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Unbounded operators in Hilbert space, duality rules, characteristic projections, and their applications

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Abstract Our main theorem is in the generality of the axioms of Hilbert space, and the theory of unbounded operators. Consider two Hilbert spaces whose intersection contains a fixed vector space $\mathscr{D}$. In the case when $\mathscr{D}$ is dense in one of the Hilbert spaces (but not necessarily in the other), we make precise an operator-theoretic linking between the two Hilbert spaces. No relative boundedness is assumed. Nonetheless, under natural assumptions (motivated by potential theory), we prove a theorem where a comparison between the two Hilbert spaces is made via a specific selfadjoint semi-bounded operator. Applications include physical Hamiltonians, both continuous and discrete (infinite network models), and the operator theory of reflection positivity.

Keywords Quantum mechanics · Unbounded operator · Closable operator · Selfadjoint extensions · Spectral theory · Reproducing kernel Hilbert space · Discrete analysis · Graph Laplacians · Distribution of point-masses · Green's functions

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Contents

1 Introduction

When realized in quantized physical systems, quantum-mechanical observables (such as Hamiltonians, momentum operators etc.) take the form of selfadjoint operators. The case of positive measurements dictate semibounded and selfadjoint realization. For this to work, two requirements must be addressed: (i) choice of appropriate Hilbert space(s); and (ii) choice of selfadjoint extension. However from the context from physics, the candidates for observables may only be formally selfadjoint (also called Hermitian), and this necessitates the second question (ii). Even if the initial Hermitian operator has a lower bound, a lower bounds for its selfadjoint extensions is not automatic. There are choices, and these choices dictate the physics (and conversely). Now, there are families of selfadjoint extensions which preserve the initial lower bound. This is the extension theory of Friedrichs and Krein; see e.g. [1,27]. Examples include free particles on an interval, particles in a number of potential fields including delta-like potentials, the one-dimensional Calogero problem, the Aharonov–Bohm problem (see e.g. [7,11,31,33]), and the relativistic Coulomb problem; and precise solutions to quantization problems must flesh out the spectral resolutions of the physical selfadjoint operators.

The setting for our main theorem (Sect. 4) is a given pair: two fixed Hilbert spaces, such that their intersection contains a fixed vector space $\mathscr{D}$. In many applications, when feasible, it is of interest to make a precise linking between such two Hilbert spaces when it is assumed that $\mathscr{D}$ is dense in one of the two; but not necessarily in the other. In the case when the two Hilbert spaces are given as $L^2(\mu_i)$ spaces, the natural means of comparison is of course via relative absolute continuity for the two measures; and then the Radon-Nikodym derivative serves the purpose, Sect. 5.

Rather, the setting for our main result below is the axioms of Hilbert space, and the theory of unbounded operators. In this generality, we will prove theorems where a comparison between the two is made instead with a specific selfadjoint semibounded operator, as opposed to a Radon-Nikodym derivative. Of course the conclusions in L^2 spaces will arise as special cases.

Our motivation comes from any one of a host of diverse applications where the initial pairs of Hilbert spaces are not given as L^2 spaces, rather they may be Dirichlet spaces, Sobolev spaces, reproducing kernel Hilbert spaces (RKHSs), perhaps relative RKHSs; or energy-Hilbert spaces derived from infinite networks of prescribed resistors; or they may arise from a host of non-commutative analysis settings, e.g. from von Neumann algebras, Voiculescu's free probability theory [6,41], and more. In [23], some applications are developed for Tomita-Takesaki theory (from the theory of von Neumann algebras) and for the Malliavin derivative (from the theory of stochastic calculus).

A particular, but important, special case where the comparison of two Hilbert spaces arises is in the theory of reflection positivity in physics. There again, the two Hilbert spaces are linked by a common subspace, dense in the first. The setting of reflection positivity, see e.g. [10,13], lies at the crossroads of the theory of representations of Lie groups, on the one hand, and constructive quantum field theory on the other; here "reflection positivity" links quantum fields with associated stochastic (Euclidean) processes. In physics, it comes from the desire to unify quantum mechanics and relativity, two of the dominating physical theories in the last century.

In the mathematical physics community, it is believed that Euclidean quantum fields are easier to understand than relativistic quantum fields. A subsequent transition from the Euclidean theory to quantum field theory is then provided by reflection positivity, moving from real to imaginary time, and linking operator theory on one side to that of the other. An important tool in the correspondence between the Euclidean side, and the side of quantum fields is a functorial correspondence between properties of operators on one side with their counterparts on the other. A benefit of the study of reflection is that it allows one to take advantage of associated Gaussian measures on suitable spaces of distributions; hence the reflection positive Osterwalder-Schrader path spaces and associated Markov processes; see [10]. Other applications to mathematical physics include [26,30,32], and to Gaussian processes with singular covariance density [2,3].

Our paper is organized as follows. Section 2 spells out the setting, and establishes notation. In Sect. 3, we study the projection onto the closure of graph (T), where T is an operator between two Hilbert spaces. We show among other things that, if T is closed, then the corresponding block matrix has vanishing Schur complements (Corollary 1). We further give a decomposition for general T into a closable and a singular part (Theorem 4). Section 4 continues the study of general operators between two Hilbert spaces; Theorem 5 is a structure theorem which applies to this general context and Theorem 6 shows how the Hilbert spaces may be linked via an intertwining unitary operator. Diverse applications are given in the remaining four sections, starting with Noncommutative Radon-Nikodym derivatives in Sect. 5, and ending with applications to discrete analysis, graph Laplacians on infinite network-graphs with assigned conductance functions.

2 The setting

In this section we recall general facts about unbounded operators from [37], and at the same time we introduce notation to be used later.

Our setting is a fixed separable infinite-dimensional Hilbert space. The inner product in $\mathscr{H}$ is denoted $\langle\cdot,\cdot\rangle$, and we are assuming that $\langle\cdot,\cdot\rangle$ is linear in the second variable. If there is more than one Hilbert space, say $\mathscr{H}_i$, $i = 1, 2$, involved, we shall use subscript notation in the respective inner products, so $\langle\cdot,\cdot\rangle_i$ is the inner product in $\mathscr{H}_i$.

Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be complex Hilbert spaces. If $\mathscr{H}_1 \xrightarrow{T} \mathscr{H}_2$ represents a linear operator from $\mathscr{H}_1$ into $\mathscr{H}_2$, we shall denote

$$dom\,(T) = \{\varphi \in \mathscr{H}_1 \mid T\varphi \text{ is well-defined}\}\,, \tag{2.1}$$

the domain of T, and

$$ran\,(T) = \{T\varphi \mid \varphi \in dom\,(T)\}\,, \tag{2.2}$$

the range of T. The closure of $ran\,(T)$ will be denoted $\overline{ran\,(T)}$, and it is called the *closed range.*

Remark 1 When $dom\,(T)$ is dense in $\mathscr{H}_1$ (as we standardly assume), then we write $T : \mathscr{H}_1 \to \mathscr{H}_2$ or $\mathscr{H}_1 \xrightarrow{T} \mathscr{H}_2$ with the tacit understanding that T is only defined for $\varphi \in dom\,(T)$.

Definition 1 Let $T : \mathscr{H}_1 \to \mathscr{H}_2$ be a densely defined operator, and consider the subspace $dom\,(T^*) \subset \mathscr{H}_2$ defined as follows:

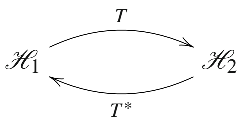
$$\begin{aligned} dom(T^*) = \Big\{ & h_2 \in \mathscr{H}_2 \mid \exists C = C_{h_2} < \infty, \text{ s.t. } \left|\langle h_2, T\varphi\rangle_2\right| \leq C\,\|\varphi\|_1 \\ & \text{holds for } \forall \varphi \in dom\,(T) \Big\}. \end{aligned} \tag{2.3}$$

Then by Riesz' theorem, there is a unique $\eta \in \mathscr{H}_1$ for which

$$\langle \eta, \varphi\rangle_1 = \langle h_2, T\varphi\rangle_2\,, \quad h_2 \in dom(T^*),\ \varphi \in dom\,(T)\,, \tag{2.4}$$

and we define the adjoint operator by $T^* h_2 = \eta$.

It is clear that T^* is an operator from $\mathscr{H}_2$ into $\mathscr{H}_1$:



Definition 2 The direct sum space $\mathscr{H}_1 \oplus \mathscr{H}_2$ is a Hilbert space under the natural inner product

$$\left\langle \begin{bmatrix}\varphi_1\\ \varphi_2\end{bmatrix}, \begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}\right\rangle := \langle\varphi_1, \psi_1\rangle_{\mathscr{H}_1} + \langle\varphi_2, \psi_2\rangle_{\mathscr{H}_2}\,, \tag{2.5}$$

and the *graph* of T is

$$G_T := \left\{ \begin{bmatrix}\varphi\\ T\varphi\end{bmatrix} \mid \varphi \in dom\,(T)\right\} \subset \mathscr{H}_1 \oplus \mathscr{H}_2. \tag{2.6}$$

Definition 3 Let $T : \mathscr{H}_1 \to \mathscr{H}_2$ be a linear operator.

(1) T is *closed* iff the graph G_T in (2.6) is closed in $\mathscr{H}_1 \oplus \mathscr{H}_2$.
(2) T is *closable* iff $\overline{G_T}$ is the graph of an operator.

(3) If (2) holds, the operator corresponding to $\overline{G_T}$, denoted $\overline{T}$, is called the *closure*, i.e.,

$$\overline{G_T} = G_{\overline{T}}. \tag{2.7}$$

Remark 2 It follows from (2.6) that T is closable iff $dom(T^*)$ is dense in $\mathscr{H}_2$, see Theorem 1. It is not hard to construct examples of operators $\mathscr{H}_1 \xrightarrow{T} \mathscr{H}_2$ with dense domain in $\mathscr{H}_1$ which are not closable [35]. For systematic accounts of closable operators and their applications, see [15,39].

Definition 4 Let V be the unitary operator on $\mathscr{H} \times \mathscr{H}$, given by

$$V \begin{bmatrix} \varphi \\ \psi \end{bmatrix} = \begin{bmatrix} -\psi \\ \varphi \end{bmatrix}.$$

Note that $V^2 = -I$, so that any subspace is invariant under V^2.

The following two results may be found in [35] or [37]; see also [38].

Lemma 1 *If $dom\,(T)$ is dense, then $G_{T^*} = (V G_T)^{\perp}$.*

Proof Direct computation:

$$\begin{aligned} \begin{bmatrix} \varphi \\ \psi \end{bmatrix} \in G_{T^*} &\iff \langle T\eta, \varphi \rangle = \langle \eta, \psi \rangle\,, \;\; \forall \eta \in dom\,(T) \\ &\iff \left\langle \begin{bmatrix} \varphi \\ \psi \end{bmatrix}, \begin{bmatrix} -T\eta \\ \eta \end{bmatrix} \right\rangle = 0, \;\; \forall \eta \in dom\,(T) \\ &\iff \begin{bmatrix} \varphi \\ \psi \end{bmatrix} \in (V G_T)^{\perp}. \end{aligned}$$

Theorem 1 *If $dom\,(T)$ is dense, then*

(1) T^* is closed.
(2) T is closable $\iff$ $dom\,(T^*)$ is dense.
(3) T is closable $\Longrightarrow$ $(\overline{T})^* = T^*$. □

Proof (1) This is immediate from Lemma 1, since $U^{\perp}$ is closed for any U.
For (2), closability gives

$$\begin{aligned} G_{\overline{T}} = \overline{G_T} = \left(G_T^{\perp}\right)^{\perp} &= \left(V^2 G_T^{\perp}\right)^{\perp} && V^2 = I \\ &= \left(V\,(V G_T)^{\perp}\right)^{\perp} && V \text{ is unitary} \\ &= (V G_{T^*})^{\perp} && \text{part } (1)\,. \end{aligned}$$

If $dom(T^*)$ is dense, then (1) applies again to give $G_{\overline{T}} = G_{T^{**}}$.
For (3), we use (1), then (2) again:

$$T^* = \overline{T^*} = \left(T^*\right)^{**} = \left(T^{**}\right)^* = \left(\overline{T}\right)^*.$$

□

Definition 5 An operator $T : \mathscr{H}_1 \to \mathscr{H}_2$ is *bounded* iff $dom\,(T) = \mathscr{H}_1$ and there is $C < \infty$ for which $\|T\varphi\|_2 \le C\,\|\varphi\|_1, \forall\varphi \in \mathscr{H}_1$. In this case, the *norm* of T is

$$\|T\| := \inf\left\{C \mid \|T\varphi\|_2 \le C\,\|\varphi\|_1\,,\ \forall \in \mathscr{H}_1\right\}, \tag{2.8}$$

and it satisfies

$$\|T\| = \left\|T^*\right\| = \left\|T^*T\right\|^{1/2}. \tag{2.9}$$

Sometimes, we clarify the notation with a subscript, e.g. $\|T\|_{\mathscr{H}_1\to\mathscr{H}_2}$ and $\|T^*\|_{\mathscr{H}_2\to\mathscr{H}_1}$.

Theorem 2 *(*von Neumann [37,40]*) Let $\mathscr{H}_i$, $i = 1, 2$, be two Hilbert spaces, and let T be a closed operator from $\mathscr{H}_1$ into $\mathscr{H}_2$ having dense domain in $\mathscr{H}_1$; then T^*T is selfadjoint in $\mathscr{H}_1$, TT^* is selfadjoint in $\mathscr{H}_2$, both with dense domains; and there is a partial isometry J from $\mathscr{H}_1$ into $\mathscr{H}_2$ such that*

$$T = J\left(T^*T\right)^{\frac{1}{2}} = \left(TT^*\right)^{\frac{1}{2}} J \tag{2.10}$$

holds on $dom\,(T)$. (Equation (2.10) is called the polar decomposition of T.)

3 The characteristic projection

While a given linear operator between a pair of Hilbert spaces, say T, may in general have subtle features (dictated by the particular application at hand), the closure of graph(T) will be a closed subspace of the direct sum-Hilbert space, and hence the orthogonal projection onto this subspace will be a block matrix, i.e., this projection is a 2×2 matrix with entries which are bounded operators. Stone suggested the name "characteristic projection". Theorem 4 shows how the characteristic projection can be used to compute the maximal closable part of T. We further show (Corollary 1) that every closed operators T has vanishing Schur-complements for its characteristic block-matrix.

The characteristic projection was introduced and studied by Marshall Stone in [39] as a means of understanding an operator via its graph. For more background, see [15,38].

If $\mathscr{H}_i$, $i = 1, 2, 3$ are Hilbert spaces with operators $\mathscr{H}_1 \xrightarrow{A} \mathscr{H}_2 \xrightarrow{B} \mathscr{H}_3$, then the domain of BA is

$$dom\,(BA) := \{\varphi \in dom\,(A) \mid A\varphi \in dom\,(B)\},$$

and for $x \in dom\,(BA)$, we have $(BA)\,x = B\,(Ax)$. In general, $dom\,(BA)$ may be $\{0\}$, even if A and B are densely defined; see Example 2.

Definition 6 (*Characteristic projection*) For a densely defined linear operator $\mathscr{H}_1 \xrightarrow{T} \mathscr{H}_2$, the *characteristic projection* $E = E_T$ of T is the projection in $\mathscr{H}_1 \oplus \mathscr{H}_2$ onto $\overline{G_T}$, where

$$E = \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix}, \tag{3.1}$$

and the components are bounded operators

$$E_{ij} : \mathscr{H}_j \longrightarrow \mathscr{H}_i, \quad i, j = 1, 2. \tag{3.2}$$

Remark 3 Since E is a projection, we have $E = E^* = E^2$, where $E = E^*$ implies

$$E_{11} = E_{11}^* \geq 0, \; E_{12} = E_{21}^*, \; E_{21} = E_{12}^*, \; E_{22} = E_{22}^* \geq 0, \tag{3.3}$$

where the ordering refers to the natural order on selfadjoint operators, and also $E = E^2$ implies

$$E_{ij} = E_{i1}E_{1j} + E_{i2}E_{2j}, \quad i, j = 1, 2. \tag{3.4}$$

Lemma 2 *If U is any unitary operator on $\mathscr{H}$ and $\mathscr{K} \subset \mathscr{H}$ is a subspace, then the orthogonal projection to $(U\mathscr{K})^\perp$ is given by*

$$proj\left[(U\mathscr{K})^\perp\right] = I - UPU^*, \tag{3.5}$$

where $P = P_{\mathscr{K}}$ is the projection to $\mathscr{K}$.

Proof It is obvious that (3.5) is selfadjoint and easy to check that it is idempotent. It is also easy to check that $\langle (I - UPU^*)\,\varphi, U\psi\rangle = 0$ whenever $\psi \in \mathscr{K}$. □

Lemma 3 *Let $E = E_T$ be the characteristic projection of a closable operator T. In terms of the components (3.2), the characteristic projection of $\mathscr{H}_2 \xrightarrow{T^*} \mathscr{H}_1$ in $\mathscr{H}_2 \oplus \mathscr{H}_1$ is given by*

$$E_{T^*} = \begin{bmatrix} I - E_{22} & E_{21} \\ E_{12} & I - E_{11} \end{bmatrix}. \tag{3.6}$$

Proof Since T is closable, we know $dom\,(T^*)$ is dense (Theorem 1). Then (3.6) follows from the identity $G_{T^*} = (VG_T)^\perp$ of Lemma 1, which indicates that $E_{T^*} = I - VEV^*$. □

Remark 4 Since the action of T can be described in terms of (3.2) as the mapping

$$\begin{bmatrix} E_{11}\varphi \\ E_{12}\psi \end{bmatrix} \xrightarrow{T} \begin{bmatrix} E_{21}\varphi \\ E_{22}\psi \end{bmatrix} \tag{3.7}$$

it is clear that

$$TE_{11} = E_{21} \quad \text{and} \quad TE_{12} = E_{22}, \tag{3.8}$$

for example, by putting $\varphi = 0$ or $\psi = 0$ in (3.8); cf. Fig. 1. Similarly, (3.6) yields

$$T^*\,(I - E_{22}) = E_{12} \quad \text{and} \quad T^*E_{21} = I - E_{11}. \tag{3.9}$$

Theorem 3 *([39, Thm. 4]) The entries of $E = E_T$ are given in terms of T by*

$$E = \begin{bmatrix} (I + T^*T)^{-1} & T^*\,(I + TT^*)^{-1} \\ T\,(I + T^*T)^{-1} & TT^*\,(I + TT^*)^{-1} \end{bmatrix}. \tag{3.10}$$

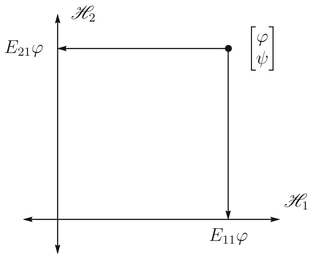


Fig. 1 A diagram indicating why $TE_{11} = E_{21}$; see (3.7) and (3.8)

Proof Applying T^* to (3.8) and then using (3.9) gives $T^*TE_{11} = T^*E_{21} = I - E_{11}$, which can be solved for E_{11} as $E_{11} = (I + T^*T)^{-1}$, whence another application of T [and (3.8)] gives $E_{21} = T(I + T^*T)^{-1}$.

Now applying T to (3.9) and then using (3.8) gives $TT^*(I - E_{22}) = TE_{12} = E_{22}$, whence $I - E_{22} = (I + TT^*)^{-1} \Longrightarrow E_{12} = T^*(I + TT^*)^{-1}$, by (3.9), and applying T to this last one gives $E_{22} = TT^*(I + TT^*)^{-1}$. □

Remark 5 Many more identities can be recovered from (3.7) in this way. For example, applying T^* to (3.8) and then using (3.9) also gives $T^*TE_{12} = T^*E_{22} = T^* - E_{12}$, which can be solved these for E_{12} to give

$$E_{12} = \left(I + T^*T\right)^{-1} T^*. \tag{3.11}$$

Now applying T to (3.9) and then using (3.8) gives

$$\begin{aligned} TT^*E_{21} &= T(I - E_{11}) = T - E_{21}, \text{ and} \\ TT^*(I - E_{22}) &= TE_{12} = E_{22}. \end{aligned}$$

Solving these for E_{22} and E_{21}, respectively, gives

$$E_{21} = \left(I + TT^*\right)^{-1} T, \quad E_{22} = \left(I + TT^*\right)^{-1} TT^*. \tag{3.12}$$

On the other hand, applying (3.8) to (3.11) gives $E_{22} = T(I + T^*T)^{-1}T^*$, and applying (3.9) to (3.12) yields

$$\begin{aligned} I - E_{11} &= T^*T\left(I + T^*T\right)^{-1}, \\ I - E_{22} &= I - \left(I + TT^*\right)^{-1} TT^*, \\ E_{11} &= I - T^*T\left(1 + T^*T\right)^{-1}, \\ E_{12} &= T^* - T^*\left(I + TT^*\right)^{-1} TT^*. \end{aligned}$$

A summary of the above:

$$
\begin{aligned}
E_{11} &= \left(I+T^*T\right)^{-1} = I - T^*T\left(1+T^*T\right)^{-1}, \\
E_{12} &= \left(I+T^*T\right)^{-1}T^* = T^*\left(I+TT^*\right)^{-1} = T^* - T^*\left(I+TT^*\right)^{-1}TT^*, \\
E_{21} &= \left(I+TT^*\right)^{-1}T = T\left(I+T^*T\right)^{-1}, \\
E_{22} &= \left(I+TT^*\right)^{-1}TT^* = TT^*\left(I+TT^*\right)^{-1} = I - \left(I+TT^*\right)^{-1}TT^*.
\end{aligned}
$$

Definition 7 For a matrix X with block decomposition

$$
X = \begin{bmatrix} A & B \\ C & D \end{bmatrix},
$$

the *Schur complements* (see [42]) are

$$
X/A := D - CA^{-1}B \quad \text{and} \quad X/D := A - BD^{-1}C. \tag{3.13}
$$

Corollary 1 *A closed operator T has Schur complements*

$$
E_T/E_{11} = E_T/E_{22} = 0.
$$

Proof Computing directly from (3.10) substituted into (3.13), we have

$$
\begin{aligned}
E_T/E_{11} &= TT^*\left(I+TT^*\right)^{-1} - T\left(I+T^*T\right)^{-1}\left(\left(I+T^*T\right)^{-1}\right)^{-1}T^*\left(I+TT^*\right)^{-1} \\
&= TT^*\left(I+TT^*\right)^{-1} - T\left(I+T^*T\right)^{-1}\left(I+T^*T\right)T^*\left(I+TT^*\right)^{-1} \\
&= TT^*\left(I+TT^*\right)^{-1} - TT^*\left(I+TT^*\right)^{-1} = 0, \quad \text{and} \\
E_T/E_{22} &= \left(I+T^*T\right)^{-1} - T^*\left(I+TT^*\right)^{-1}\left(TT^*\left(I+TT^*\right)^{-1}\right)^{-1}T\left(I+T^*T\right)^{-1} \\
&= \left(I+T^*T\right)^{-1} - T^*\left(I+TT^*\right)^{-1}\left(I+TT^*\right)\left(T^*\right)^{-1}T^{-1}T\left(I+T^*T\right)^{-1} \\
&= \left(I+T^*T\right)^{-1} - \left(I+T^*T\right)^{-1} = 0.
\end{aligned}
$$

□

Lemma 4 *([39, Thm. 2]) Let T be a densely defined linear operator and let $E = E_T$ be its characteristic projection, with components $\left(E_{ij}\right)_{i,j=1}^2$ as in (3.2). Then T is closable if and only if* $\ker\left(I - E_{22}\right) = 0$*, i.e., iff*

$$
\forall \psi \in \mathscr{H}_2, \quad E_{22}\psi = \psi \Longrightarrow \psi = 0.
$$

Proof Note that E fixes $\overline{G_T}$ by definition, so $\begin{bmatrix} 0 \\ \psi \end{bmatrix} \in \overline{G_T}$ is equivalent to

$$
\begin{bmatrix} 0 \\ \psi \end{bmatrix} = \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix}\begin{bmatrix} 0 \\ \psi \end{bmatrix} = \begin{bmatrix} E_{12}\psi \\ E_{22}\psi \end{bmatrix}
$$

which is equivalent to $\psi \in \ker(E_{12}) \cap \ker(I - E_{22})$. However, from (3.9), we have

$$T^*(\psi - E_{22}\psi) = E_{12}\psi, \quad \forall \psi \in \mathscr{H}_2,$$

and this shows that $\ker(I - E_{22}) \subset \ker(E_{12})$, whereby $\begin{bmatrix} 0 \\ \psi \end{bmatrix} \in \overline{G_T}$ iff $\psi \in \ker(I - E_{22})$. It is clear that T is closable iff such a ψ must be 0. □

Theorem 4 ([15, Thm. 3.1]) *Let $T : \mathscr{H}_1 \to \mathscr{H}_2$ be a densely defined linear operator (not assumed closable) with characteristic projection E_T as in Definition 6. Then T has a maximal closable part T_{clo}, defined on the domain $dom(T_{clo}) := dom(T)$, and given by*

$$T_{clo}x := \lim_{n\to\infty} \frac{1}{n+1} \sum_{k=1}^{\infty} k\, E_{22}^{n-k} E_{21}x, \quad x \in dom(T_{clo}). \tag{3.14}$$

Let Q be the projection onto $\overline{(I - E_{22})\mathscr{H}_2} = \ker(I - E_{22})^{\perp}$. Then the characteristic projection of T_{clo} is given by

$$E_{T_{clo}} = \begin{bmatrix} E_{11} & E_{12}Q \\ QE_{21} & E_{22}Q \end{bmatrix}. \tag{3.15}$$

Proof An application of ergodic Yosida's theorem and the associated the Cesaro mean, see [15]. □

4 A duality theorem

In this section we return to the setting where a pair of Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$ with the following property, there is a common subspace $\mathscr{D}$ which in turn defines an operator from $\mathscr{H}_1$ to $\mathscr{H}_2$. Its properties are given in Theorem 5 below.

Theorem 5 *Let $\mathscr{H}_i$ be Hilbert spaces with inner products $\langle\cdot,\cdot\rangle_i$, $i = 1, 2$. Let $\mathscr{D}$ be a vector space s.t. $\mathscr{D} \subset \mathscr{H}_1 \cap \mathscr{H}_2$, and suppose*

$$\mathscr{D} \text{ is dense in } \mathscr{H}_1. \tag{4.1}$$

Set $\mathscr{D}^* \subset \mathscr{H}_2$,

$$\mathscr{D}^* = \left\{ h \in \mathscr{H}_2 \mid \exists C_h < \infty \text{ s.t. } \left|\langle\varphi, h\rangle_2\right| \le C_h \|\varphi\|_1, \ \forall \varphi \in \mathscr{D} \right\}; \tag{4.2}$$

then the following two conditions (i)–(ii) are equivalent:

(i) $\mathscr{D}^*$ is dense in $\mathscr{H}_2$; and
(ii) there is a selfadjoint operator Δ with dense domain in $\mathscr{H}_1$ s.t. $\mathscr{D} \subset dom(\Delta)$, and

$$\langle\varphi, \Delta\varphi\rangle_1 = \|\varphi\|_2^2, \quad \forall \varphi \in \mathscr{D}. \tag{4.3}$$

Proof (i)$\Longrightarrow$(ii) Assume $\mathscr{D}^*$ is dense in $\mathscr{H}_2$; then by (4.2), the inclusion operator

$$J : \mathscr{H}_1 \longrightarrow \mathscr{H}_2, \; J\varphi = \varphi, \; \forall \varphi \in \mathscr{D} \tag{4.4}$$

has $\mathscr{D}^* \subset dom(J^*)$; so by (i), J^* has dense domain in $\mathscr{H}_2$, and J is closable. By von Neumann's theorem (see Theorem 2), $\Delta := J^*\overline{J}$ is selfadjoint in $\mathscr{H}_1$; clearly $\mathscr{D} \subset dom\,(\Delta)$; and for $\varphi \in \mathscr{D}$,

$$\text{LHS}_{(4.3)} = \left\langle \varphi, J^*J\varphi \right\rangle_1 = \langle J\varphi, J\varphi \rangle_2 \underset{\text{by}(4.4)}{=} \|\varphi\|_2^2 = \text{RHS}_{(4.3)}.$$

(Note that $J^{**} = \overline{J}$.) □

Claim $\mathscr{D}^* = dom(J^*), \;\; \mathscr{D} \subset \mathscr{H}_1 \underset{J^*}{\overset{J}{\rightleftarrows}} \mathscr{H}_2 \supset \mathscr{D}^*$

Proof $h \in dom(J^*) \Longleftrightarrow \exists C = C_h < \infty$ s.t.

$$|\langle \underbrace{J\varphi}_{=\varphi}, h\rangle_2| \leq C\,\|\varphi\|_1\,, \;\; \forall \varphi \in \mathscr{D} \Longleftrightarrow h \in \mathscr{D}^*, \text{by definition } (4.2)\,.$$

Since $dom(J^*)$ is dense, J is closable, and by von Neumann's theorem $\Delta := J^*\overline{J}$ is selfadjoint in $\mathscr{H}_1$. □

(ii)$\Longrightarrow$(i) Assume (ii); then we get a well-defined partial isometry $K : \mathscr{H}_1 \longrightarrow \mathscr{H}_2$, by

$$K\Delta^{\frac{1}{2}}\varphi = \varphi, \quad \forall \varphi \in \mathscr{D}. \tag{4.5}$$

Indeed, (4.3) reads:

$$\|\Delta^{\frac{1}{2}}\varphi\|_1^2 = \langle \varphi, \Delta\varphi \rangle_1 = \|\varphi\|_2^2\,, \quad \varphi \in \mathscr{D},$$

which means that K in (4.5) is a *partial isometry* with $dom\,(K) = K^*K = \overline{ran(\Delta^{\frac{1}{2}})}$; and we set $K = 0$ on the complement in $\mathscr{H}_1$.

Then the following inclusion holds:

$$\left\{ h \in \mathscr{H}_2 \mid K^*h \in dom(\Delta^{\frac{1}{2}}) \right\} \subseteq \mathscr{D}^*. \tag{4.6}$$

We claim that LHS in (4.6) is dense in $\mathscr{H}_2$; and so (i) is satisfied. To see that (4.6) holds, suppose $K^*h \in dom(\Delta^{\frac{1}{2}})$; then for all $\varphi \in \mathscr{D}$, we have

$$\begin{aligned} \left|\langle h, \varphi\rangle_2\right| &= \left|\langle h, K\Delta^{\frac{1}{2}}\varphi\rangle_2\right| \\ &= \left|\langle K^*h, \Delta^{\frac{1}{2}}\varphi\rangle_1\right| \quad (\text{by } (4.5)) \\ &= \left|\langle \Delta^{\frac{1}{2}}K^*h, \varphi\rangle_1\right| \leq \|\Delta^{\frac{1}{2}}K^*h\|_1 \|\varphi\|_1, \end{aligned}$$

where we used the Schwarz inequality for $\langle \cdot, \cdot \rangle_1$ in the last step. □

Corollary 2 *Let $\mathscr{D} \subset \mathscr{H}_1 \cap \mathscr{H}_2$ be as in the statement of Theorem 5, and let $J : \mathscr{H}_1 \longrightarrow \mathscr{H}_2$ be the associated closable operator; see (4.4). Then the complement*

$$\mathscr{H}_2 \ominus \mathscr{D} = \left\{ h \in \mathscr{H}_2 \mid \langle \varphi, h \rangle_2 = 0, \ \forall \varphi \in \mathscr{D} \right\}$$

satisfies $\mathscr{H}_2 \ominus \mathscr{D} = ker(J^*)$.

Proof Immediate from the theorem. □

The following result is motivated by the operator-correspondence for the case of two Hilbert spaces $\mathscr{H}_i$, $i = 1, 2$, when the second $\mathscr{H}_2$ results as a reflection-positive version of $\mathscr{H}_1$; see [13] for more details.

Theorem 6 *Let $\mathscr{D} \subset \mathscr{H}_1 \cap \mathscr{H}_2$ satisfying the condition(s) in Theorem 5, and let Δ be the associated selfadjoint operator from (4.3). Let U be a unitary operator in $\mathscr{H}_1$ which maps $\mathscr{D}$ into dom (Δ), and s.t.*

$$\Delta U \varphi = U^{-1} \Delta \varphi \left(= U^* \Delta \varphi \right) \tag{4.7}$$

holds for all $\varphi \in \mathscr{D}$.

Then there is a selfadjoint and contractive operator $\widehat{U}$ on $\mathscr{H}_2$ such that

$$\begin{aligned} \langle \widehat{U} \varphi, \psi \rangle_2 &= \langle \Delta U \varphi, \psi \rangle_1 \\ &= \langle U \varphi, \Delta \psi \rangle_1 , \quad \forall \varphi, \psi \in \mathscr{D}. \end{aligned} \tag{4.8}$$

Proof **Step 1.** We first determine $\widehat{U} \varphi \in \mathscr{H}_2$. We show that the following estimate holds for the term on the RHS in (4.8): For $\varphi, \psi \in \mathscr{D}$, we have

$$\begin{aligned} \left| \langle \Delta U \varphi, \psi \rangle_1 \right| &= \left| \left\langle U^* \Delta \varphi, \psi \right\rangle_1 \right| \quad \text{(by (4.7))} \\ &= \left| \langle \Delta \varphi, U \psi \rangle_1 \right| = \left| \langle \varphi, \Delta U \psi \rangle_1 \right| = \left| \langle \varphi, U \psi \rangle_2 \right| \le \| U \psi \|_2 \, \| \varphi \|_2 \end{aligned}$$

since $U\psi \in dom\,(\Delta)$ by the assumption. Now fix $\varphi \in \mathscr{D}$, then by Riesz, there is therefore a $h_2 \in \mathscr{H}_2$ such that $\langle \Delta U \varphi, \psi \rangle_1 = \langle \varphi, h_2 \rangle_2$, and we set $\widehat{U} \psi = h_2$.

Step 2. Relative to the $\mathscr{H}_2$-inner product $\langle \cdot, \cdot \rangle_2$, we have

$$\langle \widehat{U} \varphi, \psi \rangle_2 = \langle \varphi, \widehat{U} \psi \rangle_2, \quad \forall \varphi, \psi \in \mathscr{D}. \tag{4.9}$$

□

Proof of (4.9):

$$\begin{aligned} \text{LHS}_{(4.9)} &= \langle \Delta U \varphi, \psi \rangle_2 \\ &= \left\langle U^* \Delta \varphi, \psi \right\rangle_1 \quad \text{(by (4.7))} \\ &= \langle \Delta \varphi, U \psi \rangle_1 = \langle \varphi, \Delta U \psi \rangle_1 = \langle \varphi, \widehat{U} \psi \rangle_2 = \text{RHS}_{(4.9)} \end{aligned}$$

Hence $\widehat{U}^* = \widehat{U}$, where $*$ here refers to $\langle \cdot, \cdot \rangle_2$.

Step 3. $\widehat{U}$ is contractive in $\mathscr{H}_2$. Let $\varphi \in \mathscr{D}$, and estimate the absolute values as follows:

$$\begin{aligned}
\left|\langle\widehat{U}\varphi,\varphi\rangle_2\right| &= \left|\langle U\varphi,\Delta\varphi\rangle_1\right| \\
&\leq \langle U\varphi,\Delta U\varphi\rangle_1^{\frac{1}{2}}\,\langle\varphi,\Delta\varphi\rangle_1^{\frac{1}{2}} && \text{(by Schwarz)} \\
&= \left\langle U^2\varphi,\Delta\varphi\right\rangle_1^{\frac{1}{2}}\,\langle\varphi,\Delta\varphi\rangle_1^{\frac{1}{2}} \\
&\leq \left\langle U^4\varphi,\Delta\varphi\right\rangle_1^{\frac{1}{4}}\,\langle\varphi,\Delta\varphi\rangle_1^{\frac{1}{2}+\frac{1}{4}} && \text{(by Schwarz)} \\
&\leq \cdots && \text{(by induction)} \\
&\leq \langle U^{2^n}\varphi,\Delta\varphi\rangle_1^{\frac{1}{2^n}}\,\langle\varphi,\Delta\varphi\rangle_1^{\frac{1}{2}+\frac{1}{4}+\cdots+\frac{1}{2^n}}\,.
\end{aligned}$$

Taking the limit $n \longrightarrow \infty$, we get $|\langle\widehat{U}\varphi,\varphi\rangle_2| \leq \|\varphi\|_2^2$, since $\|\varphi\|_2^2 = \langle\varphi,\Delta\varphi\rangle_1$ by the theorem. Since $\widehat{U}^* = \widehat{U}$ by Step 2, we conclude that

$$\|\widehat{U}\varphi\|_2 \leq \|\varphi\|_2\,, \quad \forall\varphi \in \mathscr{D}. \tag{4.10}$$

Step 4. To get contractivity also on $\mathscr{H}_2$, we finally extend $\widehat{U}$, defined initially only on the closure of $\mathscr{D}$ in $\mathscr{H}_2$. By Corollary 2, we may set $\widehat{U} = 0$ on $ker(J^*)$ in $\mathscr{H}_2$. □

Corollary 3 *Let $\mathscr{D} \subset \mathscr{H}_1 \cap \mathscr{H}_2$, and suppose the condition(s) in Theorem 5 are satisfied. Set $\Delta_1 = J^*J$, and $\Delta_2 = JJ^*$, i.e., the two selfadjoint operators associated to the closed operator J from Claim 4. Let K be the partial isometry in (4.5); then*

$$\|\varphi\|_2^2 = \langle K\varphi,\Delta_2 K\varphi\rangle_2\,, \quad \forall\varphi \in \mathscr{D}. \tag{4.11}$$

Proof We shall apply Theorem 2 to the closed operator J. By Theorem 5 (ii), we have

$$\begin{aligned}
\|\varphi\|_2^2 = \langle\varphi,\Delta_1\varphi\rangle_1 &= \|J\varphi\|_2^2 \\
&= \|\Delta_2^{\frac{1}{2}}K\varphi\|_2^2 \quad \text{(by Thm. 2)} \\
&= \langle K\varphi,\Delta_2 K\varphi\rangle_2
\end{aligned}$$

which is the desired conclusion (4.11). □

5 Noncommutative Lebesgue-Radon-Nikodym decomposition

The following Examples illustrate that Theorem 5 may be considered a non-commutative Radon-Nikodym theorem. (Also see [22].)

Example 1 ($\mu_2 \ll \mu_1$) Let $(X,\mathscr{B})$ be a σ-compact measure space. Let μ_i, $i = 1, 2$, be two regular positive measures defined on $(X,\mathscr{B})$. Let $\mathscr{H}_i := L^2(\mu_i)$, $i = 1, 2$, and set $\mathscr{D} := C_c(X)$. Then the conditions in Theorem 5 hold if and only if $\mu_2 \ll \mu_1$ (relative absolute continuity).

In the affirmative case, let $f = d\mu_2/d\mu_1$ be the corresponding Radon-Nikodym derivative, and set $\Delta :=$ the operator in $L^2(\mu_1)$ of multiplication by f $(= d\mu_2/d\mu_1)$, and (4.3) from the theorem reads as follows:

$$\langle \varphi, \Delta\varphi \rangle_1 = \int_X |\varphi|^2 f \, d\mu_1 = \int_X |\varphi|^2 \, d\mu_2 = \|\varphi\|_2^2 , \quad \forall \varphi \in C_c(X) .$$

The link between Example 1 and the setting in Theorem 5 (the general case) is as follows.

Theorem 7 *Assume the hypotheses of Theorem 5. Then, for every $\varphi \in \mathscr{D}$, there is a Borel measure μ_φ on $[0, \infty)$ such that*

$$\|\varphi\|_1^2 = \mu_\varphi([0, \infty)) , \text{ and} \tag{5.1}$$

$$\|\varphi\|_2^2 = \int_0^\infty \lambda \, d\mu_\varphi(\lambda) . \tag{5.2}$$

Proof By Theorem 5, there is a selfadjoint operator $\Delta = J^*J$ satisfying (4.3). Let

$$E_\Delta : \mathscr{B}([0, \infty)) \longrightarrow \text{projections in } \mathscr{H}_1$$

be the associated projection-valued measure (i.e., $\Delta = \int_0^\infty \lambda \, E_\Delta(d\lambda)$), and set

$$d\mu_\varphi(\lambda) = \|E_\Delta(d\lambda)\varphi\|_1^2 . \tag{5.3}$$

Then it follows from the Spectral Theorem that the conclusions in (5.1) and (5.2) hold for μ_φ in (5.3). □

Example 2 ($\mu_2 \perp \mu_1$) Let $X = [0, 1]$, and consider $L^2(X, \mu)$ for measures λ and μ which are mutually singular. For concreteness, let λ be Lebesgue measure, and let μ be the classical singular continuous Cantor measure. Then the support of μ is the middle-thirds Cantor set, which we denote by K, so that $\mu(K) = 1$ and $\lambda(X \backslash K) = 1$. The continuous functions $C(X)$ are a dense subspace of both $L^2(X, \lambda)$ and $L^2(X, \mu)$ (see, e.g. [36, Ch. 2]). Define the "inclusion" operator[1] J to be the operator with dense domain $C(X)$ and

$$J : C(X) \subset L^2(X, \lambda) \longrightarrow L^2(X, \mu) \quad \text{by} \quad J\varphi = \varphi. \tag{5.4}$$

We will show that $dom(J^*) = \{0\}$, so suppose $f \in dom(J^*)$. Without loss of generality, one can assume $f \geq 0$ by replacing f with $|f|$, if necessary. By definition, $f \in dom(J^*)$ iff there exists $g \in L^2(X, \lambda)$ for which

$$\langle J\varphi, f \rangle_\mu = \int_X \overline{\varphi} f \, d\mu = \int_X \overline{\varphi} g \, d\lambda = \langle \varphi, g \rangle_\lambda , \quad \forall \varphi \in C(X) . \tag{5.5}$$

[1] As a map between sets, J is the inclusion map $C(X) \hookrightarrow L^2(X, \mu)$. However, we are considering $C(X) \subset L^2(X, \lambda)$ here, and so J is not an inclusion map between Hilbert spaces because the inner products are different. Perhaps "pseudoinclusion" would be a better term.

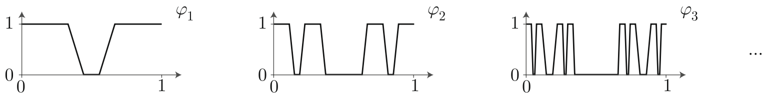


Fig. 2 A sequence $(\varphi_n)_{n=1}^{\infty} \subset C(X)$ for which $\varphi_n\big|_K = 1$ and $\lim_{n\to\infty} \int_X \varphi_n d\lambda = 0$. See Example 2

One can choose $(\varphi_n)_{n=1}^{\infty} \subset C(X)$ so that $\varphi_n\big|_K = 1$ and $\lim_{n\to\infty} \int_X \varphi_n d\lambda = 0$ by considering the appropriate piecewise linear modifications of the constant function $\mathbb{1}$. For example, see Fig. 2. Now we have

$$\left\langle \varphi_n, J^* f \right\rangle_\lambda = \langle \varphi_n, f \rangle_\mu = \langle 1, f \rangle_\mu = \int_X |f| \, d\mu, \quad \forall n \in \mathbb{N}, \tag{5.6}$$

but $\lim_{n\to\infty} \int_X \varphi_n g \, d\lambda = 0$ for any continuous $g \in L^2(X, \lambda)$. Thus $\int_X |f| \, d\mu = 0$, so that $f = 0$ μ-a.e. In other words, $f = 0 \in L^2(X, \mu)$ and hence $dom(J^*) = \{0\}$, which is certainly not dense! Thus, one can interpret the adjoint of the inclusion as multiplication by a Radon-Nikodym derivative ("$J^* f = f \frac{d\mu}{d\lambda}$"), which must be trivial when the measures are mutually singular. This comment is made more precise in Example 1 and Theorem 7. As a consequence of this extreme situation, the inclusion operator in (5.4) is not closable.

Remark 6 Using the theory of iterated function systems (IFS), it can be shown that for Example 2, the inclusion in (2.6) is actually an equality, i.e.,

$$\overline{G_T} = L^2(\lambda) \oplus L^2(\mu).$$

Note that λ and μ are both attractors of IFSs, in the sense of Hutchinson [12]. Indeed, the respective IFSs on [0, 1] are both given by

$$\left\{ S_1(x) = \frac{x}{r+1}, \quad S_2(x) = \frac{x+r}{r+1} \right\},$$

where $r = 1$ for Lebesgue measure and $r = 2$ for the Cantor measure.

6 General symmetric pairs

In this section we consider general symmetric pairs (A, B), and we show that, for every symmetric pair (A, B), there is a canonically associated single Hermitian symmetric operator L in the direct sum-Hilbert space, and we show that L has equal deficiency indices. The deficiency spaces for L are computed directly from (A, B).

Given $\mathscr{H}_1 \underset{B}{\overset{A}{\rightleftarrows}} \mathscr{H}_2$, both linear, and assume that $dom(A)$ is dense in $\mathscr{H}_1$, and $dom(B)$ is dense in $\mathscr{H}_2$. Assume further that

$$\langle Au, v \rangle_2 = \langle u, Bv \rangle_1, \quad \forall u \in dom(A), \ v \in dom(B). \tag{6.1}$$

Theorem 8 *On $\mathscr{K} := \mathscr{H}_1 \oplus \mathscr{H}_2$, set*

$$L\begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} By \\ Ax \end{bmatrix}, \quad \forall x \in dom\,(A)\,,\ \forall y \in dom\,(B)\,, \tag{6.2}$$

then L is symmetric (i.e., $L \subset L^*$) with equal deficiency indices, i.e.,

$$\langle L\xi, \eta\rangle_{\mathscr{K}} = \langle \xi, L\eta\rangle_{\mathscr{K}}\,, \tag{6.3}$$

for all $\xi, \eta \in dom\,(L) = dom\,(A) \oplus dom\,(B)$.

Proof The non-trivial part concerns the claim that L in (6.2) has equal deficiency indices, i.e., the two dimensions

$$\dim\left\{\xi_\pm \in dom\left(L^*\right) \mid L^*\xi_\pm = \pm i\xi_\pm\right\} \tag{6.4}$$

equal; we say $d_+ = d_-$.

Let $u \in \mathscr{H}_1$, $v \in \mathscr{H}_2$; then by Sect. 2, we have

$$\begin{bmatrix} u \\ v \end{bmatrix} \in dom\left(L^*\right) \Longleftrightarrow \left[u \in dom\left(B^*\right),\ v \in dom\left(A^*\right)\right];$$

and then

$$L^*\begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} A^*v \\ B^*u \end{bmatrix}. \tag{6.5}$$

Now consider the following subspace in $\mathscr{K}$,

$$DEF := \left\{\begin{bmatrix} u \\ v \end{bmatrix} \in \mathscr{K} \mid u \in dom\left(A^*B^*\right),\ v \in dom\left(B^*A^*\right),\ \text{and} \right.$$
$$\left. A^*B^*u = -u,\ B^*A^*v = -v\right\}. \tag{6.6}$$

We now prove the following claim: The vectors in (6.4) both agree with dim (DEF), see (6.6). To see this, let $\begin{bmatrix} u \\ v \end{bmatrix} \in$ DEF, and note the following equations must then hold:

$$L^*\begin{bmatrix} u \\ iB^*u \end{bmatrix} \underset{\text{by}(6.5)}{=} \begin{bmatrix} A^*\left(iB^*u\right) \\ B^*u \end{bmatrix} \underset{\text{by }(6.6)}{=} \begin{bmatrix} -iu \\ B^*u \end{bmatrix} = -i\begin{bmatrix} u \\ iB^*u \end{bmatrix}; \tag{6.7}$$

and similarly,

$$L^*\begin{bmatrix} u \\ -iB^*u \end{bmatrix} = i\begin{bmatrix} u \\ -iB^*u \end{bmatrix}. \tag{6.8}$$

The conclusions reverse, and we have proved that L is densely defined and symmetric with deficiency indices

$$\left(d_+, d_-\right) = \left(\dim\left(\text{DEF}\right), \dim\left(\text{DEF}\right)\right).$$

Since L has equal deficiency indices we know that it has selfadjoint extensions; see [9,40]. Moreover, the selfadjoint extensions of L are determined uniquely by associated partial isometries C between the respective deficiency spaces. Since we know these deficiency spaces, see (6.7) & (6.8), we get the following:

Corollary 4 *Let A, B, $\mathscr{H}_1$, $\mathscr{H}_2$, and L be as above, then TFAE:*

(i) *L is essentially selfadjoint,*
(ii) $\{h_1 \in dom\,(A^*B^*) \mid A^*B^*h_1 = -h_1\} = 0,$
(iii) $\{h_2 \in dom\,(B^*A^*) \mid B^*A^*h_2 = -h_2\} = 0.$

Example 3 (Defects $(d_+, d_-) \neq (0, 0)$) Let J be a finite open interval, $\mathscr{D} := C_c^2(J)$, i.e., compact support inside J, $\mathscr{H}_1 = L^2(J)$, and

$$\mathscr{H}_2 := \left\{ \text{functions } f \text{ on } J/\{\text{constants}\} \text{ s.t. } \|f\|^2_{\mathscr{H}_2} := \int_J \left|f'(x)\right|^2 dx < \infty \right\};$$

and $\mathscr{H}_2$ is the Hilbert space obtained by completion w.r.t. $\|\cdot\|_{\mathscr{H}_2}$.

On $\mathscr{D} \ni \varphi$, set $A\varphi := \varphi$ mod constants; and $Bf := -f'' = -\frac{d^2 f}{dx^2}$ for f such that $f'' \in L^2$ and $f' \in L^2$ (the derivatives in the sense of distribution.) Then $\langle A\varphi, f\rangle_{\mathscr{H}_2} = \langle \varphi, Bf\rangle_{\mathscr{H}_1}$ holds. So $(A, B, \mathscr{H}_1, \mathscr{H}_2)$ is a symmetric pair, and $L = \begin{bmatrix} 0 & B \\ A & 0 \end{bmatrix}$ is Hermitian symmetric with dense domain in $\mathscr{K} = \begin{bmatrix} l^2 \\ \oplus \\ \mathscr{H}_E \end{bmatrix}$. One checks that the exponential function e^x is in $dom\,(A^*B^*)$, and that $A^*B^*e^x = -e^x$.

Conclusion, the operator L has deficiency indices $(d_+, d_-) \neq (0, 0)$. In fact, $(d_+, d_-) = (2, 2)$.

Remark 7 If the finite interval J is replaced by $(-\infty, \infty)$, then the associated operator $L = \begin{bmatrix} 0 & B \\ A & 0 \end{bmatrix}$ will instead have indices $(d_+, d_-) = (0, 0)$.

Definition 8 Let $L = \begin{bmatrix} 0 & B \\ A & 0 \end{bmatrix}$ be as in (6.2) acting in $\mathscr{K} = \mathscr{H}_1 \oplus \mathscr{H}_2$. The deficiency spaces N_i and N_{-i} are as follows:

$$N_i\left(L^*\right) = \left\{\xi \in dom\left(L^*\right) \mid L^*\xi = i\xi\right\} \tag{6.9}$$

$$N_{-i}\left(L^*\right) = \left\{\eta \in dom\left(L^*\right) \mid L^*\eta = -i\eta\right\}. \tag{6.10}$$

We also set

$$N_{-1}\left(A^*B^*\right) = \left\{h \in dom\left(A^*B^*\right) \mid A^*B^*h = -h\right\}. \tag{6.11}$$

Lemma 5 *The mapping $\varphi : N_{-1}(A^*B^*) \longrightarrow N_{-i}(L^*)$ by*

$$\varphi(h) = \begin{bmatrix} h \\ iB^*h \end{bmatrix}, \quad \forall h \in N_{-1}\left(A^*B^*\right), \tag{6.12}$$

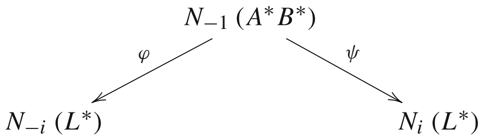
defines a linear isomorphism.

Similarly, $\psi : N_{-1}(A^*B^*) \longrightarrow N_i(L^*)$*, by*

$$\psi(h) = \begin{bmatrix} h \\ -iB^*h \end{bmatrix}, \quad \forall h \in N_{-1}\left(A^*B^*\right) \tag{6.13}$$

is a linear isomorphism from $N_{-1}(A^*B^*)$ *onto* $N_i(L^*)$*.*

Thus the two isomorphisms are both onto:



Proof Let $h \in N_{-1}(A^*B^*)$, and compute

$$L^* \begin{bmatrix} h \\ iB^*h \end{bmatrix} = \begin{bmatrix} 0 & A^* \\ B^* & 0 \end{bmatrix} \begin{bmatrix} h \\ iB^*h \end{bmatrix} = \begin{bmatrix} -ih \\ B^*h \end{bmatrix} = -i \begin{bmatrix} h \\ iB^*h \end{bmatrix}.$$

So $\varphi(N_{-1}(A^*B^*)) \subset N_{-i}(L^*)$. But φ is also onto, since

$$\begin{bmatrix} h_1 \\ h_2 \end{bmatrix} \in N_{-i}\left(L^*\right) \Longleftrightarrow \begin{bmatrix} 0 & A^* \\ B^* & 0 \end{bmatrix} \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = -i \begin{bmatrix} h_1 \\ h_2 \end{bmatrix}$$

or equivalently,

$$\begin{Bmatrix} A^*h_2 = -ih_1 \\ B^*h_1 = -ih_2 \end{Bmatrix}.$$

So we get $A^*B^*h_1 = -h_1$, and $h_2 = iB^*h_1$. Thus,

$$\begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} h_1 \\ iB^*h_1 \end{bmatrix} \in \varphi\left(N_{-1}\left(A^*B^*\right)\right)$$

which is the claim in (6.12). The proof of (6.13) is similar.

Remark 8 By von Neumann's formulae (see [9]), we have

$$dom\left(L^*\right) = dom(L) + N_i\left(L^*\right) + N_{-i}\left(L^*\right), \tag{6.14}$$

and there is a bijection between selfadjoint extensions M, i.e., $M \subset L \subset L^*$, $M = M^*$, and partial isometries $C : N_i(L^*) \to N_{-i}(L^*)$, such that $M = L_C$ has

$$dom(L_C) = \left\{\varphi + \psi_+ + C\psi_+ \mid \varphi \in dom(L),\ \psi \in N_i\left(L^*\right)\right\}. \tag{6.15}$$

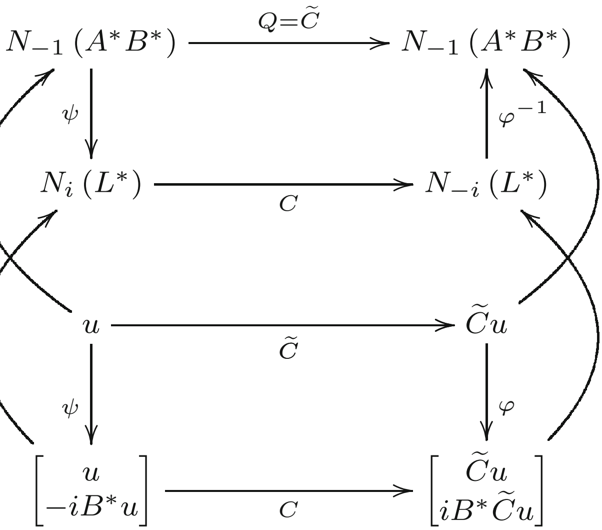


Fig. 3 The linear operator $\widetilde{C}$ in $N_{-1}\left(A^*B^*\right)$ induced by $C : N_i\left(L^*\right) \to N_{-i}\left(L^*\right)$

Remark 9 Note that if $f = \varphi + \psi_+ + \psi_- \in dom\,(L^*)$, with $\varphi \in dom\,(L)$, $\psi_\pm \in N_{\pm i}\,(L^*)$, then

$$\frac{1}{2i}\left(\left\langle f, L^* f\right\rangle - \left\langle L^* f, f\right\rangle\right) = \|\psi_+\|^2 - \|\psi_-\|^2 , \tag{6.16}$$

where the RHS of (6.16) can be seen as a generalized boundary condition. So the extensions M of L correspond to partial isometries $C : N_i\,(L^*) \to N_{-i}\,(L^*)$.

Corollary 5 *A partial isometry*

$$C = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \tag{6.17}$$

in $\mathscr{H}_1 \oplus \mathscr{H}_2$ which determines a selfadjoint extension of L satisfies

$$C_{22}C_{12}^{-1}\,(C_{11} - Q) + C_{12}^{-1}\,(C_{11} - Q)\,Q = C_{21} \tag{6.18}$$

where $Q : \ker\left(A^*B^* + I_{\mathscr{H}_1}\right) \longrightarrow \ker\left(A^*B^* + I_{\mathscr{H}_1}\right)$ is a linear automorphism. (See the diagram in Fig. 3.)

Proof By Lemma 5, the two deficiency spaces of L are

$$N_{\pm i}\left(L^*\right) := \left\{ \begin{bmatrix} u \\ \mp i B^* u \end{bmatrix} \mid u \in \ker\left(A^*B^* + 1\right) \right\}.$$

Indeed, one checks that

$$L^* \begin{bmatrix} u \\ -iB^*u \end{bmatrix} = \begin{bmatrix} 0 & A^* \\ B^* & 0 \end{bmatrix} \begin{bmatrix} u \\ -iB^*u \end{bmatrix} = i \begin{bmatrix} u \\ -iB^*u \end{bmatrix},$$

and so $\begin{bmatrix} u \\ -iB^*u \end{bmatrix} \in N_i(L^*)$, with u satisfying $A^*B^*u = -u$. The verification for $N_{-i}(L^*)$ is similar.

By the general theory of von Neumann (see [9] and Remark 8), the selfadjoint extensions $L_C \supset L$ are determined by partial isometries $C : N_i(L^*) \to N_{-i}(L^*)$, equivalently, C induces a linear operator $Q : \ker(A^*B^* + 1) \to \ker(A^*B^* + 1)$.

Use (6.6), (6.7) and (6.8) we see that every partial isometry $C = (C_{ij})_{ij=1}^2$ as in (6.17) must satisfy

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \begin{bmatrix} u \\ -iB^*u \end{bmatrix} = \begin{bmatrix} Qu \\ iB^*Qu \end{bmatrix}$$
$$\Updownarrow$$
$$C_{11}u - C_{12}iB^*u = Qu$$
$$C_{21}u - C_{22}iB^*u = iB^*Qu$$

It follows that $C_{12}iB^* = C_{11} - Q$, and $C_{22}iB^* + iB^*Q = C_{21}$. Hence

$$C_{22}C_{12}^{-1}(C_{11} - Q) + C_{12}^{-1}(C_{11} - Q)Q = C_{21},$$

which is the assertion in (6.18). □

Remark 10 Let $C : N_i(L^*) \to N_{-i}(L^*)$ be a partial isometry w.r.t. the $\mathscr{K}$ norm, i.e., $\|\cdot\|_{\mathscr{K}}^2 = \|\cdot\|_1^2 + \|\cdot\|_2^2$. We conclude that

$$\|u\|_1^2 + \left\|B^*u\right\|_2^2 = \|Qu\|_1^2 + \left\|B^*Qu\right\|_1^2, \quad \forall u \in N_{-1}\left(A^*B^*\right), \tag{6.19}$$

where $Q := \widetilde{C}$.

It may occur that A and B are not closed; if not, refer to the corresponding closures. Recall that $\overline{A}^* = A^*$, $\overline{B}^* = B^*$. Then (6.19) takes the equivalent form

$$I_1 + BB^* = Q^*Q + Q^*BB^*Q \tag{6.20}$$

as an operator identity in $N_{-1}(A^*B^*)$. Equivalently (the norm preserving property)

$$I_1 + BB^* = Q^*\left(I + BB^*\right)Q, \tag{6.21}$$

and so this is the property of Q which is equivalent to the partial isometric property of C.

Corollary 6 *Fix* $L = \begin{bmatrix} 0 & B \\ A & 0 \end{bmatrix}$*, then the selfadjoint extensions* L_Q *of* L *are determined by all operator solutions* Q *to (6.21).*

Moreover,

$$dom\left(L_Q\right) = \left\{ \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} u \\ -iB^*u \end{bmatrix} + \begin{bmatrix} v \\ -iB^*v \end{bmatrix} \right\} \tag{6.22}$$

where $\begin{bmatrix} x \\ y \end{bmatrix} \in dom\,(L)$, $u, v \in N_{-1}\,(A^*B^*)$, and $v = Qu$; and

$$L_Q \begin{bmatrix} x + u + v \\ y - iB^*u + iB^*v \end{bmatrix} = \begin{bmatrix} By + iu - iv \\ Ax + B^*u - B^*v \end{bmatrix}. \tag{6.23}$$

Proof On the domain

$$dom\,(L_C) = \left\{ \varphi + \psi_+ + C\psi_+ \mid \varphi \in dom\,(L)\,,\;\; \psi_+ \in N_i\left(L^*\right) \right\}, \tag{6.24}$$

we have

$$L_C\,(\varphi + \psi_+ + C\psi_+) = L\varphi + i\psi_+ - iC\psi_+. \tag{6.25}$$

Now apply this (6.22)–(6.23). Also see [9], and Remark 8. ◻

7 Selfadjoint extensions of semibounded operators

Many "naïve" treatments of linear operators in the physics literature are based on analogies to finite dimensions. They often result in paradoxes and inaccuracies as they miss some key issues intrinsic to unbounded operators, questions dealing with domains, closability, graphs, deficiency indices, and in the symmetric case, the distinction between formally Hermitian and selfadjoint, issues all inherent in infinite-dimensional analysis of unbounded operators and their extensions. Only when these questions are resolved for the particular application at hand, do we arrive at a rigorous spectral analysis, and get reliable predictions of scattering (from von Neumann's Spectral Theorem); see e.g. [14,24]. Since measurements of the underlying observables, in prepared states, come from the projection valued measures, which are dictated by choices (i)–(ii) (see Sect. 1), these choices have direct physical significance.

Let $\mathscr{H}$ be a complex Hilbert space. Let A be an operator in $\mathscr{H}$ with $dom\,(A) = \mathscr{D}$, dense in $\mathscr{H}$, such that

$$\|\varphi\|_A^2 := \langle \varphi, A\varphi \rangle \geq \|\varphi\|^2\,, \quad \forall \varphi \in \mathscr{D}. \tag{7.1}$$

The completion of $\mathscr{D}$ with respect to the $\|\cdot\|_A$-norm yields a Hilbert space $\mathscr{H}_A$. Let

$$J : \mathscr{H}_A \longrightarrow \mathscr{H}, \quad J\varphi = \varphi,$$

be the inclusion map. It follows from (7.1) that

$$\|J\varphi\| = \|\varphi\| \leq \|\varphi\|_A\,, \tag{7.2}$$

thus J is contractive, and so are J^*J and JJ^*.

Remark 11 The inner product in $\mathscr{H}_A$ is denoted by $\langle\cdot,\cdot\rangle_A$ with subscript A, as opposed to $\langle\cdot,\cdot\rangle$ for the original Hilbert space $\mathscr{H}$. That is,

$$\langle f, g\rangle_A := \langle f, Ag\rangle\,, \quad \forall f, g \in \mathscr{D}. \tag{7.3}$$

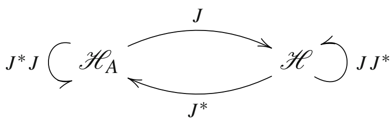
Recall the adjoint operator $J^* : \mathscr{H} \longrightarrow \mathscr{H}_A$, by

$$\langle h, Jg\rangle = \left\langle J^*h, g\right\rangle_A\,, \quad \forall h \in \mathscr{H}, g \in \mathscr{H}_A. \tag{7.4}$$

Theorem 9 *The operator $(JJ^*)^{-1}$ is unbounded, and is a selfadjoint extension of A, i.e.,*

$$\left(JJ^*\right)^{-1} \supseteq A. \tag{7.5}$$

Moreover, it coincides with the Friedrichs extension [9]. (See the diagram below.)



Proof (7.5)$\Longleftrightarrow$

$$\begin{aligned}
\left(JJ^*\right)^{-1}\varphi &= A\varphi, && \forall\varphi \in \mathscr{D},\\
&\Updownarrow\\
\varphi &= JJ^*A\varphi, && \forall\varphi \in \mathscr{D},\\
&\Updownarrow\\
\langle\psi, \varphi\rangle &= \left\langle\psi, JJ^*A\varphi\right\rangle, && \forall\psi, \varphi \in \mathscr{D}.
\end{aligned} \tag{7.6}$$

For a pair $\psi, \varphi \in \mathscr{D}$ as in (7.6), we have

$$\begin{aligned}
\text{RHS}_{(7.6)} &= \left\langle J^*\psi, J^*A\varphi\right\rangle_A && \text{by (7.4)}\\
&= \left\langle JJ^*\psi, A\varphi\right\rangle && \text{by (7.4)}\\
&= \left\langle J^*\psi, \varphi\right\rangle_A && \text{by (7.3), and } J^{**} = J \text{ from general theory}\\
&= \langle\psi, J\varphi\rangle\\
&= \langle\psi, \varphi\rangle = \text{LHS}_{(7.6)}
\end{aligned}$$

That $(JJ^*)^{-1}$ is selfadjoint follows from a general theorem of von Neumann (Theorem 2). See, e.g. [9]. $(JJ^*)^{-1}$ is the *Friedrichs extension* of A. ◻

Let q be a sesquilinear form on $\mathscr{Q} \subset \mathscr{H}$ (linear in the second variable) such that:

(i) $\mathscr{Q}$ is a dense subspace in $\mathscr{H}$.

(ii) $q(\varphi,\varphi) \geq \|\varphi\|^2$, for all $\varphi \in \mathscr{Q}$.
(iii) q is *closed*, i.e., $\mathscr{Q}$ is a Hilbert space w.r.t.

$$\langle\varphi,\psi\rangle_q := q(\varphi,\psi), \text{ and}$$
$$\|\varphi\|_q^2 := q(\varphi,\varphi), \ \forall\varphi,\psi \in \mathscr{Q}.$$

Corollary 7 *There is a bijection between sesquilinear forms q on $\mathscr{Q} \subset \mathscr{H}$ satisfying (i)–(iii), and selfadjoint operators A in $\mathscr{H}$ s.t. $A \geq 1$. Specifically, the correspondence is as follows:*

(1) Given A, set $\mathscr{Q} := dom(A^{\frac{1}{2}})$, and

$$q(\varphi,\psi) := \left\langle A^{\frac{1}{2}}\varphi, A^{\frac{1}{2}}\psi\right\rangle, \quad \forall\varphi,\psi \in dom(A^{\frac{1}{2}}). \tag{7.7}$$

(2) Conversely, if q satisfies (i)–(iii), let $J : \mathscr{Q} \to \mathscr{H}$ be the inclusion map, and set $A := (JJ^*)^{-1}$; then q is determined by the RHS of (7.7).

Proof The non-trivial part (2) ⇒ (1) follows from the proof of Theorem 9. □

Lemma 6 *Let A be a semibounded operator as in (7.1), then A is essentially selfadjoint iff $A\mathscr{D}$ is dense in $\mathscr{H}$, i.e., $\overline{ran(A)} = \mathscr{H}$. (Contrast, $\overline{A} = A^{**}$ denotes the closure of A.)*

Proof Follows from von Neumann's deficiency index theory, and the assumption that $A \geq 1$ (see (7.1).) □

By Lemma 6, if A is not essentially selfadjoint, then

$$C : A\varphi \longrightarrow \varphi \tag{7.8}$$

is contractive in $ran(A)$ (proper subspace in $\mathscr{H}$, i.e., not dense in $\mathscr{H}$.)

Proof that (7.8) is contractive: By (7.1), we have

$$\|\varphi\|^2 \underset{\text{(Schwarz)}}{\leq} \langle\varphi, A\varphi\rangle \leq \|\varphi\|\,\|A\varphi\|$$

which implies $\|\varphi\| \leq \|A\varphi\|$, for all $\varphi \in \mathscr{D}$.

We have proved that $CA\varphi = \varphi$ holds, and C is s.a. and contractive.

Theorem 10 *(*Krein [5,28,29]*) We introduce the set*

$$\mathscr{B}_A := \Big\{B \mid B^* = B,\ dom(B) = \mathscr{H},\ \|Bh\| \leq \|h\|,\ \forall h \in \mathscr{H}, \\ \textit{and } C \subset B \textit{ i.e., } CA\varphi = BA\varphi,\ \forall\varphi \in \mathscr{D};\ \textit{see } (7.8)\Big\}, \tag{7.9}$$

then $\mathscr{B}_A \neq \emptyset$.

Corollary 8 *For all $B \in \mathscr{B}_A$, we have $A \subset B^{-1}$ so B^{-1} is an unbounded selfadjoint extension of A.*

Remark 12 Krein studied $\mathscr{B}_A$ as an order lattice. Define $B_1 \leq B_2$ meaning $\langle h, B_1 h\rangle \leq \langle h, B_2 h\rangle$, $\forall h \in \mathscr{H}$. In the previous discussions we proved that $JJ^* \in \mathscr{B}_A$.

8 Application to graph Laplacians, infinite networks

We now turn to a family of semibounded operators from mathematical physics. They arose first in the study of large (infinite) networks; and in these studies entail important choices of Hilbert spaces, and of selfadjoint realizations. The best known instance is perhaps systems of resistors on infinite graphs, see e.g. [4,8,17,18,20,21]. An early paper is [34] which uses an harmonic analysis of infinite systems of resistors in dealing with spin correlations of states of finite energy of the isotropic ferromagnetic Heisenberg model.

For the discussion of the graph Laplacian Δ, we first introduce the following setting of infinite networks:

- V: the vertex set, a given infinite countable discrete set.
- $E \subset V \times V \setminus \{\text{diagonal}\}$ the edges, such that $(xy) \in E \Longleftrightarrow (yx) \in E$, and for all $x \in V$, $\#\{y \sim x\} < \infty$, where $x \sim y$ means $(xy) \in E$.
- $c : E \to \mathbb{R}_+$ a given conductance function.
- Set
$$(\Delta u)(x) := \sum_{y \sim x} c_{xy} (u(x) - u(y)), \tag{8.1}$$
defined for all functions u on V, and let
$$c(x) = \sum_{y \sim x} c_{xy}, \quad x \in V. \tag{8.2}$$
- $\mathscr{H}_E$ will be the Hilbert space of finite-energy functions on V; more precisely,
$$u \in \mathscr{H}_E \underset{\text{Def.}}{\Longleftrightarrow} \|u\|^2_{\mathscr{H}_E} = \frac{1}{2} \sum_{(xy) \in E} c_{xy} |u(x) - u(y)|^2 < \infty. \tag{8.3}$$
Set
$$\langle u, v \rangle_{\mathscr{H}_E} = \frac{1}{2} \sum_{(xy) \in E} c_{xy} (\overline{u(x)} - \overline{u(y)}) (v(x) - v(y)). \tag{8.4}$$
- We assume that (V, E, c) is connected: For all pairs $x, y \in V$, $\exists\, (x_i)_{i=0}^n \subset V$ s.t. $x_0 = x$, $(x_i x_{i+1}) \in E$, $x_n = y$.

Lemma 7 *Fix a base-point $o \in V$. Then for all $x \in V$, there is a unique $v_x \in \mathscr{H}_E$ such that*
$$f(x) - f(o) = \langle v_x, f \rangle_{\mathscr{H}_E}, \quad \forall f \in \mathscr{H}_E; \tag{8.5}$$
The vertex v_x is called a dipole.

Proof see [20,25]. □

Lemma 8 *In $\mathscr{H}_E$, we have $\delta_x = c(x)\, v_x - \sum_{y \sim x} c_{xy} v_y$, and*

$$\left| \langle \varphi, v_x \rangle_{\mathscr{H}_E} \right| = |\varphi(x) - \varphi(o)| \le \sqrt{2}\, \|\varphi\|_{l^2}, \quad \forall \varphi \in \mathscr{D}.$$

Proof See [17]. □

Remark 13 Let $\mathscr{H} = l^2(V)$, $\mathscr{D} = span\{\delta_x \mid x \in V\}$. Define the *graph Laplacian* Δ by (8.1). Let $\mathscr{H}_E$ be the energy-Hilbert space in (8.3). Then (7.1), (7.3) translate into:

$$\langle \delta_x, \Delta\delta_x \rangle_2 = c(x) = \|\delta_x\|^2_{\mathscr{H}_E}, \text{ and} \tag{8.6}$$

$$\left\langle \delta_x, \Delta\delta_y \right\rangle_2 = -c_{xy} = \left\langle \delta_x, \delta_y \right\rangle_{\mathscr{H}_E}, \ \forall (xy) \in E, \ x \neq y. \tag{8.7}$$

Let $\mathscr{H}_\Delta$ be the completion of $\mathscr{D} = span\{\delta_x\}$ with respect to $\langle \varphi, \Delta\varphi \rangle_{l^2}$, $\varphi \in \mathscr{D}$. (We have $\langle \varphi, \Delta\varphi \rangle_{l^2} = \|\varphi\|^2_{\mathscr{H}_E}$, valid for $\forall \varphi \in \mathscr{D}$.)

Conclusion. $\mathscr{H}_\Delta \hookrightarrow \mathscr{H}_E$ is an isometric inclusion, but as a subspace. The closure is $F_{in} = \mathscr{H}_E \ominus Harm$, where $Harm$ is the subspace of Harmonic functions $h \in \mathscr{H}_E$, i.e., $\Delta h = 0$.

Definition 9 (**Two unbounded closable operators**)
The graph Laplacian is denoted by Δ_2, as an operator in l^2; and by Δ_E when acting in $\mathscr{H}_E$. In both cases, Δ is given by (8.1), defined for all functions u on V.

Definition 10 Let (V, E, c) be as before. Fix a base-point $o \in V$, and let $v_x = v_{xo} =$ dipole (see Lemma 7). Let

$$\mathscr{D}_2 = span\{\delta_x\} \subset l^2 \tag{8.8}$$

$$\mathscr{D}_E = span\{v_x\}_{x \in V \setminus \{o\}} \subset \mathscr{H}_E. \tag{8.9}$$

Set

$$l^2 \supset \mathscr{D}_2 \xrightarrow{K} \mathscr{H}_E, \quad K(\delta_x) = \delta_x, \tag{8.10}$$

$$\mathscr{H}_E \supset \mathscr{D}_E \xrightarrow{L} l^2, \qquad L(v_x) = \delta_x - \delta_o. \tag{8.11}$$

Lemma 9 *We have*

$$\langle K\varphi, h \rangle_{\mathscr{H}_E} = \langle \varphi, Lh \rangle_{l^2}, \quad \forall \varphi \in \mathscr{D}_2, \forall h \in \mathscr{D}_E. \tag{8.12}$$

Proof Note $K : l^2 \to \mathscr{H}_E$ has dense domain $\mathscr{D}_2$ in l^2; and $J : \mathscr{H}_E \to l^2$ has dense domain in $\mathscr{H}_E$. Moreover, it follows from (8.12) that

(i) $K \subset L^*$, hence $dom(L^*)$ is dense in l^2; and
(ii) $L \subset K^*$, so $dom(K^*)$ is dense in $\mathscr{H}_E$. Also, both K and L are closable. See Fig. 4.

Proof of (8.12): Use (8.1) and linearity to see that it is enough to consider the special case when $\varphi = \delta_x$, $h = v_y$, so we must prove that the following holds ($x, y \in V$):

$$\left\langle K\delta_x, v_y \right\rangle_{\mathscr{H}_E} = \left\langle \delta_x, Lv_y \right\rangle_2. \tag{8.13}$$

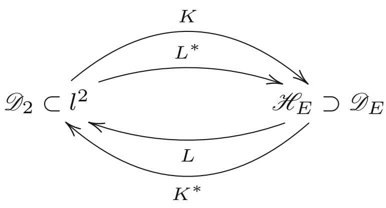


Fig. 4 *dom* $(K) = \mathscr{D}_2$, *dom* $(L) = \mathscr{D}_E$, $K \subset L^*$, and $L \subset K^*$

Note that

$$\begin{aligned} \mathrm{LHS}_{(8.13)} &= \langle \delta_x, v_y \rangle_{\mathscr{H}_E} && \text{by (8.10)} \\ &= \delta_x(y) - \delta_x(o) && \text{using the dipole property of} v_y \\ &= \delta_{xy} - \delta_{xo}; \\ \mathrm{RHS}_{(8.13)} &= \langle \delta_x, \delta_y - \delta_o \rangle_2 && \text{by (8.11)} \\ &= \delta_{xy} - \delta_{xo}. \end{aligned}$$

Thus (8.13) holds. □

The authors gratefully acknowledge the contributions of Daniel Lenz to the statement and proof of Corollary 9, which is crucial for the sequel.

Corollary 9 *The two operators below are well-defined, and selfadjoint:*

$$K^*\overline{K} \text{ is s.a. in } l^2\text{, and} \tag{8.14}$$

$$L^*\overline{L} \text{ is s.a. in } \mathscr{H}_E, \tag{8.15}$$

and both with dense domains. Here, $\overline{\cdot}$ *refers to the respective graph closures, and* $*$ *to adjoint operators, i.e.,* $K^* : \mathscr{H}_E \longrightarrow l^2$*, and* $L^* : l^2 \longrightarrow \mathscr{H}_E$*; both operators with dense domains, by (8.12).*

Moreover, (8.14)–(8.15) are selfadjoint extensions

$$\Delta_2 \subset K^*\overline{K} \text{ in } l^2, \quad \text{and} \quad \Delta_E \subset L^*\overline{L} \text{ in } \mathscr{H}_E. \tag{8.16}$$

In fact, $\overline{\Delta_2} = K^*\overline{K}$ *(non-trivial; see [16, 19]), and* $L^*\overline{L}$ *is the Krein extension of* Δ_E*.*

Proof Conclusions (8.14)–(8.15) follow from general theory; see Theorem 2. To show

$$\Delta_E \subset L^*\overline{L} \tag{8.17}$$

we must prove that

$$L^*\overline{L}v_x = \delta_x - \delta_o \, (= \Delta_E v_x), \quad \forall x \in V \setminus \{o\}. \tag{8.18}$$

We have more: $\overline{K} = L^*$, and $\overline{L} = K^*$, but this is because we have that Δ_2 is essentially selfadjoint.

To establish (8.18), we must prove that the following equation holds:

$$\left\langle v_y, L^* L v_x \right\rangle_{\mathscr{H}_E} = \left\langle v_y, \delta_x - \delta_o \right\rangle_{\mathscr{H}_E}, \quad y \neq o. \tag{8.19}$$

Note that

$$\begin{aligned}
\text{LHS}_{(8.19)} &= \left\langle L v_y, L v_x \right\rangle_2 \\
&= \left\langle \delta_y - \delta_o, \delta_x - \delta_o \right\rangle_2 \quad \text{(by (8.11))} \\
&= \delta_{xy} - \delta_{xo} - \delta_{yo} + \delta_{oo} = \delta_{xy} + 1, \\
\text{RHS}_{(8.19)} &= (\delta_x - \delta_o)(y) - (\delta_x - \delta_o)(o) = \delta_{xy} + 1.
\end{aligned}$$

Now, using $\overline{J} = K^*$, we can show that $Harm \subset dom\left(L^*\overline{L}\right) = dom\left(L^* K^*\right)$, and $L^*\overline{L}h = 0$, which means that $L^*\overline{L}$ is the Krein extension of Δ_E. □

Application of Theorem 5.

Set $\mathscr{H}_1 = l^2(V)$, $\mathscr{H}_2 = \mathscr{H}_E$, and let

$$\begin{aligned}
\mathscr{D} &:= \mathscr{D}_2 = span\left\{\delta_x\right\}_{x \in V}, \text{ and} \\
\mathscr{D}^* &:= \mathscr{D}_E = span\left\{v_x\right\}_{x \in V \setminus \{o\}};
\end{aligned}$$

see (8.8) & (8.9). Then the axioms (i)$\Longleftrightarrow$(ii) in Theorem 5 hold. Note the only non-trivial part is the dense subspace $\mathscr{D}^* \subset \mathscr{H}_2 \left(= \mathscr{H}_E\right)$.

Claim The condition in (4.2) holds; i.e., for all $h = v_x \in \mathscr{D}_E$, there exists $C_x < \infty$ s.t.

$$\left| \langle \varphi, v_x \rangle_{\mathscr{H}_E} \right| \leq C_x \left\| \varphi \right\|_{l^2}, \quad \forall \varphi \in \mathscr{D}. \tag{8.20}$$

Proof (Proof of (8.20)) We have

$$\begin{aligned}
\text{LHS}_{(8.20)} &= \left| \langle \varphi, v_x \rangle_{\mathscr{H}_E} \right| \\
&= \left| \varphi(x) - \varphi(o) \right| && \text{by (8.5)} \\
&= \left| \langle \varphi, \delta_x - \delta_o \rangle_{l^2} \right| \\
&\leq \left\| \varphi \right\|_{l^2} \left\| \delta_x - \delta_o \right\|_{l^2} && \text{by Schwarz' inequality} \\
&= \sqrt{2} \left\| \varphi \right\|_{l^2}, \ \forall \varphi \in \mathscr{D},
\end{aligned}$$

and so we may take $C_x = \sqrt{2}$. □

Remark 14 For the setting in Theorem 5 with $\mathscr{D} \subset \mathscr{H}_1 \cap \mathscr{H}_2$, note that the respective norms $\|\cdot\|_i$ on $\mathscr{H}_i$, $i = 1, 2$, induce norms $\|\cdot\|_i$ on $\mathscr{D}$. It is important that the conclusion in Theorem 5 is valid even when the two norms are not comparable; i.e., in general there are no finite constants C, D ($< \infty$) such that

$$\|\varphi\|_1 \leq C \|\varphi\|_2, \quad \forall \varphi \in \mathscr{D}; \text{ or} \tag{8.21}$$
$$\|\varphi\|_2 \leq D \|\varphi\|_1, \quad \forall \varphi \in \mathscr{D}. \tag{8.22}$$

For the application above in Corollary 9, the two Hilbert spaces are:

- $\mathscr{H}_1 = l^2(V)$
- $\mathscr{H}_2 = \mathscr{H}_E$ (the energy Hilbert space determined from a fixed conductance function c), with $\mathscr{D} = span\{\delta_x \mid x \in V\}$.

Indeed, let $x \mapsto c(x)$ be the total conductance; see (8.2), then

$$\|\delta_x\|^2_{\mathscr{H}_E} = c(x) \quad \text{and} \quad \|\delta_x\|^2_{l^2} = 1,$$

so (8.22) does not hold when $c(\cdot)$ is unbounded on V. (To see this, take $\varphi = \delta_x$.)

From the analysis above, and [19,25] there are many examples such that $spec_{l^2}(\Delta_2) = [0, \infty)$. One checks that in these examples, the estimate (8.21) also will not hold for any finite constant C, i.e., $\|\cdot\|_1 = \|\cdot\|_{l^2}$, and $\|\cdot\|_2 = \|\cdot\|_{\mathscr{H}_E}$.

Application of Theorem 8

We apply the general symmetric pair (A, B) to (V, E, c):

Notation:

- $\mathscr{D} = span\{\delta_x \mid x \in V \backslash \{o\}\}$ = finitely supported functions on $V \backslash \{o\}$
- $l^2 := l^2(V \backslash \{o\})$
- $\mathscr{H}_E$ = the corresponding energy Hilbert space
- $\mathscr{K} = l^2 \oplus \mathscr{H}_E$ $(= \mathscr{H}_1 \oplus \mathscr{H}_2)$

The pair (A, B) is maximal, where A and B are defined as follows:

$$l^2 \ni \delta_x \xrightarrow{A} \delta_x = c(x)\, v_x - \sum_{y \sim x} c_{xy} v_y \in \mathscr{H}_E \quad \text{(Lemma.8)}; \tag{8.23}$$

$$\mathscr{H}_E \ni v_x \xrightarrow{B} \delta_x - \delta_o \in l^2, \text{ i.e., } B = \Delta. \tag{8.24}$$

Then $\mathscr{D} \subset l^2 \cap \mathscr{H}_E$, and both inclusions are isometric.

Define $L = \begin{bmatrix} 0 & B \\ A & 0 \end{bmatrix}$ on $\mathscr{K} = l^2 \oplus \mathscr{H}_E$, where

$$dom\,(L) := \left\{ \begin{bmatrix} \varphi \\ f \end{bmatrix} \mid \varphi \in \mathscr{D},\ f \in dom\,(\Delta) \right\},\ \text{and} \tag{8.25}$$

$$L \begin{bmatrix} \varphi \\ f \end{bmatrix} := \begin{bmatrix} Bf \\ A\varphi \end{bmatrix} = \begin{bmatrix} \Delta f \\ \varphi \end{bmatrix},\quad \forall \begin{bmatrix} \varphi \\ f \end{bmatrix} \in dom\,(L)\,. \tag{8.26}$$

It follows that L is a Hermitian symmetric operator in $\mathscr{K}$, i.e., $L \subseteq L^*$, but we must have:

Theorem 11 *The operator L in (8.26) is essentially selfadjoint in the Hilbert space $\mathscr{K}$, i.e., it has deficiency indices $(d_+, d_-) = (0, 0)$.*

Proof **Step 1.** We have

$$\langle A\varphi, f\rangle_{\mathscr{H}_E} = \langle \varphi, Bf\rangle_{l^2}\,,\quad \forall \varphi, f \in \mathscr{D}, \tag{8.27}$$

so that $A \subseteq B^*$ and $B \subseteq A^*$.

Step 2. Define L as in (8.25)–(8.26). For the adjoint operator, set $L^* = \begin{bmatrix} 0 & A^* \\ B^* & 0 \end{bmatrix}$, with

$$dom\left(L^*\right) = \begin{bmatrix} dom\,(B^*) \\ dom\,(A^*) \end{bmatrix},\ \text{and} \tag{8.28}$$

$$L^* \begin{bmatrix} h_1 \\ h_2 \end{bmatrix} = \begin{bmatrix} A^* h_2 \\ B^* h_1 \end{bmatrix},\quad h_1 \in l^2,\ h_2 \in \mathscr{H}_E. \tag{8.29}$$

So we must be precise about A^* and B^*, and we shall need the following: □

Lemma 10 *The domains of A^* and B^* are as follows:*

$$dom\left(A^*\right) = \Big\{ f \in \mathscr{H}_E \mid \exists C_f < \infty\ s.t.\ \left|\langle \varphi, f\rangle_{\mathscr{H}_E}\right|^2 \leq C_f\,\|\varphi\|_2^2 = C_f \sum_x |\varphi_x|^2 \Big\}; \tag{8.30}$$

and

$$dom\left(B^*\right) = \Big\{ \varphi \in l^2 \mid \exists C_\varphi < \infty\ s.t.\ \left|\langle \varphi, \Delta f\rangle_{l^2}\right|^2 \leq C_\varphi\,\|f\|_{\mathscr{H}_E}^2\,,\ \forall f \in \mathscr{H}_E\ s.t.\ \Delta f \in l^2 \Big\}. \tag{8.31}$$

Proof See the definitions and (8.27). □

Remark 15 It is convenient to use Δ to act on all functions, and later to adjoint domains. See the definition in (8.1), i.e.,

$$(\Delta u)(x) := \sum_{y \sim x} c_{xy} (u(x) - u(y)), \quad f \in \mathscr{F}(V) (= \text{all functions}). \tag{8.32}$$

Proof of Theorem 11 continued **Step 3.** Recall that $dom(A^*) \subset \mathscr{H}_E$, and $dom(B^*) \subset l^2$: $l^2 \underset{B^*}{\overset{A^*}{\rightleftarrows}} \mathscr{H}_E$. It follows from Lemma 10, that

$$\left(A^* f\right)(x) = (\Delta f)(x), \quad \forall f \in dom\left(A^*\right), \ x \in V, \text{ and} \tag{8.33}$$

$$B^* \underbrace{\varphi}_{\text{in } l^2} = \varphi \in \mathscr{H}_E, \quad \forall \varphi \in dom\left(B^*\right). \tag{8.34}$$

Both sides of (8.34) are interpreted as functions on V. Also, the condition on $\varphi \in dom(B^*)$ requires $\sum\sum_{(xy) \in E} c_{cy} (\varphi(x) - \varphi(y))^2 < \infty$, and $\sum_x \varphi_x^2 < \infty$.

Step 4. Now consider Δ (in (8.32), see Remark 15), then the two eigenvalue problems:

$$\begin{Bmatrix} B^* A^* f = -f \\ A^* B^* \varphi = -\varphi \end{Bmatrix} \Longleftrightarrow \begin{Bmatrix} \Delta f = -f \\ \Delta \varphi = -\varphi \end{Bmatrix} \tag{8.35}$$

where $f \in \mathscr{H}_E$, $\Delta f \in l^2$, and $\varphi \in l^2 \cap \mathscr{H}_E$.

Apply the two isomorphisms from the general theory (see (6.6)). But (8.35) only has the solution $\varphi = 0$ in l^2. The fact that (8.35) does not have non-zero solutions follows from [16,19]. So we have that $L = \left[\begin{smallmatrix} 0 & B \\ A & 0 \end{smallmatrix}\right]$ is *essentially selfadjoint*. Indeed, this holds in the general case.

Step 5. The deficiency indices of the operator L. With the definitions,

$$L = \begin{bmatrix} 0 & B \\ A & 0 \end{bmatrix}, \quad L \begin{bmatrix} \varphi \\ f \end{bmatrix} = \begin{bmatrix} Bf \\ A\varphi \end{bmatrix} = \begin{bmatrix} \Delta f \\ \varphi \end{bmatrix}$$

where $\varphi \in l^2$, $f \in \mathscr{H}_E$ are in the suitable domains s.t.

$$\left\| L \begin{bmatrix} \varphi \\ f \end{bmatrix} \right\|^2_{\substack{l^2 \\ \oplus \\ \mathscr{H}_E}} = \|\Delta f\|^2_{l^2} + \|\varphi\|^2_{\mathscr{H}_E} < \infty. \tag{8.36}$$

So $\varphi \in l^2 \cap \mathscr{H}_E$, $f \in \mathscr{H}_E$, $\Delta f \in l^2$ defines the domain of L as an operator in $\mathscr{K} = \begin{bmatrix} l^2 \\ \oplus \\ \mathscr{H}_E \end{bmatrix}$, and we proved that L is selfadjoint, so indices $(0, 0)$. □

Corollary 10 *Viewing L as a selfadjoint operator, it follows from (8.36) that*

$$dom(L) = \left\{ \begin{bmatrix} \varphi \\ f \end{bmatrix} \in \begin{bmatrix} l^2 \\ \oplus \\ \mathscr{H}_E \end{bmatrix} \mid \varphi \in l^2 \cap \mathscr{H}_E, \ \Delta f \in l^2 \right\}.$$

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Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

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