,

$$(\boldsymbol{\gamma}, \boldsymbol{\nu}\Pi_\mathrm{D})\psi = (\boldsymbol{\gamma}\psi_0, \boldsymbol{\nu}\psi_\mathrm{D}).$$

Therefore, the surjectivity of $(\boldsymbol{\gamma}, \boldsymbol{\mu})$ follows from the separate surjectivity of the two component maps:

$$\boldsymbol{\gamma} : N(T^*) \to H^{-1/2}(\partial\Omega), \quad \boldsymbol{\nu} : D(T_\mathrm{D}) \to H^{1/2}(\partial\Omega).$$

The surjectivity of $\boldsymbol{\nu}$ has just been proved in part 1. The surjectivity of $\boldsymbol{\gamma}$ is nothing but a classical result [30] on the existence of an $L^2(\Omega)$-solution to the Laplace equation $-\Delta u = 0$ for any Dirichlet boundary condition $\boldsymbol{\gamma}u = g \in H^{-1/2}(\partial\Omega)$. □

Using the regularity result in Lemma 1, we can define the generalized Gauss–Green boundary form.

Definition 2 We define the generalized Gauss–Green boundary form

$$\Gamma : D(T^*) \times D(T^*) \to \mathbb{C}$$

such that for all $\phi, \psi \in D(T^*)$

$$\Gamma(\phi, \psi) = \langle \boldsymbol{\mu}\phi | \boldsymbol{\gamma}\psi \rangle_{H^{-1/2}(\partial\Omega)} - \langle \boldsymbol{\gamma}\phi | \boldsymbol{\mu}\psi \rangle_{H^{-1/2}(\partial\Omega)}.$$

In [19], it was proved the following result.

Proposition 1 *Let T the operator defined in (1) and let Γ the generalized Gauss–Green boundary form in Definition 2. Then,*

$$\Gamma(\phi, \psi) = \langle \phi | T^* \psi \rangle_{L^2(\Omega)} - \langle T^* \phi | \psi \rangle_{L^2(\Omega)} \quad \text{for all } \phi, \psi \in D(T^*). \tag{7}$$

Proof According to Lemma 1, every $\phi \in C^\infty(\overline{\Omega}) \subset D(T^*)$ has a unique decomposition $\phi = \phi_D + \phi_0$, with $\boldsymbol{\gamma}\phi_D = 0$ and $\Delta\phi_0 = 0$. Thus, for any $\phi, \psi \in C^\infty(\overline{\Omega})$, we get

$$\begin{aligned}
\langle \phi | T^* \psi \rangle_{L^2(\Omega)} - \langle T^* \phi | \psi \rangle_{L^2(\Omega)} &= \int_\Omega \left(\Delta\bar{\phi}_D \psi - \bar{\phi} \Delta \psi_D \right) \mathrm{d}x \\
&= \int_{\partial\Omega} \left(\frac{\partial \bar{\phi}_D}{\partial \nu} \psi - \bar{\phi} \frac{\partial \psi_D}{\partial \nu} \right) \mathrm{d}S \\
&= \langle \boldsymbol{\nu}\phi_D, \boldsymbol{\gamma}\psi \rangle_{\frac{1}{2},-\frac{1}{2}} - \langle \boldsymbol{\gamma}\phi, \boldsymbol{\nu}\psi_D \rangle_{-\frac{1}{2},\frac{1}{2}} \\
&= \langle \boldsymbol{\mu}\phi | \boldsymbol{\gamma}\psi \rangle_{H^{-1/2}(\partial\Omega)} - \langle \boldsymbol{\gamma}\phi | \boldsymbol{\mu}\psi \rangle_{H^{-1/2}(\partial\Omega)},
\end{aligned}$$

by the Gauss–Green formula and Definition 1. The result follows by density. □

Remark 6 Notice that the irregular part of the normal derivative is immaterial to the boundary conditions as it follows from the generalized Green formula; see Definition 2 and Proposition 1. It exploits a gauge freedom in Green's second identity: One can add and subtract an arbitrary boundary self-adjoint operator to the difference of the normal derivatives. It is just this freedom that was used to get rid of the irregular part of the normal derivative and to gain regularity. In other words, the Dirichlet-to-Neumann operator is a self-adjoint operator [1].

We denote by $\mathscr{H}_b := H^{-1/2}(\partial\Omega) \oplus H^{-1/2}(\partial\Omega)$.

Definition 3 Let $\mathcal{W}$ be a subspace of $\mathscr{H}_b$. We define the *Γ-orthogonal* subspace of $\mathcal{W}$ as

$$\mathcal{W}^\dagger := \left\{ (u_1, u_2) \in \mathscr{H}_b \,\middle|\, \langle u_2 | v_1 \rangle_{H^{-1/2}(\partial\Omega)} = \langle u_1 | v_2 \rangle_{H^{-1/2}(\partial\Omega)}, \ \forall (v_1, v_2) \in \mathcal{W} \right\}.$$

We say that $\mathcal{W}$ is a *maximally isotropic* subspace if $\mathcal{W} = \mathcal{W}^\dagger$.

Proposition 2 *Let $\mathcal{W}$ be a subspace of $\mathscr{H}_b$, and let $\tilde{T}$ be the restriction of T^* to the domain*

$$D(\tilde{T}) = \left\{ \phi \in D(T^*) \,|\, (\boldsymbol{\gamma}\phi, \boldsymbol{\mu}\phi) \in \mathcal{W} \right\}.$$

Then, $\tilde{T}$ is self-adjoint if and only if $\mathcal{W}$ is a closed maximally isotropic subspace.

Proof First of all, we observe that

$$\tilde{T} \text{ is self-adjoint} \iff \mathcal{G}(\tilde{T}^*) = \mathcal{G}(\tilde{T})$$

and that $D(\tilde{T}) \subset D(\tilde{T}^*) \subset D(T^*)$. The proof follows immediately by observing that the graph of $\tilde{T}$ reads

$$\mathcal{G}(\tilde{T}) = \left\{(\phi, T^*\phi) \,\middle|\, \phi \in D(\tilde{T})\right\}$$
$$= \left\{(\phi, T^*\phi) \,\middle|\, \phi \in D(T^*),\ \ (\boldsymbol{\gamma}\phi, \boldsymbol{\mu}\phi) \in \mathcal{W}\right\},$$

while the graph of $\tilde{T}^*$ is

$$\begin{aligned}\mathcal{G}(\tilde{T}^*) &= \left\{(\phi, T^*\phi) \,|\, \phi \in D(\tilde{T}^*)\right\}\\ &= \left\{(\phi, T^*\phi) \,|\, \phi \in D(T^*),\ \ \Gamma(\phi, \psi) = 0,\ \ \forall \psi \in D(\tilde{T})\right\}\\ &= \left\{(\phi, T^*\phi) \,|\, \phi \in D(T^*), \langle u_1 | \boldsymbol{\mu}\phi\rangle_{H^{-1/2}(\partial\Omega)} = \langle \boldsymbol{\gamma}\phi | u_2\rangle_{H^{-1/2}(\partial\Omega)}, \forall (u_1, u_2) \in \mathcal{W}\right\}\\ &= \left\{(\phi, T^*\phi) \,|\, \phi \in D(T^*),\ \ (\boldsymbol{\gamma}\phi, \boldsymbol{\mu}\phi) \in \mathcal{W}^\dagger\right\},\end{aligned}$$

and thus, $\mathcal{G}(\tilde{T}) = \mathcal{G}(\tilde{T}^*)$ iff $\mathcal{W} = \mathcal{W}^\dagger$. □

The closed maximally isotropic subspaces are characterized by the following theorem, whose straightforward proof can be found in [10].

Theorem 5 *A closed subspace $\mathcal{W}$ of $\mathscr{H}_b$ is a maximally isotropic subspace if and only if there exists $U \in \mathscr{U}(H^{-1/2}(\partial\Omega))$ such that*

$$\mathcal{W} = \{(u_1, u_2) \in \mathscr{H}_b \,|\, i(\mathbb{I} + U)u_1 = (\mathbb{I} - U)u_2\}.$$

We can now conclude.

Proof of Theorem 1 The proof follows immediately from Proposition 2 and Theorem 5. □

Remark 7 The proof of Theorem 1 can be translated into the language of boundary triples [10], by saying that $(\mathscr{H}_b, \boldsymbol{\gamma}, \boldsymbol{\mu})$ is a boundary triple for T^*. This follows by Proposition 1 and by assertion 3 of Lemma 1.

5 Proof of Theorem 3

Proof Let $\mathcal{X} \sqsubset H^{-1/2}(\partial\Omega)$ and $L : D(L) \subset \mathcal{X} \to \mathcal{X}^*$ a self-adjoint operator. For all $\psi \in D(T^*)$, we denote by $(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}$ the element of $\mathcal{X}^*$ defined as follows:

$$(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}} u := \langle \Lambda_{-1}\boldsymbol{\mu}\psi, u\rangle_{\frac{1}{2},-\frac{1}{2}}, \qquad \text{for all } u \in \mathcal{X},$$

and thus, we have that

$$D(T_{(\mathcal{X},L)}) = \left\{\psi \in D(T^*) \,|\, \boldsymbol{\gamma}\psi \in D(L),\ (\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}} = L\boldsymbol{\gamma}\psi\right\}.$$

The operator $\Lambda L : D(\Lambda L) \subset \mathcal{X} \to \mathcal{X}$ is self-adjoint, where $D(\Lambda L) = D(L)$. We can define

$$V = \mathscr{C}(\Lambda L) = (\Lambda L - i\mathbb{I}_{\mathcal{X}})(\Lambda L + i\mathbb{I}_{\mathcal{X}})^{-1}$$

and by Proposition 3 in Sect. 6 we have that $V \in \mathscr{U}(\mathcal{X})$. Now observe that, by assertion 3 of Proposition 3, we can rewrite $D(T_{(\mathcal{X},L)})$ as follows

$$D(T_{(\mathcal{X},L)}) = \left\{\psi \in D(T^*) \,|\, \boldsymbol{\gamma}\psi \in D(\Lambda L),\ i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}\right\}.$$

For all $\psi \in D(T^*)$, we denote by $(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}$ the element of $\mathcal{X}$ defined as follows:

$$v(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}} := \langle v, \boldsymbol{\mu}\psi\rangle_{\frac{1}{2},-\frac{1}{2}}, \quad \text{for all } v \in \mathcal{X}^*.$$

Observe that

$$\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}} = (\boldsymbol{\mu}\psi)\big|_{\mathcal{X}} \quad \text{for all } \psi \in D(T^*),$$

and therefore, $D(T_{(\mathcal{X},L)})$ can be rewritten as

$$D(T_{(\mathcal{X},L)}) = \left\{\psi \in D(T^*) \,|\, \boldsymbol{\gamma}\psi \in D(\Lambda L),\ i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}\right\}.$$

By Lemma 2 in Sect. 6, one gets that the condition $\boldsymbol{\gamma}\psi \in D(\Lambda L)$ can be dispensed with. Indeed, as long as $\boldsymbol{\gamma}\psi \in \mathcal{X}$ satisfies the equation

$$i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}},$$

then $\boldsymbol{\gamma}\psi \in D(\Lambda L)$. Therefore, we have proved that

$$D(T_{(\mathcal{X},L)}) = \left\{\psi \in D(T^*) \,|\, \boldsymbol{\gamma}\psi \in \mathcal{X},\ i(\mathbb{I}_{\mathcal{X}} + V)\boldsymbol{\gamma}\psi = (\mathbb{I}_{\mathcal{X}} - V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}\right\}.$$

Thus, by defining the operator $U := V \oplus \mathbb{I}_{\mathcal{X}^\perp} \in \mathscr{U}(H^{-1/2}(\partial\Omega))$, we have that $D(T_{(\mathcal{X},L)}) = D(T_U)$, and that $T_{(\mathcal{X},L)} = T_U$ with $U := \mathscr{C}(\Lambda L) \oplus \mathbb{I}_{\mathcal{X}^\perp}$.

Now we prove the converse. Fix $U \in \mathscr{U}(H^{-1/2}(\partial\Omega))$ and consider T_U, a self-adjoint extension of T. Let P_U the spectral projection of U on the Borel set $\{1\} \subset \mathbb{R}$. Define $\mathcal{X} := \mathrm{Ran}(P_U)^\perp \sqsubset H^{-1/2}(\partial\Omega)$ and consider the operator $V = U\restriction_{\mathcal{X}} \in \mathscr{U}(\mathcal{X})$. Clearly, 1 is not an eigenvalue of V; therefore, we can define the self-adjoint operator

$$L := \Lambda^{-1}\left[i(\mathbb{I}_{\mathcal{X}} + V)(\mathbb{I}_{\mathcal{X}} - V)^{-1}\right] : D(L) \subset \mathcal{X} \to \mathcal{X}^*.$$

We know that

$$D(T_U) = \left\{\psi \in D(T^*) \,|\, i(\mathbb{I} + U)\boldsymbol{\gamma}\psi = (\mathbb{I} - U)\boldsymbol{\mu}\psi\right\}.$$

By projecting on $\mathcal{X}$ and $\mathcal{X}^\perp$ the equation $i(\mathbb{I}+U)\boldsymbol{\gamma}\psi = (\mathbb{I}-U)\boldsymbol{\mu}\psi$, one gets

$$D(T_U) = \left\{\psi \in D(T^*) \mid \boldsymbol{\gamma}\psi \in \mathcal{X},\ i(\mathbb{I}+V)\boldsymbol{\gamma}\psi = (\mathbb{I}-V)(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}}\right\}.$$

Since $(\boldsymbol{\mu}\psi)\big|_{\mathcal{X}} = \Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}$, for all $\psi \in D(T^*)$, we have that

$$D(T_U) = \left\{\psi \in D(T^*) \mid \boldsymbol{\gamma}\psi \in \mathcal{X},\ i(\mathbb{I}+V)\boldsymbol{\gamma}\psi = (\mathbb{I}-V)\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}\right\}.$$

Again by Lemma 2, one has that

$$D(T_U) = \left\{\psi \in D(T^*) \mid \boldsymbol{\gamma}\psi \in D(\Lambda L),\ i(\mathbb{I}+V)\boldsymbol{\gamma}\psi = (\mathbb{I}-V)\Lambda(\tilde{\boldsymbol{\mu}}\psi)\big|_{\mathcal{X}}\right\}$$

and thus

$$D(T_U) = D(T_{(\mathcal{X},L)}).$$

□

6 Supplemental results

Let us recall some basic facts about the Cayley transform of self-adjoint operators. For further details, see [29].

Definition 4 Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator. We define the *Cayley transform* of A, denoted by $\mathcal{C}(A)$, as follows

$$\mathcal{C}(A) = (A - i\mathbb{I})(A + i\mathbb{I})^{-1},$$

where $\mathbb{I}$ is the identity operator on $\mathcal{H}$.

Conversely, let $U \in \mathcal{U}(\mathcal{H})$ and assume that 1 is not an eigenvalue of U. We define the *inverse Cayley transform* of U, denoted by $\mathcal{C}^{-1}(U)$, as follows

$$\mathcal{C}^{-1}(U) = i(\mathbb{I}+U)(\mathbb{I}-U)^{-1}.$$

Proposition 3 *[29] Let $A : D(A) \subset \mathcal{H} \to \mathcal{H}$ be a self-adjoint operator. Then,*

1. $\mathcal{C}(A) \in \mathcal{U}(\mathcal{H})$;
2. $\mathbb{I} - \mathcal{C}(A)$ *is injective;*
3. $\mathrm{Ran}(\mathbb{I} - \mathcal{C}(A)) = D(A)$;
4. *For all* $\phi \in D(A)$,

$$A\phi = i(\mathbb{I} + \mathcal{C}(A))(\mathbb{I} - \mathcal{C}(A))^{-1}\phi = \mathcal{C}^{-1}(\mathcal{C}(A))\phi.$$

5. *Moreover, if* $U \in \mathcal{U}(\mathcal{H})$ *such that* 1 *is not an eigenvalue of* U, *then*

$$\mathcal{C}^{-1}(U) : \mathrm{Ran}(\mathbb{I} - U) \to \mathcal{H}$$

is a self-adjoint operator and $\mathcal{C}(\mathcal{C}^{-1}(U)) = U$.

Lemma 2 *Let* $A : D(A) \subset \mathscr{H} \to \mathscr{H}$ *be a self-adjoint operator and*

$$\mathcal{G}(A) = \{(u, Au) \in \mathscr{H} \times \mathscr{H} \mid u \in D(A)\}$$

be its graph. Let

$$\Theta(A) = \{(\phi, \psi) \in \mathscr{H} \times \mathscr{H} \mid i(\mathbb{I} + \mathscr{C}(A))\,\phi = (\mathbb{I} - \mathscr{C}(A))\,\psi\}.$$

Then, $\mathcal{G}(A) = \Theta(A)$.

Proof Notice first that the inclusion $\mathcal{G}(A) \subset \Theta(A)$ follows immediately from property 3 of Proposition 3. We need to show that $\Theta(A) \subset \mathcal{G}(A)$.

Fix $(\phi, \psi) \in \mathscr{H} \times \mathscr{H}$ such that

$$i(\mathbb{I} + \mathscr{C}(A))\,\phi = (\mathbb{I} - \mathscr{C}(A))\,\psi. \tag{8}$$

Observe that

$$\mathbb{I} - \mathscr{C}(A) = 2i(A + i\mathbb{I})^{-1} \quad \text{and} \quad \mathbb{I} + \mathscr{C}(A) = 2A(A + i\mathbb{I})^{-1}.$$

Plugging these expressions in Eq. (8), we obtain:

$$A\,(A + i\,\mathbb{I})^{-1}\phi = (A + i\,\mathbb{I})^{-1}\psi.$$

The right-hand side belongs to $D(A)$, and thus, also the left-hand side belongs to $D(A)$. Then, we can multiply both sides by $A + i\,\mathbb{I}$, obtaining

$$\psi = (A + i\,\mathbb{I})\,A\,(A + i\,\mathbb{I})^{-1}\phi.$$

Since $(A+i\,\mathbb{I})^{-1}\phi \in D(A)$ and $A\,(A+i\,\mathbb{I})^{-1}\phi \in D(A)$, it follows that $(A+i\,\mathbb{I})^{-1}\phi \in D(A^2)$. The operators $(A + i\,\mathbb{I})$ and A commute on $D(A^2)$ and we get that

$$\psi = A\phi,$$

and thus $(\phi, \psi) \in \mathcal{G}(A)$. □

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