Sharp geometric bounds for eigenvalues of Schrödinger operators

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Dedication

(in the respectful spirit learned from the Good Soldier Švejk)

Said a Czech quantum expert named Exner
When checking a vexing conjecture,
“Ever since I’ve passed sixty,
With a sequence this tricky,
I forget what the heck these x_n are!

On a loop trail ….

Or on the trail of a loop?

An electron near a charged loop

Exner - Harrell - Loss, *LMP* **75**(2006)225

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

Fix the length of the loop. What shape binds the electron the least tightly? Exner conjectured some time ago that the answer is a circle.

Reduction to an isoperimetric problem of classical type.

Birman-Schwinger reduction. A negative eigenvalue of the Hamiltonian corresponds to a fixed point of the Birman-Schwinger operator:

$$\mathcal{R}^{\kappa}_{\alpha,\Gamma}\phi = \phi\,, \quad \mathcal{R}^{\kappa}_{\alpha,\Gamma}(s,s') := \frac{\alpha}{2\pi} K_0\big(\kappa|\Gamma(s)-\Gamma(s')|\big)$$

K_0 is the Macdonald function (Bessel function that is the kernel of the resolvent in 2 D).

It suffices to show that the largest eigenvalue of $\mathcal{R}^{\kappa}_{\alpha,\Gamma}$ is uniquely minimized by the circle, i.e.,

$$\int_0^L \int_0^L K_0\big(\kappa|\Gamma(s)-\Gamma(s')|\big)\,\mathrm{d}s\mathrm{d}s' \geq \int_0^L \int_0^L K_0\big(\kappa|\mathcal{C}(s)-\mathcal{C}(s')|\big)\,\mathrm{d}s\mathrm{d}s'$$

with equality only for the circle. Equivalently, show that

$$F_\kappa(\Gamma) := \int_0^{L/2} \mathrm{d}u \int_0^L \mathrm{d}s \left[K_0\big(\kappa|\Gamma(s+u)-\Gamma(s)|\big) - K_0\left(\frac{\kappa L}{\pi}\sin\frac{\pi u}{L}\right)\right]$$

is positive (0 for the circle).

Since K_0 is decreasing and strictly convex, with Jensen's inequality,

$$\frac{1}{L} F_\kappa(\Gamma) \geq \int_0^{L/2} \left[K_0\left(\frac{\kappa}{L} \int_0^L |\Gamma(s+u) - \Gamma(s)| \mathrm{d}s \right) - K_0\left(\frac{\kappa L}{\pi} \sin \frac{\pi u}{L} \right) \right] \mathrm{d}u \,,$$

where the inequality is strict unless $\int_0^L |\Gamma(s+u) - \Gamma(s)| \mathrm{d}s$ is independent of s,

i.e. for the circle. The conjecture has been reduced to:

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

A family of isoperimetric conjectures for p > 0:

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

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

Right side corresponds to circle.

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

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

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

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

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….

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 $> u$.

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 $p > 4.27898\ldots$

Polygon with many sides, $p > 6$

Polygon with rounded edges, similar.

Circle is local maximizer for all p < ∞ with respect to nice enough perturbations

Let $\Gamma(\gamma, s)$ be a closed curve in the complex plane parametrized by arc length s, of the form $(1-\gamma)e^{is} + \Theta(\gamma, s)$, where $\gamma \geq 0$. Suppose that Θ is smooth (say, C^2 in γ and s), and that for each γ, $\Theta(\gamma, s)$ is orthogonal to e^{is}. Then $\Gamma(0, s)$ is a circle of radius 1, and for any u, $0 < u < 2\pi$,

$$\left. \frac{\partial I(\Gamma(\gamma), p, u)}{\partial \gamma} \right|_{\gamma=0} < 0.$$

Reduction to an isoperimetric problem of classical type.

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

Science is full of amazing coincidences!

Mohammad Ghomi (now at **Georgia Tech**) 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.

Nanostuff - when an otherwise free electron is confined to a thin domain

The effective potential when the Dirichlet Laplacian is squeezed onto a submanifold

$- \Delta_{LB} + q,$

$$q(\mathbf{x}) = \frac{1}{4}\left(\sum_{j=1}^{d} \kappa_j\right)^2 - \frac{1}{2}\sum_{j=1}^{d} \kappa_j^2$$

d=1, $q = -\kappa^2/4 \leq 0$ d=2, $q = -(\kappa_1-\kappa_2)^2/4 \leq 0$

More loopy problems with Pavel Exner

In Prague in 1998, Exner-Harrell-Loss caricatured the foregoing operators with a family of one-dimensional Schrödinger operators on a closed loop, of the form:

$$-\frac{d^2}{ds^2} + g\kappa^2$$

where g is a real parameter and the length is fixed. What shapes optimize low-lying eigenvalues, gaps, etc., and for which values of g?

Optimizers of λ_1 for loops

- $g < 0$. Not hard to see λ_1 uniquely *max*imized by circle. No minimizer - a kink corresponds to a negative multiple of δ^2 (yikes!).
- $g > 1$. No maximizer. A redoubled interval can be thought of as a singular minimizer.
- $0 < g \leq 1/4$. E-H-L showed circle is minimizer. Conjectured that the bifurcation was at $g = 1$. (When $g=1$, if the length is 2π, both the circle and the redoubled interval have $\lambda_1 = 1$.)
- If the embedding in R^m is neglected, the bifurcation is at $g = 1/4$ (Freitas, CMP 2001).

Current state of the loop problem

- Benguria-Loss, *Contemp*. *Math*. 2004. Exhibited a one-parameter continuous family of curves with $\lambda_1 = 1$ when $g = 1$. It contains the redoubled interval and the circle.
- B-L also showed that an affirmative answer is equivalent to a standing conjecture about a sharp Lieb-Thirring constant.

Current state of the loop problem

- Burchard-Thomas, J. Geom. Analysis 15 (2005) 543. The Benguria-Loss curves are local minimizers of λ_1.
- Linde, Proc. AMS **134** (2006) 3629. Conjecture proved under an additional geometric condition. L raised general lower bound to 0.6085.
- AIM Workshop, Palo Alto, May, 2006.

Another loopy equivalence

- Another equivalence to a problem connecting geometry and Fourier series in a classical way:
  - Rewrite the energy form in the following

$$E(u) := \int_0^{2\pi} \left(|u'|^2 + \kappa^2 |u|^2 \right) ds = \int_0^{2\pi} \left| \frac{d\left(e^{i\theta(s)} u(s)\right)}{ds} \right|^2 ds$$

  - Is

$$E(u) \geq \int_0^{2\pi} u^2 \quad ?$$

Another loopy equivalence

- Replace s by $z = \exp(i\, s)$ and regard the map

  $$z \rightarrow w := u \exp(i\, \theta)$$

  as a map on C that sends the unit circle to a simple closed curve with winding number one with respect to the origin. Side condition that the mean of $w/|w|$ is 0.
- For such curves, is $\|w'\| \geq \|w\|$?

Loop geometry and Fourier series
(again)

- In the Fourier (= Laurent) representation,

$$w = \sum_{k>-\infty}^{\infty} c_k z^k$$

the conjecture is that if the mean of w/|w| is 0, then:

$$\sum_k k^2 |c_k|^2 \geq \sum_k |c_k|^2$$

Or, equivalently,

$$|c_0|^2 \leq \sum_{|k|\geq 2} (k^2 - 1) |c_k|^2$$

The effective potential when the Dirichlet Laplacian is squeezed onto a submanifold

$- \Delta_{LB} + q,$

$$q(\mathbf{x}) = \frac{1}{4}\left(\sum_{j=1}^{d} \kappa_j\right)^2 - \frac{1}{2}\sum_{j=1}^{d} \kappa_j^2$$

d=1, $q = -\kappa^2/4 \leq 0$ d=2, $q = - (\kappa_1 - \kappa_2)^2/4 \leq 0$

An effective potential that controls Schrödinger operators on submanifolds:

$$- \Delta_{LB} + q,$$

$$q(\mathbf{x}) = \frac{1}{4} \left(\sum_{j=1}^{d} \kappa_j \right)^2.$$

(Square of mean curvature)

ISOPERIMETRIC

THEOREMS

The isoperimetric theorems for $-\nabla^2 + q(\kappa)$

I. One dimension

$$-\frac{d^2}{ds^2} + g\kappa^2$$

Ω - curve.

A. Ω infinitely long, asymptotically straight

$g<0$

$\lambda_1 < 0$ unless Ω is a line

Duclos - Exner

B. Ω closed, say $|\Omega| = 1$

(i) $g \leq 0$,

λ_1 uniquely maximized by ◯

Duclos - Exner

(ii)

$g = -1$

λ_2 uniquely maximized by ◯

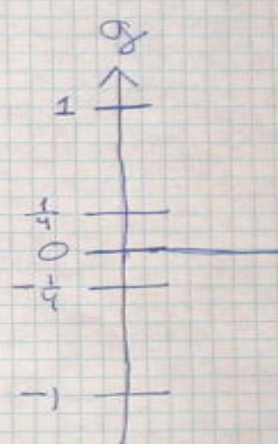
Harrell - Loss

(iii)

$0 \leq g \leq \frac{1}{4}$

λ_1 uniquely minimized by ◯

Exner - Harrell - Loss



The isoperimetric theorems for $-\nabla^2 + q(\kappa)$

C. Open.

λ_2, $g \neq -1$, $g < 0$.

λ_1, $\frac{1}{4} < g \leq 1$

Freitas, Non-embedded problem bifurcates at $\frac{1}{4}$

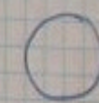
Benguria - Loss, family of curves with same λ_1 at 1

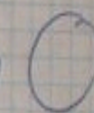
Linde, $g = 1$, lower bound under additional assumptions

II. Two dimensions

A. $q(K) = g\, K_1 K_2$ (Gauß curvature), genus$(\Omega) = 0$, $|\Omega| = 1$.

(i) Hersch 1970, $g = 0$, λ_1 trivially $= 0$

$d = 2$: λ_2 uniquely maximized by $S^2 \subset \mathbb{R}^3$ 

(ii) Harrell 1996 any g, $\lambda_{1,2}$ both uniquely maximized by 

* certain other potentials, $g\,(K_1^2 + K_2^2)$ $g < 0$.

<u>Open</u> - other genera

* Special facts in 2-D about conformal equivalence.

II. Two dimensions

A. $q(K) = g\, K_1 K_2$ (Gauß curvature), genus$(\Omega) = 0$, $|\Omega| = 1$.

False in high dim.

(i) Hersch 1970, $g = 0$, λ_1 trivially $= 0$

$d = 2$: λ_2 uniquely maximized by $S^2 \subset \mathbb{R}^3$ ○

(ii) Harrell 1996 any g, $\lambda_{1,2}$ both uniquely maximized by ○

* certain other potentials, $g(K_1^2 + K_2^2)$ $g < 0$.

__Open__ - other genera

* Special facts in 2-D about conformal equivalence.

III Two or more dimensions.

A Ω - hypersurface of codimension 1

$$-\nabla^2 - \frac{1}{\dim}\left(\sum \kappa_\ell\right)^2$$

λ_2 uniquely maximized by sphere
(Harrell - Loss '98).

$\Rightarrow$ Same for $q(\kappa) = -\sum(\kappa_\ell^2)$

B) Ω - embedded in $\mathbb{R}^{n+1}$, $\mathbb{H}^{n+1}$, $\mathbb{S}^{n+1}$

El Soufi - Ilias.

Actually show $\lambda_2(-\nabla^2 + V(x)) \le \frac{1}{|S|\dim} \int \sum \kappa_\ell^2 + V_{ave}$

Gap bounds for (hyper) surfaces

Let M be a d-dimensional manifold immersed in $\mathbb{R}^{d+1}$.

Theorem 3.1 *Let H be a Schrödinger operator on M with a bounded potential, i.e.,*

$$H = -\Delta + V, \tag{3.1}$$

where V is a bounded, measurable, real-valued function on M. If M has a boundary, Dirichlet conditions are imposed (in the weak sense that H is defined as the Friedrichs extension from $C_c^\infty(M)$). Then

$$\begin{aligned}\Gamma(H) &\leq \frac{1}{d}\int_M \left(4\left|\nabla_{||}u_1\right|^2 + h^2 u_1^2\right) dVol \\ &= \frac{4}{d}\left\langle u_1, \left(-\Delta + \frac{h^2}{4}\right) u_1\right\rangle.\end{aligned} \tag{3.2}$$

Here $\Gamma := \lambda_2 - \lambda_1$, and h := the sum of the principal curvatures. More generally:

Sum rules and Yang-type inequalities

$$1 \leq \frac{4}{dk} \sum_{j=1}^{k} \frac{\int_M \left(|\nabla u_i|^2 + \frac{|h|^2}{4} u_i^2 \right) dVol}{\lambda_{k+1} - \lambda_j}$$

$$\sum_{i=1}^{k} (\lambda_{k+1} - \lambda_i)^2 \leq \frac{4}{d} \sum_{i=1}^{k} (\lambda_{k+1} - \lambda_i) \left(\int_M \left(|\nabla u_i|^2 + \frac{|h|^2}{4} u_i^2 \right) dVol \right)$$

With the quadratic formula, the Yang-type bound:

$$\sum_{i=1}^{k}(\lambda_{k+1}-\lambda_i)^2 \leq \frac{4}{d}\sum_{i=1}^{k}(\lambda_{k+1}-\lambda_i)\left(\int_M \left(|\nabla u_i|^2 + \frac{|h|^2}{4}u_i^2\right) dVol\right)$$

implies a bound on each eigenvalue λ_{k+1} of the form:

$$\left(1+\frac{2}{d}\right)\frac{1}{k}\sum_{i=1}^{k}\lambda_i + \frac{2}{d}\frac{1}{k}\sum_{i=1}^{k}\delta_i - \sqrt{D_{nk}}$$

$$\leq \lambda_{k+1}$$

$$\leq \left(1+\frac{2}{d}\right)\frac{1}{k}\sum_{i=1}^{k}\lambda_i + \frac{2}{d}\frac{1}{k}\sum_{i=1}^{k}\delta_i + \sqrt{D_{dk}},$$

where D_{dk} depends only on the eigenvalues up through k and the dimension, and

$$\delta_i := \int_M \left(\frac{|h|^2}{4} - V\right) u_i^2.$$

The bounds on λ_{k+1} are attained for all k with $\lambda_{k+1} \neq \lambda_k$, when

1. The potential is of the form g h^2.

2. The submanifold is a sphere.

(For details see articles linked from my webpage beginning with Harrell-Stubbe Trans. AMS 349(1997)1797.)

THE

END

Benguria-Loss transformation

- One of the Lieb-Thirring conjectures is that for a pair of orthonormal functions on the line,

$$\int_{-\infty}^{\infty} \left((u_1')^2 + (u_2')^2 \right) dx \geq \frac{\pi^2}{4} \int_{-\infty}^{\infty} \left((u_1)^2 + (u_2)^2 \right) dx$$

Benguria-Loss transformation

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- Let

$$s := \pi \int_{-\infty}^{x} \left((u_1)^2 + (u_2)^2 \right) dx$$

Benguria-Loss transformation

- Also, use a Prüfer transformation of the form

$$u_1 = \sqrt{u}\cos\left(\frac{\theta}{2}\right), \quad u_2 = \sqrt{u}\sin\left(\frac{\theta}{2}\right)$$

Benguria-Loss transformation

- Also, use a Prüfer transformation of the form

$$u_1 = \sqrt{u}\cos\left(\frac{\theta}{2}\right), \quad u_2 = \sqrt{u}\sin\left(\frac{\theta}{2}\right)$$

- to obtain the conjecture in the form:

$$E(u) \geq \int_0^{2\pi} u^2 \quad ?$$