Some semiclassical and universal estimates of eigenvalues of quantum graphs

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“Universal” constraints on the spectrum

- H. Weyl, 1910, Laplace, $\lambda_n \sim n^{2/d}$
- L. Payne, G. Pólya, H. Weinberger, 1956: The gap is controlled by the average of the smaller eigenvalues:

$$\lambda_{n+1} - \lambda_n \leq \frac{4}{d} \frac{1}{n} \sum_{k \leq n} \lambda_k$$
“Universal” constraints on the spectrum with phase-space volume.

- Lieb-Thirring, 1977, for Schrödinger

\[ \varepsilon^{d/2} \sum_{\lambda_j(\varepsilon) < 0} |\lambda_j(\varepsilon)|^\rho \leq L_{\rho,d} \int_{\mathbb{R}^d} (V_-(x))^{\rho+d/2} dx \]

- Li-Yau, 1983 (Berezin 1973), for Laplace

\[ \sum_{j=1}^{k} \lambda_j \geq \frac{d}{d+2} \frac{4\pi^2 \kappa^{1+2/d}}{(C_d|\Omega|)^{2/d}} \]
“Universal” constraints on the spectrum

- Harrell 1993-present, commutator approach; with Michel, Stubbe, El Soufi and Ilias, Hermi, Yildirim.
The counting function,
\[ N(z) := \#(\lambda_k \leq z) \]

Integrals of the counting function, known as Riesz means (Safarov, Laptev, Weidl, etc.):

\[ R_\rho(z) := \sum_j (z - \lambda_j)^\rho_+ \]

Chandrasekharan and Minakshisundaram, 1952
Some models in nanophysics:

1. Schrödinger operators on curves and surfaces embedded in space. *Quantum wires and waveguides.*


3. Quantum graphs. *Nanoscale circuits*

Are the spectra of these models controlled by “sum rules,” like those known for Laplace/Schrödinger on domains or all of $\mathbb{R}^d$, or are there important differences?
Are the spectra of these models controlled by “sum rules”? If so, can we prove analogues of Lieb-Thirring, Li-Yau, PPW, etc.?
Commutators of operators

[*G, [H, G]] = 2 GHG - G^2H - HG^2

Etc., etc. Typical consequence:

$$\langle \phi_j, [G, [H, G]] \phi_j \rangle = \sum_{k: \lambda_k \neq \lambda_j} (\lambda_k - \lambda_j) |G_{kj}|^2$$

(Abstract version of Bethe’s sum rule)
A “sum rule” identity for $H=H^*$, $G=G^*$, if $J = \{\lambda_1, \ldots, \lambda_k\} \leq z \leq J^c$:

$$\frac{1}{2} \sum_{\lambda_j \in J} (z - \lambda_j)^2 \langle [G, [H, G]] \phi_j, \phi_j \rangle - \sum_{\lambda_j \in J} (z - \lambda_j) \| [H, G] \phi_j \|^2 = \sum_{\lambda_j \in J} \sum_{\lambda_k \in J^c} (z - \lambda_j)(z - \lambda_k)(\lambda_k - \lambda_j) | \langle G \phi_j, \phi_k \rangle |^2$$

For $J = \{\lambda_1 \ldots \lambda_n\}$, the right side $\leq 0!$
Basic ideas of the strategy

1. There is an exact identity involving traces including $[G, [H, G]]$ and $[H,G]*[H,G]$.

2. For the lower part of the spectrum it implies an inequality of the form:

$$\sum (z - \lambda_k)^2 (...) \leq \sum (z - \lambda_k) (...)$$
1. A good choice of G for the Laplacian is a coordinate function, because
   a) \([H,G] = -2 \frac{\partial}{\partial x_k},\) and
   b) \([G, [H, G]] = 2\)

2. For Schrödinger, sum rules connect eigenvalues with the kinetic energy.

3. Spectral information can be extracted from Riesz means with classical transforms.
**Dirichlet problem:**

*Trace identities imply differential inequalities*

\[ R_2(z) \leq \frac{4}{d} \sum_k (z - \lambda_k) T_k \]

Harrell-Hermi JFA 08: Laplacian

\[
\left(1 + \frac{4}{d}\right) R_2(z) - \frac{2z}{d} R_2'(z) \leq 0.
\]

Consequences – universal bound for \( k \geq j \):
Essentially all the universal eigenvalue relations for the Laplace problem are implied by sum-rule identities.
Quantum graphs

(With S. Demirel, Stuttgart) For which graphs is:

\[ R_{\sigma}(z) \leq L_{\sigma,1}^{cl} \int_{\Gamma} (V(x) - z)^{\sigma+1/2} \, dx \]

(Concentrate on \( \sigma=2 \).)
ON SEMICLASSICAL AND UNIVERSAL INEQUALITIES FOR EIGENVALUES OF QUANTUM GRAPHS

SEMRA DEMIREL AND EVANS M. HARRELL II

ABSTRACT. We study the spectra of quantum graphs with the method of trace identities (sum rules), which are used to derive inequalities of Lieb-Thirring, Payne-Pólya-Weinberger, and Yang types, among others. We show that the sharp constants of these inequalities and even their forms depend on the topology of the graph. Conditions are identified under which the sharp constants are the same as for the classical inequalities; in particular, this is true in the case of trees. We also provide some counterexamples where the classical form of the inequalities is false.
Quantum graphs

1. A graph (in the sense of network) with a 1-D Schrödinger operator on the edges: connected by “Kirchhoff conditions” at vertices. Sum of outgoing derivatives vanishes.
Quantum graphs

Is this one-dimensional or not? Does the topology matter?
Quantum graphs are $L-T$ one-dimensional for:

1. Trees.
2. Scottish tartans (infinite rectangular graphs):
Quantum graphs are L-T one-dimensional for:

1. Trees.
2. Infinite rectangular graphs.
3. Bathroom tiles, a.k.a. honeycombs, etc.:
Quantum graphs:

1. But not balloons! (A.k.a. tadpoles, or... )
Quantum graphs:

1. But not balloons! (A.k.a. tadpoles, or...) 

Put a soliton potential on the loop:

\[ V = \frac{-2a^2}{\cosh^2(ax)} \chi_{\text{loop}} \]

\[ \phi = \frac{\cosh(aL)}{\cosh(ax)} \text{ resp. } e^{-ax} \]

\[ \lambda_1 = -a^2 \text{ solves a transcendental equation, but } \frac{|\lambda_1|^\sigma}{\int |V|^\sigma + 1/2} \text{ is exactly determined!} \]
Quantum graphs

1. But not balloons! (A.k.a. tadpoles, or...)

$\rho = 3/2$: ratio is $3/11$ vs. $L^{\text{cl}} = 3/16$.

$\rho = 2$: ratio is messy expression $0.20092...$ vs. $L^{\text{cl}} = 8/(15\pi) = 0.169765...$
Quantum graphs

For which finite graphs is:

\[
\frac{\lambda_k}{\lambda_j} \leq \frac{4 + d}{2 + d} \left( \frac{k}{j} \right)^{2/d} \ ?
\]

e.g., is \( \lambda_2 / \lambda_1 \leq 5? \)
Quantum graphs

1. Trees.
2. Rectangular graphs/bathroom tiles with external edges:
Quantum graphs

- But not balloons!

\[ \frac{\lambda_2}{\lambda_1} \approx \frac{\pi - \arctan(1/\sqrt(2))}{\arctan(1/\sqrt(2))} \approx 16.8 \]
Quantum graphs

- Fancy balloons can have arbitrarily large $\lambda_2/\lambda_1$. 
Why?

If we can establish the analogue of the trace inequality,

\[ R_\rho(z) - \alpha \frac{2\rho}{d} \sum (z - \lambda_k)^{\rho-1} \|\nabla \phi_k\|^2 \leq 0, \]

then all the rest of the inequalities follow (LT, PPW, ratios, statistics, etc.), sometimes with modifications.

Calculate commutators with a good G.
When does a quadratic inequality hold?

If the graph can be covered by a family of transits where on each edge $G' = \text{cst}$, and for each edge there is some $G$ where this constant is not 0, then

$$\sum_j (z - \lambda_j)^+ - 4\epsilon \frac{a_{\text{max}}}{a_{\text{min}}} (z - \lambda_j)^+ + \| \phi'_j \|^2 \leq 0.$$
When does a quadratic inequality hold?

- Conjecture: This is possible unless the graph can be disconnected from all leaves by removal of one point, or contains a “Wheatstone bridge”
Some take-away messages

1. On quantum graphs, sum rules reflect the topology.

2. The QG is spectrally one-dimensional if the graph can be covered uniformly by a family of functions that resemble coordinate functions as much as possible.

3. This is not always possible: Connected with a question of classical circuit theory.

4. Full understanding of role of topology is open.
Articles related to this seminar

- E.M. Harrell, Commutators, eigenvalue gaps, and mean curvature in the theory of Schrödinger operators, Communications PDE, 2007
- E.M. Harrell and J. Stubbe, Trace identities for eigenvalues, with applications to periodic Schrödinger operators and to the geometry of numbers, Trans. AMS, to appear.