Sum rules and semiclassical limits for the spectra of some elliptic PDEs and pseudodifferential operators

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Laplace, Beltrami, and Schrödinger. $T = -\Delta = -\nabla^2 := \sum_{\alpha=1}^d \frac{\partial^2}{\partial x_{\alpha}^2}$ $\langle \phi, T\phi \rangle = \int_{\Omega} |\nabla \phi|^2$ H = T + V(x)





A Schrödinger operator with correct physical numbers.

H

 $-\frac{\hbar^2}{2m}\Delta + V(\mathbf{x})$

A Schrödinger operator with correct physical numbers.

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

 $\hbar = 6.62606896... \times 10^{-34} \text{ J-s}$ m = 9.10938215...×10⁻³¹ kg

The coefficient ε of the Laplacian is not large.

Various "semiclassical limits

+Let \hbar or equivalently ϵ tend to 0.

+ Put a large parameter in front of V.

+ Consider high energies (k large for λ_k).

+ Consider many particles, like 10²⁹.



Mathematical motivation:

Not just any sequence of positive numbers can be the spectrum of the Dirichlet Laplacian on a bounded domain. Similarly for plausible spectra of Schrödinger Operators. Laplace eigenvalues - domains in R^d

n

1	1	1	1	1	52.638	1	5.6313	1	5.7855	1	5.784	1	
2	1.438	1.43	1.404	1.435	122.82	2.3333	7.1815	1.2753	30.484	5.2689	14.684	2.5387	
3	2.04	2.027	1.961	2.037	210.55	4	12.791	2.2713	74.917	12.949	14.684	2.5387	
4	2.571	2.548	2.442	2.577	228.1	4.3333	13.094	2.3251	139.1	24.042	26.378	4.5605	
5	2.854	2.823	2.861	2.86	333.37	6.3333	17.068	3.0309	223.02	38.548	26.378	4.5605	
6	3.623	3.57	3.506	3.633	368.47	7	18.854	3.348	326.7	56.468	30.47	5.268	
7	4.184	4.153	3.924	4.18	473.74	9	19.851	3.5251	450.12	77.8	40.704	7.0373	
8	4.554	4.507	4.452	4.557	491.29	9.3333	24.18	4.2939	593.28	102.55	40.704	7.0373	
9	4.861	4.811	4.582	4.866	543.92	10.333	27.538	4.8901	756.2	130.71	49.224	8.5104	
10	5.15	5.095	5.279	5.148			30.01	5.3291	938.86	162.28	49.224	8.5104	
11				5.646									
12				6.27									
13				6.653									
14				6.984									
15				7.506									
16				8.247									
17				8.393									
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	Even-Pleransky 1999 tangrams			Sridhar- Cureton-Kuttle tangram equ. Triangle			Driscoll 1997 tangram 2		Grinfeld 128-gon	Strang			

Laplace eigenvalues - domains in R^d

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Laplace eigenvalues - domains in R^d

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27 28 29

1.435 122.82 2.3333 7.1815 1.2753 30.484 5.269 14.684 2.5387 2 1.438 1.43 1.404 3 2.04 2.027 1.961 2.037 210.55 2.571 2.548 2.442 2.577 228.1 4.3333 13.094 2.3251 139.1 24.04 26.378 4.5605 4 5 2.854 2.823 2.861 2.86 333.37 6.3333 17.068 3.0309 223.02 38.55 26.378 4.5605 6 3.623 3.57 3.506 3.633 368.47 7 4.184 4.153 3.924 4.18 473.74 4.507 4.452 4.557 491.29 9.3333 24.18 4.2939 593.28 102.5 40.704 7.0373 8 4.554 9 4.861 4.811 4.582 4.866 543.92 10.333 27.538 4.8901 756.2 130.7 49.224 8.5104 5.279 5.095 5.148 10 5.15 11 5.646 12 6.27 13 6.653 14 6.984 15 7.506 8.247 16 8.393 17 18 8.766 19 9.367 20 9.691 21 9.779

1

But according to the Ashbaugh-Benguria Theorem,

30.01 5.3291 938.86 162.3 49.224 8.5104

 $\lambda_2 / \lambda_1 \le 2.5387...!$

1 5.7855

9 19.851 3.5251 450.12

4 12.791 2.2713 74.917 12.95 14.684 2.5387

7 18.854 3.348 326.7 56.47 30.47 5.268

1 5.784

77.8 40.704 7.0373

1

(ln 2 D)

d=2 Even-Pieransky 1999 tangrams

d=2d=2 Sridhar- Cureton-Kuttler Driscoll 1997 tangram equ. Triangle tangram 2

1 52.638

10.3

10.83

11.136

11.697

d=2

1

1 5.6313

d=2 unit disc Grinfeld Strang 128-gon

Table (24) shows our estimates for the first ten simple eigenvalues on the regular 128-sided polygon.

Aha!

"Universal" constraints on the spectrum

P

+ H. Weyl, 1910, Laplace, $\lambda_n \sim n^{2/d}$

"Universal" constraints on the spectrum F. Weyl, 1910, Laplace, λ_n ~ n^{2/d} *W. Kuhn*, *F. Reiche*, *W. Thomas*, *W. Heisenberg*, 1925, *"sum rules" for atomic energies*.

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 $\frac{1}{dn} \sum_{n \neq \infty} \sum_{n$

 W. Kuhn, F. Reiche, W. Thomas, W. Heisenberg, 1925, "sum rules" for atomic energies.

 L. Payne, G. Pólya, H. Weinberger, 1956: The gap is controlled by the average of the smaller eigenvalues:

"Universal" constraints on the spectrum

 Ashbaugh-Benguria 1991, isoperimetric conjecture of PPW proved.

- H. Yang 1991, unpublished, formulae like PPW, respecting Weyl asymptotics for the first time.
- Harrell 1993-present, commutator approach; with Michel, Stubbe, El Soufi and Ilias, Hermi, Yildirim.
- Ashbaugh-Hermi, Levitin-Parnovsky, Cheng-Yang, Cheng-Chen, some others.

"Universal" constraints on the spectrum with phase-space volume. Lieb -Thirring, 1977, for Schrödinger

$$\epsilon^{\mathbf{d}/\mathbf{2}} \sum_{\lambda_{\mathbf{j}}(\epsilon) < \mathbf{0}} |\lambda_{\mathbf{j}}(\epsilon)|^{
ho} \leq \mathbf{L}_{
ho, \mathbf{d}} \int\limits_{\mathbf{R}^{\mathbf{d}}} (\mathbf{V}_{-}(\mathbf{x}))^{
ho + \mathbf{d}/\mathbf{2}} \, \mathbf{dx}$$

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

$$\sum_{j=1}^{k} \lambda_j \ge \frac{d}{d+2} \frac{4\pi^2 k^{1+2/d}}{(C_d |\Omega|)^{2/d}}$$

1. A trace formula ("sum rule") of Harrell-Stubbe '97, for H = - $\varepsilon \Delta$ + V:

$$\mathbf{R}_{\rho}(\mathbf{z}) := \sum \left(\mathbf{z} - \lambda_{\mathbf{k}}\right)_{+}^{\rho};$$

 $\mathbf{R}_{\rho}(\mathbf{z}) - \epsilon \frac{2\rho}{\mathbf{d}} \sum \left(\mathbf{z} - \lambda_{\mathbf{k}} \right)_{+}^{\rho-1} \| \nabla \phi_{\mathbf{k}} \|^{2} = \text{explicit expr} \leq \mathbf{0}.$

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2. $T_k := \langle \phi_k, -\Delta \phi_k \rangle$

1. A trace formula ("sum rule") of Harrell-Stubbe '97, for H = - $\varepsilon \Delta$ + V:

$$\mathbf{R}_{\rho}(\mathbf{z}) := \sum (\mathbf{z} - \lambda_{\mathbf{k}})_{+}^{\rho};$$

 $\begin{aligned} \mathbf{R}_{\rho}(\mathbf{z}) &- \epsilon \frac{2\rho}{\mathbf{d}} \sum \left(\mathbf{z} - \lambda_{\mathbf{k}} \right)_{+}^{\rho-1} \| \nabla \phi_{\mathbf{k}} \|^{2} = \text{explicit expr} \leq \mathbf{0}. \\ \mathbf{2.} \quad T_{k} := \left\langle \phi_{k}, -\Delta \phi_{k} \right\rangle = \frac{d\lambda_{k}}{d\epsilon} \quad \text{(Feynman-Hellman)} \end{aligned}$

Lieb-Thirring inequalities

Thus

$$\mathbf{R}_{
ho}(\mathbf{z},\epsilon) \leq -rac{2\epsilon}{\mathbf{d}}rac{\partial \mathbf{R}_{
ho}(\mathbf{z},\epsilon)}{\partial \epsilon},$$

or:

$$\frac{\partial}{\partial \epsilon} \left(\epsilon^{\frac{\mathbf{d}}{2}} \mathbf{R}_{\rho}(\mathbf{z}, \epsilon) \right) \leq \mathbf{0},$$

and classical Lieb-Thirring is an immediate consequence! Recall:

$$\lim_{\epsilon \to 0^+} \epsilon^{\frac{d}{2}} \sum_{\lambda_j(\epsilon) < 0} |\lambda_j(\epsilon)|^{\rho} = L_{\rho,d} \int |V_{\mathbf{x}}|^{\rho + \frac{d}{2}}$$

Some models in nanophysics:

- 1. Schrödinger operators on curves and surfaces embedded in space. *Quantum wires and waveguides.*
- 2. Periodic Schrödinger operators. *Electrons in crystals*.
- 3. Quantum graphs. Nanoscale circuits
- 4. Relativistic Hamiltonians on curved surfaces. *Graphene*.

Are the spectra of these models controlled by "sum rules," like those known for Laplace/Schrödinger on domains or all of 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

 Used by Heisenberg in 1925 to explain regularities in atomic energy spectra

Sum Rules

 Observations by Thomas, Reiche, Kuhn of regularities in atomic energy spectra.
 Heisenberg, 1925, Showed TRK purely algebraic, following from noncommutation of operators.
 Bethe, 1930, other identities.

Commutators of operators

+ [H, G] := HG - GH + [H, G] ϕ_k = (H - λ_k) G ϕ_k + If H=H*, < ϕ_j , [H, G] ϕ_k > = (λ_j - λ_k) < ϕ_j , G ϕ_k >

Commutators of operators

[G, [H, G]] = 2 GHG - G²H - HG²
Etc., etc. Typical consequence:

$$\langle \phi_{\mathbf{j}}, [\mathbf{G}, [\mathbf{H}, \mathbf{G}]] \phi_{\mathbf{j}}
angle = \sum_{\mathbf{k}: \lambda_{\mathbf{k}} \neq \lambda_{\mathbf{j}}} (\lambda_{\mathbf{k}} - \lambda_{\mathbf{j}}) |\mathbf{G}_{\mathbf{k}\mathbf{j}}|^2$$

(Abstract version of Bethe's sum rule)

Riesz means

The counting function,
N(z) := #(λ_k ≤ z)
Integrals of the counting function, known as *Riesz means* (Safarov, Laptev, Weidl, etc.):

$$R_{
ho}(z) := \sum_{j} (z - \lambda_j)_+^{
ho}$$

Chandrasekharan and Minakshisundaram, 1952

1st and 2nd commutators (H-S '97)

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

$$\sum_{\lambda_j \in J} \sum_{\lambda_k \in J^c} \left(z - \lambda_j \right) (z - \lambda_k) (\lambda_k - \lambda_j) |\langle G\phi_j, \phi_k \rangle|^2$$

_

The only assumptions are that H and G are selfadjoint, 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*:

$$\begin{split} &\frac{1}{2}\sum_{\lambda_{j}\in J}(z-\lambda_{j})^{2}\left(\langle[G^{*},[H,G]]\phi_{j},\phi_{j}\rangle+\langle[G,[H,G^{*}]]\phi_{j},\phi_{j}\rangle\right)\\ &-\sum_{\lambda_{j}\in J}(z-\lambda_{j})\left(\langle[H,G]\phi_{j},[H,G]\phi_{j}\rangle+\langle[H,G^{*}]\phi_{j},[H,G^{*}]\phi_{j}\rangle\right)\\ &=\\ &\sum_{\lambda_{j}\in J}\sum_{\lambda_{k}\notin J}(z-\lambda_{j})(z-\lambda_{k})(\lambda_{k}-\lambda_{j})\left(|\langle G\phi_{j},\phi_{k}\rangle|^{2}+|\langle G^{*}\phi_{j},\phi_{k}\rangle|^{2}\right),\\ \end{split}$$

What you should remember about trace formulae/sum rules in a short seminar?

What you should remember about trace formulae/sum rules in a short seminar?

- 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:

 $\sum (z - \lambda_k)^2 (...) \leq \sum (z - \lambda_k) (...)$

Universal bounds for Dirichlet Laplacians

Payne-Pólya-Weinberger, 1956:

$$\lambda_{k+1} - \lambda_k \le \frac{4}{d} \frac{1}{k} \sum_{j=1}^k \lambda_j =: \frac{4}{d} \overline{\lambda_k}$$

Hile-Protter 1980:

$$1 \le \frac{4}{d} \frac{1}{k} \sum_{j=1}^{k} \frac{\lambda_j}{\lambda_{k+1} - \lambda_j}$$

Yang 1991:

$$\sum_{j=1}^{k} \left(\lambda_{k+1} - \lambda_j\right)^2 \le \frac{4}{d} \sum_{j=1}^{k} \lambda_j \left(\lambda_{k+1} - \lambda_j\right)^2$$

Universal Bounds with Commutators

Hile-Protter vs. sum rule (H-S '97):

$$1 = \frac{4}{d} \sum_{\substack{k:\lambda_k \neq \lambda_j}} \frac{|\langle u_k, \mathbf{p} u_j \rangle|^2}{\lambda_k - \lambda_j}$$
$$1 \le \frac{4}{d} \frac{1}{n} \sum_{\substack{k \le n}} \frac{\lambda_k}{\lambda_{n+1} - \lambda_k}$$

Dirichlet problem:

Trace identities imply differential inequalities

$$R_2(z) \le \frac{4}{d} \sum_k (z - \lambda_k) T_k$$

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:

$$\frac{\overline{\lambda_k}}{\overline{\lambda_j}} \le \frac{4+d}{2+d} \left(\frac{k}{j}\right)^{2/d}$$

Statistics of spectra

$\left(\left(1+\frac{2}{d}\right)\overline{\lambda_k}\right)^2 - \left(1+\frac{4}{d}\right)\overline{\lambda_k^2} \ge 0.$

A reverse Cauchy inequality:

The variance is dominated by the square of the mean.

Statistics of spectra

$$D_{k} := \left(\left(1 + \frac{2}{d} \right) \overline{\lambda_{k}} \right)^{2} - \left(1 + \frac{4}{d} \right) \overline{\lambda_{k}^{2}} \ge 0$$
$$\lambda_{k+1} \le \left(1 + \frac{2}{d} \right) \overline{\lambda_{k}} + \sqrt{D_{k}}.$$

 $\lambda_{k+1} - \lambda_k \le 2\sqrt{D_k}$

Riesz means are related to:

Riesz means are related to

• sums of eigenvalues by Legendre transform

Riesz means are related to

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• partition functions by Laplace transform

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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
- 4. Relativistic Hamiltonians. First-order ΨDO rather than second-order.

Klein-Gordon operators, a.k.a., generators of Cauchy processes

- 1. Motivated by graphene: electrons are relativistic, albeit with c/300.
- 2. On infinite R², H = Dirac operator or $(-\Delta + m^2)^{1/2}$ (Klein Gordon).
- 3. When there are edges, imposition of BC not natural from PDE point of view.

Eigenvalue inequalities for Klein-Gordon Operators

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Abstract

We consider the pseudodifferential operators $H_{m,\Omega}$ associated by the prescriptions of quantum mechanics to the Klein-Gordon Hamiltonian $\sqrt{|\mathbf{P}|^2 + m^2}$ when restricted to a bounded, open domain $\Omega \in \mathbb{R}^d$. When the mass m is 0 the operator $H_{0,\Omega}$ coincides with the generator of the Cauchy stochastic process with a killing condition on $\partial\Omega$. (The operator $H_{0,\Omega}$ is sometimes called the *fractional Laplacian* with power $\frac{1}{2}$, cf. [15].) We prove several universal inequalities for the eigenvalues $0 < \beta_1 < \beta_2 \leq \cdots$ of $H_{m,\Omega}$ and their means $\overline{\beta_k} := \frac{1}{k} \sum_{\ell=1}^k \beta_\ell$.

$$\sqrt{-\Delta + m^2}\varphi := \mathcal{F}^{-1}\sqrt{|\xi|^2 + m^2\widehat{\varphi}(\xi)}.$$

$$\exp\left(-\sqrt{-\Delta t}\right)\left[\varphi\right](\mathbf{x}) = p_0(t, \cdot) * \varphi,$$

$$p_0(t, \mathbf{x}) := \frac{c_d t}{(t^2 + |\mathbf{x}|^2)^{\frac{d+1}{2}}}$$

Definition of K-G:

Calculate the square root of - Δ + m², and *afterwards* restrict to Ω .

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Calculate the square root of - Δ + m², and *afterwards* restrict to Ω .

• Not the same as restricting to Ω with DBC and then taking square root by spectral methods!

$$\begin{aligned} \mathcal{C}omparison \ to \ the \ free \ Laplacian \\ \langle \varphi, H_{m,\Omega}^2 \varphi \rangle &= \|H_{m,\Omega} \varphi\|^2 = \int_{\Omega} \left| \mathcal{F}^{-1} \left(\sqrt{|\xi|^2 + m^2} \hat{\varphi} \right) \right|^2 \\ &= \int_{\mathbb{R}^d} \left| \chi_{\Omega} \mathcal{F}^{-1} \left(\sqrt{|\xi|^2 + m^2} \hat{\varphi} \right) \right|^2 \\ &\leq \int_{\mathbb{R}^d} \left| \mathcal{F}^{-1} \left(\sqrt{|\xi|^2 + m^2} \hat{\varphi} \right) \right|^2 \\ &= \int_{\mathbb{R}^d} \overline{\varphi} (-\Delta + m^2) \varphi \\ &= \int_{\Omega} \overline{\varphi} (-\Delta + m^2) \varphi, \end{aligned}$$

Therefore

$$\beta_k \le \sqrt{\lambda_k + m^2}.$$

Weyl asymptotic for $H_{\Omega,m}$

Proposition 3.1 As $\beta \to \infty$,

$$N(\beta) \sim \frac{|\Omega|}{(4\pi)^{d/2} \Gamma(1+d/2)} \beta^d.$$

Equivalently, as $k \to \infty$,

$$\beta_k \sim \sqrt{4\pi} \left(\frac{\Gamma(1+d/2)k}{|\Omega|} \right)^{1/d}$$

Among the inequalities proved are:

$$\overline{\beta_k} \ge \operatorname{cst.}\left(\frac{k}{|\Omega|}\right)^{1/a}$$

for an explicit, optimal "semiclassical" constant depending only on the dimension d. For any dimension $d \ge 2$ and any k,

$$\beta_{k+1} \le \frac{d+1}{d-1}\overline{\beta_k}.$$

Furthermore, when $d \ge 2$ and $k \ge 2j$,

$$\frac{\overline{\beta}_k}{\overline{\beta}_j} \le \frac{d}{2^{1/d}(d-1)} \left(\frac{k}{j}\right)^{\frac{1}{d}}$$

Finally, we present some analogous estimates allowing for an operator including an external potential energy field, i.e, $H_{m,\Omega} + V(\mathbf{x})$, for $V(\mathbf{x})$ in certain function classes.

Calculate first and second commutators:

$$\begin{aligned} H_{m,\Omega}, x_{\alpha}] \varphi &= (H_{m,\Omega} x_{\alpha} - x_{\alpha} H_{m,\Omega}) \varphi \\ &= \chi_{\Omega} \mathcal{F}^{-1} \sqrt{|\xi|^{2} + m^{2}} \mathcal{F}[x_{\alpha} \varphi] - \chi_{\Omega} x_{\alpha} \mathcal{F}^{-1}[\sqrt{|\xi|^{2} + m^{2}} \hat{\varphi} \\ &= \chi_{\Omega} \mathcal{F}^{-1} \left[\sqrt{|\xi|^{2} + m^{2}} \frac{\partial \hat{\varphi}}{\partial \xi_{\alpha}} - \frac{\partial}{\partial \xi_{\alpha}} (\sqrt{|\xi|^{2} + m^{2}} \hat{\varphi}) \right] \\ &= -i \chi_{\Omega} \mathcal{F}^{-1} \frac{\xi_{\alpha}}{\sqrt{|\xi|^{2} + m^{2}}} \hat{\varphi}. \end{aligned}$$

Similarly,

$$[x_{\alpha}, [H_{m,\Omega}, x_{\alpha}]]\varphi = \chi_{\Omega} \mathcal{F}^{-1} \left[\left(\frac{1}{\sqrt{|\xi|^2 + m^2}} - \frac{{\xi_{\alpha}}^2}{(|\xi|^2 + m^2)^{3/2}} \right) \hat{\varphi} \right]$$

Summing over coordinates:

$$(d-1)\sum_{j=1}^{n} (z-\beta_j)^2 \langle u_j, H_{m,\Omega}^{-1} u_j \rangle - 2\sum_{j=1}^{n} (z-\beta_j) \le 0,$$

provided $z \in [\beta_n, \beta_{n+1}]$

or, equivalently,

$$(d-1)\overline{\beta_n^{-1}}z^2 - 2dz + (d+1)\overline{\beta_n} \le 0.$$

$$\beta_{n+1} \le \frac{d+1}{(d-1)\overline{\beta_n^{-1}}} \le \frac{d+1}{d-1}\overline{\beta_n}.$$

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In particular,

$$\frac{\beta_2}{\beta_1} \le \frac{d+1}{d-1},$$

Corollary 2.4 For k > 2j, Eq. (2.24) implies $\frac{\overline{\beta}_k}{\overline{\beta}_j} \le \frac{d}{2^{1/d}(d-1)} \left(\frac{k}{j}\right)^{\frac{1}{d}}.$

Quantum graphs

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

 $\mathbf{R}_{\sigma}(\mathbf{z}) \leq \mathbf{L}^{\mathbf{cl}}_{\sigma,\mathbf{1}} \int_{\Gamma} \left(\mathbf{V}(\mathbf{x}) - \mathbf{z}
ight)^{\sigma+\mathbf{1/2}}_{-} \mathrm{d}\mathbf{x}?$

(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

 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 onedimensional for:



Quantum graphs are onedimensional for:

- 1. Trees.
- 2. Scottish tartans (infinite rectangular graphs):

Quantum graphs are onedimensional for:

1. Trees.

etc.:

- 2. Infinite rectangular graphs.
- 3. Bathroom tiles, a.k.a. honeycombs,

Quantum graphs:

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

Put soliton potential on the loop. $V = \frac{-2a^2}{\cosh 24ax}$ χ_{loop} $\phi = \begin{cases} e^{-ax_s} \\ \frac{\cosh(aL)}{\cosh(aX_s)} \end{cases}$ 02 7 = - a² solves a transcendental egn, 12,16 can be determined exactly! S/1/16+1/2 dx

Quantum graphs

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

 ρ = 3/2: ratio is 3/11 vs. L^{cl} = 3/16.

ρ = 2: ratio is messy expression 0.20092...
vs. L^{cl} = 8/(15 π) = 0.169765...
For which *finite* graphs is:

$$\frac{\overline{\lambda_k}}{\overline{\lambda_j}} \le \frac{4+d}{2+d} \left(\frac{k}{j}\right)^{2/d} ?$$

e.g., is $\lambda_2/\lambda_1 \leq 5$?



1. Trees.

2. Rectangular graphs/bathroom tiles with external edges:



But not balloons!



• Fancy balloons can have arbitrarily large λ_2/λ_1 .





Why?

If we can establish the analogue of the trace inequality,

$$\mathbf{R}_{\rho}(\mathbf{z}) - \alpha \frac{2\rho}{\mathbf{d}} \sum (\mathbf{z} - \lambda_{\mathbf{k}})_{+}^{\rho-1} \|\nabla \phi_{\mathbf{k}}\|^{2} \leq \mathbf{0},$$

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

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Calculate commutators with a good G.

Suppose G'is est meach edge and \$ > 6\$ preserver vertex conditione. (In stal case this means G contin., Zox. = 0 @V.) Sum rale becomes $\sum_{j=k}^{2} \left[(z-\lambda_{k})_{+}^{2} a_{j} \|\phi_{k}\|_{p}^{2} - 4a(z-\lambda_{j})_{+}^{2} a_{j} \|\phi_{k}\|_{p}^{2} \right]$ - · · · · L O $|G'(x)|^2 = a_j \text{ on } \prod_j C \prod_j$ Where

- <u>Laj (Z-) J 119/12 - 4x (Z-) 119/12</u> k=n X Can we find a family of such 6's and sum, so that we get $\sum_{i=1}^{n} (i - i)^2 - 4\pi(2 - i) 1|4'||^2) \leq 0$



Sharpest inequalities if $a_j a$ ways 1 or, equally good, $\Xi a_j^{(4)} \chi_{p_j} = 1$. I hen: $R_2(z) := \sum_{j} (z - \lambda_j)_+^2 \leq 4 \propto \sum_{j} (z - \lambda_j)_+^T$ RG(Z) 6 26x Z(Z-Xj)+ Tj, 622 $4 \frac{1}{2} (z - \lambda_j)_{+} T_j \frac{1}{2} 642$



Commutation for loops Use non-self-adjoint trace formula with $G = e^{i\varphi x_e}, \varphi = \frac{z\pi}{L}$ cend extend by a constant on exterior parts. $T_{j} \rightarrow T_{j} + \frac{19}{4}$ systematically weakening the inequality

THE END