Geometric inequalities arising in nanophysics

Evans Harrell

Georgia Tech

www.math.gatech.edu/~harrell

Ouidah, Benin
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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.

Graphics have been suppressed in the public version of this seminar. They are easily found and viewed on line.

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 $\Gamma: R \rightarrow R^3$. $\Gamma(s)$ 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.

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:

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

$|\Gamma(s+u) - \Gamma(s)|$ 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

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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

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which in turn can be reduced to showing that:

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

A family of isoperimetric conjectures for p > 0:

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

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

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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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

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

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

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er

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

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….

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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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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?

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?

- If the thread is crumpled up, the chords can be as small as you wish.

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What about the smallest mean of chords?

- If the thread is crumpled up, the chords can be as small as you wish.
- 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.

On a (hyper) surface, what object is most like the Laplacian?

(Δ = the good old flat scalar Laplacian of Laplace)

Answer #1 (Beltrami's answer): Consider only tangential variations.

At a fixed point, orient Cartesian x_0 with the normal, then calculate

$$\sum_{j=1}^{d} \frac{\partial^2}{\partial {x_j}^2}$$

Difficulty:

- **The Laplace-Beltrami operator is an intrinsic object, and as such is unaware that the surface is immersed!**

- **Answer #2 (The nanoanswer):**

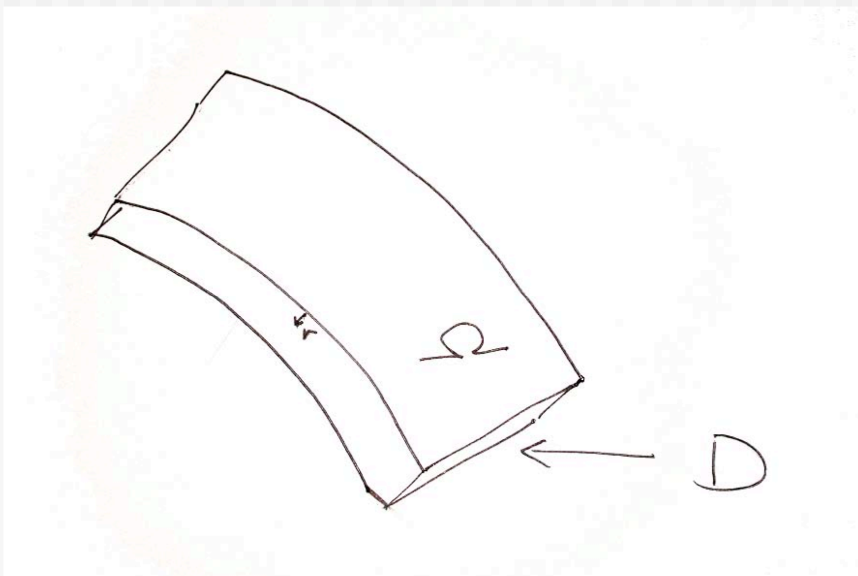
$$- \Delta_{LB} + q$$

- **Since Da Costa, PRA, 1981: Perform a singular limit and renormalization to attain the surface as the limit of a thin domain.**

Thin domain of fixed width
variable r= distance from edge

Energy form in separated variables:

$$\int_D |\nabla_{||} \zeta|^2 d^{d+1}x + \int_D |\zeta_r|^2 d^{d+1}x$$

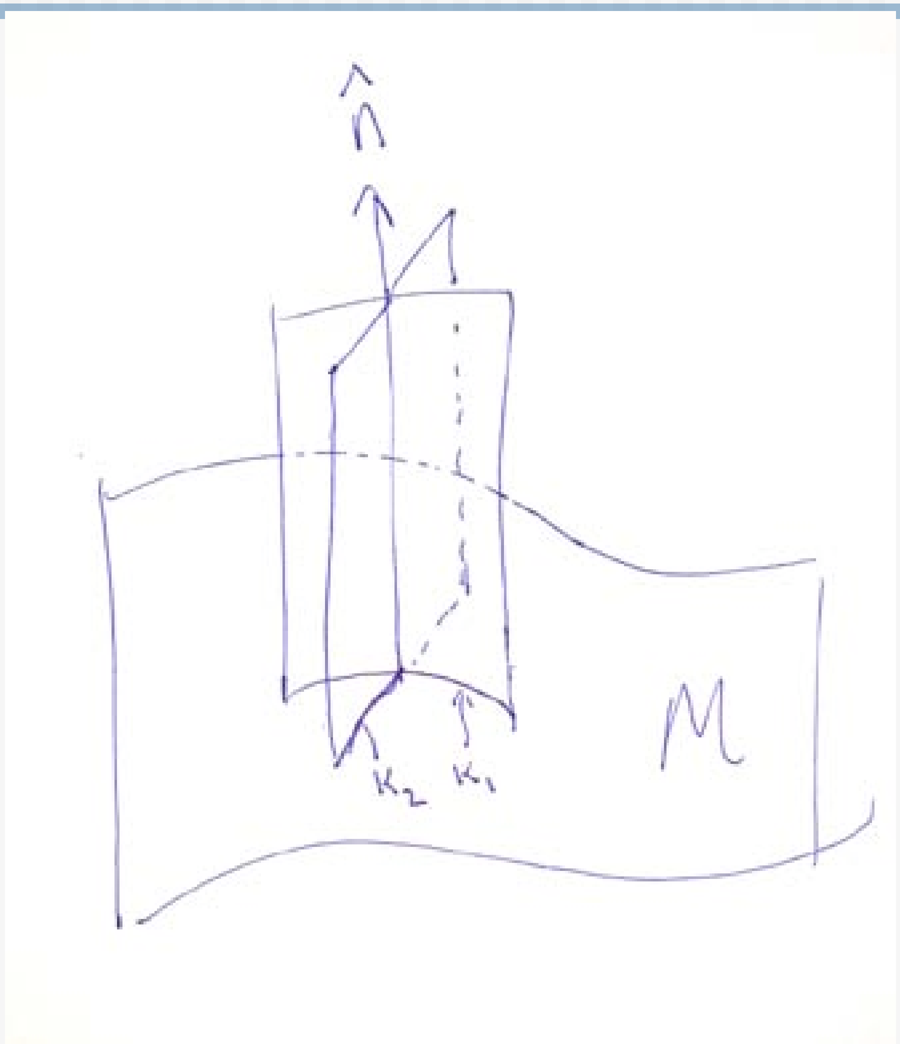


The result:

$- \Delta_{LB} + q,$

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

Principal curvatures



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

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 ○

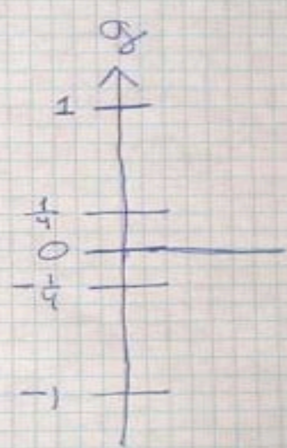
Harrell – Loss

(iii)

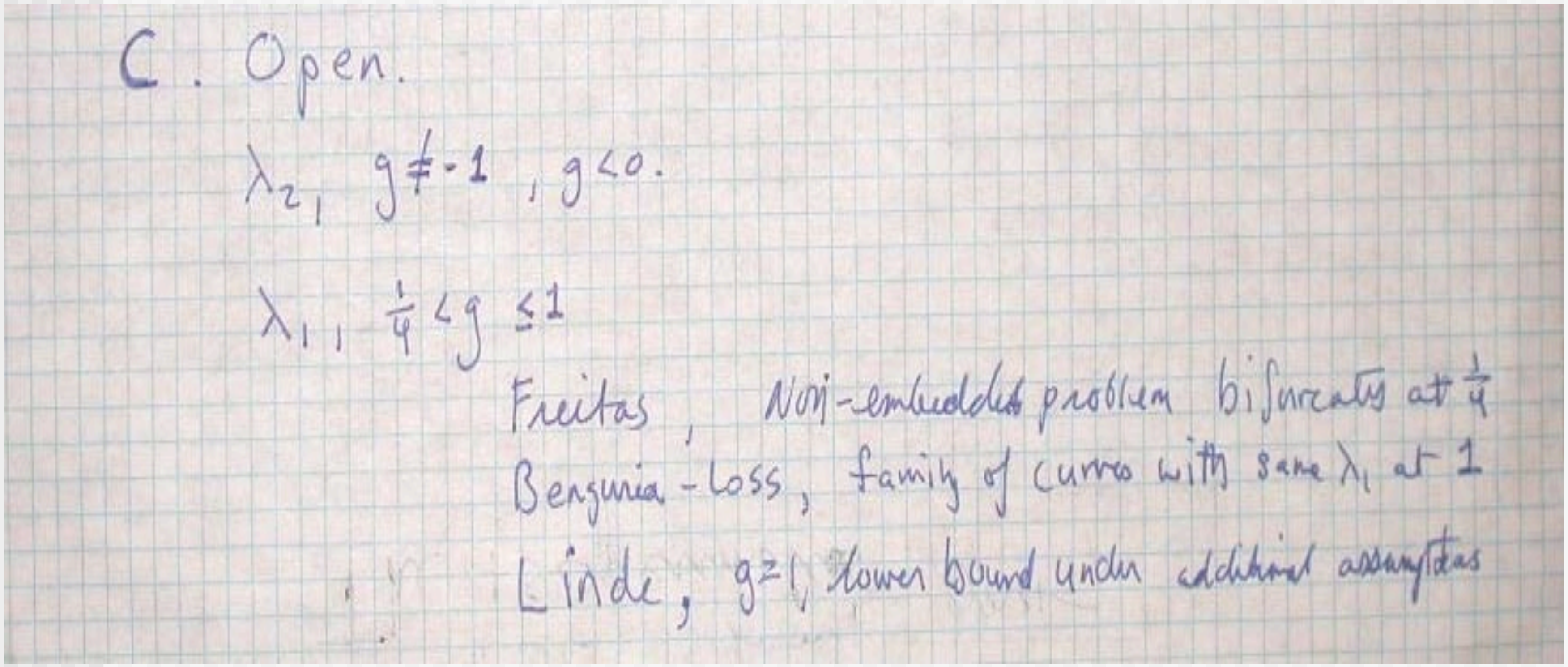
$0 \leq g \leq \frac{1}{4}$

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, $g \geq 1$, 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

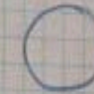
* Special facts in 2-D about conformal equivalence.

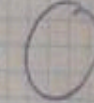
II. Two dimensions

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

False in high dim.

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

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

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

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

<u>Open</u> - other genera

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

More loopy problems

In 1999, 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

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

  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/lwl 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

END

Appendix on an electron near a charged thread

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

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Reduction to an isoperimetric problem of classical type.

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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).

About Birman-Schwinger

With a factorization due to Birman and Schwinger, an operator H will have eigenvalue λ iff a family of operators B(λ) has eigenvalue 1.

Birman - Schwinger

Consider the negative eigenvalues of $-\Delta + V(x)$ on $\mathbb{R}^n$, $V(x)$ minimally regular (Kato class) and $\to 0$ at ∞.

Suppose u is an eigenfunction,

$$(-\Delta + V(x))\,u = \lambda u, \quad \lambda < 0. \qquad ☆$$

$$(-\Delta + |\lambda|)\,u = -V(x)\,u$$

$$u = -(-\Delta + |\lambda|)^{-1} V(x)\,u.$$

Let $\phi = \sqrt{|V(x)|}\,\mathrm{sgn}\,V(x)\,u$. Then

$$\phi = \left[-\sqrt{|V(x)|}\,\mathrm{sgn}\,V(x)\,(-\Delta + |\lambda|)^{-1}\sqrt{|V(x)|}\right]\phi$$

$$=: B_\lambda \phi.$$

Simplify: $V(x) \leq 0$. Then $B_\lambda = \sqrt{|V(x)|}\,(-\Delta + |\lambda|)^{-1}\sqrt{|V(x)|}$

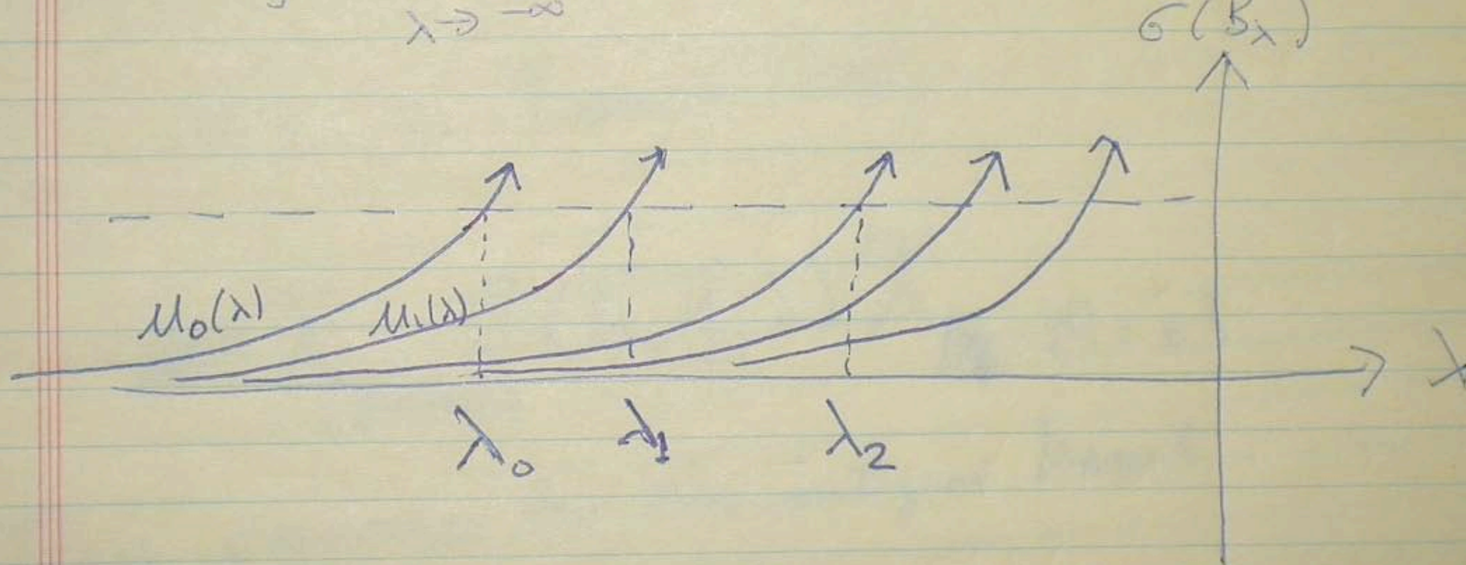
and $\boxed{\phi = B_\lambda \phi}$ (eigenvalue 1)

$\Longleftrightarrow$ ☆.

Now note that in sense of operators,

$$0 > \lambda > \lambda' \Rightarrow B_\lambda > B_{\lambda'}$$

Also, $\lim_{\lambda \to -\infty} B_\lambda = 0$



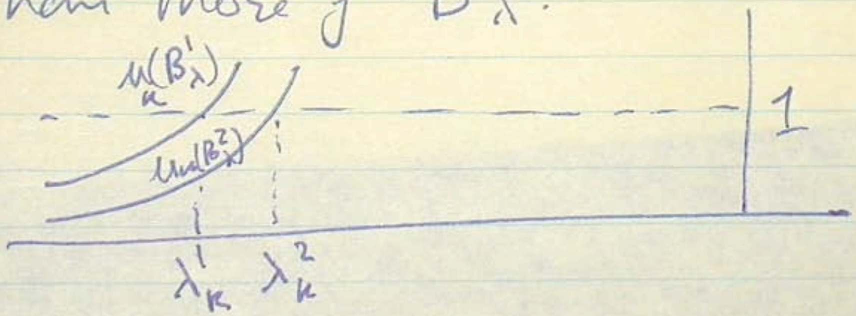
Consider now two potentials V_1, V_2,

and suppose $B^1_\lambda \geq B^2_\lambda$ for all $\lambda < 0$.

Then $\lambda^1_k(-\Delta + V_1) \leq \lambda^2_k(-\Delta + V_2)$,

because all the curves of B^1_λ are higher

than those of B^2_λ:



A positively charged thread can be modeled as

$V(x) = -\alpha\, \delta_\Gamma(\vec{x})$

Approximate by honest functions supported in $\{x : \mathrm{dist}(x, \Gamma) \le \varepsilon\}$.

B_λ has a kernel like

$$-N(\varepsilon)\, \chi_{\{|x-\Gamma| \le \varepsilon\}}\, G(\vec{x}, \vec{y}, \lambda)\, \chi_{\{|y-\Gamma| \le \varepsilon\}}$$

This converges to an integral kernel

$$G(\vec{x}, \vec{y}, \lambda)\Big|_{\vec{x}, \vec{y} \in \Gamma}$$

Specifically, with $\kappa = \sqrt{-\lambda}$,

$$\boxed{\frac{\alpha}{2\pi} K_0\left(\kappa\,|\Gamma(s) - \Gamma(s')|\right)}$$

It thus 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.

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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:

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

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.

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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,

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

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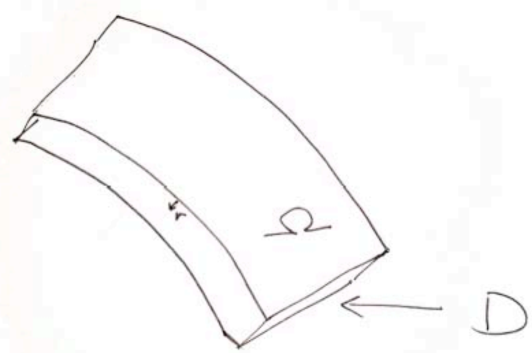
Appendix on thin structures and local geometry

Thin domain of fixed width
variable r= distance from edge

Energy form in separated variables:

$$\int_D |\nabla_{\parallel} \zeta|^2 \, d^{d+1}x + \int_D |\zeta_r|^2 \, d^{d+1}x$$



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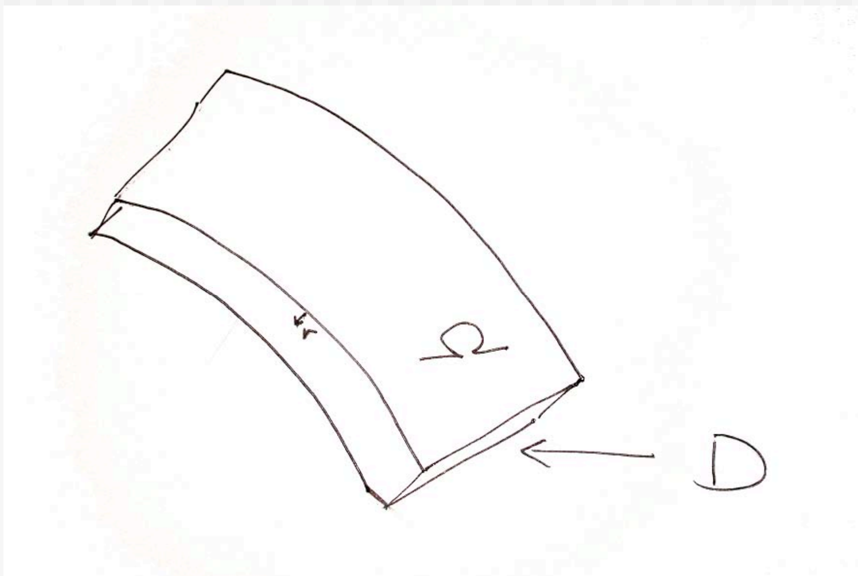

Energy form in separated variables:

$$\int_D |\nabla_{||} \zeta|^2 d^{d+1}x + \int_D |\zeta_r|^2 d^{d+1}x$$

First term is the energy form of Laplace-Beltrami.

Conjugate second term so as to replace it by a potential.

We split the components of the Dirichlet form for the Laplace operator as:

$$\int_D \left|\nabla_{||}\, \zeta\right|^2 \mathrm{d}^{\nu+1}x \;+\; \int_D \left|\zeta_r\right|^2 \mathrm{d}^{\nu+1}x$$

and transform the second term (only) as follows. Fix a coordinate system on the edge Ω, and for any point $\mathbf{x}$ in D, choose as its coordinates other than r the coordinates of the closest point on the edge. Let dV^{ν} denote the volume element on Ω. Then

$$\int_D \left|\zeta_r\right|^2 \mathrm{d}^{\nu+1}x \;=\; \int_\Omega \int_0^d \left|\zeta_r\right|^2 \rho(\mathbf{x})\mathrm{dr}\ \mathrm{dV}^{\nu},$$

We write the test function as

$$\zeta = \frac{1}{\sqrt{\rho}} \cdot (\sqrt{\rho}\,\zeta)$$

and use the product rule in the form

$$\left((fg)'\right)^2 = f^2\,(g')^2 + g^2\,(f')^2 + \frac{1}{2}\,(f^2)'(g^2)'$$

to find

$$\int_0^d |\zeta_r|^2 \rho \mathrm{dr} = \int_0^d \left(\left|(\sqrt{\rho}\zeta)_r\right|^2 + \frac{1}{4}\left(\frac{\rho_r}{\rho}\right)^2 \zeta^2 \rho + \frac{\rho}{2}\left(\frac{1}{\rho}\right)_r (\rho\zeta^2)_r \right) \mathrm{dr}.$$

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When the final term is integrated by parts, the full Dirichlet form takes on the appearance

$$\int_A |\nabla_{||}\,\zeta|^2\, \mathrm{d}^{\nu+1}x + \int_A q(\mathbf{x})\,\zeta^2\, \mathrm{d}^{\nu+1}\mathrm{x} + \int_\Omega \int_0^d |(\sqrt{\rho}\zeta)_r|^2\, \mathrm{dr}\, \mathrm{dV}^\nu. \qquad (3.1)$$

The effective potential in the middle contribution is

$$q(\mathbf{x}) := -\frac{1}{4}\left(\frac{\rho_r}{\rho}\right)^2 + \frac{1}{2}\frac{\rho_{rr}}{\rho}.$$

Some subtleties

- The limit is singular - change of dimension.
- If the particle is confined e.g. by Dirichlet boundary conditions, the energies all diverge to +infinity
- “Renormalization” is performed to separate the divergent part of the operator.

The result:

$- \Delta_{LB} + q,$

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

Appendix:
the Benguria-Loss transformation

Benguria-Loss transformation

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

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

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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:

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