Isoperimetric problems arising in the physics of thin structures and in geometry

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Nanoelectronics

- Quantum wires
- Quantum waveguides
- Designer potentials STM places individual atoms on a surface; quantum dots
- Semi- and non-conducting "threads" Simplified mathematical models

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 about 3 years that answer is circle.

Reduction to an isoperimetric problem of classical type.

Is it true that:

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

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:

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

 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 the family of operators B(λ) has eigenvalue 1.

Birman - Schwinger
Consider the negative eigenveloos of

$$-\Delta + V(X)$$
 an R^{-} , $V(X)$ minimals
 $ugular (Kato class) and $\Rightarrow c$ at ∞ .
Suppose u is an eigenfunction,
 $(-\Delta + V(X)) u = \Delta u$, $\Delta < 0$.
 $(-\Delta + I\lambda I) u = -V(X) u$
 $u = -(-\Delta + I\lambda I) - V(X) u$.
Let $\Phi = furst sgn V(X) u$. Th
 $\Phi = [-furst sgn V(X) u$. Th
 $\Phi = [-furst sgn V(X) u$. Th
 $=: B_{\lambda} \Phi$.
Simply: $V(X) < 0$. Then $B_{\lambda} = furst (-\Delta + I\lambda I)^{-1} furst$
 $and = \Phi = B_{\lambda} \Phi$. (eigensulu 1)
 $\Rightarrow A$.$

Now note that in sensed operators, $0>\lambda>\lambda' \Rightarrow B_{\lambda}>B_{\lambda'}$ Also, lim Bx = 0 6(B) Mo(x) Mulsi No A

Consider now two putentials Vi, Vz, arel suppose B' > B' > B' for all 1<0. Then $\lambda_{k}(-\Delta + V_{i}) \leq \lambda_{k}(-\Delta + V_{z})$, because all the curves and B' are highes them those of B? : M(B')/ 1 X' X'

(4) Apositively chazed thread can ke modeled as V(x)=- ~ Sr(x) Approximate by honest functions supported In $\xi : dist(x, vi) \leq \varepsilon$ By has a permit like $- \mathcal{M}_{12} X G(\overline{X}, \overline{Y}, \lambda) X$ $\{y - y \} = i \}$ This conveyes to an integral kend G (X, Y, X) XIG F Speaficilly, with K=V=, $\propto K_{o}(K[\Gamma(s)-\Gamma(s')])$

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

$$\int_0^L \int_0^L K_0 \left(\kappa |\Gamma(s) - \Gamma(s')| \right) \mathrm{d}s \mathrm{d}s' \ge \int_0^L \int_0^L K_0 \left(\kappa |\mathcal{C}(s) - \mathcal{C}(s')| \right) \mathrm{d}s \mathrm{d}s'$$

with equality only for the circle.

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with equality only for the circle. Equivalently, show that

$$F_{\kappa}(\Gamma) := \int_{0}^{L/2} \mathrm{d}u \int_{0}^{L} \mathrm{d}s \left[K_{0} \left(\kappa |\Gamma(s+u) - \Gamma(s)| \right) - K_{0} \left(\frac{\kappa L}{\pi} \sin \frac{\pi u}{L} \right) \right]$$

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:

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

A family of isoperimetric conjectures for p > 0:

$$C_{L}^{p}(u): \qquad \int_{0}^{L} |\Gamma(s+u) - \Gamma(s)|^{p} \, \mathrm{d}s \leq \frac{L^{1+p}}{\pi^{p}} \sin^{p} \frac{\pi u}{L} \,,$$

$$C_{L}^{-p}(u): \qquad \int_{0}^{L} |\Gamma(s+u) - \Gamma(s)|^{-p} \, \mathrm{d}s \geq \frac{\pi^{p} L^{1-p}}{\sin^{p} \frac{\pi u}{L}} \,,$$

Right side corresponds to circle.

Proposition. 2.1.

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

First part follows from convexity of $x \rightarrow x^a$ for a > 1:

$$\frac{L^{1+p}}{\pi^p} \sin^p \frac{\pi u}{L} \geq \int_0^L \left(|\Gamma(s+u) - \Gamma(s)|^{p'} \right)^{p/p'} ds$$
$$\geq L \left(\frac{1}{L} \int_0^L |\Gamma(s+u) - \Gamma(s)|^{p'} ds \right)^{p/p'}$$



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

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

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

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

Inequality equivalent to

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

It is therefore sufficient to prove that $|\sin nx| \le n \sin x$

Inductive argument based on

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

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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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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...

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

Stadium, small straight segments p > 4.27898...

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Polygon with rounded edges, similar.

Circle is local maximizer for all p < ∞

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 $\gamma \ge 0$. 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, $0 < u < 2\pi$,

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

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.

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Difficulty:

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

Answer #2 The nanoelectronics answer

• E.g., Da Costa, Phys. Rev. A 1981

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

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

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

Some other answers

- In other physical situations, such as reaction-diffusion, q(x) may be other quadratic expressions in the curvature, usually q(x) ≤ 0.
- The conformal answer: q(x) is a multiple of the scalar curvature.

Heisenberg's Answer (if he had thought about it)

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

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Note: $q(\mathbf{x}) \ge 0$!

Some more loopy problems

$$H(g) := -\frac{d^2}{ds^2} + g \kappa^2.$$
The isoperimetric theorems for $-\nabla^2 + q(\kappa)$



Minimality when $g \le 1/4$.

Proof. a) Assume first that 0 < g < 1/4. The minimal value of λ_1 , which we λ_* , is

$$\inf_{\kappa} \inf_{\zeta} \int \left(\left(\frac{\mathrm{d}\zeta}{\mathrm{d}s} \right)^2 + g \kappa^2 \zeta^2 \right) \mathrm{d}s,$$

Because the quantity in question is an iterated infimum, it may be calculated in the other order. By Cauchy-Schwarz's inequality

$$2\pi = \int \frac{\kappa}{\zeta} \zeta \mathrm{d}s \le \left(\int \frac{1}{\zeta^2} \mathrm{d}s\right)^{1/2} \left(\int \kappa^2 \zeta^2 \mathrm{d}s\right)^{1/2},$$

with equality only if

$$\kappa = \left(2\pi / \int \frac{1}{\zeta^2} \mathrm{d}s\right) \frac{1}{\zeta^2}.$$

A non linear functional

$$E(\zeta) := \int \left(\frac{\mathrm{d}\zeta}{\mathrm{d}s}\right)^2 \mathrm{d}s + \frac{4\pi^2 g}{\int \left(\frac{1}{\zeta^2}\right) \mathrm{d}s}.$$

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 $\lambda_* \le E(\zeta) = 4g\pi^2 < \pi^2$ for g < 1/4.

Lemma 5: If $E(\zeta) \leq \pi^2$ for a positive test function ζ normalized in L^2 , then

$$\inf_{s} \left(\zeta(\mathbf{s}) \right) > 1 - \frac{\sqrt{E(\zeta)}}{\pi}.$$

Proof of Lemma 5.

$$E(\zeta) > \int_0^1 (\zeta')^2 \, \mathrm{d}s = \int_0^1 (\zeta - \zeta_{\min})'^2 \mathrm{d}s \ge \pi^2 \int_0^1 (\zeta - \zeta_{\min})^2 \mathrm{d}s,$$

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Minimizer therefore exists. Its Euler equation is

$$-\zeta_*'' + M \frac{1}{\zeta_*^3} = C \zeta_*,$$

$$M = \frac{4\pi^2 g}{\left(\int_0^1 \frac{1}{\zeta_*^2} \, ds\right)^2}$$

Solution of Euler equation of the form:

$$\zeta_*^2 = 1 + \sqrt{1 - M/\lambda_*} \cos\left(2\sqrt{\lambda_*}(s - s_0)\right)$$

Nonconstant solution of this form excluded because $\lambda_* < \pi^2$.

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



Benguria-Loss, *Contemp. Math.* 2004
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- Linde Proc AMS 2005
- $\lambda_0 > 0.6085$ (convex, etc.)

II. J wo dimensions A. g(K)= g K, Kz (Ganß curvature), genus(2)=0, 121=1. (1) Hersch 1970, 920, 2, trivilly = 0 d=2: Iz uniquely maximized by SZCR3 (ii) Harrell 1986 any g, 2, 2 both uniquely maximized by (* certains other potentials, g (Kitki) g 40. Open - other genera * Special facts in 2-D about conformal equivalue

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113 Two or more dimensione. A R-hypnsurface of codimension 1 -72-1 (2Ke)2 12 Uniquely movimized by sphere (Hanele-Loss'98). ⇒ Same for g(K)= - Z[K2] B) D-embeddielin IRME HIME She El Soufi-Ilia Actually show h2 (-V3 V4) 4 isidim JE 12 + Vare

Universal Bounds using Commutators

• A "sum rule" identity (Harrell-Stubbe, 1997):

$$1 = \frac{4}{d} \sum_{k:\lambda_k \neq \lambda_j} \frac{\left| \langle u_k, \mathbf{p} u_j \rangle \right|^2}{\lambda_k - \lambda_j}$$

Here, H is *any* Schrödinger operator, **p** is the gradient (times -i if you are a physicist and you use atomic units)

Commutators: [A,B] := AB-BA

3a. The equations of space curves are commutators:

$$\left[\frac{d}{ds}, \mathbf{x}\right] = \mathbf{t}$$

$$\left[\frac{d}{ds}, \mathbf{t}\right] = \kappa \mathbf{n}$$

Note: curvature is defined by a second commutator

The Serret-Frenet equations as commutator relations:

$$[H, X_m] = -\frac{d^2 X_m}{ds^2} - 2 \frac{d X_m}{ds} \frac{d}{ds} = -\kappa n_m - 2t_m \frac{d}{ds}, \qquad (2.2)$$
$$[X_m [H, X_m]] = 2t_m^2. \qquad (2.3)$$

Lemma. Let *M* be a smooth curve in \mathbb{R}^d , d = 2 or 3. Then for

$$H = -\frac{d^2}{ds^2} + \mathbf{V}(\mathbf{s}) \quad and \ \varphi \in W_0^1(M),$$
$$\sum_{m=0}^{\mathbf{d}} \|[H, X_m] \ \varphi\|^2 = 4 \int_M \left(\left| \frac{d\varphi}{ds} \right|^2 + \frac{\kappa^2}{4} |\varphi|^2 \right) ds.$$

Proposition 2.1 Let
$$M$$
 be a smooth curve in \mathbb{R}^{ν} , $\nu = 2$ or 3. Then for $H = -\frac{d^2}{ds^2} + \mathbf{V}(\mathbf{s})$ and $\varphi \in W_0^1(M)$,

$$\sum_{m=0}^{\mathbf{d}} \|[H, X_m] \varphi\|^2 = 4 \int_M \left(\left| \frac{d\varphi}{ds} \right|^2 + \frac{\kappa^2}{4} |\varphi|^2 \right) ds.$$

Proof. By closure it may be assumed that $\varphi \in C_c^{\infty}(M)$. Apply (2.2) to φ and square the result, to obtain

$$4\left(t_m^2\left(\frac{d\varphi}{ds}\right)^2 + \frac{1}{4}\kappa^2 n_m^2\varphi^2 + \frac{1}{2}\kappa n_m t_m\varphi\frac{d\varphi}{ds}\right).$$

Sum on m and integrate.

QED

Interpretation:

Algebraically, for quantum mechanics on a wire, the natural H_0 is not

but rather

$$H_{1/4} := p^2 + \kappa^2/4.$$

Corollary 2.2 Let M be as in Proposition 2.1 and suppose that H is a Schrödinger Hamiltonian with a bounded measurable potential V(s). Then

$$\Gamma \le 4 \int_M \left(\left(\frac{du_1}{ds} \right)^2 + \frac{\kappa^2}{4} u_1^2 \right) ds.$$
(2.5)

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That is, the gap for *any* H is controlled by an expectation value of $H_{1/4}$.

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(2.5)

Furthermore, if H is of the form

$$H_g := -\frac{d^2}{ds^2} + g\kappa^2,$$

then

$$\Gamma \le \max\left(4, \frac{1}{g}\right)\lambda_1.$$
 (2.6)

Equivalently, the universal ratio bound

$$\frac{\lambda_2}{\lambda_1} \le \max\left(5, 1 + \frac{1}{g}\right)$$

holds.

Bound is sharp for the circle:

 $\frac{\lambda_2}{\lambda_1} = \frac{4\pi^2 \left(1+g\right)}{4\pi^2 g} = 1 + \frac{1}{g}.$

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.,

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

Here h is the sum of the principal curvatures.

Corollary 3.2 Let *H* be as in (3.1) and define $\delta := \sup_M \left(\frac{h^2}{4} - V\right)$. Then $\Gamma(H) \leq \frac{4}{d} (\lambda_1 + \delta)$.

Bound is sharp for the sphere: $\lambda_1 = qd^2, \quad \lambda_2 = qd^2 + d$ $d = \lambda_2 - \lambda_1 \le \left(\frac{gd^2}{gd}\right) = d.$

Spinorial Canonical Commutation

$$\mathbf{P} = \sum_{j=1}^{d} \left(\mathbf{t}_j \frac{\partial}{\partial s_j} \pm \frac{1}{2} \kappa_j \mathbf{n} \right)$$
(4.1)

and for a dense set of functions φ ,

$$\|\mathbf{P}\varphi\|^2 = \left\langle \varphi, H_{1/4}\varphi \right\rangle. \tag{4.2}$$

Spinorial Canonical Commutation

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and for a dense set of functions φ ,

$$\|\mathbf{P}\varphi\|^2 = \left\langle \varphi, H_{1/4}\varphi \right\rangle. \tag{4.2}$$

Thus **P** plays the rôle of a momentum operator, with which there is a version of canonical commutation (cf. (1.9)) as follows. Defining a variant commutator bracket for operators $L^2(M) \to \mathbb{R}^{d+1} \otimes L^2(M)$ by $[A; B] := A \cdot B - B \cdot A$, a calculation shows that $[\mathbf{P}; X_k \mathbf{e}_k] = \sum_{j=1}^d \mathbf{t}_j \cdot \frac{\partial X_k \mathbf{e}_k}{\partial s_j} = \mathbf{1}$ (identity operator), and by averaging on k,

$$\mathbf{1} = \frac{1}{d} \ [\mathbf{P}; \mathbf{X}] \tag{4.3}$$

which is a coordinate-independent formula.

Sum Rules

Proposition 4.1 Let H be as in (3.1), with eigenvalues $\{\lambda_k\}$ and normalized eigenfunctions $\{u_k\}$. Then

$$1 = \frac{4}{d} \sum_{\substack{k \\ \lambda_k \neq \lambda_j}} \frac{|\langle u_k, \mathbf{P} u_j \rangle|^2}{\lambda_k - \lambda_j}.$$
(4.4)

Corollaries of sum rules

- Sharp universal bounds for all gaps
- Some estimates of partition function $Z(t) = \sum \exp(-t \lambda_k)$

Speculations and open problems

- Can one obtain/improve Lieb-Thirring bounds as a consequence of sum rules?
- Full understanding of spectrum of H_g . What spectral data needed to determine the curve? What is the bifurcation value for the minimizer of λ_1 ?
- Physical understanding of H_g and of the spinorial operators it is related to.

Sharp universal bound for all gaps

Corollary 4.4 b) For H_g be of the form (1.10) on a smooth, compact submanifold. Then

$$[\lambda_n, \lambda_{n+1}] \subseteq \left[\left(1 + \frac{2\sigma}{d}\right) \overline{\lambda_n} - \sqrt{D_n}, \left(1 + \frac{2\sigma}{d}\right) \overline{\lambda_n} + \sqrt{D_n} \right],$$

with

$$D_n := \left(\left(1 + \frac{2\sigma}{d} \right) \overline{\lambda_n} \right)^2 - \left(1 + \frac{4\sigma}{d} \right) \overline{\lambda_n^2}.$$

This bound is sharp for every non-zero eigenvalue gap of $H_{\frac{1}{4}}$ on the sphere.
Partition function

$$Z(t) := tr(exp(-tH)).$$

Partition function

$$Z(t) \le \left(\frac{2t}{d}\right) \sum_{j} \left(\exp\left(-t\lambda_{j}\right)\right) \|\mathbf{P}u_{j}\|^{2},$$

which implies

- **Corollary 4.5** a) Let H be as (3.1), with M a compact, smooth submanifold. Then $t^{\frac{d}{2}} \exp(-\delta t) Z(t)$ is a nondecreasing function;
 - b) For H_g be of the form (1.10) on a smooth, compact submanifold M, $t^{\frac{d}{2\sigma}}Z(t)$ is a nondecreasing function.