Some geometric and topological inequalities arising in nanophysics

Evans Harrell

Georgia Tech

www.math.gatech.edu/~harrell

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2010 年 7 月30 日

Nanoelectronics

- Nanoscale = 10-1000 X width of atom
- Foreseen by Feynman in 1960s
- Laboratories by 1990.

Nanoelectronics

- Quantum wires
- Semi- and non-conducting “threads”
- Quantum waveguides

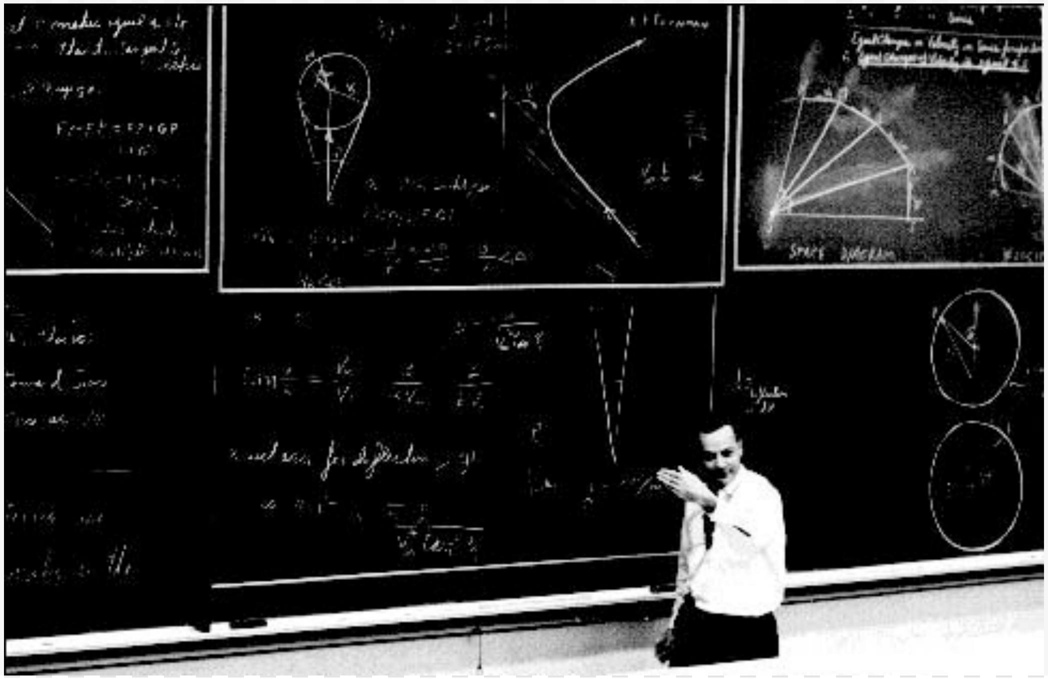
Simplified mathematical models

Some recent nanoscale objects

- Z.L. Wang, Georgia Tech, zinc oxide wire loop
- W. de Heer, Georgia Tech, carbon graphene sheets
- Semiconducting silicon quantum wires, H.D. Yang, Maryland
- UCLA/Clemson, carbon nanofiber helices
- UCLA, Borromean rings (triple of interlocking rings)
- Many, many more.

Quantum mechanics is not only weird, it's **hot**

- Nanotechnology
  - Foreseen by Feynman in 1959 at Cal Tech APS meeting:
    There's plenty of room at the bottom.



Quantum mechanics is not only weird, it's **hot**

- Nanotechnology
  - 1 nm = 10^{-9} m. The "nanoscale" refers to 1-100+ nm.
  - "Mesoscopic.": 1nm is about 10 hydrogen radii.
  - Laboratories by 1990

Quantum mechanics is not only weird, it's **hot**

Nanotechnology

- 1 nm = 10^{-9} m. The "nanoscale" refers to 1-100+ nm. "Mesoscopic."
- 1 nm is about 10 atomic radii
- Most viruses 30-200 nm
- Visible light has wavelength 400-800 nm
- Most bacteria 200-1000 nm (0.2-1 μm)
- Mammal cells 2-100 μm = 2000-100,000 nm
- Human hair 20-200 μm = 17,000-200,000 nm

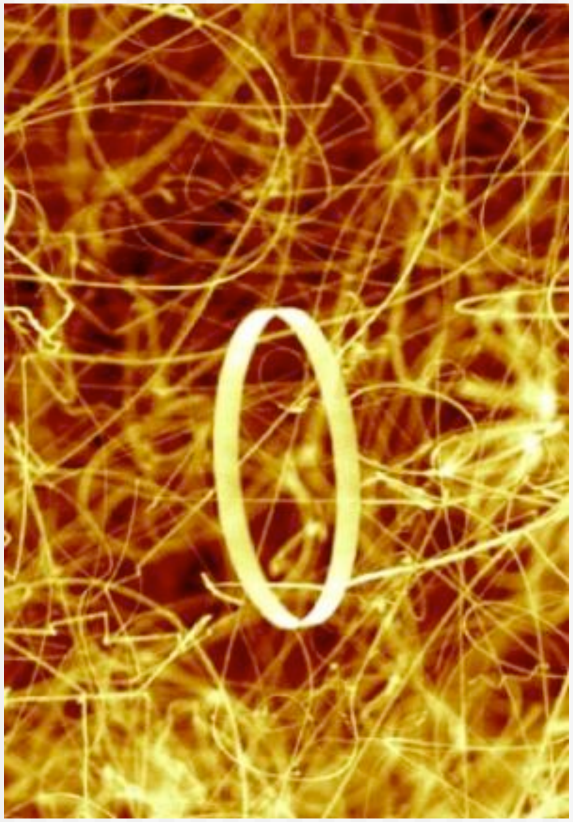
Quantum mechanics is not only weird, it's **hot**

- Nanotechnology
  - Electrical and electronic devices
    - Wires
    - Waveguides
    - Novel semiconductors
  - Motors and other mechanical devices
  - Medical applications
    - Drug delivery
    - Sensors
    - Surgical aids

Riedo, GT Physics, 2007. Lithography on polymers

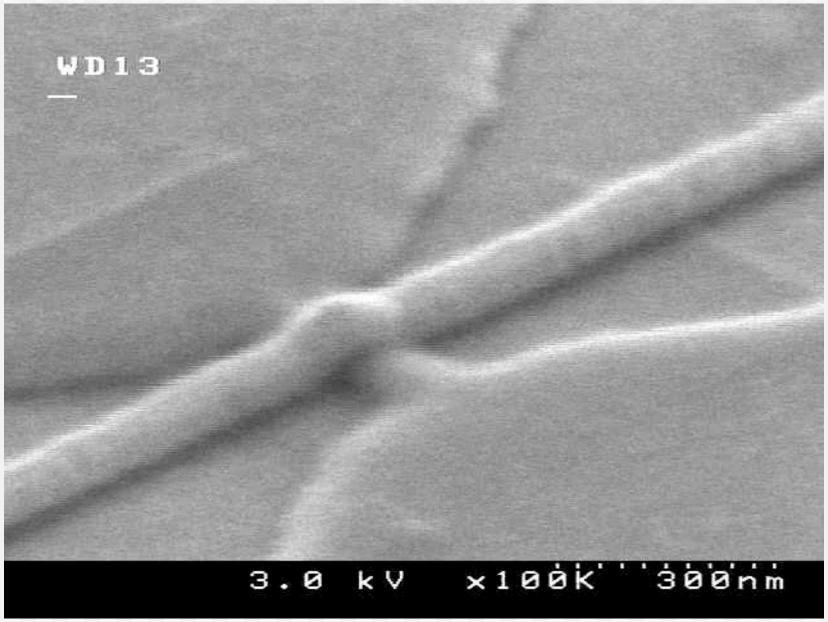
Zinc oxide quantum wire loop

- Z.L. Wang, Georgia Tech



Semiconductor quantum wire

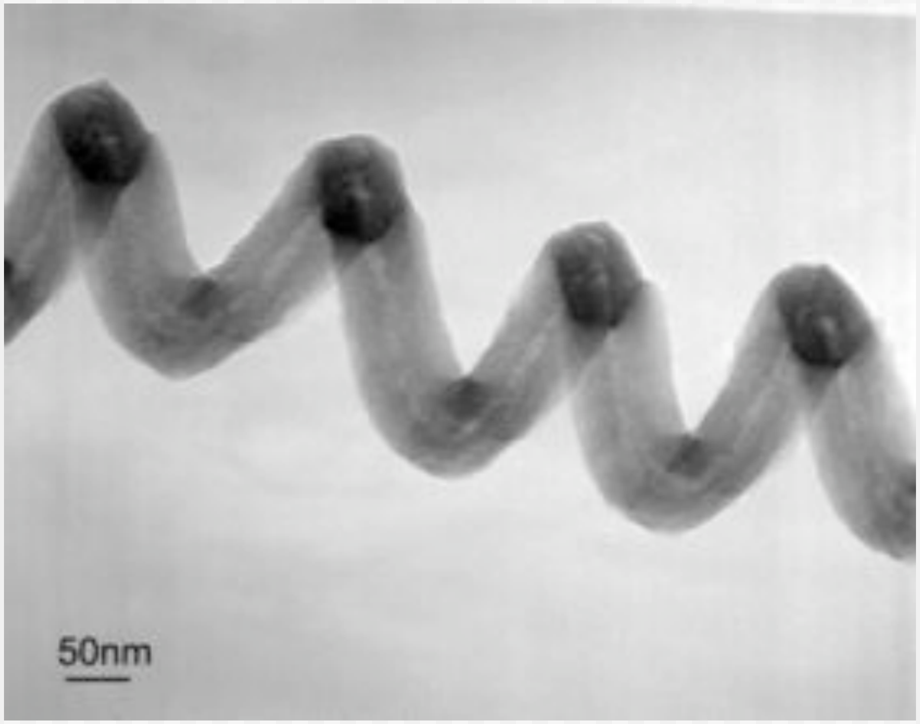
- H.D. Yang, UMD

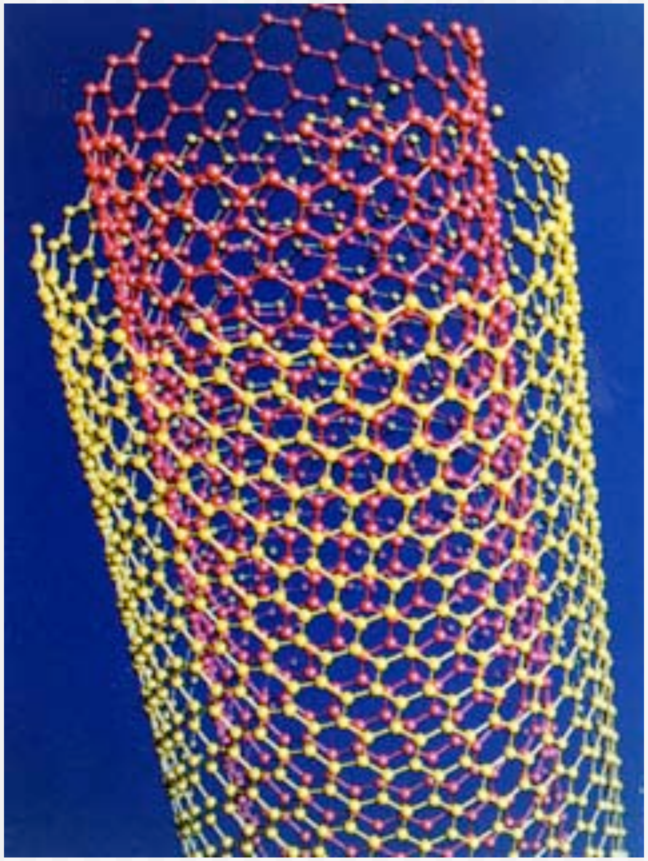


(silicon)

Carbon Nanofiber

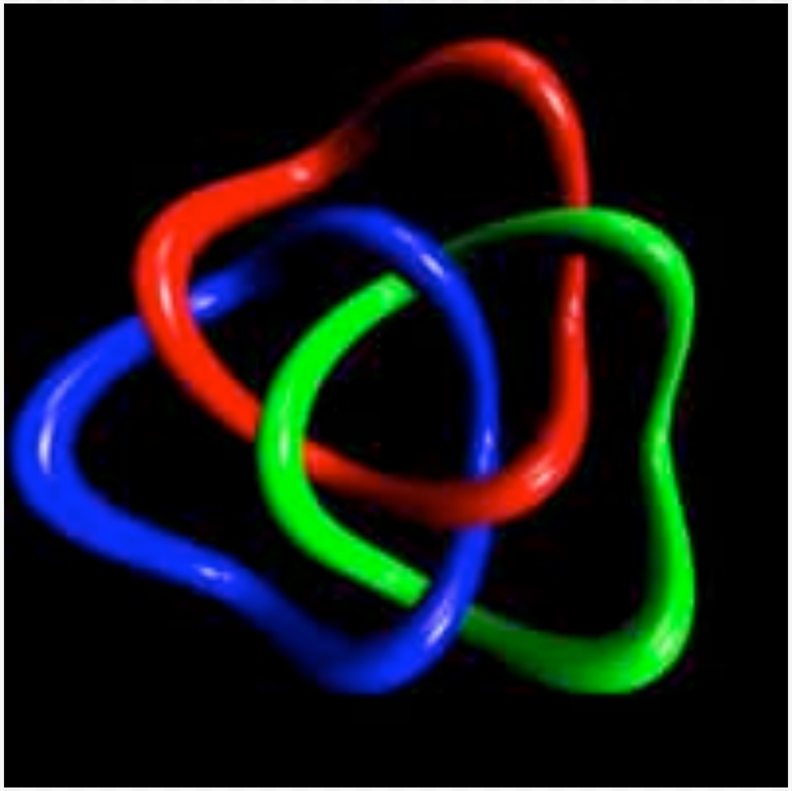
- UCSD/Clemson





Interlocking metallic rings

- UCLA Borromean rings, 2004, made of six metals. First modeled computationally, then made in the laboratory on nanoscale.

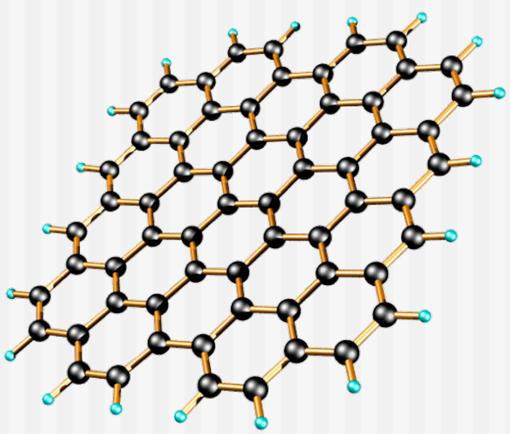


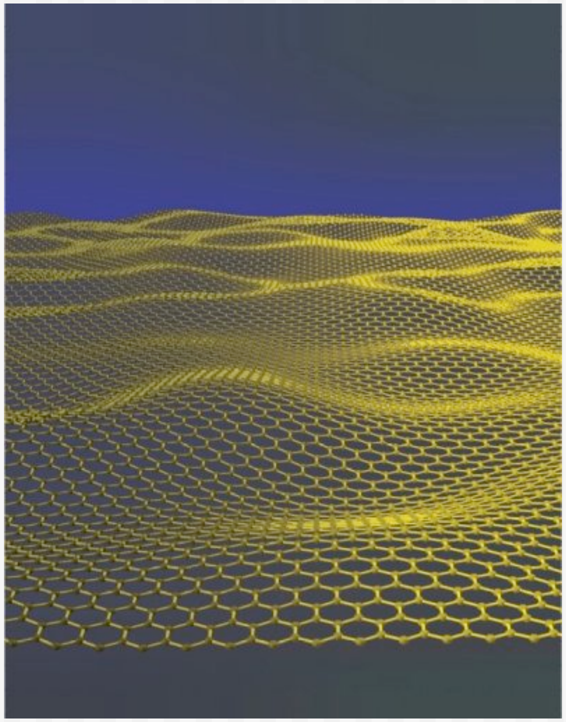
Quantum waveguides

Carbon graphene and other 2D materials.

Graphene is like graphite, but one atom thick.

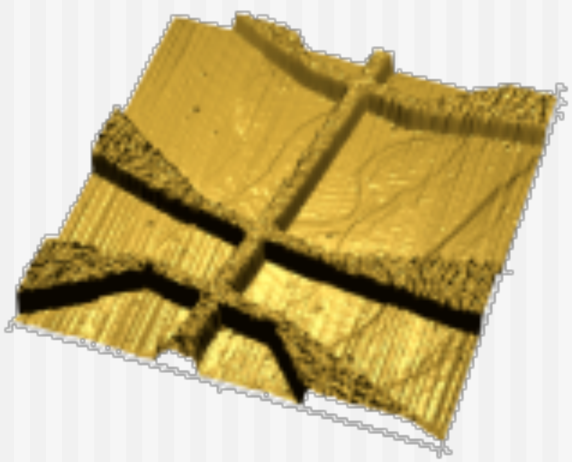
- W. de Heer, GT; A. Geim, Manchester, UK





Graphene transistors and circuit elements

- W. de Heer, GT MRSEC



Quantum wires and waveguides

- Electrons move "ballistically" except for being constrained to a narrow waveguide.

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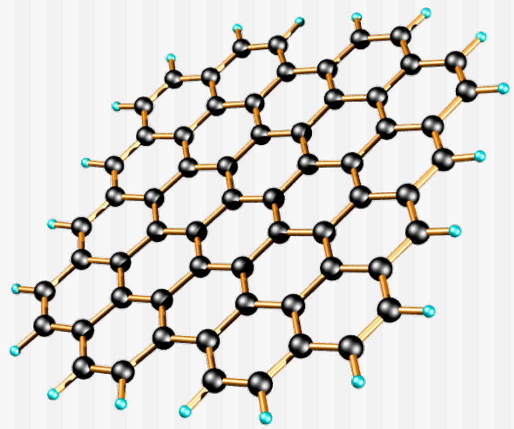
Quantum wires and waveguides

- Electrons move “ballistically” except for being constrained to a narrow waveguide.
- The only forces are the forces of constraint, and *these reflect essentially the geometry of the guide*.
- The problem of thin domains. How does a 3D PDE become 2D?

Graphene – an important new material

- How hard is it to make?



Graphene – an important new material

- How hard is it to make?

High-tech equipment for making graphene

Nanoelectronics

- Quantum wires
- Semi- and non-conducting “threads”
- Quantum waveguides

In simple but reasonable mathematical models, the Schrödinger equation responds to the geometry of the structure either through the boundary conditions or through an “effective potential.”

Graphene – Some physical properties

- Essentially a two dimensional surface
- Mean free path: 200-600 nm.
- Electrons act like massless relativistic particles but speed c/300.
- Semiconductors with 0 band gap.

Equilibrium shape of a charged thread

As a simple model, suppose the thread is a uniformly charged closed curve. We model the thread by a smooth function Γ: $R \rightarrow R^3$. $\Gamma(s)$ is a function of arc length. What is the equilibrium shape that minimizes the energy?

If the thread is flexible but not stretchable, it will seek the minimizing shape in a dissipating environment.

Some physical motivation: An electron near a charged thread

LMP 2006, with Exner and Loss

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$$

Fix the length of the thread. What shape binds the electron the least tightly? Conjectured for some years that answer is circle.

Reduction to an isoperimetric problem of classical type.

Is it true that:

$$\int_0^L |\Gamma(s+u) - \Gamma(s)|\,\mathrm{d}s \le \frac{L^2}{\pi} \sin \frac{\pi u}{L}$$

#2: An electromagnetic problem of classical type.

If a uniformly charged thread (deformable closed loop) is put into a tub of gelatin, what shape will it assume?

#2: An electromagnetic problem of classical type.

Minimize the expression:

$$\int_{C\times C} |\Gamma(s) - \Gamma(s')|^{-2} \, ds ds',$$

which after a change of variable requires minimizing the integral over u of

$$\int_C |\Gamma(s) - \Gamma(s+u)|^{-2} \, ds.$$

A family of isoperimetric conjectures for p > 0:

$$
\begin{aligned}
C_L^p(u): &\qquad \int_0^L |\Gamma(s+u)-\Gamma(s)|^p \,\mathrm{d}s \le \frac{L^{1+p}}{\pi^p}\sin^p \frac{\pi u}{L}\,, \\
C_L^{-p}(u): &\qquad \int_0^L |\Gamma(s+u)-\Gamma(s)|^{-p} \,\mathrm{d}s \ge \frac{\pi^p L^{1-p}}{\sin^p \frac{\pi u}{L}}\,,
\end{aligned}
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Right side corresponds to circle.

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\end{aligned}
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Right side corresponds to circle.

The case C^{-1} arises in an electromagnetic problem: minimize the electrostatic energy of a charged nonconducting thread.

Proposition. 2.1.

$$C_L^p(u) \;\; implies \;\; C_L^{p'}(u) \;\; if \; p \; > \; p' \; > \; 0.$$

$$C_L^p(u) \; implies \; C_L^{-p}(u)$$

First part follows from convexity of x → x^{a} for a > 1:

$$\begin{aligned}
\frac{L^{1+p}}{\pi^p}\sin^p\frac{\pi u}{L} \; &\geq \; \int_0^L \left(|\Gamma(s+u)-\Gamma(s)|^{p'}\right)^{p/p'} \mathrm{d}s \\
&\geq \; L\left(\frac{1}{L}\int_0^L |\Gamma(s+u)-\Gamma(s)|^{p'}\,\mathrm{d}s\right)^{p/p'} .
\end{aligned}$$

Proof when p = 2

$$\Gamma(s) = \sum_{0 \neq n \in \mathbb{Z}} c_n \, \mathrm{e}^{ins}$$

$$c_{-n} = \bar{c}_n \, .$$

$$\dot{\Gamma}(s) = i \sum_{0 \neq n \in \mathbb{Z}} n c_n \, \mathrm{e}^{ins} \, .$$

By assumption, $|\dot{\Gamma}(s)| = 1$, and hence from the relation

$$2\pi = \int_0^{2\pi} |\dot{\Gamma}(s)|^2 \, \mathrm{d}s = \int_0^{2\pi} \sum_{0\neq m\in\mathbb{Z}} \sum_{0\neq n\in\mathbb{Z}} nm \, c_m^* \cdot c_n \, \mathrm{e}^{i(n-m)s} \, \mathrm{d}s \,,$$

$$\sum_{0\neq n\in\mathbb{Z}} n^2 |c_n|^2 = 1 \,. \tag{2.5}$$

At first this appears to greatly weaken the condition that $\dot{\Gamma}$ is a unit vector for each s. However, since the case of equality in

$$(2\pi)^2 = \left(\int \left| \dot{\Gamma} \right| ds \right)^2 \leq 2\pi \int \left| \dot{\Gamma} \right|^2 ds$$

requires $\dot{\Gamma} = cst.a.e.$, in fact it is fully equivalent.

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$$\sum_{0\neq n\in\mathbb{Z}} n^2 |c_n|^2 = 1\,. \tag{2.5}$$

$$\int_0^{2\pi} \left| \sum_{0\neq n\in\mathbb{Z}} c_n \left(\mathrm{e}^{inu} - 1\right) \mathrm{e}^{ins} \right|^2 \mathrm{d}s = 8\pi \sum_{0\neq n\in\mathbb{Z}} |c_n|^2 \left(\sin\frac{nu}{2}\right)^2 ,$$

Inequality equivalent to

$$\sum_{0\neq n\in\mathbb{Z}} n^2|c_n|^2\left(\frac{\sin\frac{nu}{2}}{n\sin\frac{u}{2}}\right)^2 \leq 1.$$

It is therefore sufficient to prove that

$$|\sin nx| \leq n \sin x$$

Inductive argument based on

$$(n+1)\sin x \mp \sin(n+1)x = n\sin x \mp \sin nx \cos x + \sin x(1 \mp \cos nx)$$

What about $p > 2$?

Funny you should ask….

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The conjecture is false for $p = \infty$. The family of maximizing curves for $\|\Gamma(s+u) - \Gamma(s)\|_\infty$ consists of all curves that contain a line segment of length > s.

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At what critical value of p does the circle stop being the maximizer?

What about p > 2?

At what critical value of p does the circle stop being the maximizer?

This problem is open. We calculated $\|\Gamma(s+u) - \Gamma(s)\|_p$ for some examples:

Two straight line segments of length π:

$\|\Gamma(s+u) - \Gamma(s)\|_p{}^p = 2^{p+2}(\pi/2)^{p+1}/(p+1)$.

Better than the circle for $p > 3.15296\ldots$

What about $p > 2$?

Examples that are more like the circle are not better than the circle until higher p:

Stadium, small straight segments $p > 4.27898\ldots$

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Polygon with many sides, $p > 6$

What about p > 2?

Examples that are more like the circle are not better than the circle until higher p:

Stadium, small straight segments $p > 4.27898...$

Polygon with many sides, $p > 6$

Polygon with rounded edges, similar.

Circle is local maximizer for $p < p_c$

Theorem 2 *For a fixed arc length* $u \in (0, \frac{1}{2}L]$ *define*

$$p_c(u) := \frac{4 - \cos\left(\frac{2\pi u}{L}\right)}{1 - \cos\left(\frac{2\pi u}{L}\right)}, \tag{6}$$

then we have the following alternative. For $p > p_c(u)$ *the circle is either a saddle point or a local minimum, while for* $p < p_c(u)$ *it is a local maximum of the map* $\Gamma \mapsto c_\Gamma^p(u)$.

Reduction to an isoperimetric problem of classical type.

$$\int_0^L |\Gamma(s+u) - \Gamma(s)|\, \mathrm{d}s \;\le\; \frac{L^2}{\pi} \sin \frac{\pi u}{L}$$

Science is full of amazing coincidences!

Mohammad Ghomi and collaborators had considered and proved similar inequalities in a study of knot energies, A. Abrams, J. Cantarella, J. Fu, M. Ghomi, and R. Howard, *Topology*, 42 (2003) 381-394! They relied on a study of mean lengths of chords by G. Lükö, Isr. J. Math., 1966.

Equilibrium shape of a charged thread

The total energy:

$$E = \int_0^L \int_0^L \frac{ds ds'}{|\Gamma(s) - \Gamma(s')|}$$

is divergent, since the denominator is essentially |s-s´| . (The physical problem of "self-energy.") However, we may renormalize and consider instead

$$\delta(\Gamma) := \int_0^L \int_0^L \left[|\Gamma(s) - \Gamma(s')|^{-1} - |\mathcal{C}(s) - \mathcal{C}(s')|^{-1} \right] \mathrm{d}s \, \mathrm{d}s'$$

Is the circle the shape that minimizes the energy?

A change of variables $(s,s') \to (s,u=s'-s)$ simplifies the analysis and isolates the divergence:

$$\begin{aligned}\delta(\Gamma) &:= \int_0^L \int_0^L \left[|\Gamma(s)-\Gamma(s')|^{-1} - |\mathcal{C}(s)-\mathcal{C}(s')|^{-1}\right] \mathrm{d}s\, \mathrm{d}s' \\ &= 2\int_0^{L/2} \mathrm{d}u \int_0^L \mathrm{d}s\, \left[|\Gamma(s+u)-\Gamma(s)|^{-1} - \frac{\pi}{L}\csc\frac{\pi u}{L}\right].\end{aligned}$$

$|\Gamma(s+u) - \Gamma(s)|$ is the length of the chord connecting two points on the curve, separated by arc-length u.

By elementary trigonometry, for the unit circle this is

$(L/\pi) \sin(\pi u/L)$.

Is the circle the shape that minimizes the energy?

It suffices to show that for $0 < u < \pi$,

$$\int_0^L \mathrm{d}s \left[|\Gamma(s+u) - \Gamma(s)|^{-1} - \frac{\pi}{L} \csc \frac{\pi u}{L} \right] \geq 0$$

with equality only when Γ is a circle (independent of Euclidean transformations).

An electron near a charged thread

Idealizing the thread as a curve in space, the QM Hamiltonian operator for a nearby electron is:

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$$

Fix the length of the thread. What shape binds the electron the least tightly? Conjectured for about 3 years that answer is circle.

An electron near a charged thread

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$$

This is a question of showing that the *largest smallest* eigenvalue (energy) is attained when Γ is a circle,

An electron near a charged thread

$$H_{\alpha,\Gamma} = -\Delta - \alpha\delta(x - \Gamma)$$

This is a question of showing that the *largest smallest* eigenvalue (energy) is attained when Γ is a circle,

which in turn can be reduced to showing that:

$$\int_0^L |\Gamma(s+u) - \Gamma(s)| ds \le \frac{L^2}{\pi} \sin \frac{\pi u}{L}.$$

A family of isoperimetric conjectures for p > 0:

$$C_L^p(u): \qquad \int_0^L |\Gamma(s+u)-\Gamma(s)|^p \, \mathrm{d}s \overset{?}{\leq} \frac{L^{1+p}}{\pi^p} \sin^p \frac{\pi u}{L},$$

$$C_L^{-p}(u): \qquad \int_0^L |\Gamma(s+u)-\Gamma(s)|^{-p} \, \mathrm{d}s \underset{?}{\geq} \frac{\pi^p L^{1-p}}{\sin^p \frac{\pi u}{L}},$$

Right side corresponds to circle, by elementary trigonometry.
For what values of u and p are these conjectures true?

A family of isoperimetric conjectures for p > 0:

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$$C_L^{-p}(u): \qquad \int_0^L |\Gamma(s+u)-\Gamma(s)|^{-p}\, \mathrm{d}s \ge \frac{\pi^p L^{1-p}}{\sin^p \frac{\pi u}{L}},$$

These conjectures might be true for some p and u, but not for others. They are purely geometric questions that could have been considered in ancient times.

Proposition. 2.1.

$C_L^p(u)$ *implies* $C_L^{p'}(u)$ *if* $p > p' > 0.$

$C_L^p(u)$ *implies* $C_L^{-p}(u)$

Proposition. 2.1.

$$C_L^p(u) \ \ implies\ \ C_L^{p'}(u) \ \ if\ p > p' > 0.$$

Recalling that x → x^a is a convex function for a > 1, by Jensen's inequality,

(average of convex function) ≥ (convex function of average)

$$\begin{aligned} \frac{L^{1+p}}{\pi^p} \sin^p \frac{\pi u}{L} &\geq \int_0^L \left(|\Gamma(s+u) - \Gamma(s)|^{p'} \right)^{p/p'} \mathrm{d}s \\ &\geq L \left(\frac{1}{L} \int_0^L |\Gamma(s+u) - \Gamma(s)|^{p'} \, \mathrm{d}s \right)^{p/p'} . \end{aligned}$$

Proposition. 2.1, part 2.

$$C_L^p(u) \ implies \ C_L^{-p}(u)$$

As for second part, if conjecture is true for p > 0, then

$$\frac{L^2\pi^p}{L^{1+p}\sin^p\frac{\pi u}{L}} \leq \frac{L^2}{\int_0^L |\Gamma(s+u)-\Gamma(s)|^p\,ds}$$

$$\left(\int_0^L 1\right)^2 = \left(\int_0^L |\Gamma(s+u) - \Gamma(s)|^{\frac{p}{2}} |\Gamma(s+u) - \Gamma(s)|^{-\frac{p}{2}}\right)^2$$

$$\leq \int_0^L |\Gamma(s+u) - \Gamma(s)|^p \int_0^L |\Gamma(s+u) - \Gamma(s)|^{-p}$$

so

$$\int_0^L |\Gamma(s+u) - \Gamma(s)|^{-p} \geq \frac{L^2}{\int_0^L |\Gamma(s+u) - \Gamma(s)|^p}$$

Proof when p = 2

By the lemma, C^2 implies C^1 implies C^{-1}.

C^2 is the statement that the circle maximizes the chord $|\Gamma(s+u) - \Gamma(s)|$ in the mean-square sense.

C^2 is convenient because it allows theorems of Hilbert space and Fourier series.

An innocent assumption

We made the innocent assumption that $\Gamma(s)$ is a function of arc length s. This is always possible in theory, but you may recall that in elementary calculus *there are very few curves for which the formula in terms of* s *is simple*.

An innocent assumption

On the other hand a closed loop is a periodic function of, so *it can always be written as a Fourier series in* s.

Proof when p = 2

$$\Gamma(s) = \sum_{0 \neq n \in \mathbb{Z}} c_n \, \mathrm{e}^{ins}$$

(regarding the plane as the complex plane)

$$\dot{\Gamma}(s) = i \sum_{0 \neq n \in \mathbb{Z}} n c_n \, \mathrm{e}^{ins} \, .$$

By assumption, $|\dot{\Gamma}(s)| = 1$, and hence fr

$$2\pi = \int_0^{2\pi} |\dot{\Gamma}(s)|^2 \, \mathrm{d}s = \int_0^{2\pi} \sum_{0 \neq m \in \mathbb{Z}} \sum_{0 \neq n \in \mathbb{Z}} nm \, c_m^* \cdot c_n \, \mathrm{e}^{i(n-m)s} \, \mathrm{d}s \,,$$

er

$$\sum_{0 \neq n \in \mathbb{Z}} n^2 |c_n|^2 = 1 \,. \tag{2.5}$$

Recall that the exponential function exp(i (n-m) s) integrates to 0 unless n=m. This is the *orthogonality relation* of Fourier series.

By assumption, $|\dot{\Gamma}(s)| = 1$, and hence fr

$$2\pi = \int_0^{2\pi} |\dot{\Gamma}(s)|^2 \, \mathrm{d}s = \int_0^{2\pi} \sum_{0 \neq m \in \mathbb{Z}} \sum_{0 \neq n \in \mathbb{Z}} nm \, c_m^* \cdot c_n \, \mathrm{e}^{i(n-m)s} \, \mathrm{d}s \, ,$$

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$$\sum_{0 \neq n \in \mathbb{Z}} n^2 |c_n|^2 = 1 \, . \tag{2.5}$$

Square of chord length $|\Gamma(s+u) - \Gamma(s)|$ simplifies with $e^{in(s+u)} = e^{ins} \, e^{inu}$.

$$\int_0^{2\pi} \left| \sum_{0 \neq n \in \mathbb{Z}} c_n \left(\mathrm{e}^{inu} - 1 \right) \mathrm{e}^{ins} \right|^2 \mathrm{d}s = 8\pi \sum_{0 \neq n \in \mathbb{Z}} |c_n|^2 \left(\sin \frac{nu}{2} \right)^2 \, ,$$

Desired inequality equivalent to

$$\sum_{0 \neq n \in \mathbb{Z}} n^2 |c_n|^2 \left(\frac{\sin \frac{nu}{2}}{n \sin \frac{u}{2}} \right)^2 \leq 1.$$

Because if all $c_n = 0$ when $n \neq \pm 1$ are zero, $\Gamma(s)$ is a circle.
This is under the assumption that $n^2|c_n|^2$ sums to 1.

It is therefore sufficient to prove that

$$|\sin nx| \leq n \, \sin x$$

Inductive argument based on

$$(n+1)\sin x \mp \sin(n+1)x = n\sin x \mp \sin nx \cos x + \sin x(1 \mp \cos nx)$$

It is a small world!

Science is full of amazing coincidences! Mohammad Ghomi of GT and collaborators had considered and proved related inequalities in a study of knot energies, A. Abrams, J. Cantarella, J. Fu, M. Ghomi, and R. Howard, *Topology*, 42 (2003) 381-394! They relied on a study of mean lengths of chords by G. Lükö, Isr. J. Math., 1966.

In particular, the conjecture C^1 was proved earlier by Lükö, with entirely different methods.

What about p > 2?

Funny you should ask….

What about $p > 2$?

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The conjecture is false for $p = \infty$. The family of maximizing curves for $\|\Gamma(s+u) - \Gamma(s)\|_\infty$ consists of all curves that contain a line segment of length $> s$.

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Two straight line segments of length π:

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Better than the circle for $p > 3.15296\ldots$

What about p > 2?

Exner-Fraas-Harrell, 2007

Theorem 2 *For a fixed arc length $u \in (0, \frac{1}{2}L]$ define*

$$p_c(u) := \frac{4 - \cos\left(\frac{2\pi u}{L}\right)}{1 - \cos\left(\frac{2\pi u}{L}\right)}, \tag{7}$$

then we have the following alternative. For $p > p_c(u)$ the circle is either a saddle point or a local minimum, while for $p < p_c(u)$ it is a local maximum of the map $\Gamma \mapsto c_\Gamma^p(u)$.

The critical value decreases from ∞ to 5/2 as L goes from 0 to L/2.

Open questions

- Are the local isoperimetric results for $p>2$ global?
- How about means of other monotonic functions of chord length? (To model other interactions such as screened Coulomb.)
- Non-uniform densities
  - The “θ problem”.

What about the smallest mean of chords?

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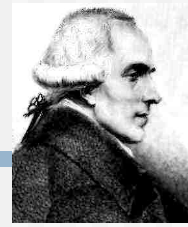
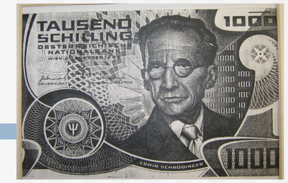
- However, if we insist that the curve bounds a convex region, this is not possible. How small can the chord be when we assume convexity? What is the optimal shape?
- Conjectures (Harrell-Henrot), if $u = \pi/m$, then m-gon. If $u = p\pi/m$, an n-gon, else no C^2 subarcs.





Discrete spectra of Laplace and Schrödinger operators.

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

$$H\,\phi_k = \lambda_k\,\phi_k$$

Semiclassical limits

1. $\lambda_k \to \infty$

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

(ε small)

“Universal” constraints on the spectrum

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

$$\lambda_{n+1} - \lambda_n \leq \frac{4}{d}\frac{1}{n}\sum_{k=1}^{n} \lambda_k$$

“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

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

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

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

Riesz means

- 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)

Stubbe's proof of sharp Lieb-Thirring for ρ≥2 (JEMS, in press)

1. A trace formula ("sum rule") of Harrell-Stubbe '97, for H = - ε Δ + V:

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

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

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2. $T_k := \langle \phi_k, -\Delta \phi_k \rangle \quad = \frac{d\lambda_k}{d\epsilon}$ (Feynman-Hellman)

Lieb-Thirring inequalities

Thus

$$\mathbf{R}_\rho(\mathbf{z},\epsilon) \le -\frac{\mathbf{2}\epsilon}{\mathbf{d}}\frac{\partial \mathbf{R}_\rho(\mathbf{z},\epsilon)}{\partial\epsilon},$$

or:

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

and classical Lieb-Thirring is an immediate consequence!

Recall:

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

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

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

Commutators of operators

- [G, [H, G]] = 2 GHG - G^2H - HG^2
- Etc., etc. Typical consequence:

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

(Abstract version of Bethe’s sum rule)

1[st] and 2[nd] commutators

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

$$=$$

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

Harrell-Stubbe TAMS 1997

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*:

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

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

$$=$$

$$\sum_{\lambda_j\in J}\sum_{\lambda_k\notin J}(z-\lambda_j)(z-\lambda_k)(\lambda_k-\lambda_j)\Big(|\langle G\phi_j,\phi_k\rangle|^2+|\langle G^*\phi_j,\phi_k\rangle|^2\Big),$$

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

For $J = \{\lambda_1 \ldots \lambda_n$, the right side ≤ 0!

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

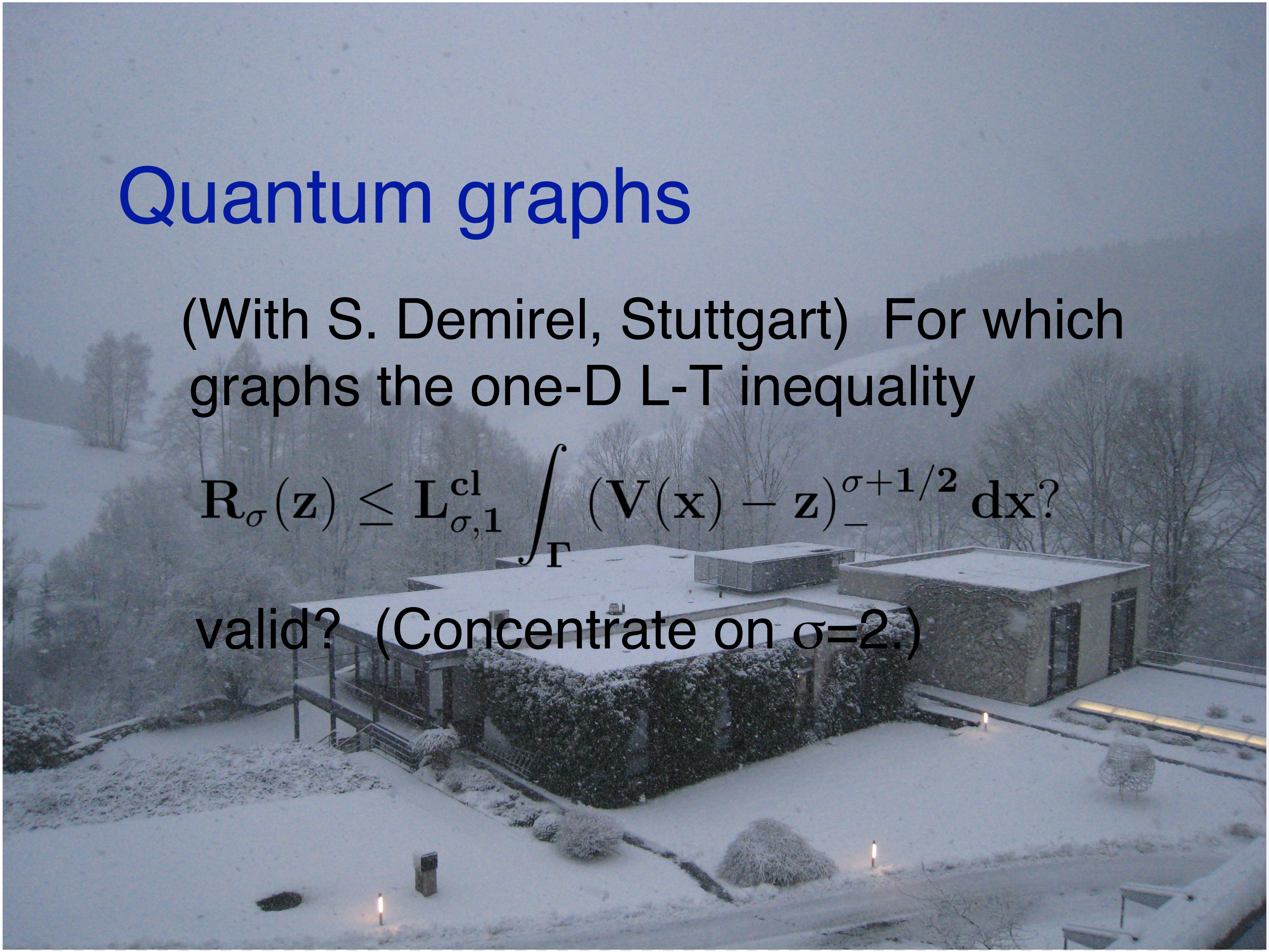
Take-away messages #1

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:

   $$\sum (z - \lambda_k)^{2} (\ldots) \quad \leq \quad \sum (z - \lambda_k) (\ldots)$$

3. ****Once this quadratic inequality is proved, the "usual correlaries," including universal bounds and Lieb-Thirring, follow*.



Quantum graphs

(With S. Demirel, Stuttgart) For which graphs the one-D L-T inequality

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

valid? (Concentrate on σ=2.)

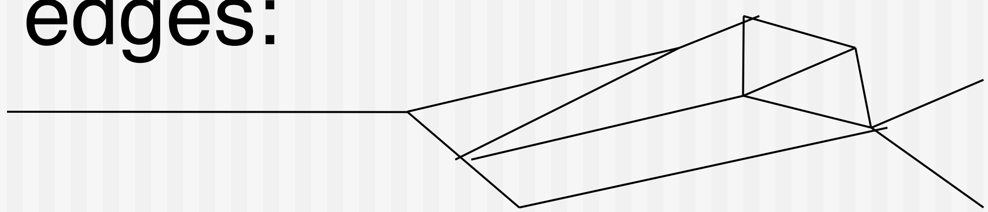
ON SEMICLASSICAL AND UNIVERSAL INEQUALITIES FOR EIGENVALUES OF QUANTUM GRAPHS

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.

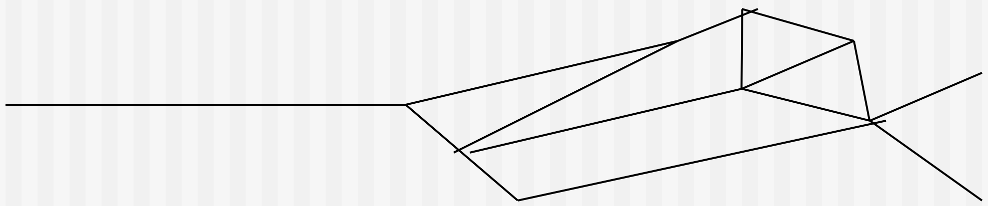
Quantum graphs

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.

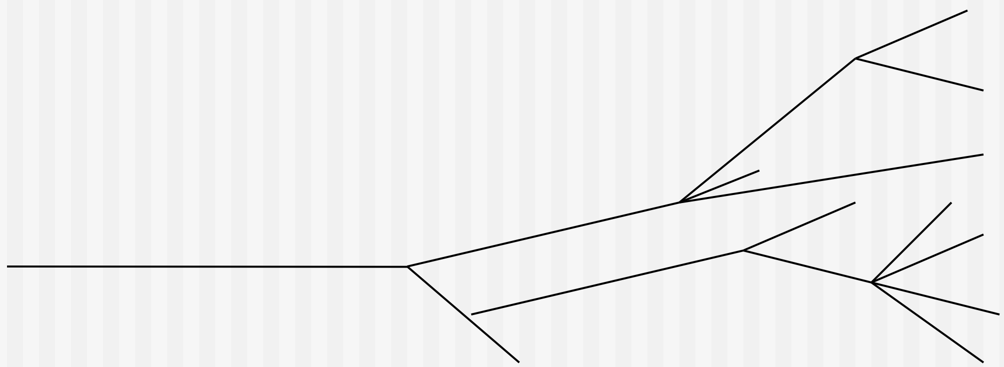
Quantum graphs



Is this one-dimensional or not? Does the topology matter?

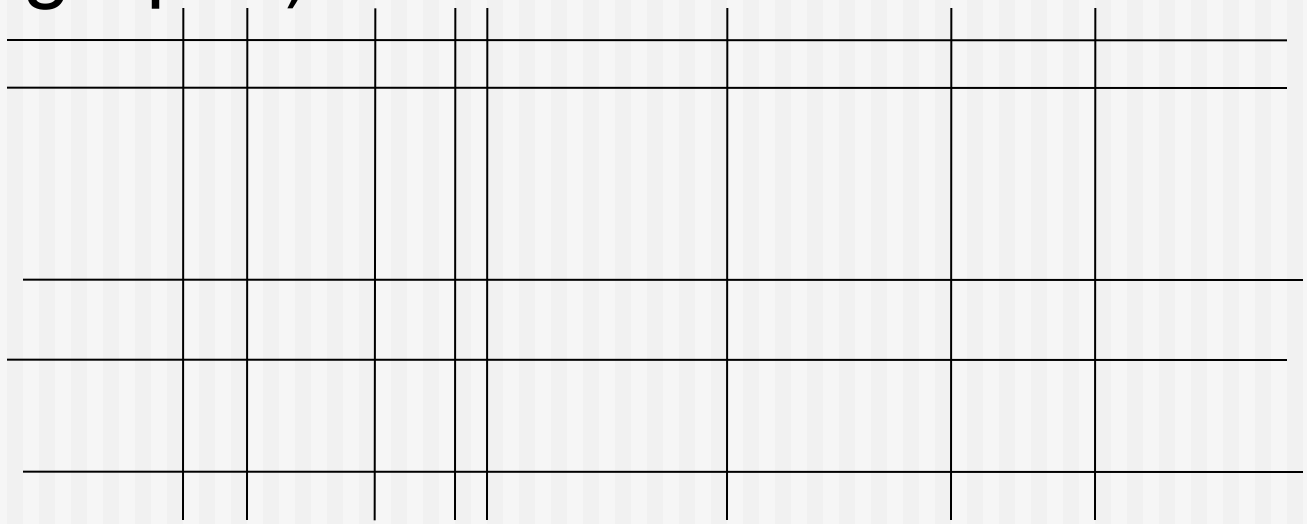
Quantum graphs satisfy the expected one-dimensional LT and universal inequalities for:

1. Trees.



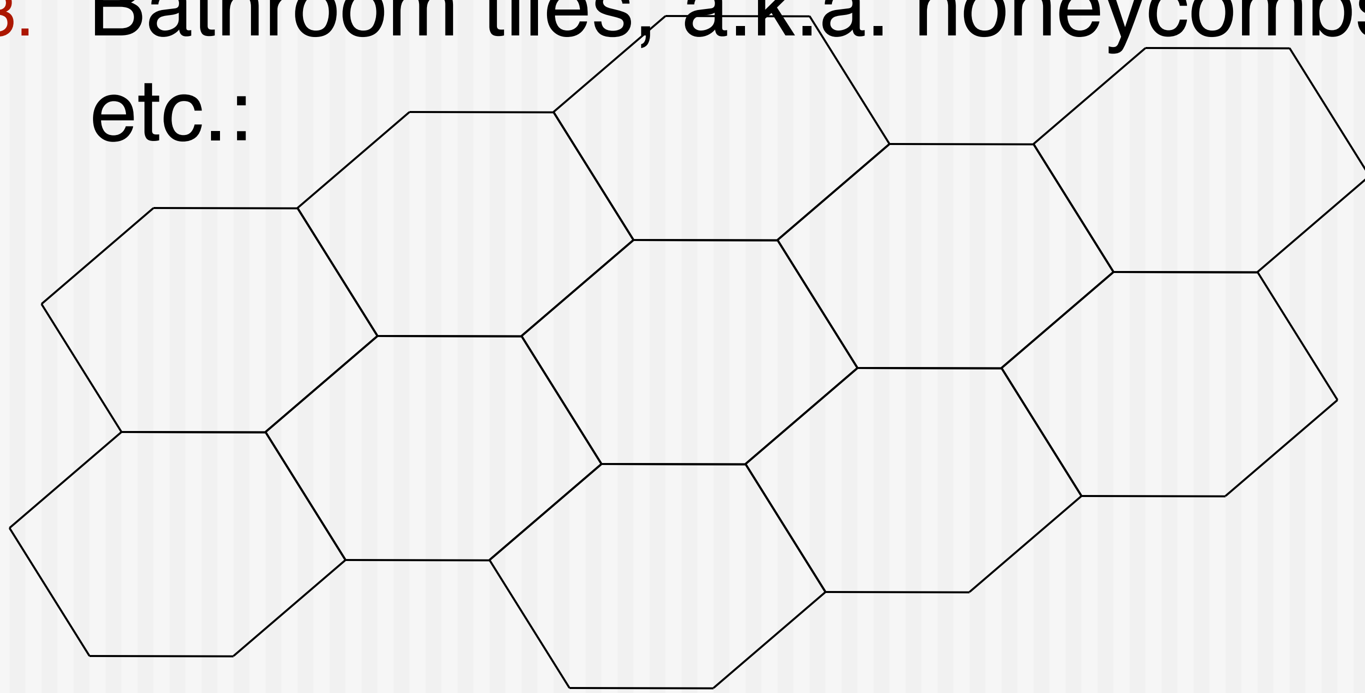
Quantum graphs satisfy the expected one-dimensional LT and universal inequalities for:

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



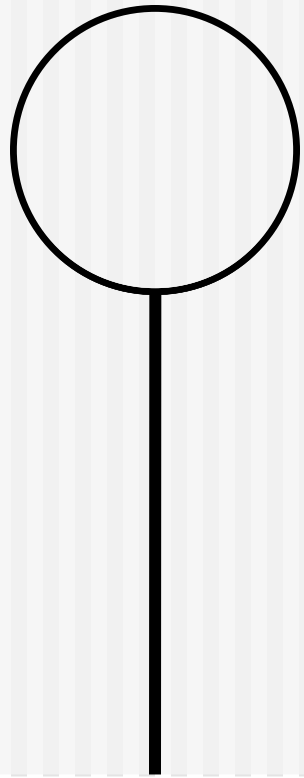
Quantum graphs satisfy the expected one-dimensional LT and universal inequalities for:

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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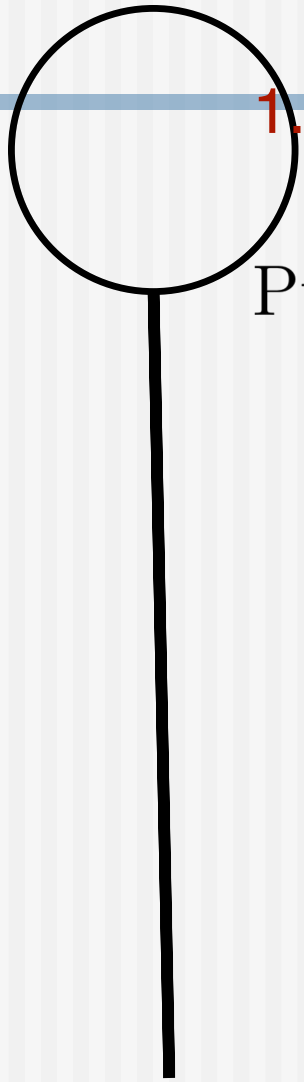


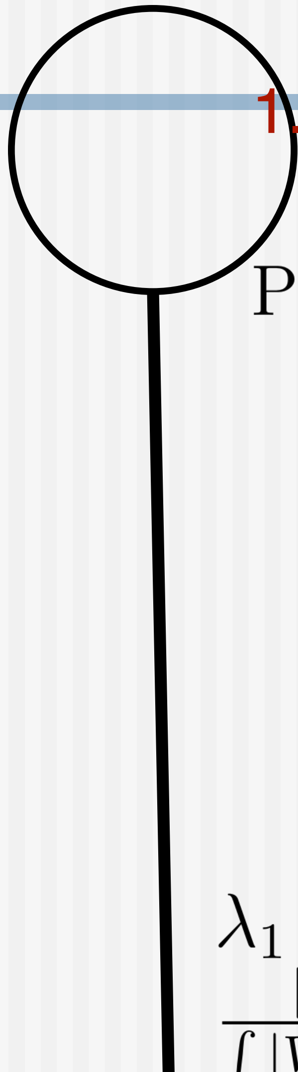
1. But not balloons! (A.k.a. tadpoles, or...)

Put a soliton potential on the loop:

$$V = \frac{-2a^2}{\cosh^2(ax)}\chi_{\mathrm{loop}}$$

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

Quantum graphs:



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

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

$\lambda_1 = -a^2$ 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. $L^{cl} = 3/16$.

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

Quantum graphs

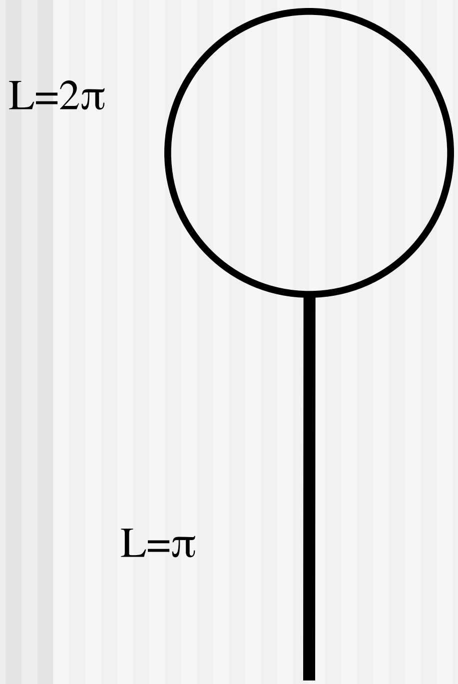
For which *finite* graphs is:

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

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

Quantum graphs

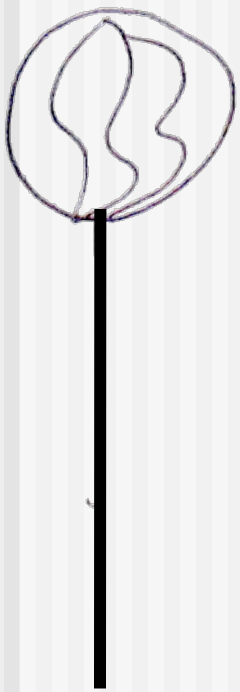
- Not balloons!

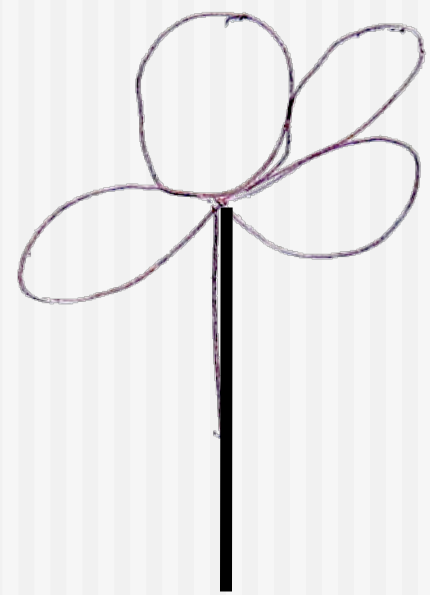


$$\frac{\lambda_2}{\lambda_1} = \left(\frac{\pi - \arctan(1/\sqrt{(}2))}{\arctan(1/\sqrt{(}2))} \right) \doteq 16.8$$

Quantum graphs

- Fancy balloons can have arbitrarily large λ_2/λ_1.





Why?

If we can establish the analogue of the trace inequality,

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

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

Calculate commutators with a good G.

Suppose G' is cst on each edge and

$\phi \to G\phi$ preserves vertex conditions.

(In std case this means G contin., $\sum \frac{\partial G}{\partial x_i} = 0$ @ V.)

Sum rule becomes

$$\sum_j \sum_k \left((z-\lambda_k)_+^2 \, a_j \|\phi_k\|_{\Gamma_j}^2 - 4\alpha (z-\lambda_j)_+ \, a_j \|\phi_k'\|_{\Gamma_j}^2 \right)$$

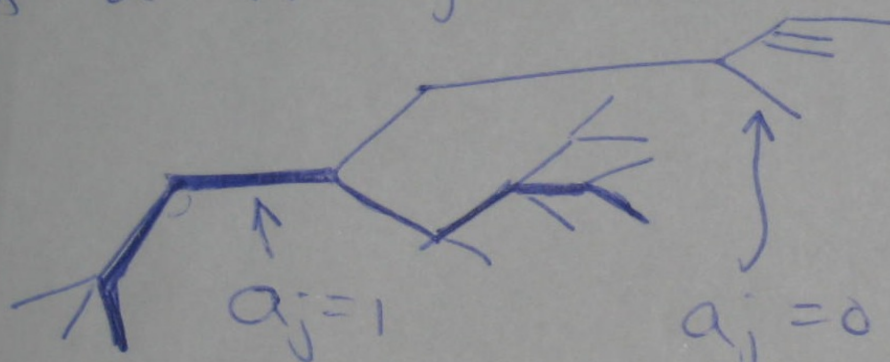
$$= \cdots \leq 0$$

where $|G'(x)|^2 = a_j$ on $\Gamma_j \subset \Gamma$.

$$\boxed{\sum_j \sum_{k\le n} a_j\left((z-\lambda_k)^2\,\|\phi_k\|^2_{\Gamma_j} - 4\alpha(z-\lambda_k)\,\|\phi_k'\|^2_{\Gamma_j}\right) \le 0}$$

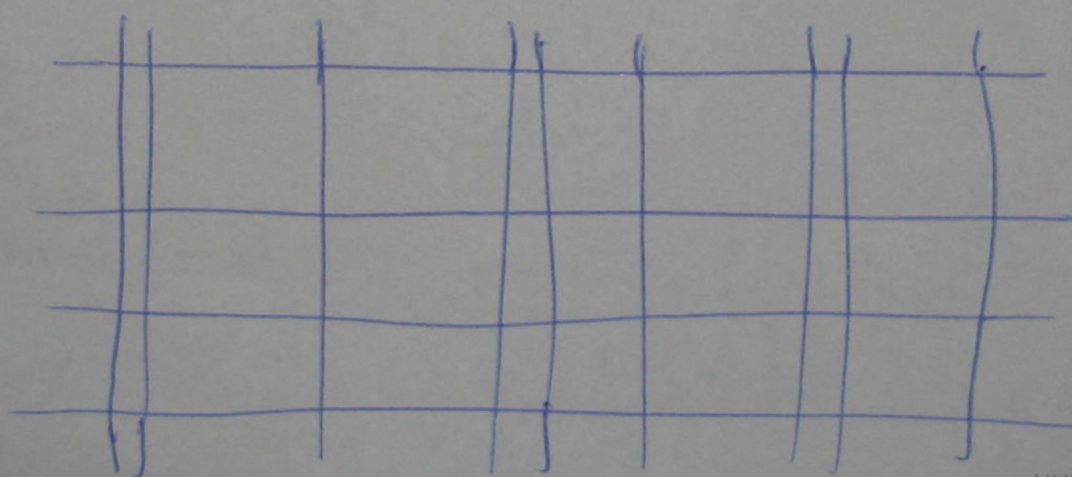
* Can we find a family of such G's and sum, so that we get $\sum_{k\le n}\left((z-\lambda_k)^2 - 4\alpha(z-\lambda_k)\,\|\phi_k'\|^2\right) \le 0$?

Example. G = distance along a "transit" in a tree, constant elsewhere.



Example. Scottish tartan, $G = x + y$

$a = 1$
(good).



Sharpest inequalities if a_j always 1

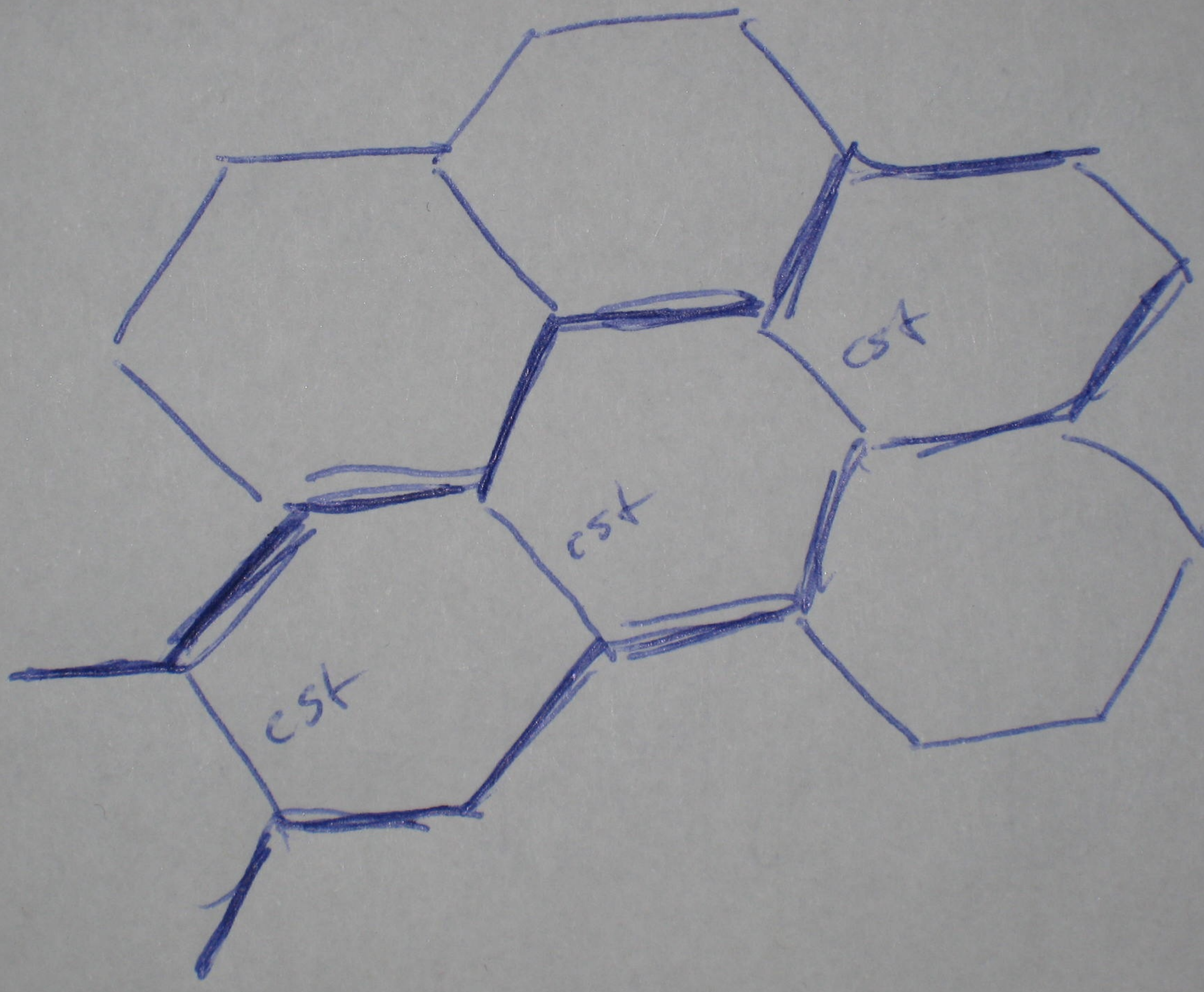
or, equally good, $\sum_{\alpha} a_j^{(\alpha)} \chi_{\Gamma_j} = 1$.

Then:

$$R_2(z) := \sum_j (z-\lambda_j)_+^2 \leq 4\alpha \sum (z-\lambda_j)_+ T_j$$

$$R_\sigma(z) \leq 2\sigma\alpha \sum (z-\lambda_j)_+ T_j, \quad \sigma \geq 2$$

$$\leq 4 \sum (z-\lambda_j)_+ T_j \quad 1 \leq \sigma \leq 2$$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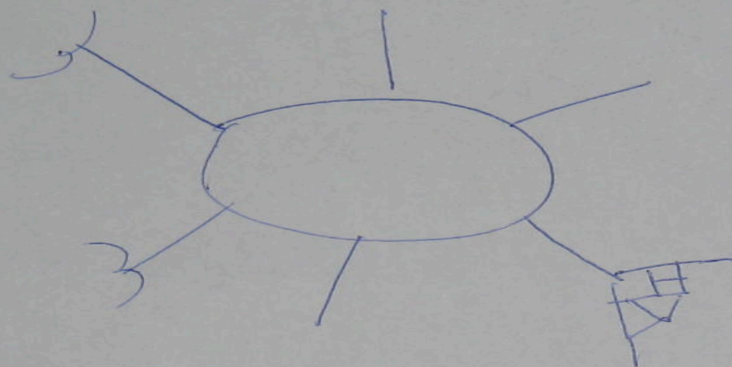
Commutation for loops



Use non-self-adjoint trace formula with $G = e^{iqx_e}$, $q = \frac{2\pi}{L}$, and extend by a constant on exterior parts.

$$T_j \to T_j + \frac{|q|^2}{4},$$

systematically weakening the inequality

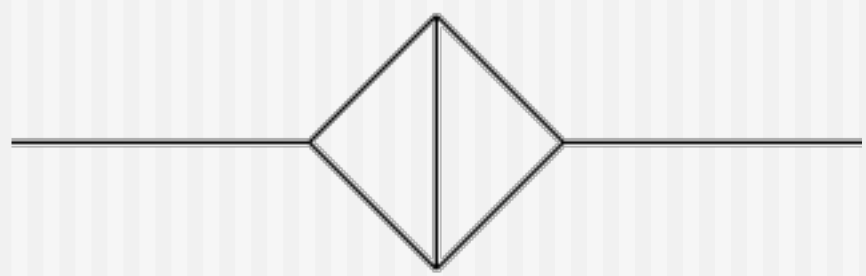
When does a quadratic inequality hold?

- If the graph can be covered by a family of transits where on each edge G' = 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

- S. Demirel and E.M. Harrell, Rev.Math. Physics, to appear.
- E.M. Harrell and J. Stubbe, On Trace Identities and Universal Eigenvalue Estimates for Some Partial Differential Operators, Trans. Amer. Math. Soc. 349(1997)1797-1809.
- E.M. Harrell, Commutators, eigenvalue gaps, and mean curvature in the theory of Schrödinger operators, Communications PDE, 2007
- A. El Soufi, E.M. Harrell, and S. Ilias, Universal inequalities for the eigenvalues of Laplace and Schrödinger operators on submanifolds, Trans AMS,2009.
- E.M. Harrell and L. Hermi, Differential inequalities for Riesz means and Weyl-type bounds for eigenvalues, J. Funct. Analysis 2008.
- E.M. Harrell and L. Hermi, On Riesz Means of Eigenvalues, preprint 2008.
- E.M. Harrell and J. Stubbe, Universal bounds and semiclassical estimates for eigenvalues of abstract Schrödinger operators, preprint 2008.
- E.M. Harrell and S. Yildirim Yolcu, Eigenvalue inequalities for Klein-Gordon Operators, J. Funct. Analysis 2009.
- 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.

THE END