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A Brief Survey on Quantum Graphs and Their Applications

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1. **Contents of the talk**
   - What is a quantum graph?
   - Origins of quantum graphs
   - Some spectral features

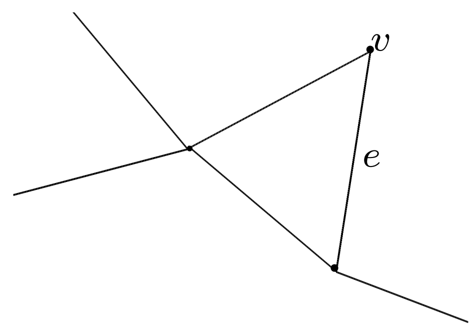
2. **Sources: V. Kostrykin and R. Schrader**, Kirchhoff's rule for quantum wires, J. Phys. A 32 (1999), 595-630.
   T. Kottos and U. Smilansky, Quantum Chaos on Graphs, Phys. Rev. Lett. **79** (1997), 4794.
   T. Kottos and U. Smilansky, Quantum Graphs: A simple model for Chaotic Scattering, J. Phys. A: Math and General **36** (2003), 3501.
   P. Kuchment, Graph models of wave propagation in thin structures, Waves in Random Media **12** (2002), no. 4, R1-R24.
   Quantum Graphs and Application, a special issue of Waves in Random Media, **14** (2004), no. 1 (and references therein)

Work done by S. Alexander, Y. Avishai, J. Avron, G. Berkolaiko, R. Blümel, R. Carlson, W. Evans, P. Exner, M. Freidlin, L. Friedlander, J. Keating, V. Kostrykin, T. Kottos, L. Kunyansky, S. Novikov, P. Ola, L. Paivarinta, B. Pavlov, J. Rubinstein, Y. Saito, H. Schanz, M. Schatzman, R. Schrader, P. Šeba, U. Smilansky, A. Sobolev, M. Solomyak, A. Wentzell, B. Winn, H. Zeng, ...

Joint Summer Research Conference in the Math. Sciences "Quantum Graphs and Their Applications", Snowbird, UT, USA, June 18 – June 24, 2005. Organizers G. Berkolaiko, R. Carlson, S. Fulling, P. Kuchment http://www.math.tamu.edu/~kuchment /src05_graphs.htm

3. **Spectral Graph Theory**

Γ - graph, V - vertices, E - edges



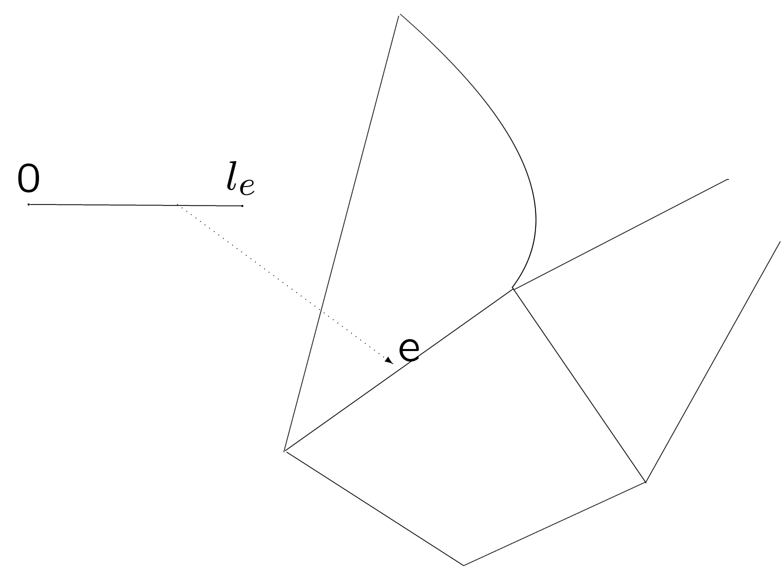
Functions f on V, Laplace operator:

$$f(v) \to \Delta f(v) = f(v) - \frac{1}{d_v} \sum_{e=(v,w)\in E} f(w)$$

Spectral properties of Δ are related to properties of Γ. Graph theory, algebra, number theory, spectral geometry, mathematical physics, Internet tomography
Books by N. Biggs, F. Chung, Y. Colin de Verdière, D. Cvetkovic et al.

4. **Metric and Quantum Graphs**

Metric graph Γ (**weighted** graph): edges e are assigned "lengths" $l_e > 0$ and identified with segments $[0, l_e]$.



Coordinate x along edges, functions $f(x)$, measure, integration, $L_2(\Gamma)$, differentiation d/dx. Sometimes a metric graph is embedded into $\mathbb{R}^n$ with induced arc length coordinates along the edges.

Quantum graph: a metric graph Γ equipped with a self-adjoint differential (sometimes pseudo-differential) operator

Example: $Hf = -\dfrac{d^2 f}{dx^2}$, or a more general Schrödinger operator

$$H = \left(\frac{1}{i}\frac{d}{dx} - A(x)\right)^2 + V(x).$$

Domain of definition: $H^2(e)$ on each edge e and **boundary conditions at vertices**.

Matrix, higher order, and pseudo-differential Hamiltonians also arise.

Example: singular Schrödinger operator on the plane (a "leaky wire"):

$$-\Delta u + \alpha\delta_\Gamma u = \lambda u.$$

Spectral/scattering properties are of interest.

Generalizations: quantum buildings, multistructures.

5. **Origin(s) of quantum graphs:**

   A. Approximations for waves propagating in thin structures:

   (a) Chemistry: π-electron orbitals in organic molecules with conjugated double bonds.

   (b) Quantum wire circuits (with nanotechnology and quantum computers applications).

   (c) Thin superconducting circuits.

   (d) Thin waveguides (quantum, acoustic, electromagnetic, optical).

   (e) Photonic crystals.

   (f) Averaging in dynamical systems.

B. Simpler models of some complex problems of math and science:

(a) Toy examples in quantum mechanics.

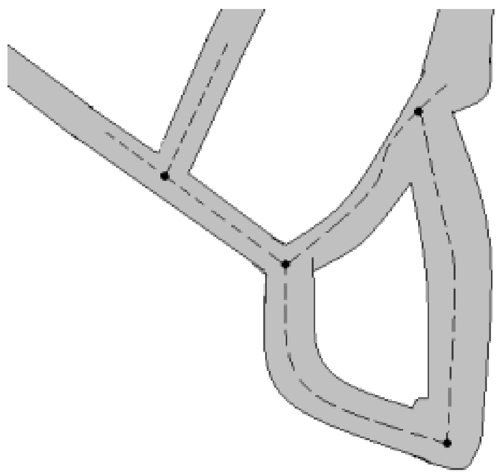
(b) Quantum chaos: conjectures concerning quantum signatures of chaos.

(c) Anderson localization.

(d) Quantum transport in multiply connected systems.

(e) Inverse problems.

Math set-up: Approximations for waves propagating in thin graph-like media



• **Neumann Laplacian** $-\Delta_{N,d}$ on Ω_d. What is behavior of $\sigma(-\Delta_{N,d})$ when $d \to 0$? (EM waveguides, superconducting structures)

• Similar question for the **Dirichlet Laplacian**. (circuits of quantum wires)

• Same question for the **Maxwell operator** $M = \nabla \times \frac{1}{\epsilon} \nabla \times$. (photonic crystals)

6. **Neumann Laplacian** (Rubinstein & Schatzman, P.K. & Zeng) $d \times p(x)$ - width of narrow tubes ($d \to 0$), areas around junctions do not decay too slowly. Then

$$\sigma\left(\left(\frac{1}{i}\frac{d}{dx} - A(x)\right)^2 + V(x)f(x)\right)$$

converges to the spectrum of the graph operator

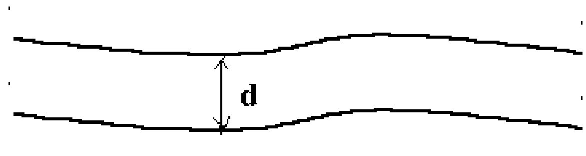
$$-\frac{1}{p}\left(\frac{d}{dx} - iA_e^\tau(x)\right)p\left(\frac{d}{dx} - iA_e^\tau(x)\right)f + Vf$$

with vertex conditions: f is continuous, at each vertex v

$$\sum_{e \in E_v} p_j(v)\left(\frac{df_j}{dx_j} - iA_j^\tau f_j\right)(v) = 0.$$

For large junctions the graph decouples into a collection of unrelated edges with Dirichlet conditions at vertices.

7. **Dirichlet Laplacian** (Duclos, Exner, Šeba, Post, ...)



Dirichlet Laplacian $-\Delta_{D,d}$ is more complex. Spectrum goes to ∞ when $d \to 0$. Subtract the first transversal eigenvalue λ_1.

The spectrum of $-\Delta_{D,d} - \lambda_1$ converges to

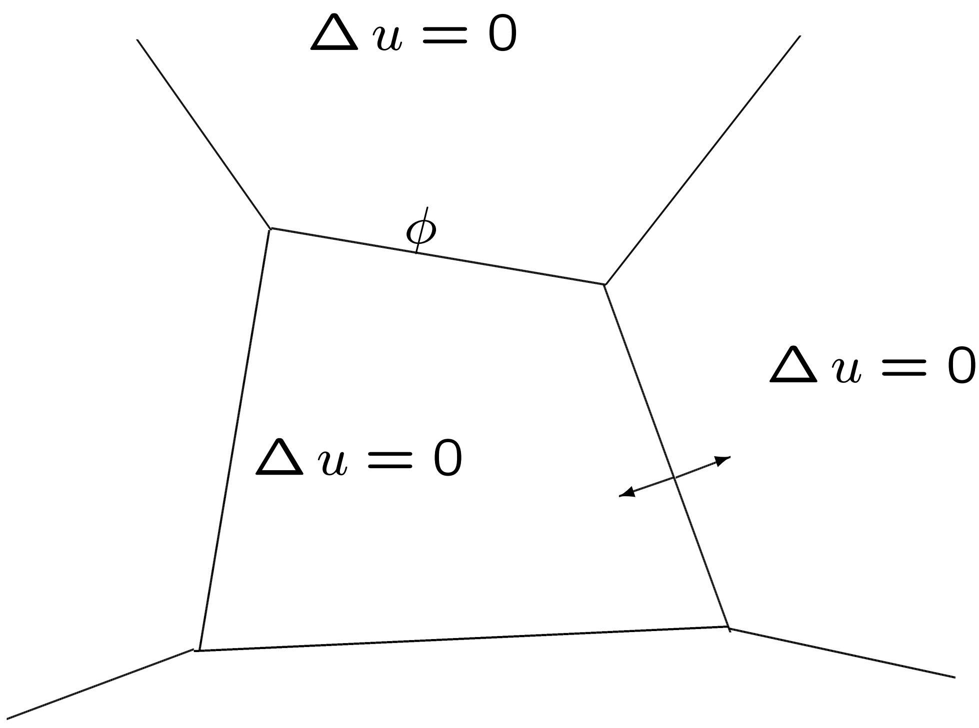
$$\sigma\left(-\frac{d^2}{dx^2} - \frac{\gamma(x)^2}{4}\right),$$

where x is the arc length coordinate on Γ, $\gamma(x)$ - curvature of Γ. **Confining electrons by bending wires**.
The case of graphs (or even a single vertex or corner) has not been understood.

8. **Maxwell operator.** $2D$ **Photonic crystals** lead to a pseudo-differential spectral problem (Figotin& P.K., P.K. & Kunyansky)

$$\Lambda_\Gamma u = \lambda u,$$

where Λ_Γ is the Dirichlet-to-Neumann operator on a planar graph.



Equivalent to: $-\Delta u = \lambda \delta_\Gamma u$
More general: $-\Delta u = \lambda \delta_\Gamma u + cu$. Leaky wires.

Some spectral features

1. **Self-adjoint BC** (Exner& Seba, Kostrykin& Schrader, Pavlov et al., Novikov, P.K.)
   $H = -\frac{d^2 f}{dx^2}$ on Γ. Examples of s.-a. BC:
   δ-**type conditions**

   $$f \text{ is continuous and at each vertex } v$$
   $$\sum_{e \in E_v} f_e'(v) = \alpha_v f(v)$$

   δ'-**type conditions**

   $$f_e'(v) \text{ is edge-independent and at each } v$$
   $$\sum_{e \in E_v} f_e(v) = \alpha_v f'(v)$$

   General self-adjoint vertex BC:

   $$P_v F(v) = 0, Q_v F'(v) + L_v F(v) = 0.$$

   Here P_v is an orthogonal projector in $\mathbb{C}^{d_v}$, $Q_v = I - P_v$, and L_v is a s.-a. operator in $Q_v \mathbb{C}^{d_v}$.
   Quadratic form: $\sum_e \int_e |\frac{df}{dx}|^2 dx - \sum_v \langle L_v F(v), F(v) \rangle$
   Complex symplectic geometry

Alternative descriptions of vertex conditions:

- (Kostrykin and Schrader)

  $$A_v F(v) + B_v F'(v) = 0,$$

  where (A_v, B_v) is of maximal rank and $A_v B_v^*$ is self-adjoint.

- (Harmer) U_v-unitary,

  $$i(U_v - \mathbb{I})F(v) + (U_v + \mathbb{I})F'(v) = 0$$

- (Kottos and Smilansky) A symmetric unitary matrix $\sigma = \sigma_v$ of size $d_v \times d_v$ that provides a transformation between the incoming and outgoing waves at the vertex. Dirichlet condition case: $\sigma_{i,j} = -\delta_{i,j}$; Neumann: $\sigma_{i,j} = -\delta_{i,j} + \frac{2}{d_v}$; in general energy dependent.

2. **Relations between quantum and combinatorial graph spectra** (S. Alexander, ...)

An example: δ-type conditions

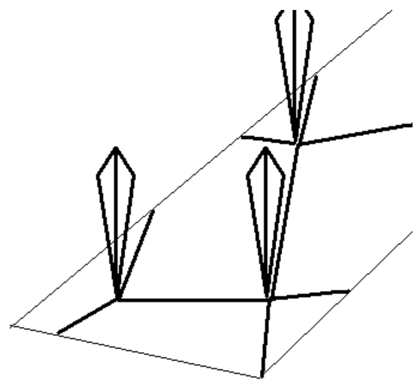
$$f \text{ is continuous and at each vertex } v$$
$$\sum_{e \in E_v} f_e'(v) = 0,$$

Γ is regular ($d_v = d = const$) and edge lengths are all same ($l_e = l = const$. The spectrum of H can be explicitly derived from the spectrum of discrete Laplacian Δ. I.e., $\lambda \in \sigma(H)$ iff $g(\lambda) \in \sigma(\Delta)$ for an explicitly written transcendental function g, which in simplest cases might look as follows:

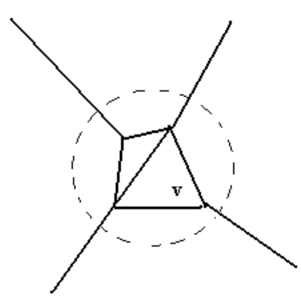
$$g(\lambda) = \left(\alpha \frac{\sin l\sqrt{\lambda}}{l\sqrt{\lambda}} + d \cos \sqrt{\lambda} \right)$$

3. **Resonant gaps**, due to small scatterers throughout the medium (Avron, Exner,& Last; Pavlov; Schenker& Aizenman, Figotin& P.K., P.K., P.K. & Kunyansky) Simplest models (work both in combinatorial and quantum cases):

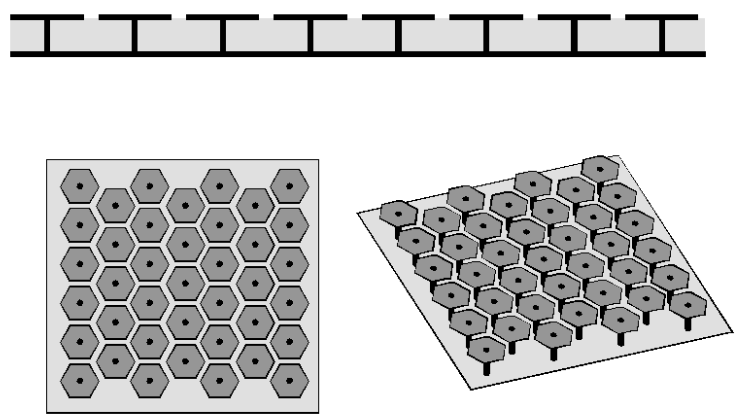
   (a) Graph decoration by “flowers”:



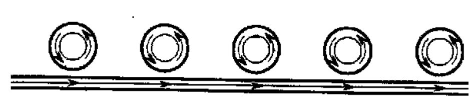
   (b) Graph decoration by “spiders”:



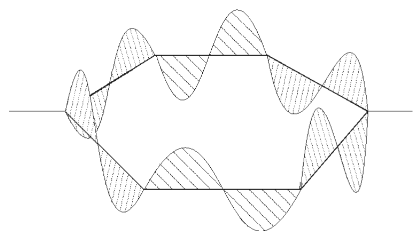
UCLA antenna ground plane:



A SCISSOR (side-coupled integrated spaced sequence of resonators):

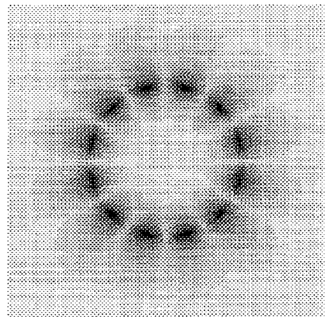


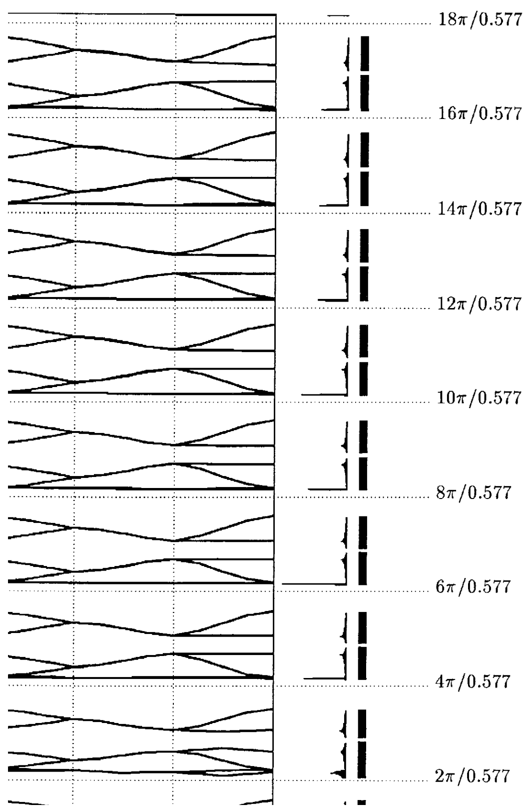
4. **Periodic graph structures** While spectra of periodic elliptic 2nd order PDEs are AC, a periodic graph Γ can have point spectrum due to topology.



Such "cycle states" are the only sources for the point spectrum on periodic combinatorial and quantum graphs (with differential Hamiltonians).

The spectrum of periodic "leaky wires" is AC. However, it may exhibit extremely flat bands with strongly localized leaky eigenfunctions and low group velocity (P.K. & Kunyansky, 1999):

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16π/0.577
14π/0.577
12π/0.577
10π/0.577
8π/0.577
6π/0.577
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2π/0.577

Suggested use for CROWs (coupled resonator optical waveguides, Yariv at al., 1999):