Semiclassical estimates of eigenvalues of quantum Hamiltonians arising in nanophysics

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Discrete spectra of Laplace and Schrödinger operators.

\[
H = -\frac{\hbar^2}{2m} \Delta + V(x)
\]

\[
H \phi_k = \lambda_k \phi_k
\]
Semiclassical limits

1. $\lambda_k \rightarrow \infty$

2. $H = \varepsilon T + V(x)$,

($\varepsilon$ small)
“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:

$$\lambda_{n+1} - \lambda_n \leq \frac{4}{d} \frac{1}{n} \sum_{k=1}^{n} \lambda_k$$
“Universal” constraints on the spectrum

- Harrell 1993-present, commutator approach; with Michel, Stubbe, El Soufi and Ilias, Hermi, Yildirim.
“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

\[ \sum_{j=1}^{k} \lambda_j \geq \frac{d}{d + 2} \frac{4\pi^2 \kappa^{1+2/d}}{(C_d |\Omega|)^{2/d}} \]
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
Stubbe’s proof of sharp Lieb-Thirring for $\rho \geq 2$  (JEMS, in press)
1. A trace formula ("sum rule") of Harrell-Stubbe ‘97, for $H = -\varepsilon\Delta + V$:

$$R_\rho(z) := \sum (z - \lambda_k)_+^{\rho};$$

$$R_\rho(z) - \varepsilon \frac{2\rho}{d} \sum (z - \lambda_k)_+^{\rho-1} \|\nabla \phi_k\|^2 = \text{explicit expr} \leq 0.$$
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2. $T_k := \langle \phi_k, -\Delta \phi_k \rangle$
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2. $T_k := \langle \phi_k, -\Delta \phi_k \rangle = \frac{d\lambda_k}{d\varepsilon}$ (Feynman-Hellman)
Lieb-Thirring inequalities

Thus

\[ R_\rho(z, \epsilon) \leq -\frac{2\epsilon}{d} \frac{\partial R_\rho(z, \epsilon)}{\partial \epsilon}, \]

or:

\[ \frac{\partial}{\partial \epsilon} \left( \epsilon^{\frac{d}{2}} R_\rho(z, \epsilon) \right) \leq 0, \]

and classical Lieb-Thirring is an immediate consequence!

Recall:

\[ \lim_{\epsilon \to 0^+} \epsilon^{\frac{d}{2}} \sum_{\lambda_j(\epsilon) < 0} |\lambda_j(\epsilon)|^\rho = L_{\rho,d} \int |V(x)|^{\rho + \frac{d}{2}} \]
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.?
Sum Rules

1. Observations by Thomas, Reiche, Kuhn of regularities in atomic energy spectra.
2. Heisenberg, 1925, Showed TRK purely algebraic, following from noncommutation of operators.
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)
The only assumptions are that $H$ and $G$ are self-adjoint, and that the eigenfunctions are a complete orthonormal sequence. (If continuous spectrum, need a spectral integral on right.)
Or even without $G=G^*$:

\[
\frac{1}{2} \sum_{\lambda_j \in J} (z - \lambda_j)^2 \left( \langle [G^*, [H, G]] \phi_j, \phi_j \rangle + \langle [G, [H, G^*]] \phi_j, \phi_j \rangle \right) \\
- \sum_{\lambda_j \in J} (z - \lambda_j) \left( \langle [H, G] \phi_j, [H, G] \phi_j \rangle + \langle [H, G^*] \phi_j, [H, G^*] \phi_j \rangle \right) \\
= \\
\sum_{\lambda_j \in J} \sum_{\lambda_k \notin J} (z - \lambda_j)(z - \lambda_k)(\lambda_k - \lambda_j) \left( |\langle G \phi_j, \phi_k \rangle|^2 + |\langle G^* \phi_j, \phi_k \rangle|^2 \right),
\]
Or even without $G = G^*$:

\[
\frac{1}{2} \sum_{\lambda_j \in J} (z - \lambda_j)^2 \left( \langle[G^*, [H, G]]\phi_j, \phi_j \rangle + \langle[G, [H, G^*]]\phi_j, \phi_j \rangle \right)
\]

\[
- \sum_{\lambda_j \in J} (z - \lambda_j) \left( \langle[H, G]\phi_j, [H, G]\phi_j \rangle + \langle[H, G^*]\phi_j, [H, G^*]\phi_j \rangle \right)
\]

\[
= \sum_{\lambda_j \in J} \sum_{\lambda_k \notin J} (z - \lambda_j)(z - \lambda_k)(\lambda_k - \lambda_j) \left( |\langle G\phi_j, \phi_k \rangle|^2 + |\langle G^*\phi_j, \phi_k \rangle|^2 \right),
\]

For $J = \{\lambda_1 \ldots \lambda_n\}$, the right side $\leq 0$!
What should you remember about trace formulae/sum rules in a short seminar?
Take-away messages #1

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:

\[
\sum (z - \lambda_k)^2 (...) \leq \sum (z - \lambda_k) (...) 
\]

3. ***Once this quadratic inequality is proved, the “usual correlaries,” including universal bounds and Lieb-Thirring, follow.
What is a good choice of $G$?

Ans: A Cartesian coordinate function, because

a) $[H, G] = -2 \frac{\partial}{\partial x_k}$, and

c) $[G, [H, G]] = 2$
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 \( k > j \):

\[
\frac{\overline{\lambda}_k}{\lambda_j} \leq \frac{4 + d}{2 + d} \left( \frac{k}{j} \right)^{2/d}
\]
How to get information about eigenvalues from information on Riesz means?

Riesz means are related to

• sums of eigenvalues by Legendre transform

• partition functions by Laplace transform
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.
Some models in nanophysics:

1. Schrödinger operators on curves and surfaces embedded in space. *Quantum wires and waveguides.*
3. Quantum graphs. *Nanoscale circuits*
In each of the four models there are new features in the trace inequality.

1. Schrödinger operators on curves and surfaces. *Explicit curvature terms.*
2. Periodic Schrödinger operators. *Geometry of the dual lattice.*
3. Quantum graphs. *Topology*
Quadratic sum rule with curvature

- A good choice of $G = x_k$, a Euclidean coordinate from $\mathbb{R}^d$ restricted to the submanifold.
Quadratic sum rule with curvature

• A good choice of $G = x_k$, a Euclidean coordinate from $\mathbb{R}^d$ restricted to the submanifold.

• There are messy terms, but when you sum the trace identity over $k = 1\ldots d$, magical cancellations occur.
Quadratic sum rule with curvature

- A good choice of $G = x_k$, a Euclidean coordinate from $\mathbb{R}^d$ restricted to the submanifold.

- There are messy terms, but when you sum the trace identity over $k = 1...d$, magical cancellations occur.

- Since there are second derivatives of $x_k$, there is a curvature contribution that doesn’t go away.
Quadratic sum rule with curvature

\[ R_2(z) \leq \frac{4}{d} \sum (z - \lambda_k)_+ T_k, \]

where now

\[ T_k := \left\langle \varphi_k, \left( -\Delta + \frac{(\sum_j \kappa_j)^2}{4} \right) \varphi_k \right\rangle \]
An interesting model

\[ H_g := -\Delta + g \left( \sum_j \kappa_j \right)^2 \]
Quadratic sum rule with curvature

Sum rules imply universal bounds on eigenvalue gaps for Schrödinger operators on closed submanifolds in terms of the lower spectrum. Let

$$\delta := \sup_M \frac{(\sum \kappa_j)^2}{4} - V(x)$$

All the same results with this systematic shift!
An explicit calculation shows that the bound is sharp for the non-zero eigenvalue gaps of the sphere, for which all the eigenvalues are known and elementary [20]: For simplicity, assume that $d = 2, g = \frac{1}{4}$, and that $M$ is the sphere of radius 1 embedded in $\mathbb{R}^3$. Then $h = 2, \sigma = 1$, and:

$$\lambda_1 = 1; \lambda_2 = \lambda_3 = \lambda_4 = 3; \ldots; \lambda_{(m-1)^2+1} = \ldots = \lambda_m = m^2 - m + 1.$$

For $n = m^2$, the calculation shows that $\overline{\lambda_n} = \frac{n+1}{2}$, and $\overline{\lambda_n^2} = \frac{n^2+n+1}{3}$. Hence $D_n = n$, and b) informs us that

$$2\overline{\lambda_m} - m = m^2 - m + 1 \leq \lambda_m = m^2 - m + 1$$

$$\leq \lambda_{m+1} = m^2 + m + 1 \leq 2\overline{\lambda_m} + m = m^2 + m + 1,$$

and thus $\lambda_m$ equals the lower bound $2\overline{\lambda_m} - m$ and $\lambda_{m+1}$ equals the upper bound $2\overline{\lambda_m} + m$. 
What about Lieb-Thirring?
What about Lieb-Thirring?

Can establish a quadratic “Yang-type inequality, either by commuting with coordinate functions, or by commuting with unitary operators

\[ G = \exp(i z.x) \]

(use modified trace identity).

Because of the curvature terms, the natural L-T inequality is not in reference to energy 0.

Harrell-Stubbe TAMS to appear
What about Lieb-Thirring?

Similar results for periodic Schrödinger. There is a shift reflecting the periodicity lattice, analogous to the mean curvatures.

Geometrically, the periodicities are connected with the curvature necessary to embed a torus in Euclidean space.
What about Lieb-Thirring?

For semiclassics we need a partial differential inequality:

$$\frac{\partial}{\partial \epsilon} \left( \epsilon^{d/2} R_2(z, \epsilon) \right) \leq \frac{gd}{2} \epsilon^{d/2} R_1(z, \epsilon)$$

$$\partial R_2 / \partial z = 2R_1$$

Harrell-Stubbe TAMS to appear
What about Lieb-Thirring?

\[ U(z, \epsilon) := \epsilon^{d/2} R_2(z, \epsilon) \]

\[ \frac{\partial U}{\partial \epsilon} \leq \frac{gd}{4} \frac{\partial U}{\partial z} \]

\[ \xi := \epsilon - \frac{4}{gd} z \quad \frac{\partial U}{\partial \xi} \leq 0 \]

(gd reflects the curvature (= sup h\^2) or, resp. periodicity.)
What about Lieb-Thirring?

For all $\epsilon > 0$ the mapping

$$\epsilon \mapsto \epsilon^{\frac{d}{2}} R_\sigma(z - \frac{\epsilon gd}{4}) = \epsilon^{\frac{d}{2}} \sum (z - \frac{\epsilon gd}{4} - \lambda_j)_+^\sigma$$

is nonincreasing, and therefore for all $z \in \mathbb{R}$ and all $\epsilon > 0$ the following sharp Lieb-Thirring inequality holds:

$$R_\sigma(z, \epsilon) \leq \epsilon^{-d/2} L^{cl}_{\sigma,d} \int_M \left(V(x) - \left(z + \frac{gd}{4\epsilon}\right)\right)^{\sigma + d/2}_{-} \, dx.$$
Extension of Reilly’s inequality (with El Soufi-Ilias)

\[ \lambda_k \leq C(d, k) \| h \|_\infty^2 \]
Take-away messages #3

1. On manifolds, sum rules involve mean curvature in an explicit way

2. Sharp for spheres where potential $= g \ h^2$.


4. Each eigenvalue dominated by mean curvature.
(With S. Demirel, Stuttgart) For which graphs the one-D L-T inequality

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

valid? (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 satisfy the expected one-dimensional LT and universal inequalities for:

1. Trees.
**Quantum graphs satisfy the expected one-dimensional LT and universal inequalities for:**

1. Trees.

2. Scottish tartans (infinite rectangular graphs):

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Quantum graphs satisfy the expected one-dimensional LT and universal inequalities 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...)

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Quantum graphs:

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

Put a soliton potential on the loop:

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

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

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Put a soliton potential on the loop:

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\[ \lambda_1 = -a^2 \] solves a transcendental equation, but

\[ \frac{|\lambda_1|^\sigma}{\int |V|^\sigma + 1/2} \] 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

• Not balloons!

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

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

$$\sum_j (z - \lambda_j)_+ - 4\epsilon \frac{a_{\max}}{a_{\min}} (z - \lambda_j)_+ \|\phi_j'\|^2 \leq 0.$$
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”
Take-away messages #4

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.