Index theorems for quantum graphs

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Abstract. In geometric analysis, an index theorem relates the difference of the numbers of solutions of two differential equations to the topological structure of the manifold or bundle concerned, sometimes using the heat kernels of two higher-order differential operators as an intermediary. In this paper, the case of quantum graphs is addressed. A quantum graph is a graph considered as a (singular) one-dimensional variety and equipped with a second-order differential Hamiltonian H (a "Laplacian") with suitable conditions at vertices. For the case of scale-invariant vertex conditions (i.e., conditions that do not mix the values of functions and of their derivatives), the constant term of the heat-kernel expansion is shown to be proportional to the trace of the internal scattering matrix of the graph. This observation is placed into the index-theory context by factoring the Laplacian into two first-order operators, $H = A^*A$, and relating the constant term to the index of A. An independent consideration provides an index formula for any differential operator on a finite quantum graph in terms of the vertex conditions. It is found also that the algebraic multiplicity of 0 as a root of the secular determinant of H is the sum of the nullities of A and A^*.

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1. Introduction

A *quantum graph* Γ is a graph (with multiple edges and loops allowed) in which each edge e is assigned a coordinate x (and hence a length) and the whole graph is equipped with a self-adjoint differential operator as Hamiltonian. For instance, if Γ is embedded nicely into a Riemannian manifold, one can use the arc length as a coordinate along an edge. In geometric language, Γ is a one-dimensional CW-complex with a Riemannian metric on each 1-cell and appropriate boundary conditions at each 0-cell to define a self-adjoint "Laplacian". We refer to [8, 12, 14, 15] for further background on quantum graphs.

Here we consider only graphs that are *compact*: the number of vertices V, the number of edges E, and the lengths of all edges are assumed to be finite. The number of edges attached to vertex v is called the *degree* of v and denoted d_v. We also assume that every vertex has at least one edge attached, since isolated vertices are negligible in the quantum graph context.

The simplest Hamiltonian for a quantum graph is the *Laplacian* with *Kirchhoff boundary conditions*, which acts as the negative second derivative along each edge,

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x_e^2}\,,$$

with the functions in its domain required to be continuous at the vertices and to satisfy the Kirchhoff condition of no net flux at each vertex:

$$\sum_{e\in E_v} \frac{\mathrm{d}f}{\mathrm{d}x_e}(v) = 0.$$

Here E_v is the set of edges incident on vertex v, and x_e is the arc-length coordinate on e outgoing from v (in other words, the distance from v of the variable point on e). For more precise definitions see [12, 15] and section 3 below.

In one of the earliest papers on quantum graphs [18], J.-P. Roth calculated the trace of the heat kernel K for the operator just described. He found an exact formula

$$\sum_{n=0}^{\infty} \mathrm{e}^{-\lambda_n t} = \operatorname{Tr} K = \int_\Gamma K(t,x,x)\,\mathrm{d}x = K_1 + K_2 + K_3\,, \tag{1}$$

where λ_n are the eigenvalues of H. Written in detail, it contains (before the integration) one term for every path in the graph Γ leading from the point x (not a vertex) to itself. These closed paths fall into three classes: The path of zero length yields the term $K_1 = L/\sqrt{4\pi t}$, the anticipated leading term in the Weyl series, where L is the total length of all edges of the graph. K_2 is the sum of the contributions of the periodic paths (where the initial and final direction of the path are the same), which are proportional to $\mathrm{e}^{-L(C)^2/4t}$, where $L(C)$ is the length of the path C. (Such terms do not contribute to the asymptotic expansion for $t \to 0$ of $\operatorname{Tr} K$ in powers of t, but they determine oscillations in the distribution of the eigenvalues $\{\lambda_n\}$.) Finally, the contributions of paths that are *closed but not periodic* (i.e., the initial and final directions are opposite) sum to the

simple form

$$K_3 = \tfrac{1}{2}(V - E), \tag{2}$$

which constitutes the entire remainder of the Weyl series for the heat kernel trace. Note that K_3 is independent of t and moreover is the *only* constant term in the formula (1).

The expression in Equation (2) is interesting because it is a half-integer and depends on the topology of Γ only (e.g., it is independent of the edge lengths). Indeed, it is the Euler characteristic of Γ regarded as a 1-complex. These features are reminiscent of *index theorems* in geometric analysis and the calculation of indexes from the constant terms in heat-kernel expansions [6, 7]. The original goal of this paper was to give an index interpretation of (2); in fact, we also generalize it to graphs with other boundary conditions and compute indexes of quite general quantum graph operators by another, very simple method.

The contents of the paper are as follows: Section 2 reviews the appearance of indexes in the heat kernel asymptotics for the case of an interval. In section 3 we introduce necessary notions and auxiliary results concerning quantum graphs. The section also contains a general formula for indexes of differential operators on quantum graphs. Section 4 contains the main results concerning the relations between the constant terms in the asymptotic expansion of the heat kernel and indexes of suitable operators on the graph. Relations to the secular determinant are discussed in section 5. The final section 6 contains some remarks and conclusions.

2. The interval

In [7, Section 1.5] P. Gilkey treats the Laplacian on an interval with Dirichlet and with Neumann boundary conditions as the prototype of the index theorem for the de Rham complex on a manifold with boundary. The index theorem for a quantum graph with Kirchhoff boundary conditions is a different generalization of this elementary example, so we shall review the latter.

Let H_D and H_N be the operator $-\mathrm{d}^2/\mathrm{d}x^2$ on the interval $(0, L)$ with Dirichlet and Neumann boundary conditions, respectively. The eigenfunctions of H_N with eigenvalue 0 are the constant functions, so the kernel of H_N has dimension 1. In contrast, H_D has trivial kernel. On the other hand [7, Subsection 3.1.3], the heat traces of these operators are

$$\operatorname{Tr} \mathrm{e}^{-tH_{D,N}} = \int_0^L K_{D,N}(t, x, x)\,\mathrm{d}x \underset{t\to 0}{\sim} \frac{L}{\sqrt{4\pi t}} \mp \frac{1}{2}\,, \tag{3}$$

where the negative sign applies to the Dirichlet case and the exponentially small terms analogous to K_2 in (1) have been omitted. Therefore,

$$\dim\ker H_N - \dim\ker H_D = 1 = \operatorname{Tr} K_N - \operatorname{Tr} K_D\,. \tag{4}$$

To identify (4) as an index theorem we must factor $H_{D,N}$ into first-order operators. Let A be the operator $\mathrm{d}/\mathrm{d}x$ acting on the domain $H^1(0, L)$, which is the Sobolev space

containing functions on $(0, L)$ that, together with their first distributional derivatives, are square-integrable. Standard integrations by parts show that the adjoint operator A^* is $-\mathrm{d}/\mathrm{d}x$ with domain $H_0^1(0, L)$ (containing functions from $H^1(0, L)$ that satisfy the Dirichlet conditions $f(0) = f(L) = 0$) and that $A^{**} = A$. One now forms two second order operators

$$H_N = A^*A, \qquad H_D = AA^*, \tag{5}$$

where in the first case the domain consists of twice differentiable ($H^2(0, L)$) functions satisfying the Neumann conditions, $f'(0) = f'(L) = 0$, so that $Af \in \operatorname{dom} A^*$ and the composition is defined; in the second case, similarly, the domain consists of functions from $H^2(0, L)$ satisfying the Dirichlet conditions.

Because $\langle f, A^*Af\rangle = \langle Af, Af\rangle = \|Af\|^2$, the kernel of A is the same as that of H_N. Similarly, $\ker A^* = \ker H_D$. Therefore, (4) can be restated as the index formula

$$\operatorname{index} A = \operatorname{Tr} K_N - \operatorname{Tr} K_D = 1. \tag{6}$$

Remark 1. By regarding the elements of $\operatorname{dom} A^*$ as 1-forms rather than scalar functions, one identifies A and A^* with the exterior derivative operator $\mathrm{d}\colon \Lambda^0(0, L) \to \Lambda^1(0, L)$ and its adjoint $\delta\colon \Lambda^1(0, L) \to \Lambda^0(0, L)$, where $\Lambda^0(0, L)$ and $\Lambda^1(0, L)$ are the spaces of L^2 functions $f(x)$ and 1-forms $g(x)\,dx$. One can combine these operators into a single operator from $\Lambda^0(0, L) \oplus \Lambda^1(0, L)$ into itself,

$$\mathrm{d} + \delta = \begin{pmatrix} 0 & \delta \\ \mathrm{d} & 0 \end{pmatrix},$$

where, in the version on the left, d annihilates the 1-forms and δ annihilates functions. Then the Hodge Laplacian is

$$(\mathrm{d} + \delta)^2 = \delta\mathrm{d} + \mathrm{d}\delta = \begin{pmatrix} H_N & 0 \\ 0 & H_D \end{pmatrix}.$$

It is this formulation that generalizes to higher-dimensional manifolds, with H_N acting on forms of even degree and H_D on forms of odd degree (or vice versa) [6, 7].

In the following sections we will extend this analysis to more general quantum graphs. In particular, a central task is to identify the analogues of the operators A and A^*.

3. Quantum graphs

3.1. Vertex conditions

As we have mentioned in section 1, appropriate vertex conditions are needed in order to turn the (negative) second derivative along the edges of a quantum graph into a self-adjoint operator in $L^2(\Gamma)$. All such choices of boundary conditions at vertices were catalogued in [12] (after prior discussion in [4]) and reformulated in [9, 15]. It will be convenient for us to follow the formulation from [15].

Let v be a vertex and $f(x)$ a function on Γ. We denote by

$$F(v) = \begin{pmatrix} f_1(v) \\ \vdots \\ f_{d_v}(v) \end{pmatrix}$$

the vector of values of the function f at the vertex v, attained along d_v edges incident to v. In particular, if f were continuous, all these values would be equal. Analogously,

$$F'(v) = \begin{pmatrix} f_1'(v) \\ \vdots \\ f_{d_v}'(v) \end{pmatrix}$$

is the vector of derivatives at v of f along these edges, where the derivatives are taken in the directions outgoing from the vertex v.

It is clear that vertex conditions for the second-derivative operator can involve only the values of the function and of its derivatives along edges. If these conditions do not mix the values attained at different vertices, they are called *local*. (On an interval, for instance, Dirichlet, Neumann, and Robin conditions are local, but the periodicity condition is nonlocal.) As we will see later, there is actually not much difference between local and nonlocal vertex conditions on a quantum graph. (For instance, the periodicity condition becomes local if the interval is replaced by a loop attached to a single vertex.)

Theorem 2. [15] *All self-adjoint realizations H of the negative second derivative on Γ with local vertex boundary conditions can be described as follows: For every vertex v, of degree d_v, there are two orthogonal (and mutually orthogonal) projectors P_v, Q_v operating in $\mathbb{C}^{d_v}$ and an invertible self-adjoint operator Λ_v operating in the subspace $(1 - P_v - Q_v)\mathbb{C}^{d_v}$. (Either P_v, Q_v, or $C_v \equiv 1 - P_v - Q_v$ might be zero.) The functions f in the operator domain are those members of the Sobolev space $\bigoplus_e H^2(e)$ that satisfy at each vertex v boundary conditions consisting of the "Dirichlet part"*

$$P_v F(v) = 0, \tag{7}$$

the "Neumann part"

$$Q_v F'(v) = 0, \tag{8}$$

and the "Robin part"

$$C_v F'(v) = \Lambda_v C_v F(v). \tag{9}$$

The quadratic form of H is

$$h[f,f] = \sum_{e\in E} \int_e \left|\frac{df}{dx}\right|^2 dx + \sum_{v\in V} (\Lambda_v C_v F, C_v F) \tag{10}$$

with the domain that consists of the functions $f(x)$ that belong to the Sobolev space $H^1(e)$ on each edge e and satisfy (7) at each vertex.

Remark 3. This theorem was formulated a little bit differently in [15]. For one thing, Λ_v was called $-L_v$ there. More importantly, there the two projectors Q_v and C_v where lumped into a single one, and thus the condition of invertibility of the operator Λ_v disappeared. The equivalent formulation provided here distinguishes between Robin and pure Neumann conditions, as is often convenient.

Remark 4. The three parts (7)–(9) of the vertex conditions can be combined into a single condition

$$A_v F(v) + B_v F'(v) = 0, \tag{11}$$

where the $d_v \times d_v$ matrices A_v and B_v are

$$A_v = P_v - \Lambda_v C_v, \quad B_v = Q_v + C_v\,. \tag{12}$$

The conditions were introduced in [12] in the form (11) (which by itself does not suffice to define the matrices A_v and B_v uniquely, however).

The most popular vertex conditions are the *Kirchhoff* ones (also called *Neumann* or *natural*), which reduce at vertices of degree 1 to Neumann conditions:

Definition 5. *The* Kirchhoff *boundary conditions are defined by the continuity condition*

$$f_1(v) = f_2(v) = \cdots = f_{d_v}(v) \equiv f(v) \tag{13a}$$

as Dirichlet part and the zero flux condition

$$\sum_{e=1}^{d_v} f_e'(v) = 0 \tag{13b}$$

as Neumann part, with no Robin part.

In other words, $(1 - P_v)\mathbb{C}^{d_v}$ is in this case one-dimensional and consists of the vectors with equal coordinates.

Another type of conditions that arises in our work is dual to the Kirchhoff type, in the sense that the roles of the values and derivatives of the function f at each vertex are switched. (At vertices of degree 1 these "anti-Kirchhoff" conditions reduce to the Dirichlet ones.)

Definition 6. *The* anti-Kirchhoff *boundary conditions are*

$$\sum_{e=1}^{d_v} f_e(v) = 0 \tag{14a}$$

as Dirichlet part and

$$f_1'(v) = f_2'(v) = \cdots = f_{d_v}'(v) \equiv f'(v) \tag{14b}$$

as Neumann part, with no Robin part.

3.2. Bonds vs edges

In what follows, we will need to use directed edges (which we will call *bonds*) rather than the undirected ones as before. Thus, each edge results in *two* directed bonds (with opposite directions), which are denoted by Greek letters. We denote by $\overline{\alpha}$ the bond α with its direction reversed.

Recall that loops (tadpoles) can always be removed from a quantum graph by inserting extra Kirchhoff vertices of degree 2. Adding such a vertex does not change the heat trace or the Euler characteristic, nor either side of any of the index formulas in this paper. Therefore, one may assume that the two ends of a bond are distinct vertices.

It is not necessary to pick either of the two directions of an edge as the canonical one. The language of differential forms makes it possible to give global meaning to the differential of a function on Γ without committing to any particular coordinate, x_e, on each edge. In discussing the behavior of functions (and their derivatives) in the neighborhood of any one vertex, therefore, we remain free to use the most convenient coordinate on each edge, namely, the outgoing arc length parameter.

3.3. Scattering matrices

In this subsection we introduce, following [12, 14], the scattering matrices and some of their properties that we will need in the rest of the text.

Let H be a self-adjoint realization of the negative second derivative $-\mathrm{d}^2/\mathrm{d}x^2$ on a finite quantum graph Γ (i.e., one of the self-adjoint vertex conditions described in Theorem 2 is imposed).

Let us consider a vertex v and the set E_v of all edges e incident to it. (Such a configuration is called a *star*; see Fig. 1.) For any edge $e_0 \in E_v$ and any real k, we

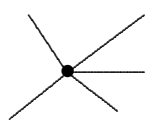

Figure 1. A star.

choose as in section 1 the coordinate x increasing away from the vertex and consider the unique solution $f(x)$ on the star E_v of the following scattering problem at v:

$$\begin{cases} -\dfrac{\mathrm{d}^2 f}{\mathrm{d}x^2} = k^2 f(x) \text{ on each edge } e \in E_v\,, \\ f(x) = e^{-ikx} + \sigma^{(v)}_{e_0 e_0} e^{ikx} \text{ on } e_0\,, \\ f(x) = \sigma^{(v)}_{e_0 e} e^{ikx} \text{ on } e \neq e_0\,, \\ \text{vertex conditions are satisfied at } v. \end{cases} \tag{15}$$

In other words, $\sigma^{(v)}_{e_0 e_0}$ is the reflection coefficient along the bond e_0, and $\sigma^{(v)}_{e_0 e}$ is the transmission coefficient from the edge e_0 to e. Notice that the coefficients $\sigma^{(v)}_{e_0 e}$ in general depend on k.

Definition 7. *The unitary $d_v \times d_v$ matrix $\sigma^{(v)}(k)$ with the entries $\sigma^{(v)}_{e_1 e_2}(k)$ for $e_j \in E_v$ is the* edge scattering matrix at the vertex v.

Notice that in defining $\sigma^{(v)}$ the direction chosen along each edge depends on the vertex considered. That is why it becomes necessary to deal with directed bonds when a scattering matrix S for the whole graph is defined. However, as explained in section 3.2, the ambiguity in x_e does not create any inconsistency in the notation. Another remark is that this matrix clearly depends upon what type of vertex conditions are imposed, and not every matrix function $\sigma^{(v)}(k)$ can necessarily be realized by one of the second-order differential Hamiltonians studied here.

It is straightforward to derive the formula [12]

$$\sigma^{(v)}(k) = -(A_v + ikB_v)^{-1}(A_v - ikB_v), \tag{16}$$

which in particular confirms that the matrix is unitary and shows that its k-dependence is tightly constrained. From (12) we get an alternative representation of σ:

$$\sigma^{(v)}(k) = P_v - Q_v + (\Lambda_v - ik)^{-1}(\Lambda_v + ik)C_v\,. \tag{17}$$

The following result will be important for what follows. A part of it was proved by Kostrykin and Schrader ([11, Proposition 2.4]), [12, Corollary 2.3], [13, Theorem 1]).

Theorem 8. *The following conditions are equivalent:*

(i) For each vertex v, $\sigma^{(v)}$ is independent of k.

(ii) For each vertex v, there is a value $k \neq 0$ such that $(\sigma^{(v)})^2 = 1$.

(iii) For each vertex v, $(\sigma^{(v)})^2 = 1$ for all k.

(iv) For each vertex v, $\sigma^{(v)}$ has the form $1 - 2Q_v$ for some orthogonal projection Q_v.

(v) There is no Robin part in the vertex conditions: $C_v = 0$ for each vertex v.

(vi) The vertex conditions are scale-invariant *(i.e., if a function $f(x)$ on neighborhood of v in the star E_v satisfies the vertex conditions at v, then after rescaling to $f(rx)$, it still satisfies the conditions).*

(vii) The Hamiltonian $H = -\frac{d^2}{dx^2}$ with the given vertex conditions can be factored as $H = A^*A$, where $A = \frac{d}{dx}$ with appropriate vertex conditions, and A^* is its adjoint operator.

Proof. Equivalence of statements (i) through (iv) was proved by Kostrykin and Schrader; it also follows rather easily from (17).

Computing $(\sigma^{(v)})^2$ using (17), we get

$$(\sigma^{(v)})^2 = P_v + Q_v + \left(\frac{\Lambda_v + ik}{\Lambda_v - ik}\right)^2 C_v\,. \tag{18}$$

If $C_v \neq 0$, then in order to get $\sigma^2 = 1$, we need that $\left(\frac{\Lambda_v + ik}{\Lambda_v - ik}\right)^2 = 1$. A straightforward calculation shows that this is impossible for an invertible operator Λ and a non-zero k. This proves equivalence of (iii) and (v).

Equivalence of (v) and (vi) is trivial.

The implication (vii) $\Rightarrow$ (v) can be established as follows. The vertex conditions for A can involve only the values of the function, not its derivatives. Thus, at any vertex v they can be written as $P_v F(v) = 0$ for some orthogonal projector P_v. Then a simple and well known (e.g., [12]) calculation, which boils down to an integration by parts, shows that for the adjoint operator $-\frac{\mathrm{d}}{\mathrm{d}x}$, the vertex conditions are given by the complementary projector $Q_v = 1 - P_v$. The equality $H = A^*A$ now implies that the vertex conditions for H have P_v as the Dirichlet and Q_v as the Neumann part, with no Robin part being present. This argument can easily be reversed to show the converse implication, (v) $\Rightarrow$ (vii). □

Corollary 9. *The scattering matrices σ for the Hamiltonian $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with Kirchhoff or anti-Kirchhoff boundary conditions satisfy the equivalent conditions of Theorem 8.*

We now introduce the *global scattering matrix* $S_{\alpha\beta}$, entries of which are indexed by the directed bonds α and β.

Definition 10. *The* $2E \times 2E$ (global) scattering matrix S *is defined as follows:*

$$S_{\beta\alpha} = \begin{cases} \sigma^{(v)}_{\beta\alpha} \text{ if } \alpha \text{ terminates at } v \text{ and } \beta \text{ starts at } v, \\ 0 \text{ otherwise,} \end{cases} \tag{19}$$

where α and β are (directed) bonds in Γ.

Proposition 11. *Let H satisfy the equivalent conditions of Theorem 8, so that it factors as $H = A^*A$ as in (vii) of the theorem. Let also $H' \equiv AA^*$. We also denote by σ' and S' the scattering matrices for H'. Then*

$$\begin{aligned} \sigma^{(v)}_{\alpha\beta} &= -(\sigma')^{(v)}_{\alpha\beta}, \\ S_{\alpha\beta} &= -(S')_{\alpha\beta} \end{aligned} \tag{20}$$

for any vertex v and any bonds α, β.

Proof. Indeed, it is clear that for H' the projectors P_v and Q_v exchange their places, while $C_v = 0$. Then formulas (17) and (19) prove the statement. □

3.4. Indexes of quantum graph operators

As it happens, one can establish a simple formula for the index of any (elliptic) differential operator on a compact quantum graph Γ, which in particular implies the index formulas for the exterior-derivative operators A introduced previously.

First we need to review the basic notions concerning the Fredholm property and the index (see, e.g., [10]). Recall that the codimension of a (closed) subspace $E \subset H$ is defined as the dimension of the quotient space H/E, or, equivalently (in a Hilbert space), the dimension of an orthogonal complement of E.

Definition 12. *A bounded operator $T\colon H_1 \to H_2$ between two Hilbert (or Banach) spaces is said to be* Fredholm*, if it has a closed range and the dimension of its kernel* $\ker T$

and the codimension of its range $\operatorname{ran} T$ *are finite. The* index *of a Fredholm operator* T *is defined as*

$$\operatorname{index} T = \dim\ker T - \operatorname{codim}\operatorname{ran} T.$$

Proposition 13. *If operator* T *is Fredholm and operator* K *is compact (in particular, of finite rank), then* $T+K$ *is also Fredholm and* $\operatorname{index}(T+K) = \operatorname{index} T$.

To formulate the main theorem for a differential operator of arbitrary order it is convenient to choose an orientation for each edge, so that the arc length parameter x_e is unambiguous.

Theorem 14. *Consider the operator on* Γ *defined by the differential expression of order* m

$$T = \sum_{j=0}^{m} c_j(x_e)\,\frac{\mathrm{d}^{m-j}}{\mathrm{d}x_e^{m-j}} \tag{21}$$

with $c_0(x)$ *continuous on each closed edge (but not necessarily on the whole graph) and never equal to* 0 *and all other* c_j *measurable and bounded. Let* T_1 *be the restriction of* T *as an operator from* $\oplus_e H^m(e)$ *into* $L^2(\Gamma)$ *to a subspace of codimension* p *(e.g., by imposing* p *vertex conditions sustainable by* H^m*, i.e., involving derivatives up to the order* $m-1$*). Then*

(i) The operator so defined is Fredholm.

(ii)
$$\operatorname{index} T_1 = mE - p. \tag{22}$$

Proof. Consider T as the naturally defined (and obviously bounded) operator from $\oplus_e H^m(e)$ into $L^2(\Gamma)$. All terms in T that involve derivatives of order less than m are compact operators and thus do not influence the Fredholm property or the index. Thus, we can assume that $T = c_0(x_e)\frac{\mathrm{d}^m}{\mathrm{d}x_e^m}$. This is now the composition of $\frac{\mathrm{d}^m}{\mathrm{d}x_e^m}$ acting from $\oplus_e H^m(e)$ to $L^2(\Gamma)$ with the invertible operator of multiplication by $c_0(x)$ in $L^2(\Gamma)$. Thus, everything reduces to the mth derivative alone. It is easy to show that it is a surjective operator from $H^m(e)$ onto the whole $L^2(e)$ (and thus from $\oplus_e H^m(e)$ onto $L^2(\Gamma)$). On each edge, it has the m-dimensional kernel consisting of polynomials of degree less than m. Thus, T is Fredholm and

$$\operatorname{index} T = \sum_e (m-0) = mE.$$

Let us now notice that by definition, T_1 is the restriction of T onto a subspace M of codimension p. Consider any (p-dimensional) complement N to M in $\oplus_e H^m(e)$ and the extension $\tilde{T}$ of T_1 from M to the whole $\oplus_e H^m(e)$ that acts as the zero operator on N. Then the difference $T-\tilde{T}$ vanishes on M and thus is a finite-dimensional operator. Hence, $\tilde{T}$ is Fredholm of the same index mE as T.

On the other hand, it is clear that the ranges of $\tilde{T}$ and T_1 are the same and the kernel of $\tilde{T}$ is p dimensions larger than the kernel of T. Hence, T is Fredholm and $\operatorname{index} T = \operatorname{index}\tilde{T} - p = mE - p$. □

This implies in particular

Corollary 15. *Let A be the exterior derivative* d *acting as a bounded operator from a subspace M of codimension p in $\bigoplus_e H^1(e)$ into $L^2(\Gamma)$. This operator is Fredholm of index $E-p$. Therefore,*

$$\operatorname{index} A = E - p = E - \sum_v \dim P_v \,, \tag{23}$$

where P_v are the orthogonal projectors describing the vertex conditions for A. Thus, in particular,

(i) Without any vertex conditions, one has $\operatorname{index} A = E$.

(ii) With continuity conditions (13a) at all vertices, one has

$$\operatorname{index} A = E - \sum_v (d_v - 1) = E - (2E - V) = V - E.$$

(iii) With the condition (14a) that the sum of values at each vertex is equal to zero, one has

$$\operatorname{index} A = E - \sum_v 1 = E - V.$$

Notice that $\sum_v \dim P_v$ arising in this corollary is just the number of vertex conditions defining H that contain only the values of the function and no derivatives (Dirichlet part of the conditions).

4. Heat kernel and index

In this section we address the relation between the heat trace asymptotics and the index on quantum graphs. Most of the considerations are independent of Theorem 14.

We will assume from now on that Γ is an arbitrary quantum graph and the Hamiltonian H satisfies the conditions of the Theorem 8, so that it factors as $H = A^*A$, where $A = \mathrm{d}/\mathrm{d}x$ with some vertex conditions on the values of functions, such conditions corresponding at any vertex v to an orthogonal projector P_v in $\mathbf{C}^{d_v}$. Then, as before, we denote by H' the operator AA^* with the vertex conditions given by the orthogonal projector $Q_v = 1 - P_v$. Let also K and K' be the corresponding heat kernels. The following proposition is standard.

Proposition 16. *In the situation just described,*

$$\operatorname{index} A = \operatorname{Tr} K - \operatorname{Tr} K'. \tag{24}$$

Proof. The non-zero eigenvalues of $H = A^*A$ and $H' = AA^*$ are the same, including their multiplicity. The only exception is that the dimensions of the eigenspaces for the eigenvalue 0 are different. Thus, the difference of the heat kernel traces is guaranteed to be independent of t. At large t this difference reduces to the difference of the nullities (i.e., dimensions of the kernels), and at small t it reduces to the difference of the constant terms in the heat-kernel expansions. See, for instance, [6] for a more

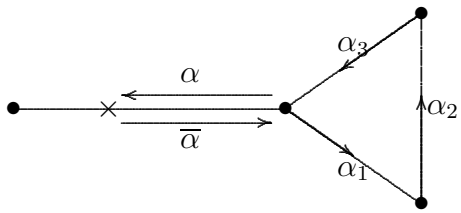

Figure 2. A bounce path $\alpha\alpha_3\alpha_2\alpha_1\overline{\alpha}$ with $n = 3$.

detailed exposition. Now, since the nullity of H is clearly equal to that of A, and that of H' coincides with that of A^*, one concludes that $\operatorname{Tr} K - \operatorname{Tr} K' = \dim\ker H - \dim\ker H' = \dim\ker A - \dim\ker A^* = \operatorname{index} A$. □

We now need to establish a formula for the constant term of a heat trace:

Theorem 17. [19, 1] *Let Γ be a finite quantum graph with scale-invariant vertex conditions defining the Laplacian. (Thus the bond-to-bond scattering matrix $S_{\alpha\beta}$ is independent of the frequency k). Let $K(t, x, y)$ be the corresponding heat kernel on Γ. Then the constant term in the asymptotic expansion at $t \to 0$ of the heat trace*

$$\sum_{n=0}^{\infty} \mathrm{e}^{-\lambda_n t} = \int_\Gamma K(t, x, x)\,\mathrm{d}x \tag{25}$$

is

$$\frac{1}{4}\sum_{\alpha} S_{\alpha\overline{\alpha}}\,. \tag{26}$$

(See Definition 10 for $S_{\alpha\beta}$.)

Sketch of proof. The theorem is proved in [1] for a different kernel, but as stressed in [19] the same argument applies to a whole class of kernels, including the heat kernel. (See also [18, 11].) Starting from the standard one-dimensional heat kernel on the real line,

$$K_0(t, x, 0) \equiv (4\pi t)^{-1/2} e^{-x^2/4t}, \tag{27}$$

by an extension of the method of images one constructs the heat kernel on the graph as a sum over all paths from y to x, which then needs to be restricted to the diagonal $y = x$. The heat trace is formed then by integrating over x. As in [18], the contributions of the periodic paths, i.e., the ones that return to the point x with the same direction as at the start, are proportional to Gaussian terms $e^{-L_{\mathbf{q}}^2/4t}$ and cannot contribute to the t-independent term of the heat-kernel expansion. The path of zero length gives the leading Weyl term, proportional to $t^{-1/2}$. The contribution of the other class of paths, which are closed but not periodic ("bounce" paths), $\alpha\mathbf{p}\overline{\alpha}$, where $\mathbf{p}$ is a cycle in Γ (see Fig. 2, where the triangle represents the cycle $\mathbf{p}$ and the point x is located on the bond α), can be reduced to the following sum:

$$\frac{1}{2}\sum_{n}\sum_{\mathbf{p}\in P_n}\sum_{\alpha} A_{\alpha\mathbf{p}\overline{\alpha}} \int_{l_{\mathbf{p}}}^{l_{\mathbf{p}}+2L_\alpha} K_0(t, x)\,dx. \tag{28}$$

(The condition of k-independence of the scattering matrix is used here.) We denote here by P_n the set of cycles of period (number of edges traversed, including multiplicity) n. E.g., in Fig. 2, the cycle $\mathbf{p} = \alpha_1\alpha_2\alpha_3$ has period 3. We also use here notations L_α for the length of the bond α and $l_\mathbf{p}$ for the metric length of the cycle $\mathbf{p}$ (e.g., $l_\mathbf{p} = L_{\alpha_1}+L_{\alpha_2}+L_{\alpha_3}$ in Fig. 2). The shorthand notation $A_{\alpha\mathbf{p}\overline{\alpha}}$ is used for the product of scattering amplitudes along the path

$$A_{\alpha\mathbf{p}\overline{\alpha}} = S_{\alpha,\alpha_n} S_{\alpha_n,\alpha_{n-1}} \cdots S_{\alpha_1,\overline{\alpha}}\,.$$

One can now make a sequence of reductions [19, 1]: The unipotency property, $\sigma^2 = 1$, of the scattering matrix (see Theorem 8) leads to

$$\sum_\alpha S_{\alpha,\alpha_n} S_{\alpha_n,\alpha_{n-1}} \cdots S_{\alpha_1,\overline{\alpha}} = \delta_{\alpha_1,\overline{\alpha}_n} S_{\alpha_n,\alpha_{n-1}} \cdots S_{\alpha_2,\alpha_1}\,.$$

This allows a massive inductive reduction of the sum (28), in the course of which one must also combine the α-dependent factors $\int_{l_\mathbf{p}}^{l_\mathbf{p}+2L_\alpha} K_0(t,x)\,dx$. One eventually arrives at the following representation of (28):

$$\frac{1}{2}\sum_\alpha S_{\alpha\overline{\alpha}} \int_0^\infty K_0(t,x)\,\mathrm{d}x. \tag{29}$$

From (29) and (27) one obtains (26) as the total contribution of all these "bounce" paths. This finishes the proof of Theorem 17. □

Example. It is well known (e.g., [14]) that at a Kirchhoff vertex of degree d_v the scattering matrix is

$$\sigma^{(v)}_{ef} = \frac{2}{d_v} - \delta_{ef}\,. \tag{30}$$

For an entirely Kirchhoff graph, therefore, we have

$$\frac{1}{4}\sum_\alpha S_{\alpha\overline{\alpha}} = \frac{1}{4}\sum_{v=1}^{V}\left(\frac{2}{d_v}-1\right)d_v = \frac{1}{2}V - \frac{1}{2}E, \tag{31}$$

since every edge is incident on two vertices. This reproduces Roth's formula (2). By a similar calculation, or by appealing to Proposition 11, one sees that in the case of a graph all of whose vertices are of the anti-Kirchhoff type, the resulting term is the negative of (31).

Proposition 18. *In the context of Proposition 16,* $\operatorname{Tr} K - \operatorname{Tr} K'$ *is equal to twice the constant term in the small-t expansion of* $\operatorname{Tr} K$.

Proof. Proposition 11 and Theorem 17 imply that the constant term in $\operatorname{Tr} K$ is the negative of that in $\operatorname{Tr} K'$. The proof of Proposition 16 shows that only these constant terms survive when the traces are subtracted. □

Corollary 19. *Under the conditions of Theorem 17 and Proposition 16, the following alternative representations hold for the index of A:*

$$\operatorname{index} A = \frac{1}{2}\sum_{\alpha} S_{\alpha\overline{\alpha}} = \operatorname{Tr} K - \operatorname{Tr} K' = E - \sum_{v} \dim P_v = E - p, \tag{32}$$

where $H = A^*A$ is the factorization of the Hamiltonian in accordance with (vii) in Theorem 8, K and K' are the heat kernels of H and A^*A, E is the number of undirected edges in Γ, P_v is the projector onto the Dirichlet part of the vertex conditions, and p is the total number of vertex conditions not involving derivatives. Furthermore, $\operatorname{Tr} K - \operatorname{Tr} K'$ can be read off from the asymptotics of a single heat kernel by virtue of Proposition 18.

Proof. The last two equalities are quoted from (23) for completeness. The rest of the corollary summarizes the results of this subsection. □

4.1. The Euler characteristic

We now look at the special situation of Kirchhoff conditions to see the implications of Corollaries 19 and 15 there.

It is convenient to consider first-order operators on quantum graphs as defined in terms of differential forms, rather than functions, introducing thus an analogue of the de Rham complex. Therefore, we henceforth identify A with $\mathrm{d}\colon \Lambda^0(\Gamma) \to \Lambda^1(\Gamma)$ and A^* with $\delta\colon \Lambda^1(\Gamma) \to \Lambda^0(\Gamma)$ (on appropriately restricted domains).

Theorem 20. *Let H_K and H_A be the Kirchhoff and anti-Kirchhoff Laplacians on a compact quantum graph Γ (acting in $\Lambda^0(\Gamma)$ and $\Lambda^1(\Gamma)$ respectively), K_K and K_A be the corresponding heat kernels, and d and $\delta = \mathrm{d}^*$ be the external derivative operators (with the domains defined by the continuity conditions for d and the sum of values equal to zero at each vertex for δ), so that*

$$H_K = \delta\mathrm{d} \quad \textit{and} \quad H_A = \mathrm{d}\delta. \tag{33}$$

Then

$$\operatorname{index} \mathrm{d} = \operatorname{Tr} K_K - \operatorname{Tr} K_A = V - E, \tag{34}$$

the Euler characteristic of Γ.

Proof. Either the first formula (with (31)) or the last formula in (32) can be used to calculate the index. □

Corollary 21. *Let C be the number of connected components of Γ. Then*

$$\dim\ker\,\mathrm{d} = \dim\ker H_K = C \tag{35}$$

and

$$\dim\ker\delta = \dim\ker H_A = E - V + C. \tag{36}$$

In particular, in the connected case

$$\dim\ker\delta = E - V + 1 = r, \tag{37}$$

the rank of the fundamental group of Γ.

Proof. Equality (35) is immediate, since the zero modes of H_K are constant on each component. Now the index theorem (34) yields (36). □

Remark 22. Equation (36) counts the locally constant differential 1-forms satisfying (14a). It is 0 for a tree graph (where (14a) must be violated at the leaves) and 1 for a cycle. In general, it counts the independent cycles in the graph.

5. Relation to the secular determinant

Kottos and Smilansky [14] derived their trace formula for the density of states of a (compact) quantum graph from a certain secular equation,

$$f(k) \equiv \det[U(k) - 1] = 0. \tag{38}$$

In terms of frequency the density of states is

$$\rho(k) = \sum_{n=0}^{\infty} \delta(k - |k_n|) \equiv N_0 \delta(k) + \rho_1(k), \tag{39}$$

where N_0 is the true *spectral multiplicity* of 0 as an eigenvalue, and $\rho_1(k)$ is the contribution of the positive eigenvalues, $\lambda_n = {k_n}^2$, appearing with multiplicity. (We assume there are no negative eigenvalues. According to [14, 17, 8, 16], for strictly positive eigenvalues the spectral multiplicity is equal to the multiplicity as a root of (38), but the situation for $k = 0$ is quite different.) The secular function f defines a distribution $\tilde{\rho}(k)$ on the entire real line by

$$\tilde{\rho}[\phi] \equiv \lim_{\epsilon \downarrow 0} \frac{1}{4\pi i} \int_{-\infty}^{\infty} \left(\frac{f'(k - i\epsilon)}{f(k - i\epsilon)} - \frac{f'(k + i\epsilon)}{f(k + i\epsilon)} \right) \phi(k)\, dk \tag{40}$$

$$= \frac{1}{2} \sum_{n=-\infty}^{\infty} \phi(k_n), \tag{41}$$

the sum being over all zeros of f (with multiplicity), including the possible one at $k = 0$, whose *algebraic multiplicity* as a root of (38) we shall denote $\tilde{N}$. If k is a nonzero root of f, then so is $-k$. The positive eigenvalues are the squares of the nonzero roots of f; thus every positive eigenvalue appears in the sum (41) twice (times its multiplicity), and hence (39) is correctly reproduced on the positive axis by $\tilde{\rho}$. The spectral multiplicity N_0, however, is generally equal neither to $\tilde{N}$ nor to $\frac{1}{2}\tilde{N}$. Furthermore, $\tilde{N}$ itself has proved difficult to calculate reliably [14, 17, 8, 16].

From the foregoing definitions and discussion it follows that

$$\rho(k) = \begin{cases} (N_0 - \frac{1}{2}\tilde{N})\delta(k) + \tilde{\rho}(k) & \text{for } k \geq 0, \\ 0 & \text{for } k < 0 \end{cases}$$

$$\equiv h(k)[(N_0 - \tfrac{1}{2}\tilde{N})\delta(k) + \tilde{\rho}(k)], \tag{42}$$

where h is the unit step function and (because the product $h\delta$ would otherwise be ambiguous) we stipulate that $h\delta[\phi] \equiv \phi(0)$ (not $\frac{1}{2}\phi(0)$). In terms of the density of states, (1) can be rewritten as

$$\int_{-\infty}^{\infty} e^{-k^2 t} \rho(k)\, dk = \operatorname{Tr} K = K_1 + K_2 + K_3\,.$$

The derivation of the trace formula [14, 17, 8, 16] makes clear that $\tilde{\rho}$ yields precisely the leading Weyl term and the oscillatory (periodic-orbit) terms in the density of states. It follows (cf. discussion following (1)) that the contribution of $\tilde{\rho}$ to the heat kernel is the terms K_1 and K_2. The remaining term in (42), proportional to $\delta(k)$, must therefore be responsible for precisely the constant term K_3 in the heat kernel. We reemphasize that the coefficient of those terms is not N_0, the coefficient of $\delta(k)$ in the spectral density ρ. That is not a paradox: The distributionally convergent periodic-orbit sum $\tilde{\rho}$ contains another $\delta(k)$ contribution to ρ that restores consistency with (39).

On the other hand, we now know from previous sections that K_3, for a scale-invariant Laplacian, is equal to half the index of the associated first-order operator, A. The index, in turn, equals $E - p$, where E is the number of (undirected) edges and p is the number of Dirichlet conditions. Furthermore, we have $\operatorname{index} A = N_0 - N_0^*$, where N_0^* is the nullity of A^* and hence of the operator dual to H. Therefore, we immediately get two interesting identities:

Corollary 23. *Let N_0 and $\tilde{N}$ be the spectral and algebraic multiplicities of $k = 0$ for a scale-invariant graph Laplacian, A^*A, and let N_0^* be the spectral multiplicity for the dual Laplacian, AA^*. Then*

$$\tilde{N} = 2N_0 - \operatorname{index} A = 2N_0 - E + p \tag{43}$$

and

$$\tilde{N} = N_0 + N_0^* \,. \tag{44}$$

Example 1: For H_K, the Laplacian of a connected Kirchhoff graph, one has $N_0 = 1$ and $\operatorname{index} A = \operatorname{index} \mathrm{d} = V - E$. Therefore, $\tilde{N} = 2 - V + E$, in agreement with [17, corrigendum] and [16].

Example 2: For the pure Neumann Laplacian H_N of section 3.4, one has $N_0 = E$ and $p = 0$, so $\tilde{N} = E$. This is correct, because 0 appears as a root of f once for each disconnected Neumann edge.

Kurasov [16] gives a convincing direct calculation of $\tilde{N}$ for the Kirchhoff case. On that basis he deduces that the Euler characteristic (2) is determined by the spectrum of H_K. Thus the direction of the logic in [16] is roughly the reverse of that in the present paper. Our derivation of Corollary 23 is simpler (as well as more general).

6. Conclusions and additional remarks

We have demonstrated that the "topological" term in the heat-kernel expansion for a Laplacian on a quantum graph does indeed have an index interpretation, if the Laplacian is of the scale-invariant class (i.e., the boundary conditions do not mix function values and derivatives, and hence the scattering matrix is independent of k). Such a Laplacian factors into two first-order operators, A and A^*, defined on domains determined by those boundary conditions.

One can calculate the index in three ways: (1) in the usual way, by subtracting the heat kernel of AA^* from that of A^*A (Proposition 16 and Theorem 20); (2) by inspection

of just the heat kernel of A^*A (Proposition 18 and Corollary 19); (3) just by counting the number of Dirichlet-type conditions (Theorem 14 and Corollary 15).

A general index formula has been derived for an arbitrary (elliptic) differential operator on a quantum graph (Theorem 14).

Along the way, we have provided some properties of the Hamiltonian that are equivalent to the scale invariance of the vertex conditions (Theorem 8).

Finally, we have determined the algebraic multiplicity of 0 as a root of the secular equation of a generic scale-invariant graph Laplacian in a novel way (Corollary 23).

We now add a few final remarks concerning the results of the paper:

- There is an elementary sense in which the integer $V - E$ encountered in (2) is associated with an operator index. A graph as a purely combinatorial object (with no lengths assigned to the edges) is described in graph theory by the *incidence matrix*, whose rows are indexed by the vertices and its columns by the edges. Each matrix entry is equal to either 0, 1, or 2, depending on whether that edge is not or is attached to that vertex or forms a loop there. Then it is easy to see that (just because of the matrix's dimensions) the index of the incidence matrix is equal to $E - V$.
- The restriction to "local" vertex conditions in Theorem 2 and elsewhere has very little content. Indeed, the structure of the graph enters the problem only through the vertex conditions, and one could *define* a vertex as a subset of edges that are related by such conditions. Alternatively, one could think that all vertices of a quantum graph have collapsed into a single one (creating a "rosette" consisting of one vertex and E cycles attached). Since all (whether previously local or nonlocal) vertex conditions refer to this single vertex, all conditions have become local. This is impossible only if we need to enforce some specific type of vertex conditions, e.g., the Kirchhoff ones; after the graph collapses to a rosette, the vertex conditions will generally no longer be of that type.
- Kirchhoff conditions on $\Lambda^0(\Gamma)$ and anti-Kirchhoff conditions on $\Lambda^1(\Gamma)$ seem to be quite natural, whereas the interchanged conditions look rather unnatural. The situation for manifolds is different: there one can either impose Neumann conditions on forms of even degree and Dirichlet conditions on forms of odd degree, or do the reverse. The two choices correspond to two different cohomology theories for the manifold, "absolute" and "relative" [6, 7].
- Carlson [2] also constructs second-order self-adjoint operators on quantum graphs in terms of first-order operators, but his construction is rather different from ours. More pertinent are the remarks of Friedman and Tillich [5] and Exner and Post [3] that derivatives on quantum graphs should be treated as 1-forms (or vector fields).
- An extension of the first-order formulation of the index theorem to operators H with a nontrivial Robin part, $C_v \neq 0$, is not to be expected. As pointed out by V. Kostrykin, in general either H or its dual will have negative spectrum, whereas operators of form A^*A and AA^* must both be positive. This impossibility

of factorization is also contained in the statement (vii) of Theorem 8. On the other hand, inserting "Robin" operators Λ_v into the definition of H does not change the t-independent terms of $\operatorname{Tr} K_H$ and its dual, which are the ingredients of the formula for the index of the second-order operator.

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