Essential selfadjointness of the graph-Laplacian

Palle E. T. Jorgensen
Department of Mathematics
University of Iowa
Iowa City, IA 52242-1419 USA

Abstract

We study the operator theory associated with such infinite graphs $G$ as occur in electrical networks, in fractals, in statistical mechanics, and even in internet search engines. Our emphasis is on the determination of spectral data for a natural Laplace operator associated with the graph in question. This operator $\Delta$ will depend not only on $G$, but also on a prescribed positive real valued function $c$ defined on the edges in $G$. In electrical network models, this function $c$ will determine a conductance number for each edge. We show that the corresponding Laplace operator $\Delta$ is automatically essential selfadjoint. By this we mean that $\Delta$ is defined on the dense subspace $D$ (of all the real valued functions on the set of vertices $G^0$ with finite support) in the Hilbert space $l^2(G^0)$. The conclusion is that the closure of the operator $\Delta$ is selfadjoint in $l^2(G^0)$, and so in particular that it has a unique spectral resolution, determined by a projection valued measure on the Borel subsets of the infinite half-line. We prove that generically our graph Laplace operator $\Delta = \Delta_c$ will have continuous spectrum. For a given infinite graph $G$ with conductance function $c$, we set up a system of finite graphs with periodic boundary conditions such the finite spectra, for an ascending family of finite graphs, will have the Laplace operator for $G$ as its limit.

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1 Introduction

The infinite graphs we consider live on a fixed countable infinite set, say $L$. Starting with such a set $L$ (subject to certain axioms, listed below), we get a notion of edges as follows: Select distinguished pairs of points in $L$, say $x$ and $y$, and connect them by a “line,” called edge. In physics, when a vertex $x$ is given, the set of vertices connected to $x$ with one “edge” is called a set of neighbors, or nearest neighbors. Initially we do not assign direction to the edges. So, as it stands, an edge $e$ is defined as a special subset $\{x, y\}$ for selected points $x, y$ in $L$. Think “nearest” neighbors!

A direction is only assigned when we also introduce a function $I$ on edges $e$, and then this function $I$ is assumed to satisfy $I(x, y) = -I(y, x)$. In electrical networks, such a function $I$ may represent a current induced by a potential which is introduced on a graph with fixed resistors. So only if a current function $I$ is introduced can we define a direction to edges, as follows: We specify source $s(e) = x$, and terminal vertex $t(e) = y$ if $I(x, y) > 0$, meaning that the current flows from $x$ to $y$.

In this paper we study the operator theory of infinite graphs $G$, with special emphasis on a natural Laplace operator associated with the graph in question. This operator will depend not only on $G$, but also on a positive real valued function $c$ defined on the edges in $G$. In electrical network models, the function $c$ will determine a conductance number for each edge $e$. If $e = (xy)$ connects vertices $x$ and $y$ in $G$, the number $c(e)$ is the reciprocal of the resistance between $x$ and $y$. Hence prescribing a conductance leads to classes of admissible flows in $G$. When they are determined from Ohm’s law, and the Kirchhoff laws, it leads to a measure of energy, and to an associated graph Laplacian. We identify the Hilbert space $\mathcal{H}(G)$ which offers a useful spectral theory, and our main result is a theorem to the effect that the graph Laplacian is essentially selfadjoint, i.e., that its operator closure is a selfadjoint operator in $\mathcal{H}(G)$.

Let $G = (G^0, G^1)$ be an infinite graph, $G^0$ for vertices, and $G^1$ for edges. Every $x$ in $G^0$ is connected to a set $\text{nbh}(x)$ of other vertices by a finite number of edges, but points in $\text{nbh}(x)$ are different from $x$; i.e., we assume that $x$ itself is excluded from $\text{nbh}(x)$; i.e., no $x$ in $G^0$ can be connected to itself with a single edge. Let $c$ be a conductance function defined on $G^1$.

Initially, the graph $G$ will not be directed, but when a conductance is fixed, and we study induced current flows, then these current flows will give a direction to the edges in $G$. But the edges in $G$ itself do not come with an intrinsic direction.

We show that the Laplace operator $\Delta = \Delta_c$ is automatically essentially
selfadjoint. By this we mean that $\Delta$ is defined on the dense subspace $\mathcal{D}$ (of all the real valued functions on $G^0$ with finite support) in the Hilbert space $\mathcal{H} = \mathcal{H}(G) := l^2(G^0)$. The explicit formula for the graph Laplacian $\Delta = \Delta_{(G,c)}$ is given in (3.6) in section 3 below which also discusses the appropriate Hilbert spaces. The conclusion is that the closure of the operator $\Delta$ is selfadjoint in $\mathcal{H}$, and so in particular that it has a unique spectral resolution, determined by a projection valued measure on the Borel subsets of the infinite half-line $\mathbb{R}_+$; i.e., the spectral measure takes values in the projections in the Hilbert space: $= l^2(G^0)$. We work out the measure.

In contrast, we note that the corresponding Laplace operator in the continuous case is not essentially selfadjoint. This can be illustrated for example with $\Delta = -(d/dx)^2$ on the domain $\mathcal{D}$ of consisting of all $C^2$-functions on the infinite half-line $\mathbb{R}_+$ which vanish with their derivatives at the end points. Then the Hilbert space is $L^2(\mathbb{R}_+)$. So our graph theorem is an instance where the analogy between the continuous case and the discrete case breaks down.

A second intrinsic issue for the operator theory of infinite graphs $G$, is that generically our graph Laplace operator $\Delta = \Delta_c$ will have continuous spectrum. We prove this by identifying a covariance system which implies that the spectrum of the corresponding Laplace operator will in fact be absolute continuous with respect to Lebesgue measure on the half-line.

In a third theorem, for a given infinite graph $G$ with conductance function $c$, we set up a system of finite graphs with periodic boundary conditions such the finite spectra, for an ascending family of finite graphs, will have the Laplace operator for $G$ as its limit.

## 2 Assumptions

In order to do computations and potential theory on infinite graphs $G$, it has been useful to generalize the continuous Laplacian $\Delta$ from Riemannian geometry [AC04] to a discrete setting [BHS05], [CS07], [Kig03], [HKK02]. However the infinities for graphs suggest an analogy to non-compact Riemannian manifolds, or manifolds with boundary.

Once the graph Laplacian is made precise as a selfadjoint operator it makes sense to ask for exact formulas for the spectrum of $\Delta$. Our Laplace operator $\Delta = \Delta_c$ is associated with a fixed system $(G, c)$ where vertices and edges are specified as usual, $G = (G^{(0)}, G^{(1)})$; and with a fixed conductance function $c : G^{(1)} \to \mathbb{R}_+$. See (3.6) below for a formula.

And as usual our Laplace operator, $\Delta = \Delta_c$ is densely defined in the
Hilbert space $\ell^2(G^{(0)})$ of all square-summable sequences on the vertices of $G$; and if $G$ is infinite, $\Delta_c$ is not defined everywhere in $\ell^2$, but rather it has a dense domain $D$ in $\ell^2$. We show in the next section that $\Delta_c$ is essentially selfadjoint for all choices of conductance function $c$.

By a graph $G$ we mean a set $G^{(0)}$ of vertices, and a set $G^{(1)}$ of edges. Edges $e$ consist of pairs $s, y \in G^{(0)}$. We write $e = (xy)$; and if $(xy) \in G^{(1)}$ we say that $x \sim y$.

Assumptions
(i) $x \not\sim x$ (i.e.; $(xx) \notin G^{(1)}$).
(ii) For every $x \in G^{(0)}$, \{ $y \in G^{(0)} | y \sim x$ \} is finite.
(iii) Points $x, y \in G^{(0)}$ for which there is a finite path $x_0, x_1, x_2, \ldots, x_n$ with $x_0 = x$, $x_n = y$, and $(x_i x_{i+1}) \in G^{(1)}$, $i = 0, \ldots n - 1$, are said to be connected.
(iv) We will assume that all connected components in $G^{(0)}$ are infinite; or else that $G^{(0)}$ is already connected.

3 The Main Theorem

3.1 The Graph Laplacian

In this section we specify a fixed graph $G$ (infinite in the non-trivial case) and an associated conductance function $c$. The associated graph Laplacian $\Delta_c$ will typically be an unbounded Hermitian operator with dense domain.

Our assumptions will be as above, and when the Hilbert spaces have been selected, our main theorem states that the graph Laplacian $\Delta_c$ is essentially selfadjoint; i.e., the operator closure, also denoted $\Delta_c$, is a selfadjoint operator. In sections 5–8 we obtain consequences and applications.

The interpretation of this results in terms of boundary conditions will be given in section 7 below. It means that $\Delta_c$ has a well defined and unique (up to equivalence) spectral resolution. Then the next objective is to find the spectrum of the operator $\Delta_c$. And a method for finding spectrum is based on “covariance.” Covariance is used on other spectral problems in mathematical physics, and it offers useful ways of getting global formulas for spectrum. As we will see, infinite models typically have graph Laplacians with continuous spectrum.

In the finite case, of course the spectrum is the set of roots in a characteristic polynomial, but unless there is some group action, it is difficult to solve for roots by “bare hands;” and even if we do, only the occurrence of groups offers insight.
A second approach to the finding spectra of graph Laplacians is “renormalization”: Renormalization of hierarchical systems of electrical networks comes into play each time one passes to a new scale (upwards or downwards). This requires additional structure, such as is found in iterated function systems (IFSs), (see [BHS05], [DJ07], [JP98], [Kig03]), i.e., specified finite systems of affine transformations in Euclidean space that are then iterated recursively.

When the mappings are so iterated on a given graph, the iterations may then be interpreted as scales in an infinite graph: (post-)composition of similarity mappings takes us further down the branches of a tree like structure in path space. We get martingale constructions as instances of renormalization.

Theorem 3.1 The graph Laplacian \( \Delta = \Delta_{(G,e)} \) is essentially selfadjoint.

Proof. To get started we recall the setting. Given:

\( G \): a fixed infinite graph. (It may be finite, but in this case the conclusion follows from finite-dimensional linear algebra.)

\( G = (G^{(0)}, G^{(1)}) \).

\( G^{(0)} \): the set of vertices in \( G \).

\( G^{(1)} \): the set of edges in \( G \).

If \( x, y \in G^{(0)} \) is a given pair, we say that \( x \sim y \) when \( e = (xy) \in G^{(1)} \).

For \( x \in G^{(0)} \), set

\[
\text{nbh} (x) = \left\{ y \in G^{(0)} | y \sim x \right\}. \tag{3.1}
\]

Our standing assumptions are as follows:

(a) \( \text{nbh} (x) \) is finite.

(b) \( x \notin \text{nbh} (x) \).

\( \mathcal{H} = \ell^2 \left( G^{(0)} \right) \) = all functions \( v : G^{(0)} \rightarrow \mathbb{C} \) such that

\[
\sum_{x \in G^{(0)}} |v(x)|^2 < \infty. \tag{3.2}
\]
Set
\[ \langle u, v \rangle = \sum_{x \in G(0)} u(x)v(x), \forall u, v \in \ell^2(G(0)). \] (3.3)

By \( \mathcal{H} \) we refer to the completed Hilbert space \( \ell^2(G(0)) \).

\[ D := \text{the set of all finitely supported } v \in \mathcal{H}; \text{i.e., } v \text{ is in } D \text{ iff } \exists F \subset G(0), \]
\[ F = F_v \text{ some finite subset such that } v(x) = 0, \forall x \in G(0) \setminus F. \]

\[ e_x := \delta_x = \text{Dirac mass, defined by} \]
\[ e_x(y) = \begin{cases} 1 & \text{if } y = x \\ 0 & \text{if } y \neq x. \end{cases} \] (3.4)

\( c : G^{(1)} \to \mathbb{R}_+ \) is a fixed function taking positive values. In network models, the function \( c \) is conductance; i.e., the reciprocal of resistance.

Assumption (symmetry): \( c(xy) = c(yx), \forall (xy) \in G^{(1)}. \)

\[ \Delta = \Delta(G,c) \] (3.5)

is the Laplacian, and is defined on \( D \) as follows:

\[ (\Delta v)(x) = \sum_{y \sim x} c(xy) (v(x) - v(y)), \forall v \in D, \forall x \in G^{(0)}. \] (3.6)

3.2 Lemmas
We will need some lemmas:

**Lemma 3.2** The operator \( \Delta \) is Hermitian symmetric on \( D \), and it is positive semidefinite. Specifically, the following two properties hold:

\[ \langle \Delta u, v \rangle_{\ell^2} = \langle u, \Delta v \rangle_{\ell^2}, \forall u, v \in D; \] (3.7)

and

\[ \langle u, \Delta u \rangle_{\ell^2} \geq 0, \forall u \in D. \] (3.8)
Proof. Both assertions are computations:

In (3.7),

\[
\langle \Delta u, v \rangle_{L^2} = \sum_{x,y \in G^{(0)}} c(x, y) (u(x) - u(y)) v(x) 
\]

\[
= \sum_{x \sim y} c(x y) u(x) v(x) - \sum_{x \sim y} u(x) c(x y) v(y) 
\]

\[
= \sum_{x \in G^{(0)}} B_c(x) (v(x) - u(y)) 
\]

Note that the summation may be exchanged since, for each \( x \in G^{(0)} \), the set of neighbors \( \text{nbh}(x) \) is finite.

In (3.8),

\[
\langle u, \Delta u \rangle_{L^2} = \sum_{x \sim y} u(x) c(x y) (u(x) - u(y)) 
\]

\[
= \sum_{x \in G^{(0)}} B_c(x) |u(x)|^2 - \sum_{x \sim y} u(x) c(x y) u(y), 
\]

where

\[
B_c(x) = \sum_{y \sim x} c(x y), \ x \in G^{(0)}. \tag{3.9}
\]

The second term in the computation may be estimated with the use of Cauchy-Schwarz as follows: Setting

\[
E_c(u) := \sum_{x,y \text{ s.t. } x \sim y} c(x y) |u(x) - u(y)|^2; \tag{3.10}
\]

we show that

\[
2\langle u, \Delta u \rangle_{L^2} = E_c(u) \geq 0. \tag{3.11}
\]

Indeed using the conditions on \( c: G^{(1)} \to \mathbb{R}^+ \)

- \( c(x y) = c(y x), \ \forall (x y) \in G^{(1)}; \)
- \( c(xx) = 0, \ \forall x \in G^{(0)}; \)
• \( c(xy) > 0, \forall (xy) \in G^{(1)}, \)

we get
\[
2\langle u, \Delta u \rangle = 2 \sum_{x \in G^{(0)}} B_c(x) |u(x)|^2 - 2 \sum_{x \sim y} u(x) c(xy) u(y) \\
= 2 \sum_{x \in G^{(0)}} B_c(x) |u(x)|^2 - 2 \text{Re} \sum_{x \sim y} u(x) c(xy) u(y) \\
= \sum_{x \sim y} c(x,y) \left( |u(x)|^2 - \overline{u(x)} u(y) - \overline{u(y)} u(x) + |u(y)|^2 \right) \\
= \sum_{xy} c(xy) |u(x) - u(y)|^2 = \mathcal{E}_c(u).
\]

For the general theory of unbounded Hermitian operators and their extensions, we refer the reader to [Jør78], [Nel69], [Sto51].

**Definition 3.3** If \( \Delta \) is an operator with dense domain \( D \) in a Hilbert space \( \mathcal{H} \), we define its adjoint operator \( \Delta^* \) by:

A vector \( v \) is in the domain \( \text{dom} (\Delta^*) \) iff there is a constant \( K \) such that
\[
|\langle v, \Delta u \rangle| \leq K \|u\|, \forall u \in D.
\]

(3.12)

When (3.12) holds, then by Riesz, there is a unique \( w := \Delta^* v \) such that
\[
\langle w, u \rangle = \langle v, \Delta u \rangle, \forall u \in D.
\]

(3.13)

Note that since \( D \) is dense in \( \mathcal{H} \), \( w (=: \Delta^* v) \) is uniquely determined by (3.12).

**Lemma 3.4** In the case of \( \Delta = \Delta_{G,c} \) and \( \mathcal{H} = \ell^2 (G^{(0)}) \), the vector \( \Delta^* v \) for \( v \in \text{dom} (\Delta^*) \) is given by the expression
\[
(\Delta^* v)(x) = \sum_{y \sim x} c(xy) (v(x) - v(y)).
\]

(3.14)

**Proof.** Since the sum in (3.13) is finite, the RHS is well defined if \( v \in \text{dom} (\Delta^*) \). Since \( \Delta^* v \in \mathcal{H} \),
\[
\sum_{x \in G^{(c)}} |(\Delta^* v)(x)|^2 < \infty.
\]

(3.15)
Set $w(x) := \sum_{y \sim x} c(xy)(v(x) - v(y))$.

We claim that (3.12) then holds. Indeed

$$
\langle w, u \rangle_{\ell^2} = \sum_{x \in G^{(0)}} \left( \sum_{y \sim x} c(xy) \left( \overline{v(x)} - \overline{v(y)} \right) \right) u(x)
$$

$$
= \sum_x v(x) \sum_{y \sim x} c(xy) (u(x) - u(y))
$$

$$
= \langle v, \Delta u \rangle_{\ell^2}
$$

(by the exchange of summation and Lemma 3.2). ■

**Lemma 3.5** Let $(G,c)$ and $\Delta = \Delta_{(G,c)}$ here as in the previous lemma. Then the equation

$$
\Delta v = -v
$$

does not have non-zero solutions $v \in \ell^2(G^{(0)})$.

**Proof.** It is immediate from (3.7) in Lemma 3.2 that eq. (3.16) does not have non-zero solutions in $\mathcal{D}$, but the assertion is that there are no non-zero solutions in any bigger subspace.

Also note that every solution in $\ell^2(G^{(0)})$ to eq. (3.16) must be in $\text{dom}(\Delta^*)$, i.e., the domain of the adjoint of $\Delta$ with $\mathcal{D}$ as domain.

If $v : G^{(0)} \to \mathbb{C}$ is a solution to (3.16), then

$$
\overline{v(x)} \Delta v(x) = -|v(x)|^2, \quad \forall x \in G^{(0)}
$$

(3.17)

which yields $\overline{v(x)} \Delta v(x) \leq 0, \forall x \in G^{(0)}$. Hence $\mathcal{E}_c(v) \leq 0$; see (3.10)-(3.11). But by (3.11), then $\mathcal{E}_c(v) = 0$.

It follows from (3.10) that $v$ must be constant on every connected component in $G^{(0)}$. Since all the connected components are infinite, $v$ must be zero. ■

**Remark 3.6** We stress that (3.16) may have non-zero solutions not in $\ell^2$. For these solutions $v$, the energy will be unbounded.

**Example 3.7** Let a graph system $(G,c)$ be determined as follows:

$G^{(0)} = \mathbb{N}_0 = \{0, 1, 2, \ldots\}$,

$G^{(1)} : \text{nbh}(0) = \{1\}$,
nbh(n) = {n − 1, n + 1} if n > 0, and
c(n, n + 1) = n + 1.

Then the Laplace operator \( \Delta_c \) will be unbounded in \( \ell^2 \) as follows from

\[
\Delta_c = \begin{pmatrix}
1 & -1 & 0 & 0 & 0 & \cdots \\
-1 & 3 & -2 & 0 & 0 & \cdots \\
0 & -2 & 5 & -3 & 0 & \cdots \\
0 & 0 & -3 & 7 & -4 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots \\
-n & 2n + 1 & -(n + 1) & \ddots & & \\
& & & & & \ddots 
\end{pmatrix}
\]

Then

\[
(\Delta u)_0 = u_0 - u_1, \text{ and} \\
(\Delta u)_n = (2n + 1)u_n - nu_{n-1} - (n + 1)u_{n+1}, \forall n \geq 1.
\]

For solving (3.16), initialize \( v_0 = 1 \). Then

\[
v_1 = 2v_0 = 2, \\
v_2 = \frac{7}{2}, \text{ and inductively} \\
v_{n+1} = 2v_n - \left(\frac{n}{n + 1}\right)v_{n-1}.
\]

We get \( v_1 < v_2 < \cdots < v_{n-1} < v_n < \cdots \) and

\[
v_{n+1} > \left(2 - \frac{n}{n + 1}\right)v_n.
\]

Hence for the truncated summations for \( \ell^2 \) and \( \mathcal{E} \) applied to this solution \( v \); we get

\[
\frac{1}{2}\mathcal{E}_N(v) = -\sum_{k=0}^{N} v_k^2 < -N
\]

which tends to \(-\infty\).

The following lemma is from the general theory of unbounded operators in Hilbert space, [Nel69], [Sto51], [vN31].
Lemma 3.8 Let \( \Delta \) be a linear operator in a Hilbert space \( \mathcal{H} \) and defined in a dense domain \( \mathcal{D} \).

Then \( \Delta \) is essentially selfadjoint (i.e., has selfadjoint closure \( \bar{\Delta} \)) if the following conditions hold:

(i) \( \langle u, \Delta u \rangle \geq 0, \forall u \in \mathcal{D} \)

(ii) \( \dim \{ v \in \text{dom}(\Delta^*) | \Delta^* v = -v \} = 0 \).

Proof. This is in the literature, e.g. [vN31]. The idea is the following, if (i) is assumed, then there is a well defined bounded operator

\[
T = (I + \Delta)^{-1}
\]

precisely when (ii) is satisfied. \( \blacksquare \)

In our analysis of the graph Laplacian \( \Delta_c \) in (3.6) we shall need one more:

Lemma 3.9 Let \( \Delta_c \) be as in (3.6). Then for all \( v \in \mathcal{D} \),

\[
\sum_{x \in \mathcal{G}(0)} (\Delta_c v)(x) = 0. \tag{3.18}
\]

In fact, when \( v \) is fixed, the number of non-zero terms in (3.18) is finite.

Proof. The finiteness claim follows from the assumptions on \((G,c)\) we listed in section 2.

A direct computation yields the result:

\[
\sum_{x \in \mathcal{G}(0)} (\Delta_c v)(x) = \sum_x \sum_{y \sim x} c(xy)(v(x) - v(y)) \\
= \sum_x v(x) \sum_{y \sim x} c(xy) - \sum_y v(y) \sum_{x \sim y} c(xy) \\
= \sum_x v(x) B_c(x) - \sum_y v(y) \sum_{x \sim y} c(yx) \\
= \sum_x v(x) B_c(x) - \sum_y v(y) B_c(y) \\
= 0.
\]

\( \blacksquare \)
4 Operator Theory

Once the operator theoretic tools are introduced, we show in section 5 below that class of infinite graph systems \((G, c)\) where \(G\) is a graph and \(c\) is a conductance function (the pair \((G, c)\) satisfying the usual axioms as before), have the spectrum of the associated Laplace operator \(\Delta_c\) continuous. This refers to the \(\ell^2\) space of \(G(0)\), i.e., the Hilbert space is \(\ell^2(G(0))\) where as usual \(G(0)\) denotes the set of vertices.

It is important that \(G(0)\) is infinite. Otherwise of course the spectrum is just the finite set of zeros of the characteristic polynomial. See Example 6.6 below.

We give an operator theory/spectral theory analysis, with applications, of a class of graph Laplacians; and we have been motivated by a pioneering paper [Pow76] which in an exciting way applies graphs and resistor networks to a problem in quantum statistical mechanics. In one of our results we establish the essential selfadjointness of a large class of graph Laplacians on graphs of infinite networks. (A Hermitian symmetric operator with dense domain in Hilbert space is said to be \textit{essentially selfadjoint} if its closure is selfadjoint, i.e., if the deficiency indices are \((0,0)\). See Definition 4.1 below! There are many benefits from having the graph Laplacian \(\Delta\) essentially selfadjoint.

Here is a partial list:

(a) We get the benefit of having the spectral resolution for the selfadjoint closure, also denoted \(\Delta\) for notational simplicity.

(b) We get a spectral representation realization of the operator \(\Delta\), i.e., a unitarily equivalent form of \(\Delta\) in which an equivalent operator \(\Delta^\sim\) may occur in applications. See e.g., [Arv02], [PS72].

(c) We get a scale of Hilbert spaces, \(\mathcal{H}_s\) for \(s\) in \(\mathbb{R}\), defined from the graph of the operator \(\Delta^s\) where the fractional power \(\Delta^s\) is defined by functional calculus applied to the selfadjoint realization of \(\Delta\). See [Jor04].

(d) Gives us a way of computing scales of resistance metrics on electrical networks realized on infinite graphs, extending tools available previously only for finite graphs; see [BD49].

(e) The case \(s = 1/2\) yields an exact representation of the energy Hilbert space associated with a particular system \((G, c)\) and the corresponding graph Laplacian \(\Delta = \Delta(G, c)\).

(f) Gives us a way of computing fractional Brownian motion on graphs, allowing an analytic continuation in the parameter \(s\), and with \(s = 1/2\) corresponding to the standard Brownian motion; see e.g., [DJ07], [Jor06].

In the course of the proofs of our main results, we are making use of...
tools from the theory of unbounded operators in Hilbert space: von Neumann’s deficiency indices, operator closure, graphs of operators, operator domains, operator adjoints; and extensions of Hermitian operators with a dense domain in a fixed complex Hilbert space. Our favorite references for this material include: [AC04], [Jør77], [Jør78], [JP00], [Nel69], [vN31], [Sto51]. For analysis on infinite graphs and on fractals, see e.g., [BHS05], [CS07], [DJ06], [HKK02], [Hut81], [JP98], [JKS07], [Kig03], [BD49].

**Definition 4.1** Let $\Delta$ be a Hermitian linear operator with dense domain $\mathcal{D}$ in a complex Hilbert space $\mathcal{H}$. Set

$$\mathcal{D}_\pm := \{v_\pm \in \text{dom}(\Delta^*) \mid \Delta^* v_\pm = \pm i v_\pm\},$$

where $i = \sqrt{-1}$. Then the two numbers $n_\pm := \dim \mathcal{D}_\pm$ are called the deficiency indices.

Von-Neumann’s theorem states that the initial operator $\Delta$ is essentially selfadjoint on $\mathcal{D}$ if and only if $n_+ = n_- = 0$. It has selfadjoint extensions defined on a larger domain in $\mathcal{H}$ if and only if $n_+ = n_-$. The following two conditions on a Hermitian operator, (A) and (B), individually imply equal deficiency indices, i.e., $n_+ = n_-:

(A) For all $v \in \mathcal{D}$, we have the estimate

$$\langle v, \Delta v \rangle \geq 0,$$

i.e., $\Delta$ is semibounded.

(B) There is an operator $J : \mathcal{H} \to \mathcal{H}$ satisfying the following four conditions:

(i) $J (u + \alpha v) = J u + \bar{\alpha} J v$, for $\forall u, v \in \mathcal{H}, \alpha \in \mathbb{C}$

(ii) $\langle J u, J v \rangle = \langle v, u \rangle \ \forall u, v \in \mathcal{H}$; ($J$ is called a conjugation!)

(iii) $J$ maps the subspace $\mathcal{D}$ into itself, and

$$J \Delta v = \Delta J v, \ \forall v \in \mathcal{D}.$$

(iv) $J^2 = \text{id}$; $J$ is of period 2.

**Remark 4.2** There are many examples (see the Appendix) where either (A) or (B) is satisfied but where the operator $\Delta$ is not essentially selfadjoint.
Both conditions (A) and (B) hold for a graph Laplacians $\Delta_c$, and Theorem 3.1 states that $\Delta_c$ is essentially selfadjoint.

For Riemannian manifolds with boundary, there is a close analogue of the graph Laplacian $\Delta_c$ above; but it is known (see section 7) that these continuous variants are typically not essentially selfadjoint.

Indeed the obstruction to essential selfadjointness in these cases captures a physical essence of the metric geometry behind the use of Laplace operators in Riemannian geometry.

5 The Energy Form

5.1 Operators

In section 3 we proved essential selfadjointness of the graph Laplacians $\Delta_c$. This refers to sequence space $\ell^2$, the Hilbert space of all square-summable sequences indexed by the points in $G^{(0)}$, and equipped with the usual $\ell^2$-inner product.

This means that the axioms for $\Delta_c$ are such that boundary conditions at infinity in $G$ are determined by computations on finite subsets of the vertices in $G$. (In the Appendix, we will contrast this state of affairs with related but different boundary conditions from quantum mechanics.) Recall that $\Delta_c$ is generally a densely defined Hermitian and unbounded operator. So in principle there might be non-trivial obstructions to selfadjointness (other than simply taking operator closure.) Recall (Definition 4.1) that a given Hermitian operator with dense domain is essentially selfadjoint if and only if the dimension of each of the two “defect eigenspaces” is zero.

So that is why we look at the “minus 1 eigenspaces” for the adjoint operator, $\Delta^* u = -u$.

For potential theoretic computations we need an additional Hilbert space, the Energy Hilbert space $\mathcal{H}_E$ (details below.) For example the voltage potentials associated with a fixed graph Laplacian are typically not in $\ell^2(G^{(0)})$ but rather in an associated Energy Hilbert space. Our Laplace operator $\Delta$ is formally Hermitian in both the Hilbert spaces $\ell^2$ and $\mathcal{H}_E$ (the energy Hilbert space). We show that the Laplace operator $\Delta$ is essentially selfadjoint both in $\ell^2$ and in $\mathcal{H}_E$. In both cases, we take for dense domain $\mathcal{D}$ the linear subspace of all finitely supported functions $G^{(0)} \rightarrow \mathbb{R}$.

Our setting and results in this section are motivated by [Pow76] and [BD49].

There are several distinctions between the two Hilbert spaces: For example, the Dirac functions $\{\delta_x | x \in G^{(0)}\}$ form an orthonormal basis (ONB)
in $\ell^2$, but not in $\mathcal{H}_E$. The implication of this is that our graph Laplacians have different matrix representations in the two Hilbert spaces. In speaking of “matrix representation” for an operator in a Hilbert space, we will always be referring to a chosen ONB.

We shall need the operator $\Delta$ in both guises. One reason for this is that for infinite graphs, typically the potential function $v$ solving $\Delta v = \delta_x - \delta_y$, for pairs of vertices will not be in $\ell^2$, but nonetheless $v$ will have finite energy, i.e., $\mathcal{E}(v) < \infty$, meaning that the energy form applied to $v$ is finite. Caution: The sequence $v$ might not be in the $\ell^2$-space. Specifics in Example 5.2 below!

When we study the Laplace operator $\Delta$, our questions concern its spectrum, and its spectral resolution. The spectrum will be contained in the half-line $[0, \infty)$, but (as we show in examples) it can be unbounded, and it can have continuous parts mixed in with discrete parts. In case the conductance function is “very unbounded,” as an operator in $\ell^2$, it may be necessary to pass to a proper operator extension in an enlarged Hilbert space to get a different selfadjoint realization of $\Delta$.

These operator issues only enter in case $\Delta$ is unbounded. The unboundedness of the operator $\Delta$ is tied in closely with unboundedness of the conductance function $c$ which is used. Recall $\Delta = \Delta_c$ depends on the choice of $c$. If $c$ is unbounded “at infinity” (on the set $G^{(1)}$ of edges), then the resistors tend to zero at distant edges. Intuitively, this means that “the current escapes to infinity,” and we make this precise in the language of operator theory. Our general setup here will be as in [Pow76].

We will need a second Hilbert space, the energy Hilbert space $\mathcal{H}_E$. Here the inner product is the energy quadratic form. Since the energy form evaluated on a function $v$ is defined in terms of the square of differences $v(x) - v(y)$, it follows that the elements in $\mathcal{H}_E$ are really sequences modulo constants.

Let $G = (G^{(0)}, G^{(1)})$ be a graph satisfying the axioms in section 3 with vertices $G^{(0)}$ and edges $G^{(1)}$. Let

$$c : G^{(1)} \to \mathbb{R}_+ \quad (5.1)$$

be a fixed function (called conductance.) If $e = (xy) \in G^{(1)}$, we say that $x \sim y$, and the function $c$ must satisfy $c(xy) = c(yx)$, symmetry. In particular, for a pair of vertices $x, y$, $c(xy)$ is only defined if $x \sim y$, i.e., if $(xy) \in G^{(1)}$. For every $x \in G^{(0)}$, we assume that

$$\text{nbh}(x) = \left\{ y \in G^{(0)} \mid y \sim x \right\} \quad (5.2)$$
is finite, and that $x \notin \text{nbh} (x)$.

Following eq. (3.9), we study functions $v : G^{(0)} \to \mathbb{C}$ for which

$$E_c (v) = \sum_{\text{all } x, y \text{ s.t. } x \sim y} c (xy) |v (x) - v (y)|^2 < \infty. \quad (5.3)$$

Clearly we must work with functions on $G^{(0)}$ modulo constants. Setting

$$E_c (u, v) := \sum_{\text{all } x, y \text{ s.t. } x \sim y} c (xy) \left( \overline{u (x)} - \overline{u (y)} \right) \left( v (x) - v (y) \right), \quad (5.4)$$

we get

$$|E_c (u, v)|^2 \leq E_c (u) E_c (v), \quad \forall u, v \in D, \quad (5.5)$$

by Schwarz’ inequality.

Setting

$$\langle u, v \rangle_E := E_c (u, v) \quad (5.6)$$

we get an inner-product, and an associated Hilbert space $\mathcal{H}_E$ of all functions $v$ for which (5.3) holds.

The triangle inequality

$$E_c (u + v)^{\frac{1}{2}} \leq E_c (u)^{\frac{1}{2}} + E_c (v)^{\frac{1}{2}} \quad (5.7)$$

holds; or equivalently

$$\|u + v\|_E \leq \|u\|_E + \|v\|_E, \quad \forall u, v \in \mathcal{H}_E.$$

In the next result we give a characterization of the Hilbert space $\mathcal{H}_E$ directly in terms of the selfadjoint operator $\Delta_c$ from section 3.

Recall $\Delta_c$ is the closure of the operator $\Delta_c$ with dense domain $D$ in $\ell^2 (G^{(0)})$. It will be convenient to write simply $\Delta_c$ for the closure. Since it is selfadjoint, we have a Borel functional calculus; i.e., if $f$ is a Borel function on $\mathbb{R}$, and if $P (\cdot)$ is a projection valued measure for $\Delta_c$, then

$$\Delta_c = \int_0^\infty \lambda P (d\lambda), \quad (5.8)$$

and

$$f (\Delta_c) := \int f (\lambda) P (d\lambda). \quad (5.9)$$

For the corresponding (dense) domains, we have

$$\text{dom} (\Delta_c) = \left\{ v \in \ell^2 (G^{(0)}) \mid \int_0^\infty |\lambda|^2 \|P (d\lambda) v\|^2 < \infty \right\}, \quad (5.10)$$
and
\[
\text{dom } (\Delta_c) = \left\{ v \in \ell^2 \left( G^{(0)} \right) \mid \int_0^\infty |f(\lambda)|^2 \| P(d\lambda) v \|^2 < \infty \right\}. \tag{5.11}
\]

**Theorem 5.1** Let \( G = (G^{(0)}, G^{(1)}) \) and \( c: G^{(1)} \to \mathbb{R}_+ \) be as described, and let \( \mathcal{H}_E \) be the energy Hilbert space. Let \( \Delta_c \) be the selfadjoint graph Laplacian in \( \ell^2 \left( G^{(0)} \right) \) from Section 3.

(a) Then
\[
\text{dom } \left( \Delta_c^{1/2} \right) = \mathcal{H}_E \cap \ell^2 \left( G^{(0)} \right). \tag{5.12}
\]

(b) In general the right hand side is a proper subspace of \( \ell^2 \left( G^{(0)} \right) \).

**Proof.** We proved in (3.11), Lemma 3.2, that
\[
\mathcal{E}_c(u, v) = 2\langle u, \Delta_c v \rangle \tag{5.13}
\]
for all functions \( u, v \) on \( G^{(0)} \) for which the two sides in (5.13) are finite. If \( u = v \), then the expression on the RHS in (5.13) is \( 2 \| \Delta_c^{1/2} v \|^2 \) iff \( v \in \text{dom } \left( \Delta_c^{1/2} \right) \). This follows from (5.11) applied to
\[
f(\lambda) := \sqrt{\lambda}, \ \lambda \in [0, \infty).
\]
Since \( \text{dom } (\Delta_c) \subset \text{dom } \left( \Delta_c^{1/2} \right) \subset \ell^2 \left( G^{(0)} \right) \) the desired conclusion (5.12) holds.

To see that \( \text{dom } \left( \Delta_c^{1/2} \right) \) may be a proper subspace of
\[
\mathcal{H}_E = \left\{ v \mid \mathcal{E}_c(v) < \infty \right\}, \tag{5.14}
\]
consider the following example \((G, c)\) built on the simplest infinite graph \( G^{(0)} := \mathbb{Z} \).

**Example 5.2**
\[
G^{(0)} = \mathbb{Z},
G^{(1)} = \{(n, n \pm 1) \mid n \in \mathbb{Z}\}, \text{ and } c: G^{(1)} \to \mathbb{R}_+, \ c \equiv 1 \text{ on } G^{(1)}.
\]

The corresponding graph Laplacian is
\[
(\Delta v)(n) = 2v(n) - v(n - 1) - v(n + 1), \ \forall n \in \mathbb{Z}. \tag{5.15}
\]
If \( k \in \mathbb{Z}_+ \) is given, we claim that there is a unique function \( v \in \mathcal{H}_E \) solving
\[
\Delta v = \delta_0 - \delta_k. \tag{5.16}
\]
Existence: Set

\[ v(n) := \begin{cases} 
0 & \text{if } n \leq 0 \\
-n & \text{if } 0 < n \leq k \\
-k & \text{if } k \leq n.
\end{cases} \] (5.17)

A substitution shows that the function \( v \) in (5.17) satisfies (5.16).

Uniqueness: Let \( w \in \mathcal{H}_\mathcal{E} \) be a solution to (5.16). Then

\[ \mathcal{E}_c(u, v - w) = 0, \quad \forall u \in \mathcal{D}. \]

Since \( G = (G^{(0)}, G^{(1)}) \) is connected, \( \mathcal{D} \) is dense in \( \mathcal{H}_\mathcal{E} \); and so the difference \( v - w \) must be a constant function. But the Hilbert space \( \mathcal{H}_\mathcal{E} \) is defined by moding out with the constants. Hence, \( v = w \) in \( \mathcal{H}_\mathcal{E} \).

The following three facts follow directly from (5.17):

(i) \( v \) is non-constant;
(ii) \( v \notin \ell^2(\mathbb{Z}) \); and
(iii) \( \mathcal{E}_c(v) < \infty \).

In fact, an application of (5.13) yields

\[ \mathcal{E}_c(v) = 2k. \] (5.18)

Proof of (5.18):

\[ \mathcal{E}_c(v) = 2\langle v, \Delta v \rangle \text{ by (5.13)} \]
\[ = 2\langle v, \delta_0 - \delta_k \rangle \]
\[ = 2 (v(0) - v(k)) \]
\[ = 2k \text{ by (5.17)}. \]

Theorem 5.3 Let \( G = (G^{(0)}, G^{(1)}) \) and \( c : G^{(1)} \to \mathbb{R}_+ \) be a graph system as in the previous theorem, and in section 3 i.e., we assume that the pair \((G, c)\) satisfies the axioms listed there. Let \( \Delta_c \) be the corresponding graph Laplacian with a choice \( c \) for conductance.

Let \( \alpha, \beta \in G^{(0)} \) be a fixed pair of vertices. Then there is a unique function \( v \in \mathcal{H}_\mathcal{E} \), i.e., \( \mathcal{E}_c(v) < \infty \) satisfying

\[ \Delta_c v = \delta_\alpha - \delta_\beta. \] (5.19)

The solution to (5.19) is called a voltage potential. Moreover,

\[ \mathcal{E}_c(v) = 2(v(\alpha) - v(\beta)). \] (5.20)
Proof. The argument for uniqueness is the same as in the previous proof.

To prove existence, we will appeal to Riesz’ theorem for the energy Hilbert space $\mathcal{H}_E$.

Hence, we must show that there is a finite constant $K$ such that

$$|u(\alpha) - u(\beta)| \leq KE_c(u)^{\frac{1}{2}} \text{ for all } u \in \mathcal{D}. \quad (5.21)$$

Motivated by Ohm’s law, we set $\Omega(e) : = c(e)^{-1}, \forall e \in G^{(1)}$. By the assumptions in section 3, we may pick a finite subset $x_0, x_1, x_2, \ldots, x_n$ in $G^{(0)}$ such that

$$\left\{ \begin{array}{l}
x_0 = \alpha, \ x_n = \beta, \text{ and} \\
e_i = (x_i x_{i+1}) \in G^{(1)}, \ i = 0, 1, \ldots, n - 1.
\end{array} \right. \quad (5.22)$$

Then

$$|u(\alpha) - u(\beta)| \leq \sum_{i=0}^{n-1} |u(x_i) - u(x_{i+1})| 
\leq \left( \sum_{i=0}^{n-1} \Omega(e_i) \right)^{\frac{1}{2}} \left( \sum_{i=0}^{n-1} c(e_i) |u(x_i) - u(x_{i+1})|^2 \right)^{\frac{1}{2}} \quad \text{(by Schwarz)} 
\leq \left( \sum_{i=1}^{n-1} \Omega(e_i) \right)^{\frac{1}{2}} E_c(u)^{\frac{1}{2}}. \quad (by \ Schwarz)$$

To get a finite constant $K$ in (5.21), we may take the infimum over all paths subject to conditions (5.22), connecting $\alpha$ to $\beta$.

An application of Riesz’ lemma to $\mathcal{H}_E$ yields a unique $v \in \mathcal{H}_E$ such that for all $u \in \mathcal{D}$, we have the following identity:

$$u(\alpha) - u(\beta) = \frac{1}{2} E_c(v, u) = \langle \Delta_c v, u \rangle \quad \text{(by (5.13))}. \quad (5.23)$$

Using again density of $\mathcal{D}$ in $\mathcal{H}_E$, we get the desired conclusion

$$\Delta_c v = \delta_\alpha - \delta_\beta. \quad (5.23)$$

\[ \blacksquare \]

Corollary 5.4 Let $(G, c)$ satisfy the conditions in the theorem. Let $\alpha, \beta \in G^{(0)}$, and let $v \in \mathcal{H}_E$ be the solution (potential) to

$$\Delta_c v = \delta_\alpha - \delta_\beta. \quad (5.23)$$
Then
\[ E_c(v) \leq 2 \inf_{(e_i)} \sum_{i=0}^{n-1} \Omega(e_i) \] (5.24)

where \( e_0, e_1, \ldots, e_{n-1} \in G^{(1)} \) is a system of edges connecting \( \alpha \) to \( \beta \), i.e., satisfying the conditions listed in (5.22).

**Proof.** This follows from the previous proof combined with the fact that
\[ \sup_{E_c(u)=1} |E_c(u,v)|^2 = E_c(v). \] (5.25)

### 5.2 A matrix representation

While \( \Delta_c \) may be understood as an operator, it is also an \( \infty \times \infty \) matrix. Since the set \( \text{nbh}(x) \subset G^{(0)} \) is finite for all \( x \in G^{(0)} \), \( \Delta_c \) is a banded matrix.

To see this, note that when \( x \in G^{(0)} \) is fixed, the summation
\[ (\Delta_c v)(x) = \sum_{y \sim x} c(xy)(v(x) - v(y)) \] (5.26)

is finite for all functions \( v : G^{(0)} \rightarrow \mathbb{C} \).

Since \( G \) is assumed connected, the only bounded solutions \( v \) to the equation
\[ \Delta_c v = 0 \] (5.27)

are the constants.

Solutions \( v \) to (5.27) are called harmonic, or \( c \)-harmonic.

There are examples of systems \( (G, c) \) which are connected and have unbounded non-constant harmonic functions, e.g., models with \( G^{(0)} = \mathbb{Z}^3 \), or tree-models.

In the general case, introducing
\[ B_c(x) := \sum_{y \sim x} c(xy), \quad x \in G^{(0)}; \] (5.28)

we see that (5.26) takes the following form
\[ (\Delta_c v)(x) = B_c(x)(v(x) - \sum_{y \sim x} c(xy)v(y)). \] (5.29)
Hence eq. (5.27) may be rewritten as
\[ v(x) = \frac{1}{B_c(x)} \sum_{y \sim x} c(xy) v(y). \] (5.30)

It follows that harmonic functions on \( G(0) \) satisfy a mean value property. At every \( x \in G(0) \) formula (5.30) expresses \( v(x) \) as a convex combination of its values on the set nbh (\( x \)).

In matrix language, \( x \rightarrow B_c(x) \) represents the diagonal matrix-entries; and \( c(xy) \) the off-diagonal entries. Since \( \{ y \in G(0) | c(xy) \neq 0 \} \) is finite, we say that the matrix for \( \Delta_c \) is \emph{banded}. It is clear that products of banded matrices are again banded; and in particular that the summations involved in matrix-products of banded matrices are all finite. Hence, each of the operators \( \Delta_c, \Delta_c^2, \Delta_c^3, \ldots \), is banded. Since by Theorem 3.1 \( \Delta_c \) is selfadjoint as an operator in \( \ell^2 (G(0)) \), the fractional power \( \Delta_c^{1/2} \) is well defined by the Spectral Theorem. The matrix-entries of \( \Delta_c^{1/2} \) are the numbers
\[ \langle \delta_x, \Delta_c^{1/2} \delta_y \rangle_{\ell^2} = \left( \Delta_c^{1/2} \delta_y \right)(x), \ x, y \in G(0). \] (5.31)

It can be checked that if \( G \) is infinite, the matrix for \( \Delta_c^{1/2} \) is typically \emph{not} banded. The same conclusion applies to \( \Delta_c^s \) when \( s \in \mathbb{R} \setminus \mathbb{N} \).

5.3 Example 5.2 revisited

The system \((G, c)\) in Example 5.2 does not have non-constant harmonic functions. This can be seen from the representation of \( \Delta \) (in Ex. 5.2) as a \( \mathbb{Z} \times \mathbb{Z} \) double infinite matrix, i.e.,

\[ (\Delta v)(n) = 2v(n) - v(n - 1) - v(n + 1) \]
\[ = v(n) - v(n - 1) + v(n) - v(n + 1) \]
\[ = \sum_{m \sim n} v(m) - v(m), \ n \in \mathbb{Z}. \]

In matrix form, \( \Delta \) from Example 5.2 is as follows:
Using Fourier series

\[ f(x) = \sum_{n \in \mathbb{Z}} v(n) e^{inx} \in L^2(-\pi, \pi); \quad (5.32) \]

\[ \sum_{n \in \mathbb{Z}} |v(n)|^2 = \frac{1}{2\pi} \int_{-\pi}^{\pi} |f(x)|^2 \, dx; \quad (5.33) \]

we arrive at the representation

\[ \left( \tilde{\Delta} f \right)(x) = 2 \left( 1 - \cos x \right) f(x) \quad (5.34) \]

\[ = 4 \sin^2 \left( \frac{x}{2} \right) f(x), \]

proving that \( \Delta \) has Lebesgue spectrum, and

\[ \text{spec}_{\ell^2}(\Delta) = \text{spec}_{L^2}(\tilde{\Delta}) = [0, 4]. \quad (5.35) \]

### 5.4 Banded Matrices (A Preview)

It is immediate from the matrix representation for \( \Delta_c \) in Example 5.2 that it has a **banded** form. We will take up banded infinite matrices in detail in section 8 below.

Since \( \Delta_c \) is selfadjoint, its square-root \( \Delta_c^{1/2} \) is a well defined operator. However its matrix representation is typically **not** banded; see (5.31). For \( \Delta_c^{1/2} \) in Ex. 5.2 one can check that the \((m,n)\)-matrix entries are

\[ \left( \Delta_c^{1/2} \right)_{m,n} \sim \frac{1}{4 \cdot (n-m)^2 + 1}. \]
5.5 Extended Hilbert Spaces

To understand solutions \( v \) to operator equations like

\[
\Delta_c v = \delta_\alpha - \delta_\beta
\]

as in (5.23), potential functions it is convenient to extend the Hilbert space \( \ell^2 \left( G^{(0)} \right) \). Indeed we saw in Example 5.2 that the solutions \( v \) to equations like (5.23) are typically not in \( \ell^2 \left( G^{(0)} \right) \).

Definition 5.5 The space \( \mathcal{H}_c (s) \).

A function \( v : G^{(0)} \to \mathbb{C} \) is said to belong to the space \( \mathcal{H}_c (s) \) if there is a finite constant \( K = K (s) \) such that the following estimate holds:

\[
\left| \sum_{x \in G^{(0)}} v (x) (\Delta_s^c u) (x) \right|^2 \leq K (s) \sum_{x \in G^{(0)}} |u (x)|^2 \quad \text{for all } u \in \mathcal{D}. \tag{5.36}
\]

If (5.36) holds, then by Riesz, there is a unique \( w \in \ell^2 \left( G^{(0)} \right) \) such that

\[
\sum_{x \in G^{(0)}} v (x) (\Delta_s^c u) (x) = \langle w, u \rangle_{\ell^2} \quad \text{for all } u \in \mathcal{D} \subset \ell^2; \tag{5.37}
\]

and we set

\[
\| v \|_{\mathcal{H}_c (s)} := \| w \|_{\ell^2 \left( G^{(0)} \right)}. \tag{5.38}
\]

By abuse of notation, we will write \( \Delta_s^c v = w \) when \( v \in \mathcal{H}_c (s) \).

If two functions \( v_i \) for \( i = 1, 2 \) are in \( \mathcal{H}_c (s) \), and if \( \Delta_s^c v_i = w_i \in \ell^2 \left( G^{(0)} \right) \),

we set

\[
\langle v_1, v_2 \rangle_{\mathcal{H}_c (s)} := \langle w_1, w_2 \rangle_{\ell^2} \tag{5.39}
\]

\[
= \sum_{x \in G^{(0)}} w_1 (x) w_2 (x). \]

Remark 5.6 We proved in section \( \text{X} \) that

\[
\sum_{x \in G^{(0)}} (\Delta_c u) (x) = 0 \quad \text{for } \forall u \in \mathcal{D}.
\]

Hence the constant function \( v_1 (x) \equiv 1 \) on \( G^{(0)} \) is in \( \mathcal{H}_c (1) \), and \( \| v_1 \|_{\mathcal{H}_c (1)} = 0 \). Hence in considering the extension spaces, we shall work modulo the constant functions on \( G^{(0)} \).
Theorem 5.7 For every \( s \in \mathbb{R} \), the space \( \mathcal{H}_c(s) \) is a Hilbert space when equipped with the inner product \((5.39)\), and the norm \((5.38)\).

Proof. The idea in the proof follows closely the construction of Sobolev spaces, by analogy to the continuous case. The key step in the verification of completeness of \( \mathcal{H}_c(s) \) is the essential selfadjointness of \( \Delta_c \) as an operator in \( \ell^2(G^{(0)}) \). As before, we use the same notation \( \Delta_c \) for the closure of \( \Delta_c \), defined initially only on the subspace \( \mathcal{D} \) in \( \ell^2(G^{(0)}) \). Formulas \((5.9)-(5.11)\) above now allow us to define the selfadjoint operator \( \Delta_s \); and this operator is closed in the sense that its graph is closed in \( \ell^2(G^{(0)}) \times \ell^2(G^{(0)}) \). The completeness of \( \mathcal{H}_c(s) \) now follows from this, and an application of Riesz; see the estimate \((5.37)\).

Corollary 5.8 Let \((G,c)\) be an infinite graph, and let \( c : G^{(1)} \to \mathbb{R}_+ \) be a conductance function satisfying the axioms above. Let \( \alpha, \beta \in G^{(0)} \), and let \( v : G^{(0)} \to \mathbb{C} \) be a solution to \( \Delta_cv = \delta_\alpha - \delta_\beta \); i.e., to \((5.23)\).

Assume \( v \in \mathcal{H}_c \). Then

\[
v \in \mathcal{H}_c \left( \frac{1}{2} \right) \cap \mathcal{H}_c(1);
\]

and we have

\[
\|v\|_{1/2}^2 = \frac{1}{2} \mathcal{E}_c(v),
\]

and

\[
\|v\|_1^2 = 2.
\]

Proof. To prove \((5.40)\), we must check the \textit{a priori} estimate \((5.36)\) for \( s = 1/2 \), and \( s = 1 \):

Verification of \((5.36)\) for \( s = 1/2 \)

Let \( v \) satisfy the stated conditions, and let \( u \in \mathcal{D} \). Then

\[
\left| \sum_{x \in G^{(0)}} v(x) \left( \Delta_c^{1/2} u \right)(x) \right| = \left| \sum_{x \in G^{(0)}} v(x) \Delta_c\Delta_c^{-1/2}u(x) \right| = \frac{1}{2} \left| \mathcal{E}_c \left( v, \Delta_c^{-1/2}u \right) \right| \leq \frac{1}{2} \mathcal{E}_c(v)^{1/2} \mathcal{E}_c \left( \Delta_c^{-1/2}u \right)^{1/2} \quad \text{(Schwarz)}
\]

\[
= \frac{1}{\sqrt{2}} \mathcal{E}_c(v)^{1/2} \|u\|_{\ell^2(G^{(0)})},
\]

25
where we used the identity

\[
E_c \left( \Delta_c^{\frac{1}{2}} u \right) = 2 \| u \|_{L^2(G(0))}^2
= 2 \sum_{x \in G(0)} |u(x)|^2
\]
valid for \( \forall u \in \mathcal{D} \).

**Verification of (5.36) for \( s = 1 \)**

With \( v \) and \( u \) as before, we must estimate the summation:

\[
\left| \sum_{x \in G(0)} v(x) \left( \Delta_c u \right)(x) \right| = \left| \sum_{x \in G(0)} \left( \Delta_c v \right)(x) u(x) \right|
= \left| \sum_{x \in G(0)} \left( \delta_\alpha(x) - \delta_\beta(x) \right) u(x) \right|
= |u(\alpha) - u(\beta)|
\leq 2 \| u \|_{L^2(G(0))}, \ \forall u \in \mathcal{D}.
\]

Once (5.40) has been checked, the exact formulas (5.41) and (5.42) follow:

Firstly,

\[
\| v \|_1^2 = \left\| \Delta_c^{\frac{1}{2}} v \right\|_{L^2}^2
= \langle \Delta_c^{\frac{1}{2}} v, \Delta_c^{\frac{1}{2}} v \rangle
= \frac{1}{2} E_c(v);
\]

and secondly

\[
\| v \|_1^2 = \| \Delta_c v \|_{L^2}^2
= \| \delta_\alpha - \delta_\beta \|_{L^2}^2
= 2.
\]

\[\blacksquare\]
Remark 5.9 In conclusion (5.40) in Corollary 5.8 is not best possible. In fact, the optimal range of the fraction $s$ for which the potentials $v$ are in $\mathcal{H}_c(s)$ may be computed explicitly in Example 5.2 and related examples. Details in the next subsection.

In Example 5.2, $G^{(0)} = \mathbb{Z}$, $G^{(1)} = \{ (n, n \pm 1) \mid n \in \mathbb{Z} \}$, and $c \equiv 1$. Let $k \in \mathbb{N}$. The graph Laplacian $\Delta$ is given in formula (5.15).

Let $v$ be the unique solution to the potential equation

$$\Delta v = \delta_0 - \delta_k.$$  \hspace{1cm} (5.43)

Then $v \in \mathcal{H}(s)$ if and only if $s > 1/4$.

Proof. Setting

$$v(z) = \sum_{n \in \mathbb{Z}} v_n z^n, \text{ and } z = e^{ix},$$  \hspace{1cm} (5.44)

we get

$$v(z) = \frac{z (z^k - 1)}{(z - 1)^2};$$  \hspace{1cm} (5.45)

and therefore

$$|v(x)| = \left| \frac{\sin \left( \frac{kx}{2} \right)}{\sin^2 \left( \frac{x}{2} \right)} \right|.$$  \hspace{1cm} (5.46)

Since, in the spectral representation, the graph Laplacian $\Delta$ is multiplication by $4 \sin^2 (x/2)$, the question: “For what exponents $s$ is

$$v \in \mathcal{H}(s)?$$  \hspace{1cm} (5.47)

is decided by the asymptotics near $x = 0$ of the function $(\Delta^s v)(x)$. Using (5.46), we see that $\Delta^s v$ is in $L^2(-\pi, \pi)$ if and only if $x^{2k-1} \in L^2$ near $x = 0$; and this hold if and only if

$$s > \frac{1}{4}$$  \hspace{1cm} (5.48)

as claimed. $\blacksquare$

5.6 Lattice Models

Example 5.10 We proved that potential functions are often not in $\ell^2(G^{(0)})$, but in general the problem is more subtle.

The setting is as follows:

$$G = (G^{(0)}, G^{(1)}) \text{ a given graph;}$$
\[ c : G^{(1)} \to \mathbb{R}^+ \text{ a given conductance function;} \]
\[ \Delta_c = \text{the corresponding graph Laplacian;} \]
\[ \alpha, \beta \in G^{(0)} \text{ a fixed pair of vertices, } \alpha \neq \beta. \]

With this, we say that a function \( v : G^{(0)} \to \mathbb{R} \) is a potential if

\[ \Delta_c v = \delta_\alpha - \delta_\beta. \quad (5.49) \]

In the next result we show that lattice models \( \mathbb{Z}^D \) with \( D > 2 \) have \( \ell^2 \) potentials.

### 5.7 Preliminaries

By \( \mathbb{Z}^D \) we mean the rank \( D \)-lattice of vertex points \( n = (n_1, n_2, \ldots, n_D), \)
\( n_i \in \mathbb{Z}, i = 1, 2, \ldots, D. \) Every point \( n \in \mathbb{Z}^D \) has \( 2D \) distinct nearest neighbors

\[ (n_1, \ldots, n_i \pm 1, n_{i+1}, \ldots, n_D), \quad (5.50) \]

so \( \text{nbh} (n) \) consists of these \( 2D \) points; and \( G^{(1)} \) is the corresponding set of edges. In the discussion below, we pick the constant conductance \( c \equiv 1 \), i.e., a system of unit-resistors arranged in nearest-neighbor configurations. See Fig. 1 for an illustration of the simplest lattice configuration, \( D = 1, 2, \) and 3.

Fig. 1a: \( D = 1 \)
Fig. 1b: $D = 2$

Fig. 1c: $D = 3$

Fig. 1. Lattice configurations in the rank-$D$ lattices $\mathbb{Z}^D$ with nearest-neighbor resistors.

**Proposition 5.11** The potential functions $v$, i.e., solutions to (5.49) with $c \equiv 1$ are in $\ell^2(\mathbb{Z}^D)$ if $D > 2$.

**Proof.** Recall that the $D$-torus $\mathbb{T}^D$ is the compact dual of the rank-$D$ lattice. Pick coordinates in $\mathbb{T}^D$ s.t. $x = (x_1, \ldots, x_D)$, $-\pi < x_i \leq \pi$, $i = 1, 2, \ldots, D$.  

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Then, by Parseval,

\[ \ell^2(\mathbb{Z}^D) \simeq L^2(T^D). \]

By the argument from Example 5.2, we see that \( \Delta \) has the following spectral representation in \( L^2((-\pi, \pi] \times \cdots \times (-\pi, \pi]) \) \( D \) times

\[ (\Delta v)(x) = 4 \sum_{k=1}^{D} \sin^2 \left( \frac{x_k}{2} \right) v(x). \] (5.51)

Introducing spherical coordinates in \( \mathbb{R}^D \), we get the representation

\[ dx = \rho^{D-1} dS_1 \] (5.52)

where

\[ \rho : = \left( \sum_{k=1}^{D} x_k^2 \right)^{\frac{1}{2}}, \]

and whence \( dS_1 \) denotes the rotationally invariant measure on the sphere in \( \mathbb{R}^D \).

The question of deciding when the solution \( v \) to (5.49) is in \( \ell^2(\mathbb{Z}^D) \) can be better understood in the spectral representation \( v(x) \) for \( x = (x_1, \ldots, x_D) \) close to 0, i.e., \( \rho(x) \sim 0 \).

Using (5.51)-(5.52), we see that the potential function \( v \) is in \( \ell^2 \) if \( D > 2 \).

More generally, the argument from Example 5.2 proves that in \( \mathbb{Z}^D \), the potential function \( v \) is in \( \mathcal{H}(s) \) if \( s > \frac{2-D}{4} \).

The next results illustrate new issues entering the analysis of \( \mathbb{Z}^D \)-graphs when \( D > 1 \), compared to the \( D = 1 \) case.

**Corollary 5.12** For the case \( D = 3 \) in the lattice model in Example 5.10, consider \( k = (k_1, k_2, k_3) \in \mathbb{Z}^3 \setminus \{0\} \) fixed, and let

\[ v_k : \mathbb{Z}^3 \to \mathbb{R} \]

the solution to the potential equation

\[ \Delta v_k = \delta_0 - \delta_k. \] (5.53)

Then

\[ \lim_{n \to \infty} v_k(n) = 0. \] (5.54)
Proof. Our notation is as follows: \( n = (n_1, n_2, n_3) \in \mathbb{Z}^3 \) and by “\( n \to \infty \)” we mean:

\[
|n| = \sqrt{n_1^2 + n_2^2 + n_3^2} \to \infty.
\]

Moreover,

\[
\delta_k : \mathbb{Z}^3 \to \mathbb{R}
\]

is the usual Dirac mass

\[
\delta_k(n) = \delta_{k_1,n_1} \delta_{k_2,n_2} \delta_{k_3,n_3}.
\]

(5.55)

We proved in Proposition 5.11 \((D = 3)\) that

\[
\sum_{n \in \mathbb{Z}^3} |v_k(n)|^2 = \|v_k\|^2 < \infty;
\]

(5.56)

and so in particular, the conclusion (5.54) must hold. □

Our next example illustrates that the potential equation (5.53) has unbounded solutions in case \( D \geq 3 \). This will also provide concrete cases of unbounded harmonic functions, i.e., functions \( w : \mathbb{Z}^D \to \mathbb{R} \) for which \( \Delta w = 0 \).

To aid the construction, we include the following lemma which is about the general case of systems \((G,c)\) as analyzed in sections 3-4 above.

Lemma 5.13 Let \( G = (G^{(0)}, G^{(1)}) \), and \( c : G^{(1)} \to \mathbb{R}_+ \), be a graph system as described in Theorem 5.1, and let \( \Delta_c \) be the graph Laplacian.

Let \( \alpha, \beta \in G^{(0)} \) be given, \( \alpha \neq \beta \). Then there is a 1-1 correspondence between two classes of functions \( v : G^{(0)} \to \mathbb{R} \), and functions \( I : G^{(1)} \to \mathbb{R} \), where the two classes are given as follows:

Class 1.

\[
\Delta_c v = \delta_\alpha - \delta_\beta
\]

(5.57)

Class 2. \( I : G^{(1)} \to \mathbb{R} \) satisfying (Kirchoff’s Laws):

\[
(a) \sum_{y \sim x} I(x,y) = (\delta_\alpha - \delta_\beta)(x), \ \forall x \in G^{(0)}; \text{ and}
\]

\[
(b) \sum_i c(x_i,x_{i+1})^{-1} I(x_i,x_{i+1}) = 0 \text{ for all } x_0, x_1, x_2, \ldots, x_n \in G^{(0)} \text{ subject to } x_0 = x_n, \text{ and } x_i \sim x_{i+1}, \text{ i.e., all closed loops in } G^{(0)}.
\]

The connection between the two classes is given by the following formula:

\[
c(xy)^{-1} I(xy) = v(x) - v(y), \ \forall (xy) \in G^{(1)}.
\]

(5.58)
The function \( v \) is determined from \( I \) uniquely, up to a constant, when \( I \) is known to satisfy (a)-(b). Moreover,

\[
\sum_{e \in G^{(1)}} \frac{(I(e))^2}{c(e)} = \mathcal{E}_c(v). \tag{5.59}
\]

**Proof.** Left to the reader. The arguments are included in the proof of Theorem 5.1. \( \blacksquare \)

**Example 5.14** The \( D = 2 \) lattice model; i.e., \( G^{(0)} = \mathbb{Z}^2 \), edges given by nearest neighbors as in Fig. 1b; and \( c \equiv 1 \).

We consider the equation (5.57) for \( \alpha = (0,0) \) and \( \beta = (1,1) \). The two different solutions \( v \) to (5.57) will be presented in the form of Class 2 in Lemma 5.13, i.e., in terms of current functions defined on the edges in \( G \).

First recall that the Laplace operator \( \Delta \) in the \( \mathbb{Z}^2 \)-model is

\[
(\Delta v) (m,n) = 4v(m,n) - v(m-1,n) - v(m+1,n) - v(m,n-1) - v(m,n+1), \ \forall (m,n) \in \mathbb{Z}^2.
\]

Eq. (5.56) then takes the form

\[
\Delta v = \delta_{(0,0)} - \delta_{(1,1)}. \tag{5.60}
\]

We now describe the two current functions \( I \) which correspond to the two solutions to (5.60).
Fig. 2. The function $I$ for the first solution $v$ to (5.60).

Flow design for the current function $I$. The symbols “>” indicate arrows in the direction of the current flow. An arrow points in the direction of voltage drop.
And now the (different) function $I$ for the second solution to (5.60):

\[
\begin{array}{cccccc}
\vdots \\
0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 \\
0 & 0 & 0 & 0 & \frac{1}{2} & < \frac{1}{2} & < \frac{1}{2} \\
0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 \\
0 & 0 & 0 & \frac{1}{2} & < \frac{1}{2} & < \frac{1}{2} & 0 \\
\vdots \\
\end{array}
\]

\[
\begin{array}{cccccc}
\vdots \\
0 & 0 & 0 & \frac{1}{2} & < \frac{1}{2} & 0 & 0 \\
0 & 0 & \frac{1}{4} & \frac{1}{2} & \frac{1}{2} & 0 & 0 \\
0 & \frac{1}{4} & \frac{1}{4} & \frac{1}{2} & 0 & 0 & 0 \\
0 & \frac{1}{4} & (1,1) & \frac{1}{4} & 0 & 0 & 0 \\
\vdots \\
0 & (0,0) & \frac{1}{2} & \frac{1}{4} & \frac{1}{2} \rightarrow \frac{1}{2} \rightarrow \frac{1}{2} \rightarrow \frac{1}{2} \rightarrow \frac{1}{2} \rightarrow \frac{1}{2} \rightarrow \frac{1}{2} > \\
0 & 0 & 0 & 0 & 0 & 0 & \ldots \\
\vdots \\
\end{array}
\]

Fig. 3.

Flow design for the current function $I$. The symbols “>” indicate arrows in the direction of the current flow. An arrow points in the direction of voltage drop.

5.8 The Resistance Metric

Let $G = (G^{(0)}, G^{(1)})$ be a graph satisfying the axioms from section 2 and let

\[
c : G^{(1)} \rightarrow \mathbb{R}_+
\]

be a conductance function. Let $\mathcal{E}_c(\cdot)$ be the corresponding energy form, and let $\Delta_c$ be the graph Laplacian.

Pick a definite point $0$ in the vertex set $G^{(0)}$. Now for every $x \in G^{(0)}$ let $v_x \in \mathcal{H}_{\mathcal{E}_c}$ be the solution to

\[
\Delta_c v_x = \delta_0 - \delta_x.
\]

(5.61)
Set
\[
dist_c(x, y) := \mathcal{E}_c(v_x - v_y)^{\frac{1}{2}}
\]
for \(x, y \in G^{(0)}\). We say that \(x, y \rightarrow \dist_c(x, y)\) is the resistance metric on \(G^{(0)}\). It is immediate from (5.61) that it satisfies the triangle inequality.

**Proposition 5.15** The following formula holds for the resistance metric:
\[
dist_c(x, y) = \sqrt{2} (v_x(y) + v_y(x) - v_x(x) - v_y(y))^{\frac{1}{2}}.
\]

**Proof.** In view of (5.62), it is enough to compute \(\mathcal{E}_c(v_x - v_y)\) for pairs of points \(x, y\).

Let \(x, y \in G^{(0)}\) be given, and let \(v_x, v_y\) be the potential functions from (5.61). Then
\[
\mathcal{E}_c(v_x - v_y) = 2(\Delta_c(v_x - v_y), v_x - v_y)_{\ell^2} \\
= 2(\delta_0 - \delta_x - (\delta_0 - \delta_y), v_x - v_y)_{\ell^2} \\
= 2((v_x - v_y)(y) - (v_x - v_y)(x)) \\
= 2(v_x(y) + v_y(x) - v_x(x) - v_y(y)).
\]

**Example 5.16** (See also Example 3.7) Let \(\Delta_c\) be given by the following \(\infty \times \infty\) matrix:
\[
\begin{pmatrix}
1 & -1 & 0 & 0 & \cdots \\
-1 & 5 & -2^2 & 0 & \cdots \\
0 & -2^2 & 2^2 + 3^2 & -3^2 & \cdots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
0 & -n^2 & n^2 + (n + 1)^2 & -(n + 1)^2 & \cdots \\
0 & \cdots & \cdots & \cdots & \cdots
\end{pmatrix}
\]

So \(G^{(0)} = \mathbb{N}_0, G^{(1)} = \{(0, 1), \cdots, (n - 1, n), (n, n + 1), \cdots\}, \) and \(c(n, n + 1) = (n + 1)^2\). The first vertex has one neighbor, and the later two.
The potential equation \((5.62)\) may be solved by inspection, and we get
the following formula for the resistance metre \(\text{dist}_c\) in Proposition 5.15: If \(m < n\) (in \(\mathbb{N}_0\)) then
\[
\text{dist}_c(m, n) \simeq \left(\frac{1}{(m+1)^2} + \frac{1}{(m+2)^2} + \cdots + \frac{1}{n^2}\right)^{\frac{1}{2}}.
\]
Since \(\sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}\), we conclude that \((G^{(0)}, \text{dist}_c)\) is a bounded metric space.

Further, the resistance is bounded at infinity; or equivalently the voltage drop is “very” slow at infinity for the current flow induced by the experiment which inserts 1 amp at a particular place in \(G^{(0)} = \mathbb{N}_0\).

The reason is that the conductance is “very” unbounded, or equivalently or more precisely, the resistance is \(O(n^{-2})\) for this particular \((G, c)\) system.

Some conclusions: The finite-energy solution \(v\) to \((5.60)\) is the function \(v: \mathbb{Z}^2 \to \mathbb{R}\), beginning with the values 0, \(-1/2\), and \(-1\) as follows: In Figs. 2–3 we list the values of \(v\) on the points in the interior square in \(G^{(0)} (= \mathbb{Z}^2)\). The three values are prescribed in the centered square; and they then propagate into the quarter planes, with the value \(-1/2\) in the NW and the SE quarter planes.

6 Finite Dimensional Approximation

6.1 Systems of Graphs

Let \(G = (G^{(0)}, G^{(1)})\) be an infinite graph satisfying the axioms from section 2. In particular, we assume for every \(x\) in \(G^{(0)}\) that \(x\) itself is excluded from \(\text{nbh}(x)\); i.e., no \(x\) in \(G^{(0)}\) can be connected to itself with a single edge. Let \(c\) any conductance function defined on \(G^{(1)}\) and satisfying our usual axioms.

In section 3 we showed that the corresponding Laplace operator \(\Delta = \Delta_c\) is automatically essentially selfadjoint. By this we mean that when \(\Delta\) is initially defined on the dense subspace \(\mathcal{D}\) (of all the real valued functions on \(G^{(0)}\) with finite support) in the Hilbert space \(\mathcal{H} := \ell^2(G^{(0)})\), then the closure of the operator \(\Delta\) is selfadjoint in \(\mathcal{H}\), and so in particular it has a unique spectral resolution, determined by a projection valued measure on the Borel subsets the infinite half-line \(\mathbb{R}_+\).

In contrast, we note (Example 7.1) that the corresponding Laplace operator in the continuous case is not essential selfadjoint.

This can be illustrated with \(\Delta = -(d/dx)^2\) on the domain \(\mathcal{D}\) of consisting of all \(C^2\)-functions on the infinite half-line \(\mathbb{R}_+\) which vanish with their
derivatives at the end points. Then the Hilbert space is \( L^2(\mathbb{R}_+) \).

So this is an instance where the analogy between the continuous case and the discrete case breaks down.

In the study of infinite graphs \( G = (G^{(0)}, G^{(1)}) \) and the corresponding Laplacians, it is useful to truncate and consider first a nested system of finite graphs \( G_N \); then compute in the finite case and, in the end, take the limit as \( N \to \infty \). Our approximation results here continue work started in [Jør77], [Jør78].

**Definition 6.1** In this section we prove specific results showing that the procedure works. While there are several candidates for designing the finite approximating graphs \( G^N = (G^{(0)}_N, G^{(1)}_N) \), we will concentrate here on the simplest: Starting with an infinite \( G = (G^{(0)}, G^{(1)}) \), pick finite subsets of vertices as follows:

\[
G^{(0)}_1 \subset G^{(0)}_2 \subset G^{(0)}_3 \subset \cdots \subset G^{(0)}_N \subset \cdots \subset G^{(0)}
\]

such that

\[
\bigcup_{N=1}^{\infty} G^{(0)}_N = G^{(0)}.
\]

Set \( \mathcal{H} := \ell^2(G^{(0)}) \), and \( \mathcal{H}_N = \ell^2(G^{(0)}_N) \). Then the projection \( P_N \) of \( \mathcal{H} \) onto \( \mathcal{H}_N \) is multiplication by the indicator function \( \chi_{G^{(0)}_N} \); and the projection onto the complement \( \mathcal{H} \ominus \mathcal{H}_N \) is multiplication with \( \chi_{(G^{(0)}_N)^c} \) where \( (G^{(0)}_N)^c = G^{(0)} \setminus G^{(0)}_N \) is the complement of \( G^{(0)}_N \).

The edges \( G^{(1)}_N \) in \( G_N \) are simple the edges in \( G \), for which the vertices lie in \( G^{(0)}_N \); i.e., if \( x, y \in G^{(0)}_N \), then:

\[
(xy) \in G^{(1)}_N \iff (xy) \in G^{(1)} \text{ and } x, y \in G^{(0)}_N.
\]

If a system \( (G_N)_{N \in \mathbb{N}} \) of graphs is given as in (6.1)·(6.3), and if \( c : G^{(1)} \to \mathbb{R}_+ \) is a conductance function; we denote by \( c_N \) the restriction of \( c \) to \( G^{(1)}_N \).

**Lemma 6.2** Let \( G = (G^{(0)}, G^{(1)}) \) and \( c : G^{(1)} \to \mathbb{R}_+ \) be given as above. Let \( G_N \) be a system of graphs determined subject to conditions (6.1)·(6.3).

Let \( \Delta_N \) be the graph Laplacian associated to \( (G_N, c_N) \). Then

\[
P_N \Delta P_N = \Delta_N, \text{ for } \forall N \in \mathbb{N}.
\]

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Proof. For \( v \in \mathcal{D} = \text{finite linear combinations of } \{ \delta_x | x \in G^{(0)} \} \), we have

\[
(P_N \Delta P_N v) (x) = \chi_{G_N} (x) \sum_{y \sim x} c(xy) ((\chi_{G_N} v) (x) - (\chi_{G_N} v) (y)) = \sum_{y \sim x \text{ in } G_N} c_N (xy) (v (x) - v (y)) = (\Delta_N v) (x);
\]

proving the formula (6.4).

Lemma 6.3 Let \( G = (G^{(0)}, G^{(1)}) \), and \( c : G^{(1)} \to \mathbb{R}_+ \), be as in Lemma 6.2 and Definition 6.1. Then for all \( v \in \mathcal{D} \) and \( x \in G^{(0)} \), we have the following formula for the difference operator \( \Delta - \Delta_N \), \( N = 1, 2, \ldots \):

\[
(\Delta v) (x) - (\Delta_N v) (x) = -\chi_{G_N} (x) \sum_{y \sim x \text{ in } G_N} c(xy) v (y) .
\]

(6.5)

In other words, the contribution to \( \Delta - \Delta_N \) comes from the boundary of \( G_N = \text{the edges } e \in G^{(1)} \text{ s.t. one vertex in } e \text{ is in } G^{(0)} \text{ and the other in the complement.} \)

Proof. Using the previous lemma, we get

\[
(\Delta v) (x) - (\Delta_N v) (x) = \sum_{y \sim x} (c(xy) - c_N(xy)) (v(x) - v(y)) = -\chi_{G_N} (x) \sum_{y \sim x \text{ in } G_N} c(xy) v (y) .
\]

Definition 6.4 Let \( G = (G^{(0)}, G^{(1)}) \), and \( c : G^{(1)} \to \mathbb{R}_+ \) be given as in Theorem 5.1; and denote by \( \Delta = \Delta_c \) the corresponding selfadjoint graph Laplacian. Setting

\[
S(t) = \int_0^\infty e^{-t\lambda} P(d\lambda) \quad (\text{see } (5.9) - (5.10)) \quad (6.6)
\]

\[
e^{-t\Delta}, \quad t \in \mathbb{R}_+ ;
\]

we see that \( t \mapsto S(t) \) is a contractive semigroup of selfadjoint operators in \( \ell^2 (G^{(0)}) \); in particular,

\[
S(s + t) = S(s) S(t), \quad \forall s, t \in \mathbb{R}_+ \text{ and } S(0) = I_{\ell^2} .
\]

(6.7)
The semigroup consists of bounded operators while the infinitesimal generator $\Delta = \Delta_c$ is typically unbounded, albeit with dense domain in $\ell^2(G(0))$. Moreover, the semigroup helps us identify dynamics as infinite graphs of resistors.

Returning to approximations, as in Definition 6.1, we now get a sequence of Laplacians $\Delta_N, N = 1, 2, \ldots$, and a corresponding sequence of dynamical semigroups, $S_N(t) = e^{-t\Delta_N}, N = 1, 2, \ldots$.

Let $N$ be fixed, and let $\partial G_N$ be the boundary of $G_N$ (Definition 6.1). Then the finite matrix

$$T_N := (c(xy))_{x,y \in \partial G_N}$$

(6.8)

is positive, and has a Perron-Frobenius eigenvalue $\lambda_N = \lambda_N(PF) = \text{the spectral radius of } T_N$.

**Theorem 6.5** Let $(G, c)$ be a graph/conductance system, and let $(G_N)_{N \in \mathbb{N}}$ ascending system of graphs such that (6.2) is satisfied. Let $S(t)$, and $S_N(t), N = 1, 2, \ldots$, be the corresponding semigroups of bounded operators.

Then for all $v \in \ell^2(G(0))$, we have the following estimate:

$$\|S(t)v - S_N(t)v\|_{\ell^2} \leq \lambda_N(PF) t \|v\|_{\ell^2}, \forall t \in \mathbb{R}_+, N = 1, 2, \ldots \quad (6.9)$$

**Proof.** With the use of (5.8)-(5.9), we get the integral formula:

$$e^{-t\Delta} - e^{-t\Delta_N} = \int_0^t e^{-(t-s)\Delta} (\Delta - \Delta_N) e^{-s\Delta_N} \, ds. \quad (6.10)$$

Since the operators on both sides in (6.10) are bounded, it is enough to verify the estimate (6.9) for vectors $v$ in the dense domain $D$.

Using new Lemma (6.3) we get the following estimates on the respective $\ell^2$-norms:

$$\|S(t)v - S_N(t)v\|_{\ell^2} \leq \int_0^t \|\Delta - \Delta_N\| S_N(s)v\|_{\ell^2} \quad \text{(by (6.10))}$$

$$\leq \lambda_N(PF) \int_0^t \|S_N(s)v\| \, ds \quad \text{(by Lemma 6.3 and (6.8))}$$

$$\leq \lambda_N(PF) \|v\|_{\ell^2} \int_0^t \, ds$$

$$= \lambda_N(PF) t \|v\|_{\ell^2},$$

which is the desired conclusion.
6.2 Periodic boundary conditions

Example 6.6 We now compare Example 5.2 with an associated family of finite graphs $G_N$ where $N \in \mathbb{N}$. Let $\mathbb{Z}_N = \mathbb{Z}/N\mathbb{Z} \simeq \{0,1,2,\ldots,N-1\}$ be the cyclic group of order $N$. Introduce nearest neighbors as in Example 5.2 (the $\mathbb{Z}$-case) with the modification for $G_N$ given by $0 \sim (N-1)$, in other words that there is an edge connecting $0$ to $N-1$.

It follows that the graph Laplacian $\Delta_N$ for $G_N$ is given by the finite matrix

$$
\begin{bmatrix}
2 & -1 & 0 & 0 & 0 & \cdots & 0 & -1 \\
-1 & 2 & -1 & 0 & 0 & \cdots & 0 & 0 \\
0 & -1 & 2 & -1 & 0 & \cdots & 0 & 0 \\
\vdots & & & & & & \vdots & \\
0 & 0 & \cdots & 2 & -1 & 0 \\
0 & 0 & \cdots & -1 & 2 & -1 \\
-1 & 0 & \cdots & \cdots & 0 & -1 & 2
\end{bmatrix}.
$$

The spectrum of $\Delta_N$ is as follows:

$$
\text{spec} (\Delta_N) = \left\{ 2 \left( 1 - \cos \left( \frac{2\pi k}{N} \right) \right) | k = 0, 1, \ldots, N - 1 \right\} \quad (6.11)
$$

$$
= \left\{ 4 \sin^2 \left( \frac{\pi k}{N} \right) | k = 0, 1, \ldots, N - 1 \right\}.
$$

Comparing with (5.34)-(5.35), we see that the spectra converge in a natural sense; with the infinite model in Ex 5.2 being a limit of $N$-periodic boundary condition as $N \to \infty$. 

40
Fig. 4. The vertices and edges in $G_N$ for $N = 3, 4$ and $5$.

The spectrum of the cyclic graph Laplacian $\Delta_N$ of the graphs $G_N$, $N = 3, 4$ and $6$ (in Fig. 3) may have multiplicity; see (6.11). This holds in fact for all values of $N$. Specifically,

spec($\Delta_3$) = \{0, 3\} with $\lambda = 3$ having multiplicity 2.

spec($\Delta_4$) = \{0, 2, 4\} with $\lambda = 2$ having multiplicity 2.

spec($\Delta_6$) = \{0, 1, 3, 4\} now with $\lambda = 1$ and $\lambda = 3$ each having multiplicity 2.

Hence for $D = 1$, we get the following distinction between the spectral theory of the cyclic graph Laplacians $\Delta_N$ for $N < \infty$ on the one hand and $\Delta$ in Example 5.2 on the other: The commutant of $\Delta$ is an abelian algebra of operators in $\ell^2(\mathbb{Z})$, while the operators in $\ell^2(\mathbb{Z}_N)$ which commute with $\Delta_N$ form a non-abelian algebra.

**Proposition 6.7** (Cyclic graphs) Let $N \in \mathbb{N}$, $N \geq 3$; and let $G_N$ be the corresponding cyclic graph with graph Laplacian $\Delta_N$; i.e., with

$$G_N^{(0)} = \{0, 1, 2, \ldots, N - 1\}.$$
Then the voltage potential \( v \in \ell^2(\mathbb{Z}_N) \) solving \( \Delta_N v = \delta_0 - \delta_1 \) is

\[
\begin{align*}
    v_0 & = 0 \\
    v_1 & = -\frac{N-1}{N} \\
    v_2 & = -\frac{2}{N} \\
    \vdots  \\
    v_{N-2} & = -\frac{N-2}{N} \\
    v_{N-1} & = -\frac{1}{N}.
\end{align*}
\]

**Proof.** A direct computation; see also Fig. 4, and eq. (6.10). 

7 Boundary Conditions

In the study of infinite graphs \( G \), boundary conditions play an important role; for example if a current escapes to infinity in “finite time,” conditions must then be assigned “at infinity.”

One way to do this is to first do computations in a system of finite graphs \( G_N \) which exhausts the given graph \( G \) in a suitable way. Do computations on each finite subgraph \( G_N \) of the fixed infinite graph \( G \), and then take the limit as \( N \) tends to infinity. There are several ways one may do the computations on each individual \( G_N \), for example look for symmetry, or look for a suitable periodicity, or similarity up to scale. In the simplest cases, this allows the use of a finite Fourier transform, thus making \( G_N \) periodic, or cyclic. The case of \( G = \mathbb{Z} \) (the rank-1 integer graph), and \( G_N = \) the cyclic group of order \( N \) is done in all detail in Example 6.6 above.

Some advantages of the cyclic approach: One, the spectrum comes out given explicitly by a closed formula, thus making it clear how the limit \( N \to \infty \) works also for spectra, getting the continuous spectrum in the infinite limit.

**Example 7.1** In this section we compare the two cases, continuous vs. discrete. As noted, our graph Laplacians are second order (or more than second order) difference operators in a generalized sense.

They have spectrum contained in the half-line \([0, \infty)\), so generalizing

\[
(\Delta v)(x) := -\left(\frac{d}{dx}\right)^2 v(x)
\]

with the Hilbert space \( \mathcal{H} := L^2(0, \infty) \), and dense domain

\[
\mathcal{D} := \{ v \in C^2(0, \infty) \mid v, v', v'' \in L^2(0, \infty), \text{ and } v(0) = v'(0) = 0 \}; \quad (7.2)
\]
i.e., with vanishing boundary conditions on $v$ and $v'(x) = \frac{dv}{dx}$ at $x = 0$.

We get the spectral estimate:

$$\langle v, \Delta v \rangle_{L^2} \geq 0, \forall v \in \mathcal{D}. \quad (7.3)$$

A simple verification shows that for the adjoint operator $\Delta^*$ we have:

$$\text{dom}(\Delta^*) = \{ v \in L^2(0, \infty) \mid v', v'' \in L^2(0, \infty) \}. \quad (7.4)$$

Comparing (7.2) and (7.4) we see that $\Delta$ results from $\Delta^*$ by “removing” the two boundary conditions which specify the domain $\mathcal{D}$ of $\Delta$.

Moreover, the defect space

$$\mathcal{D}_+ := \{ v \in \text{dom}(\Delta^*) \mid \Delta^* v = -v \} \quad (7.5)$$

is one-dimensional; in fact,

$$\mathcal{D}_+ = \mathbb{C}e^{-x}. \quad (7.6)$$

The selfadjoint extensions of $\Delta$ on $\mathcal{D}$ are parametrized by pairs of numbers $A, B \in \mathbb{R}$, not both zero, such that

$$Av(0) + Bv'(0) = 0. \quad (7.7)$$

**Example 7.2** Let $G = (G^{(0)}, G^{(1)})$ be the following graph generalizing the continuous example:

$$G^{(0)} := \mathbb{N}_0 = \{0, 1, 2, 3, \ldots\}, \quad (7.8)$$

$$G^{(1)} := \{(01), (n, n \pm 1) \mid n \in \mathbb{N}\}.$$

Pick $\lambda > 1$, and set

$$c(n, n+1) = \lambda^{n+1}. \quad (7.9)$$

Then the corresponding graph Laplacian is unbounded; and

$$\langle \Delta v \rangle (0) = \lambda v_0 - \lambda v_1; \quad (7.10)$$

$$(\Delta v) (n) = -\lambda^n v_{n-1} + \lambda^n (1 + \lambda) v_n - \lambda^{n+1} v_{n+1}, \forall n \in \mathbb{N}. \quad (7.11)$$
For domain $D$, we take all $v \in \ell^2(N_0)$ s.t. $v_n = 0$ except for a finite set of values of $n$. The matrix representation of $\Delta$ is presented in Fig. 4:

$$
\begin{pmatrix}
\lambda & -\lambda & 0 & 0 & 0 & \cdots \\
-\lambda & \lambda(1 + \lambda) & -\lambda^2 & 0 \\
0 & -\lambda^2 & \lambda^2(1 + \lambda) & -\lambda^3 \\
0 & & & & \ddots \\
0 & & & & -\lambda^n \\
0 & & & & -\lambda^n(1 + \lambda) & -\lambda^{n+1} & \cdots \\
0 & & & & -\lambda^{n+1}
\end{pmatrix}
$$

Fig. 4.

By Parseval’s formula, we have the isometric isomorphism $\ell^2(N_0) = \mathcal{H}_+ = \text{the Hardy space of analytic functions on } D = \{z \in \mathbb{C}; |z| < 1\}$

$$v(z) := \sum_{n=0}^{\infty} v_n z^n;$$

and

$$||v||^2_{\mathcal{H}_+} = \sum_{n=0}^{\infty} |v_n|^2. \quad (7.12)$$

In the Hardy space representation we have

$$(\Delta v)(z) = (1 + \lambda) v(\lambda z) - \lambda z v(\lambda z) - z^{-1} v(\lambda z) \quad (7.13)$$

on the dense space of functions $v$ on $\mathbb{C}$ which extend analytically to $D_\lambda := \{z \in \mathbb{C}; |z| < \lambda\}$.

We now show that there are no non-zero solutions to

$$\Delta^*_\lambda v = -v, \quad (7.14)$$

i.e., $v \in \text{dom}(\Delta^*_\lambda)$; equivalently $\mathcal{D}_+(\lambda) = \{0\}$; the defect space for the operator $\Delta_\lambda$ is trivial. So this is a direct verification that $\Delta_\lambda$ is essentially selfadjoint; and contrasting with $(7.6)$ above.

To see this, combine $(7.13)$ and $(7.14)$. It follows that every solution $v$ to $(7.14)$ must have an infinite-product representation given by

$$v(z) = \frac{(z-1)(\lambda z - 1)}{\lambda z} v(\lambda z); \quad (7.15)$$
and the limit of finite products as follows

\[
(z - 1) \prod_{k=1}^{n-1} (\lambda^k z - 1)^2 (\lambda^n z - 1) \quad \frac{z^n \lambda^{-\frac{n(n+1)}{2}}}{}. \]

These products do not have a non-zero representation consistent with the isomorphism (7.12), and with (7.12).

8 Appendix

A Heisenberg’s Infinite Banded Matrices

We proved in sections 3 through 5 that in general, graph Laplacians \( \Delta_c \) are essentially selfadjoint operators in the \( \ell^2 \) sequence-Hilbert space. Recall that the axioms for our graph Laplacians include the following given data: A graph \( G = (G^{(0)}, G^{(1)}) \) and a fixed positive conductance function \( c \) defined on the set of edges \( G^{(1)} \). Every vertex \( x \) of \( G \) is connected to a finite set of neighbors in \( G^{(0)} \). For every fixed \( x \) in \( G^{(0)} \), this implies finiteness of the set of \( y \) in \( G^{(0)} \) for which \( c(xy) \) is nonzero. This means in turn that the natural matrix representation of the operator \( \Delta_c \) is banded; see section 5 for the Definition. Note however that we place no boundedness restrictions on the conductance function \( c \).

Our proof of essentially selfadjoint for the operator \( \Delta_c \) uses this bandedness property in an essential way. In fact, starting with an infinite by infinite matrix, it is generally difficult to turn it into a linear operator in a Hilbert space unless it is assumed banded, see section 4 and the references cited there.

The purpose of this section is three-fold.

First to make precise the operator theory of banded infinite by infinite matrices; and second to show that the infinite matrices used in representing the operator algebra generated by Heisenberg’s quantum mechanical momentum and position observables consists of (infinite) banded matrices. Thirdly, we use Heisenberg’s (and Born’s) computations to exhibit such banded operators which are not essentially selfadjoint. The simplest such matrix \( M \) is as follows: let \( P \) be Heisenberg’s momentum operator and \( Q \) the (dual) position operator. Then we show that the monomial \( M = PQP \) is banded, but not essentially selfadjoint. In fact, its deficiency indices are \((1, 1)\).
Definition A.1 Let $L$ be a countable (typically infinite) set, and let $m : L \times L \to \mathbb{C}$ be a function on $L \times L$. We say that $m$ is banded iff for every $x \in L$, the set
\[ \{ y \in L | m(x, y) \neq 0 \} \tag{A.1} \]
is finite.

Let $\ell^2(L)$ be the sequence space with norm
\[ \|v\|_{\ell^2}^2 : = \sum_{x \in L} |v(x)|^2 < \infty. \tag{A.2} \]
The sum on the right is the supremum of all the numbers $\sum_{x \in F} |v(x)|^2$ as $F$ ranges over all finite subsets in $L$.

Let $D$ be the dense subspace of all functions $v : L \to \mathbb{C}$ such that the support set
\[ \{ x \in L | v(x) \neq 0 \} \tag{A.3} \]
is finite. Equivalently, setting
\[ \delta_x(y) = \begin{cases} 1 & y = x \\ 0 & y \neq x \end{cases}; \tag{A.4} \]
the space $D$ is then the linear span of the set of functions $\{ \delta_x | x \in L \}$; and these functions form an orthonormal basis for $\ell^2(L)$. Moreover, every Hilbert space $\mathcal{H}$ is isomorphic to $\ell^2(L)$ for some set $L$. The set $L$ is countable if and only if $\mathcal{H}$ is separable.

Lemma A.2 Let $m : L \times L \to \mathbb{C}$ be a banded function. For $v \in D \subseteq \ell^2(L)$, set
\[ (Mv)(x) = \sum_{y \in L} m(x, y) v(y). \tag{A.5} \]
Then $M$ defines a linear operator $M : D \to D$, with a well defined adjoint operator $M^*$. Moreover,
\[ D \subseteq \text{dom}(M^*) \tag{A.6} \]
where $\text{dom}(M^*)$ is the domain of $M^*$.

Proof. When $x \in L$ is fixed, the sum in (A.5) is finite because the set (A.1) is finite by assumption. Using finiteness of both sets (A.1) and (A.3) we conclude that $Mv$ in (A.5) is in $D$ if $v$ is. And so, in particular, $Mv \in \ell^2(L)$; see (A.2) and (A.4).
To establish the inclusion “⊆” in (A.6), we must show that for every \( v \in \mathcal{D} \), there is a constant \( K = K(v) \) such that the following estimate holds:

\[
|\langle Mu, v \rangle_{\ell^2}| \leq K \|u\|_{\ell^2}, \quad \forall u \in \mathcal{D}.
\]  

(A.7)

The expression on the left in (A.7) is

\[
\sum_{x,y \in L} m(x,y)u(y)v(x).
\]  

(A.8)

But the terms in this double-sum vanish outside a finite subset in \( L \times L \) an account of assumptions (A.1) and (A.3).

The modulus-square of the sum in (A.8) is estimated by Schwarz by:

\[
\sum_{y \in L} |u(y)|^2 \sum_{y \in L} \sum_{x} m(x,y)v(x)^2
\]

which yields the desired estimate (A.7).

**Corollary A.3** Let \( M \) be a linear operator in a Hilbert space \( \mathcal{H} \). Then \( M \) has a banded matrix representation if and only if there is an orthonormal basis \( \{ e_x | x \in L \} \) such that the linear space \( \mathcal{D} \) spanned by \( (e_x)_{x \in L} \) is mapped into itself by \( M \).

**Corollary A.4** In that case the matrix entries of \( M \) are indexed by \( L \times L \) as follows:

\[
m( x, y ) := \langle e_x, Me_y \rangle.
\]  

(A.9)

**Proof.** Only the conclusion (A.9) is not contained in the lemma. Now suppose some operator \( M \) in \( \mathcal{H} \) satisfies the conditions, and let \( (e_x)_{x \in L} \) be the associated ONB. Then \( Me_y \in \mathcal{H} \cong \ell^2(L) \), so \( Me_y = \sum_{x \in L} \langle e_x, Me_y \rangle e_x \), and

\[
\|Me_y\|^2_{\mathcal{H}} = \sum_{x \in L} |\langle e_x, Me_y \rangle|^2
\]  

(A.10)

holds by Parseval’s formula. The conclusion (A.9) follows.

**Corollary A.5** Let \( G = (G^{(0)}, G^{(1)}) \) and

\[
c : G^{(1)} \to \mathbb{R}_+
\]
be a graph system satisfying the axioms in section 2. Let \( \{ \delta_x | x \in G^{(0)} \} \) be the canonical ONB in \( \ell^2(G^{(0)}) \). Then the graph Laplacian has a corresponding banded matrix representation as follows:

\[
\langle \delta_x, \Delta_c \delta_y \rangle = \begin{cases} 
- c(xy) & \text{if } y \neq x \text{ and } y \sim x \\
B_c(x) & \text{if } y = x \\
0 & \text{if } y \not\sim x \text{ and } y \neq x.
\end{cases}
\] (A.11)

**Proof.** Recall the function

\[
B_c(x) := \sum_{y \sim x} c(xy)
\] (A.12)

on the right-hand side in (A.11).

Since, for \( v \in D \), we have

\[
(\Delta_c v)(x) := \sum_{y \sim x} c(xy) (v(x) - v(y))
\] (A.13)

setting \( v = \delta_y \), we get

\[
(\Delta_c \delta_y)(x) = \begin{cases} 
B_c(x) & \text{if } y = x \\
- c(xy) & \text{if } y \sim x \\
0 & \text{if } y \not\sim x
\end{cases}
\]
from which the desired formula (A.11) follows. ■

Heisenberg introduced \( \infty \times \infty \) matrix representations for the operators of momentum \( P \) and position \( Q \) in quantum mechanics.

In the simplest case of one degree of freedom, they are as follows:

\[
\begin{pmatrix}
1 & 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 & \cdots \\
0 & \sqrt{2} & 0 & 0 & \cdots & \cdots & \cdots & \sqrt{n-2} & 0 & \cdots \\
0 & 0 & \sqrt{n-2} & 0 & \cdots & \cdots & \cdots & \sqrt{n-1} & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & 0 & \sqrt{n-1} & \cdots & \cdots & \cdots & \sqrt{n-1} & \cdots & \cdots \\
\frac{1}{\sqrt{n}} & \cdots & \cdots & \cdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & \cdots & \cdots & \cdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & \ddots & \ddots & \ddots & \ddots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots
\end{pmatrix}
\]
Set $N_0 := \{0, 1, 2, \ldots\} = \mathbb{Z}_+ \cup \{0\}$, and $\mathcal{H} := \ell^2(N_0)$. Then the two matrices $P$ and $Q$ are represented by the following second order difference operators, having the same form as our graph Laplacians (A.13).

$$
\left( \begin{array}{ccccccc}
0 & -1 & 0 & \cdots & \cdots & \cdots & \\
1 & 0 & -\sqrt{2} & \cdots & \cdots & \cdots & \\
0 & \sqrt{2} & 0 & -\sqrt{n-2} & 0 & 0 & \\
& & \ddots & \ddots & \ddots & \ddots & \\
\frac{1}{2i} & \ddots & \ddots & \ddots & \ddots & \ddots & \\
\. & \ddots & \ddots & \ddots & \ddots & \ddots & \\
\cdots & \ddots & \ddots & \ddots & \ddots & \ddots & \\
\cdots & \ddots & \ddots & \ddots & \ddots & \ddots & \\
\end{array} \right).
$$

It is well known that both $P$ and $Q$, as in (A.14) and (A.15), are essentially selfadjoint.

It follows by the above lemma that

$$M := PQ$$

is also a banded operator., referring to the canonical ONB $\{e_n|n \in N_0\}$ in $\ell^2(N_0)$.

Caution: All the operators $P, Q$, and $M$ are unbounded, but densely defined; see [Jør77], [Jør78], [Sto51].

**Proposition A.6** The operator $M$ in (A.16) is Hermitian, and has deficiency indices $(1, 1)$; in particular is not essentially selfadjoint. In fact, it has many selfadjoint extensions; a one-parameter family indexed by $\mathbb{T}$.

**Proof.** By the Stone-von Neumann uniqueness theorem, the two operators $P$ and $Q$ in (A.14) and (A.15) are unitarily equivalent to the following pair in the Hilbert space $L^2(\mathbb{R})$ of all square-integrable functions on the red line:

$$
(Pf) (x) = \frac{1}{2i} \frac{d}{dx} f (x),
$$

(A.17)
and

$$(Qf)(x) = xf(x), \text{ for } \forall f \in L^2(\mathbb{R}), \ x \in \mathbb{R}. \quad (A.18)$$

For domain $D$ in (A.17) and (A.18), we may take $D := C_c^\infty(\mathbb{R})$, or the span of the Hermite functions.

From the representations (A.14)-(A.15), it follows that the operator $M := PQPQ$ in (A.16) commutes with a conjugation in the Hilbert space; and so by von Neumann’s theorem (see Remark 4.2), it has deficiency indices $(n, n)$. We will show that $n = 1$. Hence we must show that each of the equations $M^*v_\pm = \pm i v_\pm$ has a one-dimensional solution space in $\mathcal{H}$.

Taking advantage of Schrödinger’s representation (A.17)-(A.18), we arrive at the corresponding pair of ODEs in $L^2(\mathbb{R})$:

$$x \frac{d}{dx}(xf) = \pm f(x). \quad (A.19)$$

By symmetry, we need only to treat the first one.

A direct integration shows that

$$f(x) = \begin{cases} \exp\left(\frac{-1}{x}\right) & \text{if } x > 0 \\ 0 & \text{if } x \leq 0 \end{cases} \quad (A.20)$$

solves (A.19) in the case of “+” on the right hand side. Also note that (A.20) is meaningful as all the derivatives of $x^{-1}\exp(-\frac{1}{x})$ for $x \in \mathbb{R}_+$ tend to 0 when $x \to 0_+$. This means that the two separate expressions on the right-hand side in (A.20) “patch” together differently at $x = 0$.

By the reasoning alone, we conclude that $M$ has indices $(1, 1)$. As a result of von Neumann’s extension theory, the distinct selfadjoint extensions of $M$ are then indexed by $\mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\}$. If $z \in \mathbb{T}$, and if $f_\pm$ are normalized solutions to (A.19), then the extension $M_z$ is determined by

$$M_z(f_+ + zf_-) = i(f_+ - zf_-).$$

Example A.7 Let $P$ and $Q$ be the canonical momentum and position operators; see (A.14)-(A.15), and let

$$H := P^2 - Q^4 \quad (A.21)$$

be the Hamiltonian of a “particle-wave” in one degree of freedom, corresponding to a repulsive $x^4$ potential. Then the reasoning from above shows that $H$ is a banded $\infty \times \infty$ matrix. As an operator in $\ell^2(\mathbb{Z})$, $H$ has deficiency indices $(2, 2)$. 

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