An Inverse Spectral Theorem

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Abstract

We prove a substantial extension of an inverse spectral theorem of Ambarzumyan, and show that it can be applied to arbitrary compact Riemannian manifolds, compact quantum graphs and finite combinatorial graphs, subject to the imposition of Neumann (or Kirchhoff) boundary conditions.

Keywords: inverse problems, Ambarzumyan, spectral geometry, heat kernel, heat trace asymptotics, quantum graph
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1 Introduction

Let $X$ be a compact metric space provided with a finite measure $dx$. Let $H_0$ be a non-negative self-adjoint operator acting on $L^2(X, dx)$. We assume that $H_0$ has discrete spectrum $\{\lambda_n\}_{n=1}^\infty$, where the eigenvalues are written in increasing order and repeated according to multiplicity, and that its smallest eigenvalue $\lambda_1 = 0$ has multiplicity 1 with corresponding eigenfunction $\phi_1 = |X|^{-1/2}$, where $|X|$ is the volume of $X$. Given a bounded real potential $V$ on $X$, we put $H = H_0 + V$, so that $H$ also has discrete spectrum, which we denote by $\{\mu_n\}_{n=1}^\infty$. The problem is to write down a general list of abstract conditions on $H_0$ which imply that if $H$ and $H_0$ have the same spectrum, taking multiplicities into account, then $V$ is identically zero.

The classical theorem of Ambarzumyan solved this problem when $X = [a, b]$ and $H_0 f = -\frac{d^2 f}{dx^2}$, subject to Neumann boundary conditions at $a$ and $b$. The result is also known for periodic boundary conditions, but the corresponding result for Dirichlet boundary conditions is false; the best known inverse spectral theorem in this context depends on knowing the spectrum of $H$ for
two different sets of boundary conditions at $a, b$. Ambarzumyan’s theorem has been extended to trees with a finite number of edges, \cite{4, 11, 12}, by combining the Sturm-Liouville theory with a careful boundary value analysis. The present paper extends it to a much broader context by adapting a range of classical techniques from the theory of the heat equation in several dimensions. Theorem \cite{7} establishes that if $\mu_1 \geq 0$ and $\limsup_{n \to \infty} (\mu_n - \lambda_n) \leq 0$ then $V = 0$, subject to certain generic conditions on the heat kernels involved.

This theorem can be applied to arbitrary compact Riemannian manifolds, compact quantum graphs and finite combinatorial graphs, subject to Neumann (or Kirchhoff) boundary conditions. Our proof depends on a list of abstract hypotheses that are known to be satisfied in a wide variety of situations. The hypotheses are by no means the weakest possible; the strategy of our proof is more important than the detailed assumptions, and can be adapted to other cases.

The material in Sections 2 and 3 is of a general character, and the reader may prefer to start in Section 4. In Section 5 we prove that all of the hypotheses hold for a finite connected quantum graph $X$, subject to Kirchhoff boundary conditions at every vertex.

Before proceeding, I should like to thank Professor Chun-Kong Law for a very stimulating lecture in the Isaac Newton Institute in July 2010, where the author learned about this problem.

## 2 Properties of $H_0$

We start by listing the hypotheses that will be used in the proofs.

- **(H1)** The operator $e^{-H_0 t}$ has a non-negative integral kernel $K_0(t, x, y)$ for $t > 0$, which is continuous on $(0, \infty) \times X \times X$.

- **(H2)** There exist constants $c > 0$ and $d > 0$ such that $0 \leq K_0(t, x, x) \leq ct^{-d/2}$ for all $t \in (0, 1)$.

- **(H3)** There exists a constant $a > 0$ such that $\lim_{t \to 0} t^{d/2} K_0(t, x, x) = a$ for all $x \notin N$, where $N$ is a set of zero measure.

- **(H4)** The smallest eigenvalue $\lambda_1$ of the operator $H_0$ equals 0 and has multiplicity 1. The corresponding eigenfunction is $\phi_1 = |X|^{-1/2}$.

We do not assume that $H_0$ is a second order elliptic differential operator, because we wish to allow other possibilities. For example $H_0$ could be a fractional
power of a Laplacian. The case in which $H_0$ is a discrete Laplacian on $l^2(X)$ for some finite set $X$ is discussed in Example 8. The conditions (H1) to (H4) have been examined in some detail in [6], from which we quote the following consequences of (H1) and (H4).

The quadratic form defined on $\text{Quad}(H_0) = \text{Dom}(H_0^{1/2})$ by
\[
Q_0(f) = \langle H_0^{1/2}f, H_0^{1/2}f \rangle
\]
is a Dirichlet form; see [6, Theorem 1.3.2]. The one-parameter semigroup $T_t = e^{-H_0 t}$ on $L^2(X, dx)$ is an irreducible symmetric Markov semigroup. It extends to a one-parameter contraction semigroup on $L^p(X, dx)$ for all $1 \leq p \leq \infty$, with the proviso that for $p = \infty$ the semigroup is not strongly continuous; see [6, Prop. 1.4.3]. Mercer’s theorem, [10, Prop. 5.6.9], implies that the operator $e^{-H_0 t}$ is trace class for all $t > 0$ and
\[
\text{tr}[e^{-H_0 t}] = \int_X K_0(t, x, x) \, dx.
\]

In particular
\[
\sum_{n=1}^{\infty} e^{-\lambda_n t} < \infty
\]
for all $t > 0$, where $\{\lambda_n\}_{n=1}^{\infty}$ are the eigenvalues of $H_0$ written in increasing order and repeated according to multiplicities. If $\phi_n$ are the corresponding normalized eigenfunctions then by applying the formula
\[
e^{-\lambda_n t} \phi_n(x) = \int_X K_0(t, x, y) \phi_n(y) \, dy
\]
we deduce that every eigenfunction $\phi_n$ is bounded and continuous on $X$. The semigroup $T_t$ is ultracontractive in the sense of [6, Section 2.1] and the series
\[
K_0(t, x, y) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \phi_n(x) \phi_n(y)
\]
converges uniformly on $[\alpha, \infty) \times X \times X$ for every $\alpha > 0$; see [6, Theorem 2.1.4]. This implies that $K_0(t, x, y)$ converges uniformly to $|X|^{-1}$ on $X \times X$ as $t \to \infty$, so
\[
\frac{1}{2|X|} \leq K_0(t, x, y) \leq \frac{3}{2|X|}
\]
for all large enough $t > 0$.

The condition (H2) is much more specific, but necessary and sufficient conditions for its validity are now classical.
Proposition 1 Let $H$ be a self-adjoint operator acting in $L^2(X, dx)$. If $H$ is bounded below and $e^{-Ht}$ is positivity preserving for all $t \geq 0$ then the following are equivalent, the constant $d > 0$ being the same in all cases.

1. The operator $e^{-Ht}$ satisfies
   \[ \|e^{-Ht}f\|_\infty \leq c_1 t^{-d/4} \|f\|_2 \]
   for some $c_1 > 0$, all $f \in L^2(X, dx)$ and all $t \in (0, 1)$.

2. The bound
   \[ \int_X f^2 \log(f) dx \leq \varepsilon Q(f) + \beta(\varepsilon) \|f\|_2^2 + \|f\|_2^2 \log(\|f\|_2) \]
   holds for all $0 \leq f \in \text{Quad}(H) \cap L^1 \cap L^\infty$ and all $\varepsilon \in (0, 1)$, where $\beta(\varepsilon) = c_2 - (d/4) \log(\varepsilon)$ for some $c_2 > 0$. See [6, Example 2.3.3].

3. The bound
   \[ \|f\|_2^{4/d} \leq c_3 \left( Q(f) + \|f\|_2^2 \right) \|f\|_4^{4/d} \]
   holds for some $c_3 > 0$ and all $0 \leq f \in \text{Quad}(H) \cap L^1$. See [6, Corollary 2.4.7].

4. Assuming $d > 2$, the bound
   \[ \|f\|_2^{2d/(d-2)} \leq c_4 \left( Q(f) + \|f\|_2^2 \right) \]
   holds for some $c_4 > 0$ and all $f \in \text{Quad}(H)$. See [6, Corollary 2.4.3].

All of the above conditions imply that $e^{-Ht}$ has a measurable heat kernel $K$ that satisfies
\[ 0 \leq K(t, x, y) \leq c_5 t^{-d/2} \quad (2) \]
for some $c_5 > 0$, almost all $x, y \in X$ and all $t \in (0, 1)$. Conversely, if $\|e^{-Ht}\|_{L^\infty \to L^\infty} \leq c_6$ for all $t \in (0, 1)$ then (2) implies the previous conditions. See [6, Lemma 2.1.2].

An important feature of all these conditions is that they depend on the quadratic form $Q$ and can therefore be transferred from one operator to another if the quadratic forms are comparable.

Example 2 Let $H_0 = -\frac{d^2}{dx^2}$ act in $L^2((0, \infty), dx)$ subject to Neumann boundary conditions at 0. Then
\[ K_0(t, x, y) = (4\pi t)^{-1/2} \left( e^{-(x-y)^2/(4t)} + e^{-(x+y)^2/(4t)} \right) \]
so

\[ 0 \leq K_0(t, x, y) \leq 2(4\pi t)^{-1/2} \]

for all \( t > 0 \) and \( x, y \in (0, \infty) \). Moreover

\[
\lim_{t \to 0} (4\pi t)^{1/2} K_0(t, x, x) = \begin{cases} 
1 & \text{if } x > 0, \\
2 & \text{if } x = 0.
\end{cases}
\]

This explains the need for an exceptional set of zero measure in (H3).

One may also solve the corresponding example in \( \mathbb{R}^N_+ = (0, \infty)^n \) subject to Neumann boundary conditions on the boundary. In this case the possible values of \( \lim_{t \to 0} (4\pi t)^{1/2} K_0(t, x, x) \) are the integers \( 2r \) where \( 0 \leq r \leq n \). A related result for general convex sets is given in [9, Theorem 12]. □

3 Properties of \( H = H_0 + V \)

Given a self-adjoint operator \( H_0 \) satisfying the hypotheses (H1) to (H4), we put \( H = H_0 + V \) where \( V \) is a bounded real-valued potential; this condition can surely be weakened. An application of the Trotter product formula or a perturbation expansion imply that

\[
\|e^{-Ht}\|_{L^p \to L^p} \leq e\|V\|_\infty t
\]

for all \( p \in [1, \infty] \) and \( t \geq 0 \). By using standard variational methods one sees that \( H \) has discrete spectrum and that its eigenvalues \( \{\mu_n\}_{n=1}^\infty \), written in increasing order and repeated according to multiplicity, satisfy

\[
\lambda_n - \|V\|_\infty \leq \mu_n \leq \lambda_n + \|V\|_\infty
\]

for all \( n \geq 1 \). Hence

\[
0 \leq e^{-\|V\|_\infty t} \text{tr}[e^{-H_0t}] \leq \text{tr}[e^{-Ht}] \leq e^{\|V\|_\infty t} \text{tr}[e^{-H_0t}]
\]

for all \( t > 0 \).

The proof of the following theorem involves standard ingredients, [5, 6], but we write it out in detail for the sake of completeness.

**Theorem 3** The operator \( e^{-Ht} \) has a non-negative continuous kernel \( K \) for all \( t > 0 \) and \( x, y \in X \). The kernel satisfies

\[
0 \leq e^{-\|V\|_\infty t} K_0(t, x, y) \leq K(t, x, y) \leq e^{\|V\|_\infty t} K_0(t, x, y)
\]

(3)

for all \( t > 0 \). The smallest eigenvalue \( \mu_1 \) of \( H \) has multiplicity 1.
Proof We will assume throughout the proof that $0 < t < 1$; once (3) has been proved in this case it can be extended to larger $t$ by using the semigroup property. Since the quadratic form

$$Q(f) = Q_0(f) + \int_X V(x)|f(x)|^2 \, dx$$

is a Dirichlet form in the sense of [6, Theorem 1.3.2], the operators $e^{-Ht}$ are all positivity preserving. The quadratic forms of $H_0$ and $H$ are comparable, so we may use Proposition 1 to deduce that for every $t \in (0, 1)$ there is a bounded, measurable integral kernel $K(t, x, y)$ satisfying $0 \leq K(t, x, y) \leq ct^{-d/2}$ if $0 < t < 1$ and

$$(e^{-Ht} f)(x) = \int_X K(t, x, y)f(y) \, dy$$

for all $f \in L^2$. Since $e^{-Ht} = e^{-H_0 t} e^{-H} e^{-H_0} t$ for all $\varepsilon > 0$ and $t > 2\varepsilon$, we can use the norm analyticity of $e^{-H(t-2\varepsilon)}$ in $L^2$ to deduce the norm analyticity of $e^{-Ht}$ from $L^1$ to $L^\infty$. This implies that $K(t, \cdot, \cdot)$ depends analytically on $t$ in the $L^\infty(X \times X)$ norm for $0 < t < \infty$.

The upper and lower bounds in (3) are now direct applications of the Trotter product formula. (1) and (3) together imply that the operator $A = e^{-Ht}$ is irreducible for all large enough $t > 0$. Therefore its largest eigenvalue has multiplicity 1 by a direct application of [10, Theorem 13.3.6] to $A/\|A\|$. The operator $e^{-Ht}$ has an operator norm convergent infinite series expansion involving $e^{-H_0 t}$ and $V$, but we will use the more compact expression

$$e^{-Ht} = e^{-H_0 t} - A(t) + B(t)$$

(4)

where

$$A(t) = \int_{s=0}^t e^{-H_0(t-s)} V e^{-H_0 s} \, ds,$$

$$B(t) = \int_{s=0}^t \int_{u=0}^s e^{-H_0(t-s)} V e^{-H(s-u)} V e^{-H_0 u} \, du \, ds.$$

The integrands are norm continuous in $\{s : 0 < s < t\}$, resp. $\{(s, u) : 0 < u < s < t\}$, and they are uniformly bounded in norm, so the integrals are norm convergent and $A(t), B(t)$ depend norm continuously on $t$.

The equation (4) has a version involving integral kernels, namely

$$K(t, x, y) = K_0(t, x, y) - L(t, x, y) + M(t, x, y)$$

(5)
for all $t > 0$ and $x, y \in X$, where

$$L(t, x, y) = \int_{s=0}^{t} \int_{z \in X} K_0(t-s, x, z)V(z)\, K_0(s, z, y) \, dz,$$

and we will prove that

$$|M(t, x, y)| \leq ct^{2-d/2} \quad (6)$$

for all $t \in (0, 1)$ and $x, y \in X$.

We will also prove that all the kernels on the right-hand side of (5) are continuous on $(0, 1) \times X \times X$, and this will establish that $K$ is continuous on the same set. The estimates below involve the uniform norm $\| \cdot \|_\infty$ on $B = C(X \times X)$.

The integral kernel of $A(t)$ is

$$L(t, x, y) = \int_{s=0}^{t} L_{s,t}(x, y) \, ds \quad (7)$$

where $L_{s,t} : X \times X \to \mathbb{R}$ is defined by

$$L_{s,t}(x, y) = \int_{X} K_0(t-s, x, z)V(z)\, K_0(s, z, y) \, dz.$$

Now $L_{s,t} \in B$ for all $0 < s < t$ and $L_{s,t}$ depends norm continuously on $s, t$ subject to these conditions. We have to prove that the integral (7) is norm convergent in $B$. This follows from

$$\int_{s=0}^{t} \|L_{s,t}\|_\infty \, ds \leq \|V\|_\infty \int_{s=0}^{t} \sup_{x, y} \left\{ \int_{X} K_0(t-s, x, z)V(z)\, K_0(s, z, y) \, dz \right\} \, ds$$

$$= \|V\|_\infty \int_{s=0}^{t} \sup_{x, y} \{K_0(t, x, y)\} \, ds$$

$$\leq c\|V\|_\infty t^{1-d/2}$$

provided $0 < t < 1$.

The integral kernel of $B(t)$ is

$$M(t, x, y) = \int_{s=0}^{t} \int_{u=0}^{s} M_{u, s, t}(x, y) \, du \, ds \quad (8)$$

where $M_{u, s, t} : X \times X \to \mathbb{R}$ is defined by

$$M_{u, s, t}(x, y) = \int_{X^2} K_0(t-s, x, z)V(z)\, K(s-u, z, w)V(w)\, K_0(u, w, y) \, dw \, dz.$$

Without assuming that $K(s-u, z, w)$ is continuous in $z, w$, one sees by (3) that $M_{u, s, t} \in B$ for all $0 < u < s < t$, and that $M_{u, s, t}$ depends norm continuously.
on \( u, s, t \) subject to these conditions. We have to prove that the integral (8) is norm convergent in \( B \). We have
\[
\| M_{u,s,t} \|_\infty \leq \| V \|_\infty^2 \| N_{u,s,t} \|_\infty
\]
where
\[
N_{u,s,t}(x,y) = \int_{X^2} K_0(t - s, x, z) K(s - u, z, w) K_0(u, w, y) \, dw \, dz
\]
\[
\leq e^{\| V \|_\infty t} \int_{X^2} K_0(t - s, x, z) K_0(s - u, z, w) K_0(u, w, y) \, dw \, dz
\]
\[
= e^{\| V \|_\infty t} K_0(t, x, y)
\]
\[
\leq e^{\| V \|_\infty ct^{-d/2}}.
\]
provided \( 0 < t < 1 \). Therefore
\[
\int_{s=0}^{t} \int_{u=0}^{s} \| M_{u,s,t} \|_\infty \, du \, ds \leq bt^{2-d/2}
\]
where \( b \) depends on \( \| V \|_\infty \).

\[\square\]

**Corollary 4** One has
\[
\text{tr}[e^{-H}] = \text{tr}[e^{-H_0 t}] - t \int_X K_0(t, x, x) V(x) \, dx + \rho(t) \tag{9}
\]
where \( \rho(t) = O(t^{2-d/2}) \) as \( t \to 0 \).

**Proof** One puts \( x = y \) in (5) and integrates with respect to \( x \). The bound on \( \rho(t) \) follows from (6).

\[\square\]

## 4 The main results

In this section we assume that \( H_0 \) satisfies (H1) to (H4) and that \( H = H_0 + V \) where \( V \) is a real bounded potential on \( X \). Both operators have discrete spectrum, and their eigenvalues are denoted by \( \{ \lambda_n \}_{n=1}^\infty \), respectively \( \{ \mu_n \}_{n=1}^\infty \), written in increasing order and repeated according to multiplicity. We assumed that \( \lambda_1 = 0 \) and proved that \( \mu_1 \) has multiplicity 1; see Theorem 3. Our following theorem has something in common with [15, Theorems 2.5, 3.4], which obtain a related result for Schrödinger operators in one and two dimensions subject to (10).
Theorem 5 If \( \mu_1 \geq 0 \) and
\[
\int_X V(x) \, dx \leq 0 \tag{10}
\]
then \( V = 0 \).

Proof The variational estimate
\[
\mu_1 \leq Q(\phi_1) = |X|^{-1} \int_X V(x) \, dx \leq 0,
\]
where \( \phi_1(x) = |X|^{-1/2} \), shows that \( \mu_1 = 0 \) under the stated conditions. We apply the results of the last section to \( H_s = H_0 + sV \) where \( s \) is a real parameter. The smallest eigenvalue \( F(s) = \mu_1(s) \) of \( H_s \) has multiplicity 1 for all \( s \in \mathbb{R} \) and therefore is an analytic function of \( s \) by a standard argument in perturbation theory. It is also concave by a variational argument. Finally \( F(0) = 0 \) and
\[
F'(0) = \langle V\phi_1, \phi_1 \rangle = |X|^{-1} \int_X V(x) \, dx \leq 0.
\]
Since \( F(1) = 0 \), its concavity implies that \( F(s) \) must equal 0 for all \( s \in [0, 1] \). By its analyticity, \( F(s) = 0 \) for all \( s \in \mathbb{R} \).

If \( V \) does not vanish identically then (10) implies that its negative part cannot vanish identically. Therefore there exists a function \( \psi \in L^2(X, dx) \) such that \( \langle V\psi, \psi \rangle < 0 \). An approximation argument allows us to assume that \( \psi \in \text{Quad}(H_0) \). We now conclude that
\[
F(s) = Q_0(\psi) + s\langle V\psi, \psi \rangle < 0
\]
for all large enough \( s > 0 \). The contradiction implies that \( V = 0 \). \( \square \)

The following is our main inverse spectral theorem.

Theorem 6 If \( \mu_1 \geq 0 \) and \( \limsup_{t \to 0} \sigma(t) \leq 0 \) where
\[
\sigma(t) = t^{d/2-1} \sum_{n=1}^\infty \left( e^{-\lambda_n t} - e^{-\mu_n t} \right)
\]
then \( V = 0 \).

Proof We rewrite (11) in the form
\[
t^{d/2} \int_X K_t(x, x) V(x) \, dx
= t^{d/2-1} \left\{ \text{tr}[e^{-H_0 t}] - \text{tr}[e^{-H t}] \right\} + t^{d/2-1} \rho(t)
= \sigma(t) + t^{d/2-1} \rho(t)
\]
and then take the limit of both sides as \( t \to 0 \). The left hand side converges to 
\[ a \int_X V(x) \, dx \]
where \( a > 0 \), by (H2) and (H3). We deduce that \( \int_X V(x) \, dx \leq 0 \) and may therefore apply Theorem 5.

The following corollary of Theorem 6 contains the original Ambarzumyan theorem as a special case.

**Theorem 7** If \( \mu_1 \geq 0 \) and \( \limsup_{n \to \infty} (\mu_n - \lambda_n) \leq 0 \) then \( V = 0 \).

**Proof** Given \( \varepsilon > 0 \) there exists \( N = N(\varepsilon) \) such that \( \mu_n - \lambda_n \leq \varepsilon \) for all \( n \geq N \). We then have

\[
\sigma(t) = \sigma_1(t) + \sigma_2(t)
\]

where

\[
\sigma_1(t) = t^{d/2-1} \sum_{n=1}^{N-1} (e^{-\lambda_n t} - e^{-\mu_n t}) \\
\leq t^{d/2} \sum_{n=1}^{N-1} |\lambda_n - \mu_n|,
\]

and

\[
\sigma_2(t) = t^{d/2-1} \sum_{n=N}^{\infty} (e^{-\lambda_n t} - e^{-\mu_n t}) \\
\leq t^{d/2} \sum_{n=N}^{\infty} \left( e^{-\lambda_n t} - e^{-\varepsilon t} \right) \\
\leq \varepsilon t^{d/2} \sum_{n=1}^{\infty} e^{-\mu_n t} \\
\leq c\varepsilon
\]

for all \( t \in (0, 1) \), by an application of (H2). We conclude that \( \limsup_{t \to 0} \sigma(t) \leq c\varepsilon \) for all \( \varepsilon > 0 \), and may therefore apply Theorem 6.

**Example 8** Let \( H_0 \) be a (non-negative) discrete Laplacian on \( l^2(X) \) for some finite, combinatorial graph \( X \), with \( |X| = n \). One can bypass many of our calculations by using the elementary formula

\[
\sum_{r=1}^{n} \mu_r - \sum_{r=1}^{n} \lambda_r = \text{tr}[H - H_0] = \text{tr}[V] = \sum_{x \in X} V(x).
\]

The relevant conditions on the eigenvalues in this case are

\[
\mu_1 \geq 0 \text{ and } \sum_{r=1}^{n} \mu_r \leq \sum_{r=1}^{n} \lambda_r.
\]
However the analysis of the function \( F \) in Theorem 5 requires the assumptions (H1) and (H4), and the use of the theory of irreducible symmetric Markov semigroups.

Theorem 9  The hypotheses (H1) to (H4) and therefore the conclusions of Theorems 4 and 7 are valid if \( H_0 \) is the Laplace-Beltrami operator on a compact, connected Riemannian manifold \( X \), subject to Neumann boundary conditions if \( X \) has a boundary \( \partial X \); the boundary should satisfy the Lipschitz condition.

Proof  All of the hypotheses except (H2) and (H3) are minor variations on results in [6]. the Lipschitz boundary condition is needed to obtain (H2), \( d \) being the dimension of \( X \). This is a result of a general principle that bounded changes of the metric, and therefore of the local coordinate system, do not affect bounds such as (H2), [9]. The precise heat kernel asymptotics required in (H3) holds for all \( x \not\in \partial X \), and is a small part of classical results of Minakshisundaram, Pleijel and others concerning the small time asymptotics of the heat kernel; see [3, 5, 11, 13]. In this context the nature of the boundary is irrelevant by the principle of ‘not feeling the boundary’; see Theorem 12 and [8].

5  Finite quantum graphs

In this section we prove that Theorems 6 and 7 are applicable when \( X \) is a finite connected quantum graph. We assume that \( X \) is the union of a finite number of edges \( e \in \mathcal{E} \), each of finite length. Each edge terminates at two vertices out of a finite set \( V \), and we assume that the graph as a whole is connected. The operator \( H_0 \) acts in \( L^2(X, dx) \) by the formula \( H_0 f(x) = -\frac{d^2}{dx^2} \), subject to Kirchhoff boundary conditions at each vertex; more precisely we require that all functions in the domain of \( H_0 \) are continuous and that the sum of the outgoing derivatives vanishes at each vertex. All of our calculations depend on the fact that the quadratic form associated with \( H_0 \) is given by

\[
Q_0(f) = \int_X |f'(x)|^2 \, dx
\]

with domain \( \text{Quad}(H_0) = \text{Dom}(H_0^{1/2}) = W^{1,2}(X) \) where this is the space of all functions \( f \) whose restriction to any edge \( e \) lies in \( W^{1,2}(e) \), together with the requirement that \( f \) is continuous at every vertex. We observe that \( W^{1,2}(X) \) is continuously embedded in \( C(X) \). It is immediate from its definition that \( Q_0 \) is a Dirichlet form, so the operators \( e^{-H_0 t} \) are positivity preserving for all \( t \geq 0 \). The identity \( H_0 1 = 0 \) implies that \( e^{-H_0 t} 1 = 1 \) for all \( t \geq 0 \), so \( e^{-H_0 t} \) is a symmetric Markov semigroup.
Lemma 10  The operator $H_0$ on $L^2(X, dx)$ satisfies (H1), (H2) and (H4).

Proof  If we disconnect $X$ by imposing Neumann boundary conditions independently at the end of each edge, then we obtain a new operator $H_1$ associated a quadratic form $Q_1$; this has the same formula as $Q_0$, but a larger domain, consisting of all functions $f \in L^2(X, dx)$ such that the restriction of $f$ to any edge $e$ lies in $W^{1,2}(e)$. The operator $H_1$ acts independently in each $L^2(e, dx)$ and its heat kernel in $e$ is of the form

$$K_e(t, x, y) = \frac{1}{a} + \frac{2}{a} \sum_{n=1}^{\infty} e^{-\pi^2 n^2 t/a^2} \cos(\pi nx/a) \cos(\pi ny/a),$$

where we parametrize $e$ by $(0, a)$. One readily sees that each $K_e$ is continuous and that

$$|K_e(t, x, y)| \leq c_1 t^{-1/2}$$

for some $c_1 > 0$, all $x, y \in e$ and all $0 < t < 1$. Moreover $K_e(t, x, y) \geq 0$ because $Q_1$ is a Dirichlet form. It follows from these observations that the various equivalent conditions of Proposition [1] hold for $Q_1$ with $d = 1$. Since $Q_0$ is a restriction of $Q_1$, Proposition [1] implies that

$$0 \leq K_0(t, x, y) \leq c_2 t^{-1/2}$$

for some $c_2 > 0$, all $x, y \in X$ and all $0 < t < 1$. This completes the proof of (H2).

To prove (H1) we note that if $\{\phi_n\}_{n=1}^{\infty}$ is an orthonormal basis of eigenfunctions of $H_0$ and $\lambda_n$ are the corresponding eigenvalues, then

$$\phi_n \in \text{Dom}(H_0) \subseteq \text{Dom}(H_0^{1/2}) = W^{1,2}(X) \subset C(X).$$

Since the series

$$K_0(t, x, y) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \phi_n(x) \phi_n(y)$$

converges uniformly on $[\alpha, \infty) \times X \times X$ for every $\alpha > 0$ by [6] Theorem 2.1.4, we deduce that $K_0$ is continuous on $(0, 1) \times X \times X$.

The proof of (H4) depends on the observation that $H_0 \phi = 0$ if and only if $\phi \in W^{1,2}(X) \subset C(X)$ and

$$0 = Q_0(\phi) = \int_X |\phi'(x)|^2 \, dx.$$

This implies that $\phi$ is constant. Therefore 0 is an eigenvalue of multiplicity 1.

□

Our final task is to prove (H3).
Lemma 11 Let \( K_a(t, x, y) \) be the heat kernel of the operator \(-\frac{d^2}{dx^2}\) acting in \( L^2(-a, a) \) subject to Dirichlet boundary conditions at \( \pm a \). Then
\[
0 \leq K_a(t, x, y) \leq K_\infty(t, x, y) = (4\pi t)^{-1/2}e^{-|x-y|^2/(4t)}
\] (11)
for all \( t > 0 \) and \( x, y \in (-a, a) \). Moreover
\[
1 \geq \int_{-a}^{a} K_a(t, 0, x) \, dx \geq 1 - 4e^{-a^2/(8t)}
\] (12)
and
\[
(4\pi t)^{-1/2} \geq K_a(t, 0, 0) \geq (4\pi t)^{-1/2}
\left(1 - 15e^{-a^2/(4t)}\right)
\] (13)
for all \( t > 0 \).

**Proof** The inequality (11) follows directly from the monotonicity of the Dirichlet heat kernel as a function of the region. Sharper versions of the inequalities (12) and (13) may be proved by applying the Poisson summation formula to the explicit eigenfunction expansion of \( K_a \), [16]. An alternative proof of (12) based on the properties of the underlying Brownian motion is given in [7, Lemma 6.5].

One may prove (13) from (12) as follows. We define \( f, g : \mathbb{R} \to (0, \infty) \) by
\[
f(x) = \begin{cases} 
K_a(t, 0, x) & \text{if } |x| \leq a, \\
0 & \text{otherwise},
\end{cases}
\]
\[
g(x) = K_\infty(t, 0, x) = (4\pi t)^{-1/2}e^{-x^2/(4t)}.
\]
so that \( 0 \leq f(x) \leq g(x) \leq (4\pi t)^{-1/2} \) for all \( x \in \mathbb{R} \) and \( \int_{\mathbb{R}} g(x) \, dx = 1 \). Therefore
\[
0 \leq (8\pi t)^{-1/2} - K_a(2t, 0, 0)
= K_\infty(2t, 0, 0) - K_a(2t, 0, 0)
= \int_{\mathbb{R}} \{ g(x)^2 - f(x)^2 \} \, dx
\leq \int_{\mathbb{R}} \{ g(x) - f(x) \} 2g(x) \, dx
\leq (\pi t)^{-1/2} \int_{\mathbb{R}} \{ g(x) - f(x) \} \, dx
= (\pi t)^{-1/2}
\left(1 - \int_{-a}^{a} f(x) \, dx\right)
\leq (\pi t)^{-1/2}4e^{-a^2/(8t)}.
\]
by (H2). We finally obtain (13) upon replacing \( t \) by \( t/2 \). \( \square \)

We prove (H3) by using the principle of ‘not feeling the boundary’, [8].
Theorem 12 The operator $H_0$ on $L^2(X, dx)$ satisfies (H3), the exceptional set $N$ being the set of all vertices on $X$.

Proof This repeats the argument used to prove (13). We assume that $z \in X$ is not a vertex and that $a > 0$ is its distance from the closest vertex. We then let $K_a$ denote the Dirichlet heat kernel for the interval $I$ with centre $z$ and length $2a$. Our task is to compare the heat kernel $K$ of $X$ with $K_a$. We use the following facts.

$$0 \leq K_a(t, x, y) \leq K_0(t, x, y)$$

for all $t > 0$ and $x, y \in X$, where we put $K_a(t, x, y) = 0$ if $x$ or $y$ does not lie in the interval $I$. In addition $0 \leq K_0(t, x, y) \leq ct^{-1/2}$ for all $0 < t < 1$ and all $x, y \in X$. Finally

$$\int_X K_0(t, x, y) \, dy = 1$$

for all $t > 0$ and $x \in X$.

Let $f(x) = K_a(t, z, x)$ and $g(x) = K_0(t, z, x)$ so that $0 \leq f(x) \leq g(x)$ for all $x \in X$. We have

$$0 \leq \int_X \{g(x) - f(x)\} \, dx = 1 - \int_I K_a(t, z, x) \, dx$$

$$\leq 4e^{-a^2/(8t)}$$

by (12). Therefore

$$K_0(2t, z, z) - K_a(2t, z, z) = \int_X \{g(x)^2 - f(x)^2\} \, dx$$

$$\leq \int_X \{g(x) - f(x)\} 2g(x) \, dx$$

$$\leq c_1 t^{-1/2} e^{-a^2/(8t)}.$$

The theorem follows by combining this with (13). □

References


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