Spectra of Quantum Graphs

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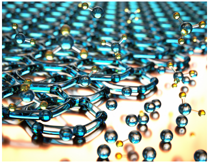
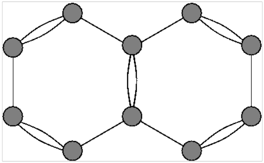


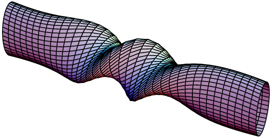
Jointly with Pavel Kurasov (Stockholm University)

Layout

Motivation

Quantum graph is a linear network-like structure. It was first employed in 30's to model the motion of free electrons in molecules (eg. naphthalene, graphene).





- They may arise when solving various problems: quantum waveguides, quantum chaos, photonic crystals, periodic structures.

Layout

Historical remarks

References:

- P. Exner and P. Šeba, *Free quantum motion on a branching graph*, Rep. Math. Phys., 28 (1989), **7-26**.
- P. Kuchment, *Quantum Graphs I: Some Basic Structures*, Waves Random Media, 14, **107-128**, 2004.
- V. Kostrykin, P. Schrader, *Kirchhoff's Rule for Quantum Wires*, J. Phys. A, 32, **595-630**, 1999.
- T. Kottos, U. Smilansky, *Periodic Orbit Theory and Spectral Statistics for Quantum Graphs*, Ann. Physics, 274, no. 1, **76-124**, 1999.
- P. Kurasov, *Quantum Graphs: Spectral Theory and Inverse Problems*, in preparation.

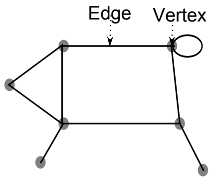
Definition

Definition of a quantum graph consists of three parts:

- metric graph
- differential operator acting on the edges
- matching and boundary conditions at internal and external vertices respectively

Metric graph

Metric graph is a collection of vertices and edges characterized by its length.



Edges and vertices are defined as follows:

$$E_n = \begin{cases} [x_{2n-1}, x_{2n}], & n = 1, 2, \ldots, N_c \\ [x_{2n-1}, \infty), & n = N_c + 1, \ldots, N_c + N_i = N, \end{cases}$$

$$\mathbf{V} = \{x_{2n-1}, x_{2n}\}_{n=1}^{N_c} \cup \{x_{2n-1}\}_{n=N_c+1}^{N},$$

Differential operator

Magnetic Schrödinger operator

$$L_{q,a} = \left(i\frac{d}{dx} + a(x) \right)^2 + q(x),$$

where $q(x), a(x) \in \mathbb{R}$.

Maximal operator L^{max} is defined on $H^2(\Gamma \setminus V)$ and minimal operator L^{min} on $C_0^\infty(\Gamma \setminus V)$.

Extended normal derivatives

$$\partial u(x_j) = \begin{cases} \lim_{x \to x_j} \left(\frac{d}{dx} u(x) - ia(x)u(x) \right), & x_j \text{ left endpoint}, \\ -\lim_{x \to x_j} \left(\frac{d}{dx} u(x) - ia(x)u(x) \right), & x_j \text{ right endpoint}, \end{cases}$$

Matching and boundary conditions

The maximal Laplace operator $(a, q = 0)$ is self-adjoint if the form

$$\langle L^{\max} u, v \rangle - \langle u, L^{\max} v, \rangle = \sum_{x_j \in \mathbf{V}} \left(\partial u(x_j) \overline{v(x_j)} - u(x_j) \overline{\partial v(x_j)} \right)$$

is equal to zero.

Matching and boundary conditions

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is equal to zero.

Standard matching conditions in each V_m

$$\begin{cases} u \text{ is continuous at } V_m \\ \sum_{x_j \in V_m} \partial u(x_j) = 0. \end{cases}$$

- for two edges- the middle point may be removed
- define **free (standard) Laplace operator**

Layout

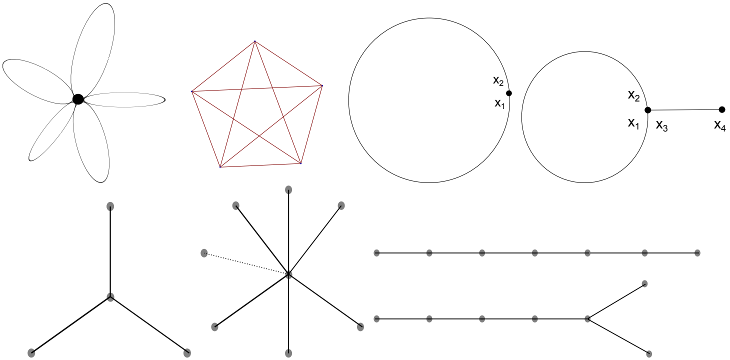
Spectrum

In quantum mechanics, physical observables are described by eigenvalues of self-adjoint operators. For Hamiltonian, they correspond to energy levels.

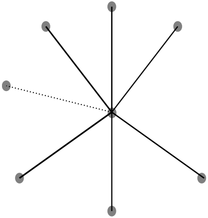
Basic properties

- If Γ is compact and finite, then the spectrum is purely discrete with unique accumulation point $+\infty$.
- Given $k_n^2 \neq 0$ is an eigenvalue of a Laplace operator L on graph Γ consisting of basic lengths ($l_j = n_j \Delta$). Then $(k_n + \frac{2\pi}{\Delta})^2$ also belongs to the spectrum.
- 0 is the first eigenvalue of the free Laplacian with multiplicity equal to number of connected components.

Explicitly solvable cases



Example: Equilateral star graph

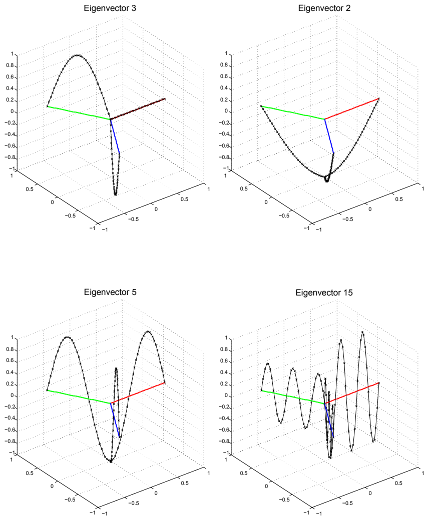


Star graph's eigenvalues:

$$k_p = \begin{cases} \frac{\pi}{2\ell} + \frac{p\pi}{\ell}, & \text{multiplicity } n-1, \\ \frac{\pi p}{\ell}, & \text{multiplicity } 1, \end{cases}$$

where n is the number of edges and ℓ is the edge length.

Equilateral star graph



Layout

Spectral gap for discrete graphs

Definition

Spectral gap is the difference between smallest two eigenvalues of an operator.

Formerly investigated on discrete (combinatorial) graphs:
Laplacian L for discrete graph is defined as $L = V - A$ where

$$A_{ij} = \begin{cases} 1 & \text{if the vertices } i \text{ and } j \text{ are connected,} \\ 0 & \text{otherwise,} \end{cases}$$

$$V = \operatorname{diag}(v_1, v_2, \ldots, v_n),$$

v_k being the kth vertex valency.

- for Laplacian sometimes called Fiedler value or algebraic connectivity on discrete graphs
- measure of synchonizability and robustness
- internet, neuron networks, signal transfer, social interaction

Layout

Quantum and discrete graphs- adding an edge

Let us consider a quantum graph with free Laplacian and a discrete graph. Provided we have the same set of vertices.

Discrete graph

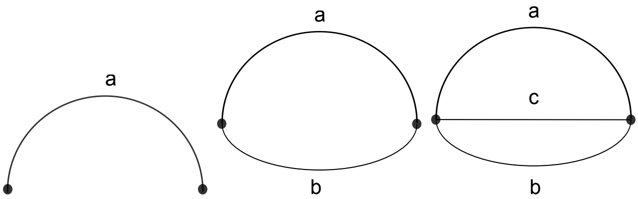
Adding one edge always *increases* the spectral gap or keeps it unchanged.

Quantum graph

Adding one edge between nodes m_1 and m_2 might cause either *increase* or *decrease* in the spectral gap. Sufficient condition for λ_1 to drop is to be able to choose the eigenfunction u_1 corresponding to the spectral gap such that

$$u_1(m_1) = u_1(m_2).$$

Example



$$\lambda_n(\Gamma) = \left(\frac{\pi}{a}\right)^2 n^2, \qquad \lambda_n(\Gamma') = \left(\frac{2\pi}{a+b}\right)^2 n^2.$$

Any relation between these values is possible:

$$b > a \;\Rightarrow\; \lambda_1(\Gamma) > \lambda_1(\Gamma'),$$
$$b < a \;\Rightarrow\; \lambda_1(\Gamma) < \lambda_1(\Gamma').$$

Always:

$$\lambda_1(\Gamma'') \leq \lambda_1(\Gamma').$$

Quantum and discrete graphs- adding a pending edge

Let us consider a quantum graph with free Laplacian and a discrete graph. Adding a pending edge gives the same result for both types.

Discrete & quantum graph

Adding one pending edge always *decreases* the spectral gap or keeps is unchanged.

Quantum graphs- adding an edge

Let Γ be a connected finite compact metric graph of length $\mathcal{L}(\Gamma)$ and let Γ' be a graph constructed from Γ by adding an edge of length ℓ between certain two vertices. If

$$\ell > \mathcal{L}(\Gamma),$$

then the eigenvalues of the corresponding free Laplacians satisfy the estimate

$$\lambda_1(\Gamma) \geq \lambda_1(\Gamma').$$

Layout

Minimizing the spectral gap

Rayleigh estimate (P. Kurasov, S. Naboko 2012)

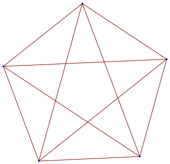
The *string graph* Δ has the smallest spectral gap among all quantum graphs with the same total length, i.e. for all graphs Γ:

$$\lambda_1(\Gamma) \geq \lambda_1(\Delta).$$

Maximizing the spectral gap

Conjecture

The *complete graph* has the highest spectral gap among all quantum graphs with the same total length and fixed number of vertices.



Papers

- P. Kurasov, S. Naboko, *Rayleigh Estimates for Differential Operators on Graphs*, in preparation.
- P. Kurasov, G. Malenova, S. Naboko, *Spectral gap for quantum graphs and their edge connectivity*, J. Phys. A: Math. Theor. 46 (2013) 275309.

Conclusion

Conclusion:

- Spectra of quantum graphs have been investigated
- Main focus on spectral gap
- In the pipeline: Maximization problem? Third eigenvalue?

On the audience

THANK YOU FOR YOUR ATTENTION