Commutators, eigenvalues, and quantum mechanics on surfaces.

Evans Harrell

Georgia Tech

www.math.gatech.edu/~harrell

Tucson and Tours,
2004

Dramatis personae

$$\Delta := \nabla^2 := \sum_j \frac{}{\partial {x_j}^2}$$

Schrödinger:

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

Dramatis personae

- Commutator $[A,B] = AB - BA$

Dramatis personae

- Commutator $[A,B] = AB - BA$
- The “nano” world

Dramatis personae

- Commutator $[A,B] = AB - BA$
- The “nano” world
- Curvature

Eigenvalues

- $H\ u_k = \lambda\ u_k$
- For simplicity, the spectrum will often be assumed to be discrete. For example, the operators might be defined on bounded regions.

Eigenvalues

- Laplacian - squares of frequencies of normal modes of vibration (acoustics/electromagnetics, etc.)

Eigenvalues

- Laplacian - squares of frequencies of normal modes of vibration (acoustics/electromagnetics, etc.)
- Schrödinger Operator - energies of an atom or quantum system.

The spectral theorem for a general self-adjoint operator

- The spectrum can be any closed subset of R.

The spectral theorem for a general self-adjoint operator

- For each u, there exists a measure μ, such that

$$\langle u, f(A)u \rangle = \int_{sp} f(\lambda) d\mu(\lambda)$$

The spectral theorem for a general self-adjoint operator

- Implication:
  - If $f(\lambda) \geq g(\lambda)$ on the spectrum, then
  - $\langle u, f(H)\, u\rangle \geq \langle u, g(H)\, u\rangle$

The spectrum of H

- For Laplace or Schrödinger not just any old set of numbers can be the spectrum!

“Universal” constraints on the spectrum

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

“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.

“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:

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

“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:
- E. Lieb and W. Thirring, 1977, P. Li, S.T. Yau, 1983, sums of powers of eigenvalues, in terms of the phase-space volume.

“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:
- E. Lieb and W. Thirring, 1977, P. Li, S.T. Yau, 1983, sums of powers of eigenvalues, in terms of the phase-space volume.
- Hile-Protter, 1980, Like PPW, but more complicated.

PPW vs. HP

- L. Payne, G. Pólya, H. Weinberger, 1956:

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

- Hile-Protter, 1980:

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

The universal industry after PPW

- Ashbaugh-Benguria 1991, proof of the isoperimetric conjecture of PPW.

PPW:

$$\frac{\lambda_2}{\lambda_1} \leq 1 + \frac{4}{d}$$

Ashbaugh-Benguria:

$$\frac{\lambda_2}{\lambda_1} \leq \frac{\lambda_2(\text{ball})}{\lambda_1(\text{ball})}$$

"Universal" constraints on eigenvalues

- Ashbaugh-Benguria 1991, isoperimetric conjecture of PPW proved.
- H. Yang 1991-5, unpublished, complicated formulae like PPW, respecting Weyl asymptotics.
- Harrell, Harrell-Michel, Harrell-Stubbe, 1993-present, commutators.
- Hermi PhD thesis
- Levitin-Parnovsky, 2001?

In this industry….

In this industry….

1. The arguments have varied, but always essentially algebraic.

In this industry….

1. The arguments have varied, but always essentially algebraic.

2. Geometry often shows up - isoperimetric theorems, etc.

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 nanophysicists' answer

- E.g., Da Costa, Phys. Rev. A 1981

Answer #2:

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

Where the effective potential q responds to how the surface is immersed in space.

Nanoelectronics

- Nanoscale = 10-1000 X width of atom

Nanoelectronics

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

Nanoelectronics

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

Nanoelectronics

- Quantum wires - etched semiconductors, wires of gold in carbon nanotubes.

Nanoelectronics

- Quantum wires
- Quantum waveguides - macroscopic in two dimensions, nanoscale in the width

Nanoelectronics

- Quantum wires
- Quantum waveguides
- Designer potentials - STM places individual atoms on a surface

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

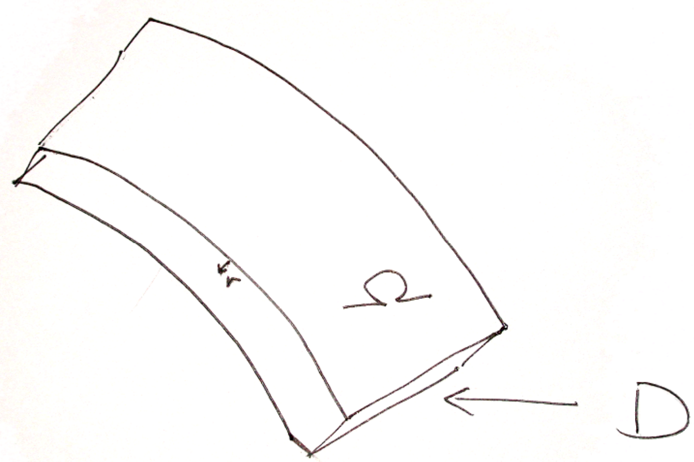
$$- \Delta_{LB} + q$$

- **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:

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



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.

Some subtleties

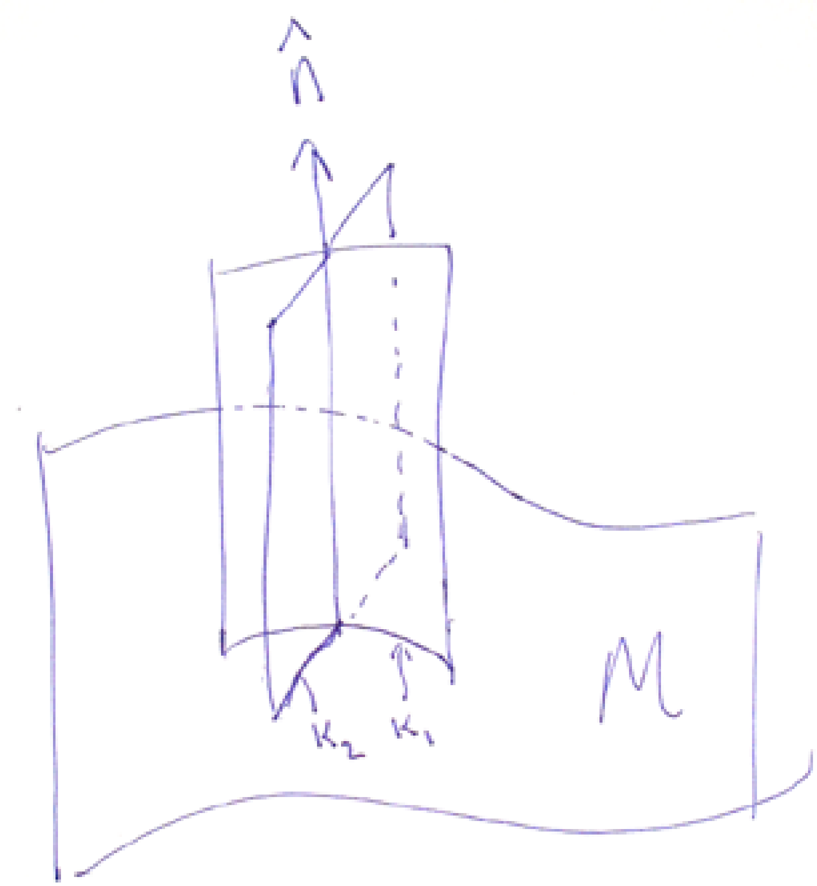
- The limit is singular - change of dimension.
- If the particle is confined e.g. by Dirichlet boundary conditions, the energies all diverge to +infinity
- “Renormalization” is performed to separate the divergent part of the operator.

The result:

$- \Delta_{LB} + q,$

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

Principal curvatures



The result:

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

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

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

Consequence of $q(x) \leq 0$:

Consequence of $q(x) \leq 0$:

- If there is any bending at all, and the wire or waveguide is large and asymptotically flat, then there is always a bound state below the conduction level.

Consequence of $q(x) \leq 0$:

- If there is any bending at all, and the wire or waveguide is large and asymptotically flat, then there is always a bound state below the conduction level.
- By bending or straightening the wire, current can be switched off or on.

Difficulty:

- **Tied to a particular physical model - other effective potentials arise from other physical models or limits.**

Some other answers

- **In other physical situations, such as reaction-diffusion, $q(x)$ may be other quadratic expressions in the curvature, usually $q(x) \le 0$.**

- **The conformal answer: $q(x)$ is a multiple of the scalar curvature.**

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

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

Heisenberg's Answer

(if he had thought about it)

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

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

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

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

1. Quantum mechanics is the effect that observables do not commute:

- Canonical commutation:

$[Q, P] = i\hbar$

- Equations of motion, “Heisenberg picture”

$$\frac{\partial A}{\partial t} = \frac{i}{\hbar}[H, A]$$

Canonical commutation

Set $\hbar = 1$

$[Q, P] = i$

Represented by $Q = x$, $P = -i\, d/dx$
Canonical commutation is then just
the product rule:

$$x i \frac{d}{dx} f(x) - i \frac{d}{dx} \left(x f(x) \right) = i f(x)$$

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

2. Eigenvalue gaps are connected to commutators:

$H u_k = \lambda_k u_k$, H self-adjoint

Elementary gap formula:

$$\langle u_j, [H,G] u_k \rangle = (\lambda_j - \lambda_k) \langle u_j, G u_k \rangle .$$

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

Elementary gap formula:

$$[H, G]u_k = (H - \lambda_k)Gu_k,$$

$$\Longrightarrow$$

$$\langle u_j, [H, G]u_k \rangle = (\lambda_j - \lambda_k) \langle u_j, Gu_k \rangle .$$

What do you get when you put canonical commutation together with the gap formula?

Commutators and gaps

Elementary gap formula:

$$\langle u_j, [H,G]u_k\rangle = (\lambda_j - \lambda_k)\langle u_j, Gu_k\rangle\,. \tag{1.2}$$

Since $[H,G]u_k = (H - \lambda_k)Gu_k,$

$$\|[H,G]u_k\|^2 = \left\langle Gu_k, (H-\lambda_k)^2\,Gu_k\right\rangle, \tag{1.3}$$

and more generally

$$\langle [H,G]u_j, [H,G]u_k\rangle = \langle Gu_j, (H-\lambda_j)\,(H-\lambda_k)\,Gu_k\rangle\,. \tag{1.4}$$

Second commutator formula:

$$\langle u_j \mid [G,[H,G]]\,u_k\rangle = \langle Gu_j \mid (2H - \lambda_j - \lambda_k)\,Gu_k\rangle\,. \tag{1.5}$$

In particular,

$$\langle u_j \mid [G,[H,G]]\,u_j\rangle = 2\,\langle Gu_j \mid (H - \lambda_j)\,Gu_j\rangle\,. \tag{1.6}$$

The fundamental eigenvalue gap

$$\Gamma \;:=\; \lambda_2 - \lambda_1$$

- In quantum mechanics, an excitation energy
- In "spectral geometry" a geometric quantity

  small gaps indicate decoupling (dumbbells)

  (Cheeger, Yang-Yau, etc.)

  large gaps indicate convexity/isoperimetric

  (Ashbaugh-Benguria)

Gap Lemma

$$\Gamma \langle u_1, [G, [H, G]]\, u_1 \rangle \leq 2\|[H, G] u_1\|^2.$$

H = your favorite self-adjoint operator, u_1 the fundamental eigenfunction, and G is whatever you want.

Gap Lemma

$$\Gamma \langle u_1, [G, [H, G]]\, u_1 \rangle \leq 2 \| [H, G] u_1 \|^2.$$

H = your favorite self-adjoint operator, u_1 the fundamental eigenfunction, and G is whatever you want. *CHOOSE IT WELL!*

Commutators and gaps

Elementary gap formula:

$$\langle u_j, [H,G]u_k\rangle = (\lambda_j - \lambda_k)\,\langle u_j, Gu_k\rangle\,. \tag{1.2}$$

Since $\quad [H,G]u_k = (H-\lambda_k)Gu_k,$

$$\|[H,G]u_k\|^2 = \left\langle Gu_k, (H-\lambda_k)^2\, Gu_k\right\rangle, \tag{1.3}$$

and more generally

$$\langle [H,G]u_j, [H,G]u_k\rangle = \langle Gu_j, (H-\lambda_j)\,(H-\lambda_k)\,Gu_k\rangle\,. \tag{1.4}$$

Second commutator formula:

$$\langle u_j \mid [G,[H,G]]\,u_k\rangle = \langle Gu_j \mid (2H-\lambda_j-\lambda_k)\,Gu_k\rangle\,. \tag{1.5}$$

In particular,

$$\langle u_j \mid [G,[H,G]]\,u_j\rangle = 2\,\langle Gu_j \mid (H-\lambda_j)\,Gu_j\rangle\,. \tag{1.6}$$

Commutators and gaps

Since $[H,G]u_k = (H-\lambda_k)Gu_k,$

$$\|[H,G]u_k\|^2 = \left\langle Gu_k, (H-\lambda_k)^2\, Gu_k \right\rangle, \qquad (1.3)$$

$$\langle u_j \mid [G,[H,G]]\, u_j \rangle = 2\,\langle Gu_j \mid (H-\lambda_j)\, Gu_j \rangle\,. \qquad (1.6)$$

Commutators and gaps

Since $[H, G]u_k = (H - \lambda_k)Gu_k,$

$$\|[H, G]u_k\|^2 = \left\langle Gu_k, (H - \lambda_k)^2 \, Gu_k \right\rangle, \qquad (1.3)$$

$$\langle u_j \mid [G, [H, G]] \, u_j \rangle = 2 \, \langle Gu_j \mid (H - \lambda_j) \, Gu_j \rangle \, . \qquad (1.6)$$

Proof

Because

$$\langle u_k \mid [G,[H,G]]\, u_k\rangle = 2\,\langle Gu_k \mid (H-\lambda_k)\, Gu_k\rangle\,.$$

and

$$\|[H,G]u_k\|^2 = \Big\langle Gu_k, (H-\lambda_k)^2\, Gu_k \Big\rangle$$

the inequality

$$\Gamma\,\langle u_1, [G,[H,G]]\, u_1\rangle \leq 2\|[H,G]u_1\|^2. \qquad (1.7)$$

is equivalent to

$$\langle Gu_1 \mid (H-\lambda_1)\,(\lambda_2-\lambda_1)\, Gu_1\rangle \leq \Big\langle Gu_1 \mid (H-\lambda_1)^2 Gu_1 \Big\rangle$$

Proof

Because

$$\langle u_k \mid [G,[H,G]]\, u_k \rangle = 2 \langle G u_k \mid (H-\lambda_k)\, G u_k \rangle .$$

and

$$\|[H,G]u_k\|^2 = \left\langle G u_k, (H-\lambda_k)^2\, G u_k \right\rangle$$

the inequality

$$\Gamma \langle u_1, [G,[H,G]]\, u_1 \rangle \leq 2\|[H,G]u_1\|^2. \qquad (1.7)$$

is equivalent to

$$\langle G u_1 \mid (H-\lambda_1)\,(\lambda_2-\lambda_1)\, G u_1 \rangle \leq \left\langle G u_1 \mid (H-\lambda_1)^2 G u_1 \right\rangle$$

But on the spectrum,

$$(\lambda - \lambda_1)\,(\lambda_2 - \lambda_1) \leq (\lambda - \lambda_1)^2$$

Universal Bounds using Commutators

- Play off canonical commutation relations against the specific form of the operator:

$$H = p^2 + V(x)$$

- Insert projections, take traces.

Universal Bounds using Commutators

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

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

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

Universal Bounds with Commutators

- Compare with Hile-Protter:

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

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

Universal Bounds with Commutators

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

- No sum on j - multiply by $f(\lambda_j)$, sum and symmetrize
- Numerator only kinetic energy - no potential.

Among the consequences:

- All gaps: $[\lambda_n, \lambda_{n+1}] \subseteq [\lambda_-(n), \lambda_+(n)]$, where

$$\lambda_\pm := \left(1 + \frac{2\sigma}{d}\right) \frac{1}{n} \sum_{k=1}^{n} \lambda_n \pm \sqrt{D_n}$$

- The constant σ is a bound for the kinetic energy/total energy. ($\sigma=1$ for Laplace, but 1/2 for the harmonic oscillator)

Among the consequences:

- All gaps: $[\lambda_n,\lambda_{n+1}] \subseteq [\lambda_-(n),\lambda_+(n)]$, where

$$\lambda_\pm := \left(1+\frac{2\sigma}{d}\right)\frac{1}{n}\sum_{k=1}^{n}\lambda_n \pm \sqrt{D_n}$$

- D_n is a statistical quantity calculated from the lower eigenvalues.

Among the consequences:

- All gaps: $[\lambda_n, \lambda_{n+1}] \subseteq [\lambda_-(n), \lambda_+(n)]$, where

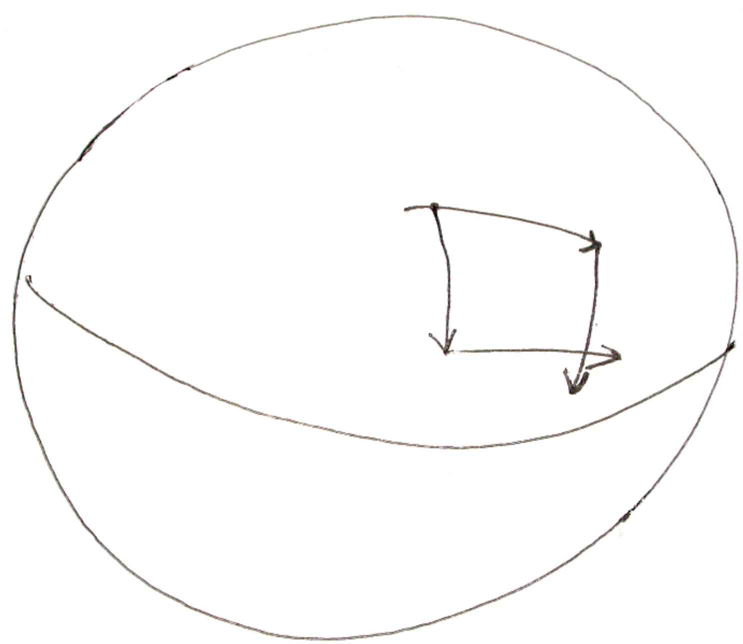
$$\lambda_\pm := \left(1 + \frac{2\sigma}{d}\right) \frac{1}{n} \sum_{k=1}^{n} \lambda_n \pm \sqrt{D_n}$$

- Sharp for the harmonic oscillator for all n!

And now for some completely different commutators….

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

3. Curvature is the effect that motions do not commute:



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

- More formally (from, e.g., Chavel, *Riemannian Geometry, A Modern Introduction*: Given vector fields X,Y,Z and a connection ∇, the curvature tensor is given by:

$$R(X,Y) = [\nabla_Y, \nabla_X] - \nabla_{[Y,X]}$$

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

3a. The equations of space curves are commutators:

$$\frac{d\mathbf{x}}{ds} = \mathbf{t}$$

$$\frac{d\mathbf{t}}{ds} = \kappa \mathbf{n}$$

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

3a. The equations of space curves are commutators:

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

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

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:

$$[H, X_m] = -\frac{d^2 X_m}{ds^2} - 2\,\frac{dX_m}{ds}\frac{d}{ds} = -\kappa n_m - 2t_m\frac{d}{ds}, \tag{2.2}$$

$$[X_m\,[H, X_m]] = 2t_m^2. \tag{2.3}$$

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

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

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

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

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

$$\mathbf{p}^2,$$

but rather

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

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*

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

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*

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

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

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*

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

Furthermore, if H is of the form

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

then

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

Equivalently, the universal ratio bound

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

holds.

Bound is sharp for the circle:

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

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.,*

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

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

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:

$$\lambda_1 = gd^2, \quad \lambda_2 = gd^2 + d$$

$$d = \lambda_2 - \lambda_1 \le \left(\frac{gd^2}{gd} \right) = d.$$

Spinorial Canonical Commutation

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

and for a dense set of functions φ,

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

Spinorial Canonical Commutation

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

and for a dense set of functions φ,

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

Thus $\mathbf{P}$ 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*

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

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

$$Z(t) := \mathrm{tr}(\exp(-tH)).$$

Partition function

$$Z(t) \leq \left(\frac{2t}{d}\right) \sum_j \left(\exp\left(-t\lambda_j\right)\right) \left\|\mathbf{P} u_j\right\|^2,$$

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.*