Index Theorems for Quantum Graphs

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S A. Fulling, P. Kuchment, & J. H. Wilson*

Departments of Mathematics and Physics,
Texas A&M University

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* Undergraduate Research Fellow; now at University of Maryland

Credits

- National Science Foundation
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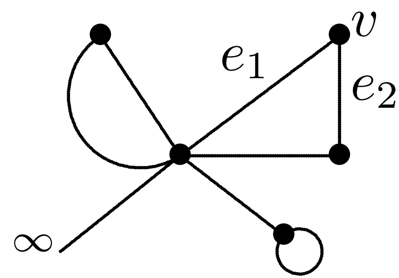
- Participants there: Jens Bolte, Vadim Kostrykin, Audrey Terras, ...
- Other members of the quantum graph group at TAMU: Gregory Berkolaiko, Jonathan Harrison, Brian Winn

What is a quantum graph?

A quantum graph combines the features of one-dimensional and multidimensional systems.



A quantum graph is a Riemannian 1-complex equipped with a self-adjoint second-order Laplacian operator:

On each edge: $\quad -\dfrac{d^2}{dx_{\mathrm{e}}^2}u = k^2 u \equiv \lambda u.$

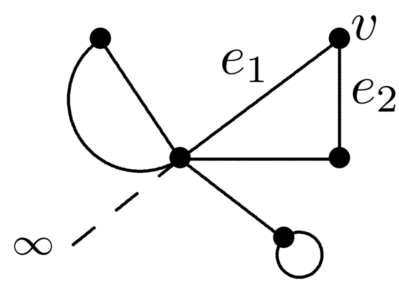
At each vertex: Boundary conditions that make it self-adjoint. *Example:* u is continuous and

$$\sum_{\mathrm{e}} \frac{du}{dx_e} = \alpha_v u(v).$$

Note: This is a *metric graph*, not a *combinatorial graph* where the edges are inert and

$$\Delta u(v) \equiv (\mathrm{const})\, u(v) - \sum_{\text{neighbors}} u(v_e)\,.$$

For today: *compact* graphs (finitely many edges, each of finite length). No isolated vertices. Multiple links are allowed, as are loops (tadpoles).



Applications of quantum graphs

1. Modeling thin structures in 3 dimensions (quantum wires)
   e.g., Kuchment, *Waves Random Media* **12** (2002) R1
2. Abstract model of quantum chaos
   e.g., Kottos & Smilansky, *Phys. Rev. Lett.* **24** (1997) 4794
3. Symbolic dynamics for wave propagation in piecewise homogeneous media
   e.g., Dabaghian et al., *Phys. Rev. E* **63** (2001) 066201

4. Lungs, veins, . . .
e.g., Carlson, 2005 Snowbird conference (*Contemp. Math.* **415** (2006) 65)

5. Modeling of multidimensional (continuum) quantum-mechanical systems
   - Melnikov & Pavlov, *J. Math. Phys.* **42** (2001) 1202
   - Exner, Hejčík, & Šeba, *Rep. Math. Phys.* **57** (2006) 445

More about boundary conditions

Kostrykin & Schrader (1999): $A\mathbf{u}(v) + B\mathbf{u}'(v) = 0$ with some technical conditions on matrices A and B.

Kuchment (2004): At each vertex v, of degree d_v , there are orthogonal projectors P_v and Q_v operating in $\mathbf{C}^{d_v}$ and a self-adjoint matrix Λ_v operating in the complementary subspace, $(1 - P_v - Q_v)\mathbf{C}^{d_v}$. (Any of the three subspaces might be zero.) The functions u in the operator domain are those members of the Sobolev space $\bigoplus_e H^2(e)$ that satisfy, at each vertex, boundary conditions consisting of the "Dirichlet part"

$$P_v \mathbf{u}(v) = 0,$$

the "Neumann part"

$$Q_v \mathbf{u}'(v) = 0,$$

and the "Robin part"

$$(1 - P_v - Q_v)\mathbf{u}'(v) = \Lambda_v (1 - P_v - Q_v)\mathbf{u}(v),$$

$u'_e \equiv \dfrac{du}{dx_e}$ being the derivative along edge e in the outgoing direction. The domain of $H = -\dfrac{d^2}{d{x_e}^2}$ as a quadratic form consists of the functions $u(x_e)$ that belong to the Sobolev space $H^1(e)$ on each edge and satisfy $P_v\mathbf{u}(v) = 0$ (the Dirichlet part of the BC) at each vertex. The Robin matrices Λ_v arise from boundary terms in the quadratic form defining the operator.

Nongeometer's point of view

Each edge has an initial point ($x_e = 0$) and a terminal point ($x_e = L_e$).

$$u_e'(v) = \begin{cases} u_e'(0), \text{ or} \\ -u_e'(L_e), \end{cases} \qquad \text{depending.}$$

Geometer's point of view

u_e' is a one-form (or a vector field). $du_e = \frac{du}{dx_e}\, dx_e$ is unambiguous. At each vertex we understand $u_e'(v)$ to be the outgoing (from the vertex) derivative.

Kirchhoff boundary conditions

Dir.: $$u_e(v) = \text{same for all } e \quad \text{(continuity);}$$

Neu.: $$\sum_{e=1}^{d_v} u_e'(v) = 0 \quad \text{(no net flux);}$$

no Robin part.

Dual (anti-Kirchhoff) boundary conditions

Dir.: $\displaystyle\sum_{e=1}^{d_v} w_e(v) = 0 \quad$ (average value at vertex $= 0$);

Neu.:

$w_e'(v) =$ same for all $e \quad$ (continuity of divergence).

These conditions are natural for $w \in \Lambda^1(\Gamma)$, $w' = {*d*w} \in \Lambda^0(\Gamma)$.

The heat kernel of a quantum graph

J.-P. Roth (1983): For Kirchhoff BC,

$$\sum_{n=0}^{\infty} e^{-\lambda_n t} = \operatorname{Tr} K \equiv \int_\Gamma K(t,x,x)\,dx$$

$$= \text{sum over closed paths} = K_1 + K_2 + K_3\,.$$

1. Zero length: $\quad K_1 = \dfrac{L}{\sqrt{4\pi t}} \quad$ (Weyl's law).

   $L \equiv$ total length of Γ.

2. Periodic: $$K_2 = \frac{1}{\sqrt{4\pi t}} \sum_C \mathcal{A}(C) L(C_p) e^{-L(C)^2/4t}.$$

$L(C), L(C_p) \equiv$ path lengths.
$\mathcal{A}(C) \equiv$ an amplitude you don't want to know.

3. Closed, nonperiodic:
"Ce calcul est un peu plus délicat."

$$K_3 = \frac{1}{2}(V - E)$$

(rest of the Weyl series; the **only** constant term).
$V \equiv$ number of vertices, $E \equiv$ number of edges.

$V - E$ is

- an integer;
- "topological" (Euler characteristic of a 1-complex).

So what? . . .

Let's generalize Gilkey, *Asymptotic Formulae in Spectral Geometry*, which treats this graph: $0 \bullet\!\!-\!\!\!-\!\!\!-\!\!\bullet\, \pi$

Let $d \equiv \frac{d}{dx} \colon \Lambda^0(\Gamma) \to \Lambda^1(\Gamma)$ with Kirchhoff conditions

- Dirichlet part: $u_e(v)$ independent of e;
- Neumann part: $\sum_e u_e'(v) = 0$.

Then $d^\dagger = -\frac{d}{dx} \colon \Lambda^1(\Gamma) \to \Lambda^0(\Gamma)$ with dual conditions

- Dirichlet part: $\sum_e w_e(v) = 0$;
- Neumann part: $w_e'(v)$ independent of e.

$$d^\dagger d \equiv H_K = \text{Kirchhoff Laplacian};$$

$$dd^\dagger \equiv H_A = \text{dual Laplacian}.$$

$$d^\dagger d \equiv H_K; \quad dd^\dagger \equiv H_A\,.$$

(Outer operator on form domain $\oplus_e H^1(e)_{\mathrm{Dir}}$;
inner operator on operator domain $\oplus_e H^2(e)_{\mathrm{Dir,Neu}}$.)

Let K_K and K_A be the respective heat kernels.

$$\operatorname{Tr} K_K = \frac{L}{\sqrt{4\pi t}} + \frac{1}{2}(V-E) + \cdots.$$

$$\operatorname{Tr} K_A = \frac{L}{\sqrt{4\pi t}} + \frac{1}{2}(E-V) + \cdots.$$

There follows:

Index theorem (simplest case)

$$\operatorname{index} d = \operatorname{Tr} K_K - \operatorname{Tr} K_A = V - E = \chi(\Gamma).$$

COROLLARY

Let C be the number of connected components of Γ. Then

$$\dim\ker d = \dim\ker H_K = C,$$

$$\dim\ker d^\dagger = \dim\ker H_A = E - V + C.$$

In particular, in the connected case

$$\dim\ker d^\dagger = E - V + 1 = r,$$

the rank of the fundamental group. (Number of locally constant anti-Kirchhoff vector fields = number of independent cycles in graph.)

More general boundary conditions

A choice of self-adjoint extension dictates an internal *scattering matrix* $\sigma(k)$ for the graph (unitary; number of indices $= 2E$; $k = \sqrt{\lambda}$).

Theorem (Kostrykin & Schrader; Kuchment): These are equivalent:

- There is no "Robin part" in the boundary conditions: $1 - P_v - Q_v = 0$.
- σ is independent of k (scale invariance).
- $\sigma^2 = I$, so $\sigma = I - 2P$ ($P = \sum P_v =$ orthogonal projection).
- The Laplacian can be factored: $H = A^\dagger A$ where $A = \frac{d}{dx}$ with some vertex conditions.

Theorem (Kostrykin, Putthoff & Schrader; Wilson): For any scale-invariant graph Laplacian H,

$$\operatorname{Tr} K_H = \frac{L}{\sqrt{4\pi t}} + \frac{1}{4}\operatorname{tr}\sigma + \text{exponential terms.}$$

As before, there is a dual Laplacian (interchanging Dirichlet and Neumann conditions), and its scattering matrix is $-\sigma$. There follows:

Index theorem (general case)

Define A with the BC defining H and hence $A^\dagger$ with the dual BC. Then $H = A^\dagger A$ and

$$\operatorname{index} A = 2 \operatorname{Tr} K_H .$$

But also . . .

Index theorem (rendered trivial by Kuchment)

For any scale-invariant graph Laplacian H,

$$\operatorname{index} A = E - p,$$

where $p \equiv \dim \operatorname{ran} P$, the number of Dirichlet conditions in the definition of H.

The proof is an elementary exercise in changing the codimension of the domain of a Fredholm operator by a finite amount.

Example:

$$p = \begin{cases} 2E - V & \text{for Kirchhoff,} \\ V & \text{for anti-Kirchhoff.} \end{cases}$$

So

$$\operatorname{index} d = E - p = V - E,$$

$$\operatorname{index} d^{\dagger} = E - V.$$

The secular determinant

Kottos & Smilansky (1999): The nonzero eigenvalues satisfy a secular equation $\det[U(k) - I] = 0$. But the algebraic multiplicity of $k = 0$ may be greater than its true spectral multiplicity.

Previous methods of determining these multiplicities have proved difficult and error-prone.

Corollary of index theorem

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

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

and $\tilde{N} = N_0 + N_0^*$.

Example 1: For H_K , the Laplacian of a connected Kirchhoff graph, $N_0 = 1$ and index $d = V - E$. Therefore, $\tilde{N} = 2 - V + E$, as proved earlier by Kurasov.

Example 2: For a graph consisting of disconnected Neumann edges, one has $N_0 = E$ and $p = 0$, so $\tilde{N} = E$. This is correct, because $k = 0$ appears as a root once for each edge. The dual has disconnected Dirichlet edges and has $N_0^* = 0$ and $p = 2E$. (This pair is the starting point of the elementary Fredholm exercise.)

Conclusions

1. The "topological" term in the heat kernel does have an index interpretation, for scale-invariant boundary conditions.
2. Namely, H has the form $A^\dagger A$, and the index of A can be calculated in three ways:
   (a) as usual, from $\operatorname{Tr} K_{A^\dagger A} - \operatorname{Tr} K_{AA^\dagger}$.
   (b) by inspection of $K_{A^\dagger A}$ by itself;
   (c) just by counting the number of Dirichlet-type boundary conditions.

3. The geometer's viewpoint (one-forms versus functions) is helpful.
4. The algebraic multiplicity of 0 as a root of the secular equation is related to the spectral multiplicities for the Laplacian ($A^\dagger A$) and its dual ($AA^\dagger$).

A simultaneous related paper

Olaf Post, First order approach and index theorems for discrete and metric graphs, *Ann. H. Poincaré* **10** (2009) 823–866.

At the Dartmouth conference I learned from Ralf Rueck-riemen about an earlier paper:

B. Gaveau and M. Okada, Differential forms and heat diffusion on one-dimensional singular varieties, *Bull. Sci. Math.* **115** (1991) 61–79.

They introduce the first-order formalism and state the simplest index theorem under the name of "Gauss–Bonnet theorem".