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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, heat kernel, heat trace asymptotics, quantum graph.*

MSC (2010): 35R30, 34A55, 58J53, 35P20, 34L15.

INTRODUCTION

Let X be a compact metric space provided with a finite measure $\mathrm{d}x$. Let H_0 be a non-negative self-adjoint operator acting on $L^2(X, \mathrm{d}x)$. 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 $H_0 f = -\mathrm{d}^2 f/\mathrm{d}x^2$, subject to Neumann boundary conditions at a and b, [1]. 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, [2]. Ambarzumyan's theorem has recently been extended to trees with a finite number of edges, [4], [16], [14], by combining the Sturm–Liouville theory with a careful boundary value analysis. It was also extended to compact symmetric spaces many years ago by Harrell [12], citing even earlier work by Guillemin and Weinstein. The present paper extends it to a much broader context by adapting a range of standard techniques from the theory of the heat equation in several dimensions. Theorem 3.3 establishes that if $\mu_1 \geqslant 0$ and $\limsup_{n\to\infty}(\mu_n - \lambda_n) \leqslant 0$ then $V = 0$, subject to certain generic conditions on the heat kernels involved.

We apply our general theorem to arbitrary compact Riemannian manifolds in Theorem 3.5, to compact quantum graphs in Section 4 and to finite combinatorial graphs in Example 3.4, 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.

In Sections 1 and 2 we prove some general facts about heat kernels, and the reader may prefer to start in Section 3. In Section 4 we prove that all of the hypotheses hold for a finite connected quantum graph X, subject to Kirchhoff boundary conditions at every vertex.

1. PROPERTIES OF H_0

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

(H1): The operator $\mathrm{e}^{-H_0 t}$ 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 $0 \leqslant K_0(t,x,x) \leqslant ct^{-d/2}$ 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 λ_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 3.4. The case of the Laplace–Beltrami operator on a compact Riemannian manifold is discussed in Theorem 3.5. 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 $\mathrm{Quad}(H_0) = \mathrm{Dom}(H_0^{1/2})$ by

$$Q_0(f) = \langle H_0^{1/2} f, H_0^{1/2} f\rangle$$

is a Dirichlet form; see Theorem 1.3.2 of [6]. The one-parameter semigroup $T_t = \mathrm{e}^{-H_0 t}$ on $L^2(X,\mathrm{d}x)$ is an irreducible symmetric Markov semigroup. It extends to a one-parameter contraction semigroup on $L^p(X,\mathrm{d}x)$ for all $1 \leqslant p \leqslant \infty$, with the proviso that for $p = \infty$ the semigroup is not strongly continuous; see Proposition 1.4.3 of [6]. Mercer's theorem ([9], Proposition 5.6.9) implies that the operator $\mathrm{e}^{-H_0 t}$ is trace class for all $t > 0$ and

$$\mathrm{tr}[\mathrm{e}^{-H_0 t}] = \int_X K_0(t,x,x)\,\mathrm{d}x.$$

In particular

$$\sum_{n=1}^{\infty} \mathrm{e}^{-\lambda_n t} < \infty$$

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 ϕ_n are the corresponding normalized eigenfunctions then by applying the formula

$$\mathrm{e}^{-\lambda_n t}\phi_n(x) = \int_X K_0(t,x,y)\phi_n(y)\,\mathrm{d}y$$

we deduce that every eigenfunction ϕ_n is bounded and continuous on X. The semigroup T_t is ultracontractive in the sense of Section 2.1 in [6] and the series

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

converges uniformly on $[\alpha,\infty) \times X \times X$ for every $\alpha > 0$; see Theorem 2.1.4 of [6]. This implies that $K_0(t,x,y)$ converges uniformly to $|X|^{-1}$ on $X \times X$ as $t \to \infty$, so

$$\frac{1}{2|X|} \leqslant K_0(t,x,y) \leqslant \frac{3}{2|X|} \tag{1.1}$$

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 1.1. *Let H be a self-adjoint operator acting in $L^2(X,\mathrm{d}x)$. If H is bounded below and e^{-Ht} is positivity preserving for all $t \geqslant 0$ then the following are equivalent, the constant $d > 0$ being the same in all cases.*

(i) *The operator e^{-Ht} satisfies*

$$\|\mathrm{e}^{-Ht}f\|_\infty \leqslant c_1 t^{-d/4}\|f\|_2$$

for some $c_1 > 0$, all $f \in L^2(X,\mathrm{d}x)$ and all $t \in (0,1)$.

(ii) *The bound*

$$\int_X f^2\log(f)\mathrm{d}x \leqslant \varepsilon Q(f) + \beta(\varepsilon)\|f\|_2^2 + \|f\|_2^2\log(\|f\|_2)$$

holds for all $0 \leqslant f \in \mathrm{Quad}(H) \cap L^1 \cap L^\infty$ and all $\varepsilon \in (0,1)$, where $\beta(\varepsilon) = c_2 - (d/4)\log(\varepsilon)$ for some $c_2 > 0$; see Example 2.3.3 *of* [6].

(iii) *The bound*

$$\|f\|_2^{2+4/d} \leqslant c_3(Q(f) + \|f\|_2^2)\|f\|_1^{4/d}$$

holds for some $c_3 > 0$ *and all* $0 \leqslant f \in \mathrm{Quad}(H) \cap L^1$*; see Corollary* 2.4.7 *of* [6].

(iv) *Assuming* $d > 2$, *the bound*

$$\|f\|_{2d/(d-2)}^2 \leqslant c_4(Q(f) + \|f\|_2^2)$$

holds for some $c_4 > 0$ *and all* $f \in \mathrm{Quad}(H)$*; see Corollary* 2.4.3 *of* [6].

All of the above conditions imply that e^{-Ht} *has a measurable heat kernel* K *that satisfies*

$$0 \leqslant K(t,x,y) \leqslant c_5 t^{-d/2} \tag{1.2}$$

for some $c_5 > 0$, *almost all* $x, y \in X$ *and all* $t \in (0,1)$. *Conversely, if* $\|\mathrm{e}^{-Ht}\|_{L^\infty \to L^\infty} \leqslant c_6$ *for all* $t \in (0,1)$ *then* (1.2) *implies the previous conditions; see Lemma* 2.1.2 *of* [6].

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 1.2. Let $H_0 = -\mathrm{d}^2/\mathrm{d}x^2$ act in $L^2((0,\infty), \mathrm{d}x)$ subject to Neumann boundary conditions at 0. Then

$$K_0(t,x,y) = (4\pi t)^{-1/2}(\mathrm{e}^{-(x-y)^2/(4t)} + \mathrm{e}^{-(x+y)^2/(4t)})$$

so

$$0 \leqslant K_0(t,x,y) \leqslant 2(4\pi t)^{-1/2}$$

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 2^r where $0 \leqslant r \leqslant n$. A related result for general convex sets is given in Theorem 12 of [7].

2. 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, measurable, real-valued potential; this condition can surely be weakened. An application of the Trotter product formula or a perturbation expansion imply that

$$\|\mathrm{e}^{-Ht}\|_{L^p \to L^p} \leqslant \mathrm{e}^{\|V\|_\infty t}$$

for all $p \in [1,\infty]$ and $t \geqslant 0$. 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

$$\lambda_n - \|V\|_\infty \leqslant \mu_n \leqslant \lambda_n + \|V\|_\infty$$

for all $n \geqslant 1$. Hence

$$0 \leqslant \mathrm{e}^{-\|V\|_\infty t} \mathrm{tr}[\mathrm{e}^{-H_0 t}] \leqslant \mathrm{tr}[\mathrm{e}^{-Ht}] \leqslant \mathrm{e}^{\|V\|_\infty t} \mathrm{tr}[\mathrm{e}^{-H_0 t}]$$

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

$$0 \leqslant \mathrm{e}^{-\|V\|_\infty t} K_0(t,x,y) \leqslant K(t,x,y) \leqslant \mathrm{e}^{\|V\|_\infty t} K_0(t,x,y) \tag{2.1}$$

for all $t > 0$. *The smallest eigenvalue* μ_1 *of* H *has multiplicity* 1.

Proof. We will assume throughout the proof that $0 < t < 1$; once (2.1) has been proved in this case it can be extended to larger t by using the semigroup property. Since the quadratic form

$$Q(f) = Q_0(f) + \int_X V(x)|f(x)|^2 \,\mathrm{d}x$$

is a Dirichlet form in the sense of Theorem 1.3.2 of [6], the operators e^{-Ht} are all positivity preserving. The quadratic forms of H_0 and H are comparable, so we may use Proposition 1.1 to deduce that for every $t \in (0,1)$ there is a bounded, measurable integral kernel $K(t,x,y)$ satisfying $0 \leqslant K(t,x,y) \leqslant ct^{-d/2}$ if $0 < t < 1$ and

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

for all $f \in L^2$. Since

$$\mathrm{e}^{-Ht} = \mathrm{e}^{-H\varepsilon} \mathrm{e}^{-H(t-2\varepsilon)} \mathrm{e}^{-H\varepsilon}$$

for all $\varepsilon > 0$ and $t > 2\varepsilon$, we can use the norm analyticity of $\mathrm{e}^{-H(t-2\varepsilon)}$ in L^2 to deduce the norm analyticity of e^{-Ht} from L^1 to L^∞. 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 (2.1) are now direct applications of the Trotter product formula. (1.1) and (2.1) together imply that the operator $A = \mathrm{e}^{-Ht}$ is irreducible for all large enough $t > 0$. Therefore its largest eigenvalue has multiplicity 1 by a direct application of Theorem 13.3.6 of [9] to $A/\|A\|$.

The operator e^{-Ht} has an operator norm convergent infinite series expansion involving $\mathrm{e}^{-H_0 t}$ and V, but we will use the more compact expression

$$\mathrm{e}^{-Ht} = \mathrm{e}^{-H_0 t} - A(t) + B(t) \tag{2.2}$$

where

$$A(t) = \int_{s=0}^{t} \mathrm{e}^{-H_0(t-s)} V \mathrm{e}^{-H_0 s}\, \mathrm{d}s, \quad B(t) = \int_{s=0}^{t} \int_{u=0}^{s} \mathrm{e}^{-H_0(t-s)} V \mathrm{e}^{-H(s-u)} V \mathrm{e}^{-H_0 u}\, \mathrm{d}u\mathrm{d}s.$$

The integrands are norm continuous in $\{s : 0 < s < t\}$, respectively $\{(s,u) : 0 < u < s < t\}$, 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 (2.2) has a version involving integral kernels, namely

$$K(t,x,y) = K_0(t,x,y) - L(t,x,y) + M(t,x,y) \tag{2.3}$$

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

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

and we will prove that

$$|M(t,x,y)| \leqslant c t^{2-d/2} \tag{2.4}$$

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 (2.3) 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 $\mathcal{B} = C(X \times X)$.

The integral kernel of $A(t)$ is

$$L(t,x,y) = \int_{s=0}^{t} L_{s,t}(x,y)\, \mathrm{d}s \tag{2.5}$$

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

$$L_{s,t}(x,y) = \int_X K_0(t-s,x,z) V(z) K_0(s,z,y)\, \mathrm{d}z.$$

Now $L_{s,t} \in \mathcal{B}$ 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 (2.5) is norm convergent in $\mathcal{B}$. This follows from

$$\begin{aligned} \int_{s=0}^{t} \|L_{s,t}\|_\infty\, \mathrm{d}s &\leqslant \|V\|_\infty \int_{s=0}^{t} \sup_{x,y} \Big\{ \int_X K_0(t-s,x,z) K_0(s,z,y)\, \mathrm{d}z \Big\} \mathrm{d}s \\ &= \|V\|_\infty \int_{s=0}^{t} \sup_{x,y} \{K_0(t,x,y)\}\, \mathrm{d}s \leqslant c \|V\|_\infty t^{1-d/2} \end{aligned}$$

provided $0 < t < 1$.

The integral kernel of $B(t)$ is

$$M(t,x,y) = \int_{s=0}^{t} \int_{u=0}^{s} M_{u,s,t}(x,y)\, \mathrm{d}u \mathrm{d}s \tag{2.6}$$

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

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

Without assuming that $K(s-u,z,w)$ is continuous in z,w, one sees by (2.1) that $M_{u,s,t} \in \mathcal{B}$ 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 (2.6) is norm convergent in $\mathcal{B}$. We have

$$\|M_{u,s,t}\|_\infty \leqslant \|V\|_\infty^2 \|N_{u,s,t}\|_\infty$$

where

$$\begin{aligned} N_{u,s,t}(x,y) &= \int_{X^2} K_0(t-s,x,z)K(s-u,z,w)K_0(u,w,y)\, \mathrm{d}w\mathrm{d}z \\ &\leqslant \mathrm{e}^{\|V\|_\infty t} \int_{X^2} K_0(t-s,x,z)K_0(s-u,z,w)K_0(u,w,y)\, \mathrm{d}w\mathrm{d}z \\ &= \mathrm{e}^{\|V\|_\infty t} K_0(t,x,y) \leqslant \mathrm{e}^{\|V\|_\infty} c t^{-d/2}, \end{aligned}$$

provided $0 < t < 1$. Therefore

$$\int_{s=0}^{t} \int_{u=0}^{s} \|M_{u,s,t}\|_\infty \, \mathrm{d}u\mathrm{d}s \leqslant b t^{2-d/2}$$

where b depends on $\|V\|_\infty$. ∎

COROLLARY 2.2. *One has*

$$\mathrm{tr}[\mathrm{e}^{-Ht}] = \mathrm{tr}[\mathrm{e}^{-H_0 t}] - t \int_X K_0(t,x,x)V(x)\, \mathrm{d}x + \rho(t) \tag{2.7}$$

where $\rho(t) = O(t^{2-d/2})$ *as* $t \to 0$.

Proof. One puts $x = y$ in (2.3) and integrates with respect to x. The bound on $\rho(t)$ follows from (2.4). ∎

3. 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, measurable 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 μ_1 has multiplicity 1; see Theorem 2.1. Our following theorem has something in common with Theorems 2.5, 3.4 of [17], which obtain a related result for Schrödinger operators in one and two dimensions subject to (3.1).

THEOREM 3.1. *If* $\mu_1 \geqslant 0$ *and*

$$\int_X V(x)\,\mathrm{d}x \leqslant 0 \tag{3.1}$$

then $V = 0$.

Proof. The variational estimate

$$\mu_1 \leqslant Q(\phi_1) = |X|^{-1} \int_X V(x)\,\mathrm{d}x \leqslant 0,$$

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. The variational formula

$$F(s) = \inf\{\langle (H + sV)\phi, \phi\rangle : \phi \in \mathrm{Dom}(H) \text{ and } \|\phi\| = 1\}$$

implies that F is concave, as the infimum of a family of linear functions; see Section 4.5 of [8]. Finally $F(0) = 0$ and

$$F'(0) = \langle V\phi_1, \phi_1\rangle = |X|^{-1} \int_X V(x)\,\mathrm{d}x \leqslant 0.$$

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 (3.1) implies that its negative part cannot vanish identically. Therefore there exists a function $\psi \in L^2(X, \mathrm{d}x)$ such that $\langle V\psi, \psi\rangle < 0$. An approximation argument allows us to assume that $\psi \in \mathrm{Quad}(H_0)$. 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 $V = 0$. ∎

The following is our main inverse spectral theorem.

THEOREM 3.2. *If* $\mu_1 \geqslant 0$ *and* $\limsup_{t\to 0} \sigma(t) \leqslant 0$ *where*

$$\sigma(t) = t^{d/2-1} \sum_{n=1}^{\infty} (\mathrm{e}^{-\lambda_n t} - \mathrm{e}^{-\mu_n t})$$

then $V = 0$.

Proof. We rewrite (2.7) in the form

$$t^{d/2}\int_X K_0(t,x,x)V(x)\mathrm{d}x = t^{d/2-1}\{\mathrm{tr}[\mathrm{e}^{-H_0 t}] - \mathrm{tr}[\mathrm{e}^{-Ht}]\} + t^{d/2-1}\rho(t) = \sigma(t) + t^{d/2-1}\rho(t)$$

and then take the limit of both sides as $t \to 0$. The left hand side converges to $a \int_X V(x)\,\mathrm{d}x$ where $a > 0$, by (H2) and (H3). We deduce that $\int_X V(x)\,\mathrm{d}x \leqslant 0$ and may therefore apply Theorem 3.1. ∎

The following corollary of Theorem 3.2 contains the original Ambarzumyan theorem as a special case.

THEOREM 3.3. *If* $\mu_1 \geqslant 0$ *and* $\limsup_{n\to\infty}(\mu_n - \lambda_n) \leqslant 0$ *then* $V = 0$.

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

$$\sigma(t) = \sigma_1(t) + \sigma_2(t)$$

where

$$\sigma_1(t) = t^{d/2-1}\sum_{n=1}^{N-1}(\mathrm{e}^{-\lambda_n t} - \mathrm{e}^{-\mu_n t}) \leqslant t^{d/2}\sum_{n=1}^{N-1}|\lambda_n - \mu_n|,$$

and

$$\begin{aligned}\sigma_2(t) &= t^{d/2-1}\sum_{n=N}^{\infty}(\mathrm{e}^{-\lambda_n t} - \mathrm{e}^{-\mu_n t}) \leqslant t^{d/2-1}\sum_{n=N}^{\infty}(\mathrm{e}^{-\lambda_n t}(1-\mathrm{e}^{-\varepsilon t}))\\ &\leqslant \varepsilon t^{d/2}\sum_{n=1}^{\infty}\mathrm{e}^{-\lambda_n t} \leqslant c\varepsilon\end{aligned}$$

for all $t \in (0,1)$, by an application of (H2). We conclude that $\limsup_{t\to 0}\sigma(t) \leqslant c\varepsilon$ for all $\varepsilon > 0$, and may therefore apply Theorem 3.2. ∎

EXAMPLE 3.4. 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

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

The relevant conditions on the eigenvalues in this case are

$$\mu_1 \geqslant 0 \quad \text{and} \quad \sum_{r=1}^{n}\mu_r \leqslant \sum_{r=1}^{n}\lambda_r.$$

However the analysis of the function F in Theorem 3.1 requires the assumptions (H1) and (H4), and the use of the theory of irreducible symmetric Markov semi-groups.

THEOREM 3.5. *The hypotheses* (H1) *to* (H4) *and therefore the conclusions of Theorems* 3.2 *and* 3.3 *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 ∂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), [7]. The precise heat kernel asymptotics required in (H3) holds for all $x \notin \partial X$, 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], [15]. One only obtains a complete asymptotic expansion if the potential is smooth, but we only need the second coefficient in the full heat expansion, which is known to satisfy

$$a_1(g,V) = a_1(g,0) - \int_X V \,\mathrm{d}x.$$

See [11]. In this context the nature of the boundary is irrelevant by the principle of "not feeling the boundary"; see Theorem 4.3 and [13]. ∎

4. COMPACT QUANTUM GRAPHS

In this section we prove that Theorems 3.2 and 3.3 are applicable when X is a compact 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 $\mathcal{V}$, and we assume that the graph as a whole is connected. The operator H_0 acts in $L^2(X, \mathrm{d}x)$ by the formula $H_0 f(x) = -\mathrm{d}^2 f/\mathrm{d}x^2$, 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

$$Q_0(f) = \int_X |f'(x)|^2 \,\mathrm{d}x$$

with domain $\mathrm{Quad}(H_0) = \mathrm{Dom}(H_0^{1/2}) = W^{1,2}(X)$ 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 $\mathrm{e}^{-H_0 t}$ are positivity preserving for all $t \geqslant 0$. The identity $H_0 1 = 0$ implies that $\mathrm{e}^{-H_0 t} 1 = 1$ for all $t \geqslant 0$, so $\mathrm{e}^{-H_0 t}$ is a symmetric Markov semigroup.

LEMMA 4.1. *The operator H_0 on $L^2(X, \mathrm{d}x)$ 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 to a quadratic form Q_1; this has the same formula as Q_0, but a larger domain, consisting of all functions $f \in L^2(X, \mathrm{d}x)$ such that the restriction of f to any edge e lies in $W^{1,2}(e)$. The operator H_1 acts independently in each $L^2(e, \mathrm{d}x)$ and its heat kernel in e is of the form

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

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

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

for some $c_1 > 0$, all $x, y \in e$ and all $0 < t < 1$. Moreover $K_e(t, x, y) \geqslant 0$ because Q_1 is a Dirichlet form. It follows from these observations that the various equivalent conditions of Proposition 1.1 hold for Q_1 with $d = 1$. Since Q_0 is a restriction of Q_1, Proposition 1.1 implies that

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

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 λ_n are the corresponding eigenvalues, then

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

Since the series

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

converges uniformly on $[\alpha, \infty) \times X \times X$ for every $\alpha > 0$ by Theorem 2.1.4 of [6], 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

$$0 = Q_0(\phi) = \int_X |\phi'(x)|^2 \, \mathrm{d}x.$$

This implies that ϕ is constant. Therefore 0 is an eigenvalue of multiplicity 1. ∎

Our final task is to prove (H3).

LEMMA 4.2. *Let $K_a(t, x, y)$ be the heat kernel of the operator $-\mathrm{d}^2/\mathrm{d}x^2$ acting in $L^2(-a, a)$ subject to Dirichlet boundary conditions at $\pm a$. Then*

$$0 \leqslant K_a(t, x, y) \leqslant K_\infty(t, x, y) = (4\pi t)^{-1/2} \mathrm{e}^{-|x-y|^2/(4t)} \tag{4.1}$$

for all $t>0$ and $x,y\in(-a,a)$. Moreover

$$1\geqslant\int_{-a}^{a}K_a(t,0,x)\,\mathrm{d}x\geqslant 1-4\mathrm{e}^{-a^2/(8t)} \tag{4.2}$$

and

$$(4\pi t)^{-1/2}\geqslant K_a(t,0,0)\geqslant(4\pi t)^{-1/2}(1-15\mathrm{e}^{-a^2/(4t)}) \tag{4.3}$$

for all $t>0$.

Proof. The inequality (4.1) follows directly from the monotonicity of the Dirichlet heat kernel as a function of the region. Sharper versions of the inequalities (4.2) and (4.3) may be proved by applying the Poisson summation formula to the explicit eigenfunction expansion of K_a, [18]. An alternative proof of (4.2) based on the properties of the underlying Brownian motion is given in Lemma 6.5 of [10].

One may prove (4.3) from (4.2) as follows. We define $f,g:\mathbb{R}\to(0,\infty)$ by

$$f(x)=\begin{cases}K_a(t,0,x) & \text{if } |x|\leqslant a,\\ 0 & \text{otherwise,}\end{cases}$$

$$g(x)=K_\infty(t,0,x)=(4\pi t)^{-1/2}\mathrm{e}^{-x^2/(4t)},$$

so that $0\leqslant f(x)\leqslant g(x)\leqslant(4\pi t)^{-1/2}$ for all $x\in\mathbb{R}$ and $\int_{\mathbb{R}} g(x)\,\mathrm{d}x=1$. Therefore

$$\begin{aligned}0&\leqslant(8\pi t)^{-1/2}-K_a(2t,0,0)=K_\infty(2t,0,0)-K_a(2t,0,0)\\&=\int_R\{g(x)^2-f(x)^2\}\,\mathrm{d}x\leqslant\int_R\{g(x)-f(x)\}2g(x)\,\mathrm{d}x\\&\leqslant(\pi t)^{-1/2}\int_R\{g(x)-f(x)\}\,\mathrm{d}x=(\pi t)^{-1/2}\Big(1-\int_{-a}^{a}f(x)\,\mathrm{d}x\Big)\\&\leqslant(\pi t)^{-1/2}4\mathrm{e}^{-a^2/(8t)},\end{aligned}$$

by (H2). We finally obtain (4.3) upon replacing t by $t/2$. ∎

We prove (H3) by using the principle of "not feeling the boundary", [13].

THEOREM 4.3. *The operator H_0 on $L^2(X,\mathrm{d}x)$ satisfies* (H3)*, the exceptional set N being the set of all vertices on X.*

Proof. This repeats the argument used to prove (4.3). 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:

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

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 $0 \leqslant K_0(t,x,y) \leqslant ct^{-1/2}$ for all $0 < t < 1$ and all $x, y \in X$. Finally

$$\int_X K_0(t,x,y)\,\mathrm{d}y = 1$$

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 $0 \leqslant f(x) \leqslant g(x)$ for all $x \in X$. We have

$$0 \leqslant \int_X \{g(x) - f(x)\}\,\mathrm{d}x = 1 - \int_I K_a(t,z,x)\,\mathrm{d}x \leqslant 4\mathrm{e}^{-a^2/(8t)}$$

by (4.2). Therefore

$$\begin{aligned} K_0(2t,z,z) - K_a(2t,z,z) &= \int_X \{g(x)^2 - f(x)^2\}\,\mathrm{d}x \\ &\leqslant \int_X \{g(x) - f(x)\}2g(x)\,\mathrm{d}x \\ &\leqslant c_1 t^{-1/2}\mathrm{e}^{-a^2/(8t)}. \end{aligned}$$

The theorem follows by combining this with (4.3). ∎

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