Mathematics of Quantum Mechanics on Thin Structures

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United Nations
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Lecture 1

Quantum Mechanics for the Impatient

The five-minute history

- Quanta hypothesized around 1900
  - Black-body radiation, Planck
  - Atomic levels, Bohr
  - Photoelectric effect, Einstein
- 1925 Schrödinger turns QM into PDE
- 1925 Heisenberg turns QM into algebra
- 1932 von Neumann shows it's all operator algebra, represented on Hilbert space.

Quantum mechanics is truly weird

Spukhafte Fernwirkung!

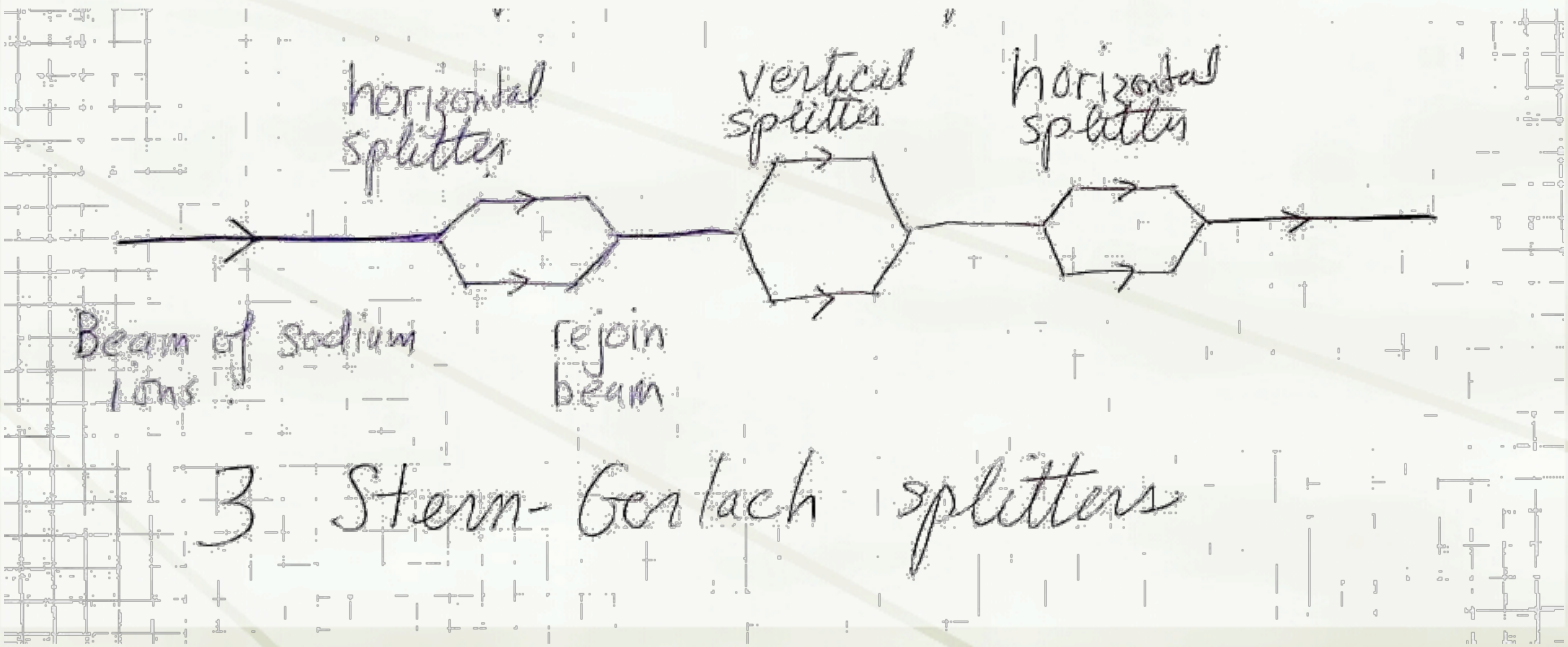
- Stern-Gerlach
- Double-slit
- EPR paradox, “entanglement”

Stern-Gerlach experiment

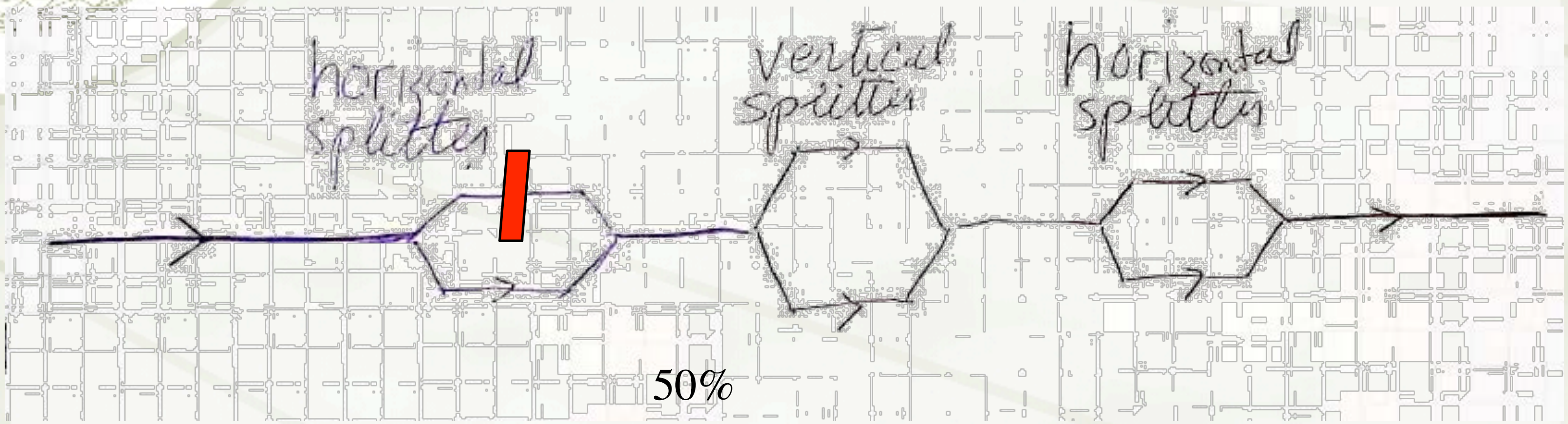
- The observable "spin" can be measured by using a magnetic field to split a beam of ions. For "spin ½" particles, there are precisely two beams, whether split horizontally or vertically. In quantum physics, however, a vertical polarization ("up-down") is incompatible with a horizontal polarization ("right-left")

Stern-Gerlach experiment

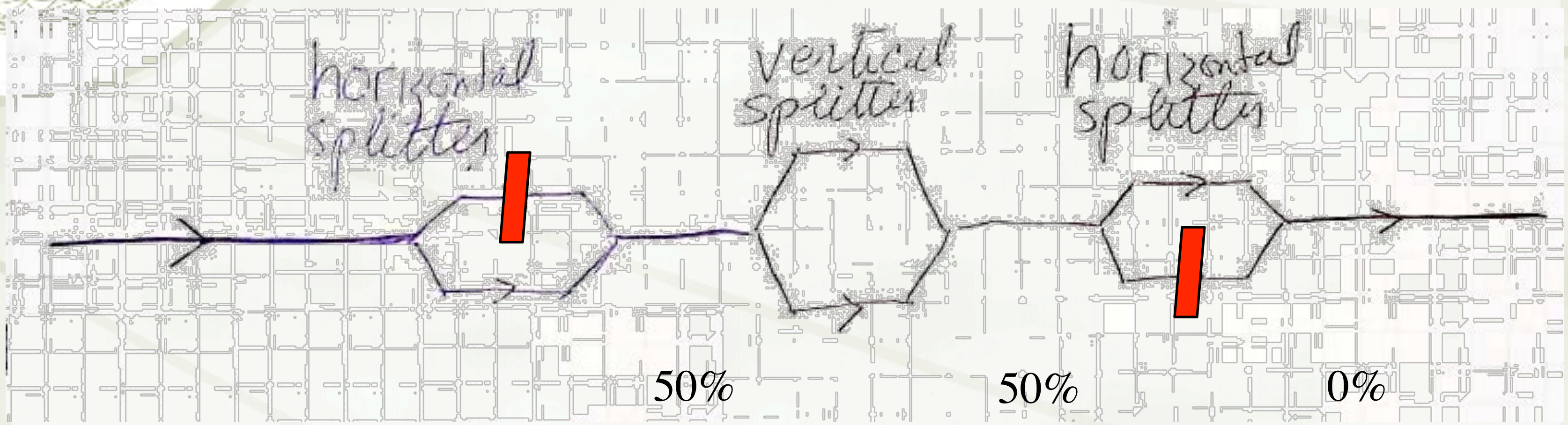
(Following discussion in Feynman's lectures on quantum mechanics.)



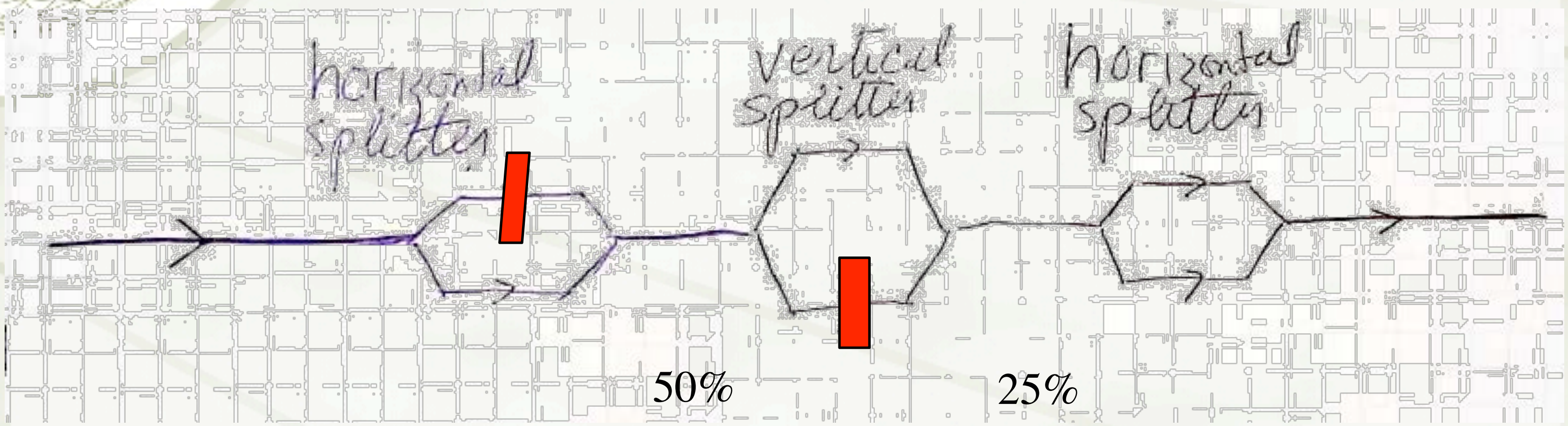
Stern-Gerlach experiment



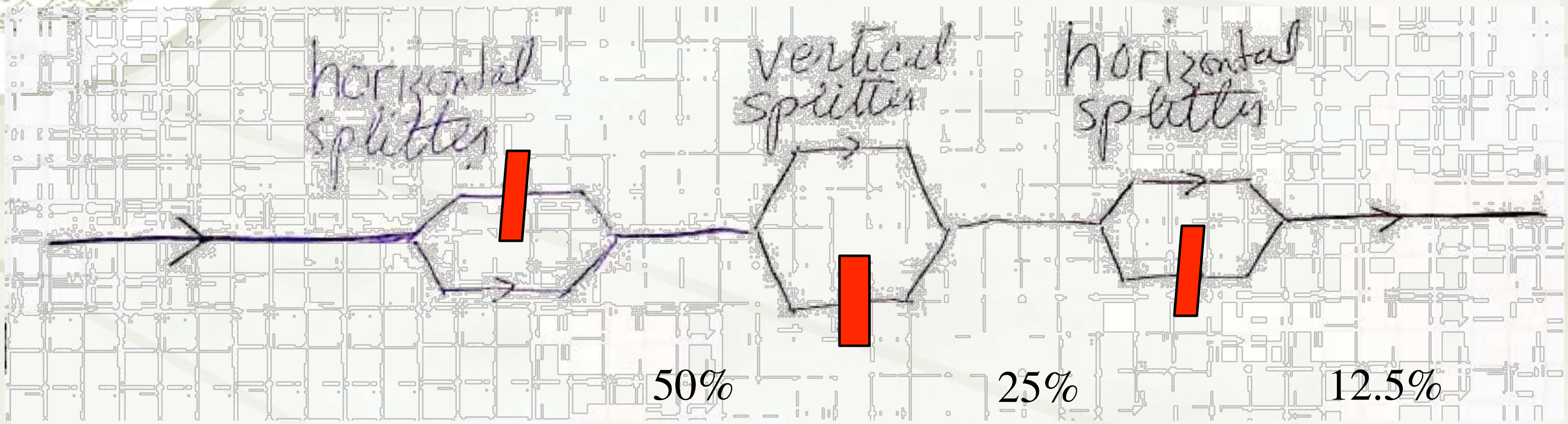
Stern-Gerlach experiment

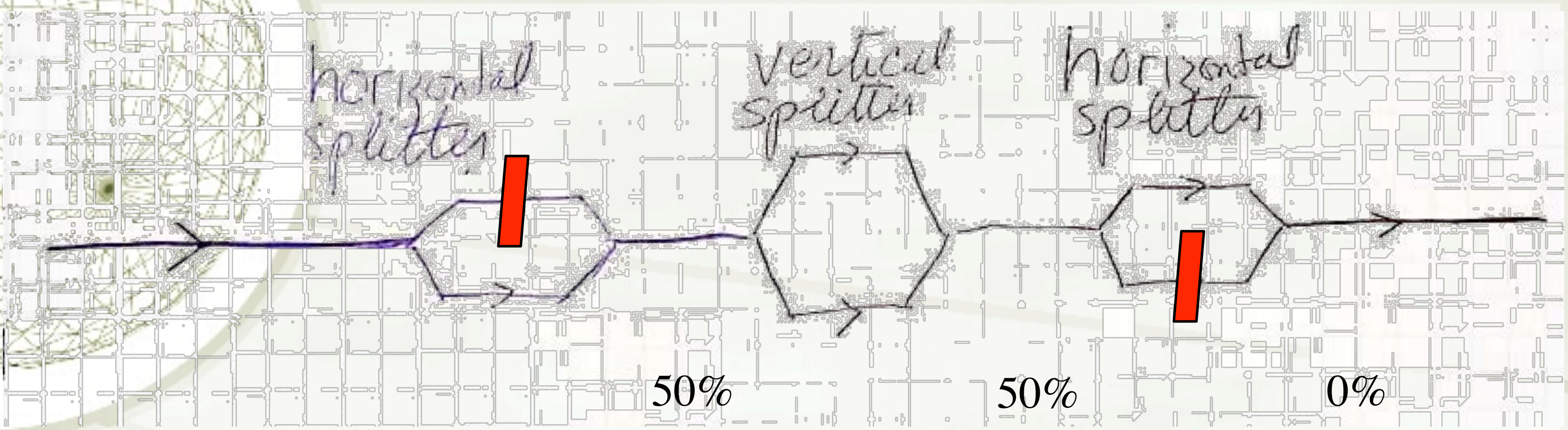


Stern-Gerlach experiment



Stern-Gerlach experiment

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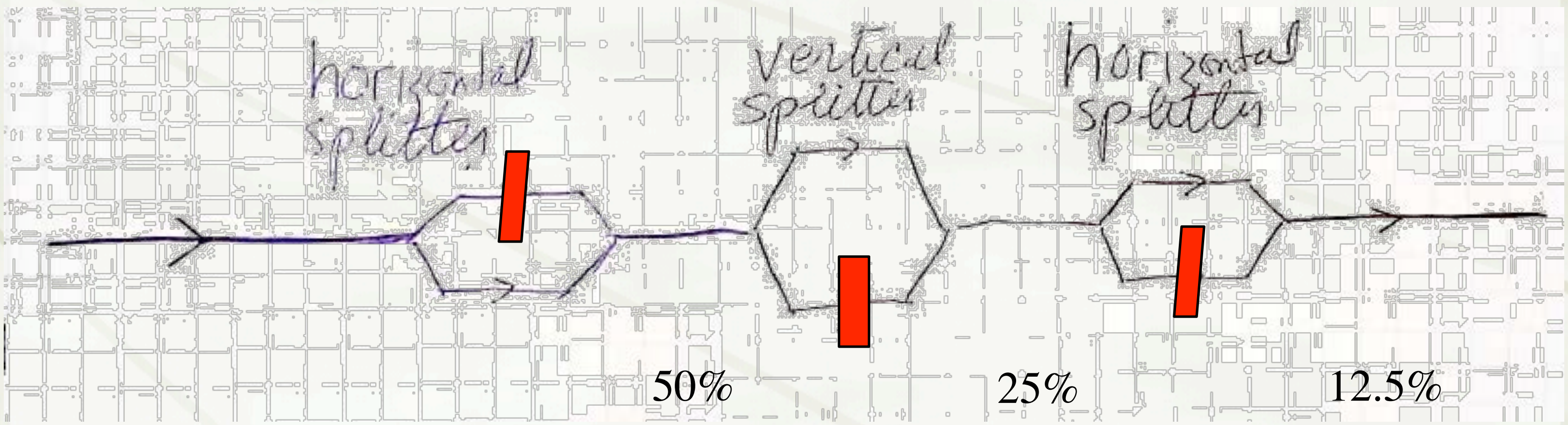
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Quantum mechanics is truly weird

Spukhafte Fernwirkung!

- Stern-Gerlach
- Double-slit
  - interference patterns as for waves, but only particles are measured
- EPR paradox, “entanglement”
  - measurements in one place instantaneously affect measurements somewhere else.

The parts of QM that are weird

- Measurement theory
- Action at a distance
- Interference
- Wave-particle duality
- Tunneling

Discussion break

- Quantum mechanics is the effect that measurement disturbs the system. True or false?

The parts of QM that are not weird

- Solving for the wave function.
- Calculating probabilities
- Calculating the effect of a measurement
- Dealing with probability distributions

The Schrödinger equation

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(x)\Psi$$

$=: \mathrm{H}\,\Psi,$

$\mathrm{H} = \mathrm{H}^*$

The Schrödinger equation

Why is it reasonable to expect the quantity

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

to arise in a theory in which there is both a **local interaction** (potential energy V(**x**)) and an **averaging effect** that delocalizes the state over a small region?

How does $f(x_0)$ relate to averages of $f(x)$ at nearby positions?

Let $\mathbf{x}_0 \to 0$ and set $f_\epsilon(0) := \frac{\int_{|\mathbf{x}|=\epsilon} f(\mathbf{x})dS}{|\partial B_\epsilon|}$.

$$\frac{d}{d\epsilon} f_\epsilon(0) := \frac{|\partial B_\epsilon| \left(\int_{|\mathbf{x}|=\epsilon} \mathbf{e}_r \cdot \nabla f(\mathbf{x})dS + \int_{|\mathbf{x}|=\epsilon} f(\mathbf{x})\sigma dS \right) - \int_{|\mathbf{x}|=\epsilon} f(\mathbf{x})dS \int_{|\mathbf{x}|=\epsilon} \sigma dS}{|\partial B_\epsilon|^2}$$

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Therefore

$$\frac{d}{d\epsilon} f_\epsilon(0) = \frac{\int_{|\mathbf{x}|=\epsilon} \mathbf{n} \cdot \nabla f(\mathbf{x})dS}{|\partial B_\epsilon|} = \frac{\int_{|\mathbf{x}|\leq\epsilon} \nabla^2 f(\mathbf{x})dV}{|\partial B_\epsilon|}$$

How does $f(x_0)$ relate to averages of $f(x)$ at nearby positions?

Therefore $f_\varepsilon(0) = f(0) + (\varepsilon/d)\ \nabla^2 f(0) + \ldots$

The Laplacian provides a measure of how the spherical average of a function changes as the radius increases.

Quantum mechanics is a mystery, but in so far as a classical interaction V(x) at a point is augmented by some isoptropic averaging of a state function over a small neighborhood, the Schrödinger operator

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

is a reasonable quantity to use in a mathematical model.

Challenges

- Use this interpretation of the Laplacian to derive the mean value theorem for solutions of Laplace's eqn.
- Does this argument need to be modified if f(x) is defined on a manifold?

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

- Quantum information
  - The issues of entanglement and measurement are the basis for quantum computation and quantum cryptography.

*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

Some recent nanoscale objects

- Z.L. Wang, Georgia Tech, zinc oxide wire loop
- W. de Heer, Georgia Tech, carbon graphene sheets
- E. Riedo, GT Physics, 2007. Lithography on polymers
- 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.

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?

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.

The weak form of a differential operator

One of the ways analysts understand partial differential operators is to consider the *quadratic forms* they define on *test functions*. Suppose H is a linear differential operator (not necessarily Schrödinger), acting on functions defined in a region Ω. The coefficients in H and the boundary of Ω may not be very nice, so we can begin by asking how H acts on functions $\varphi \in \mathbf{C}_{\mathbf{c}}^{\infty}(\mathbf{\Omega})$, the set of infinitely smooth functions that vanish in a neighborhood of ∂Ω.

The weak form of a differential operator

Defining an inner product as

$$\langle \psi, \varphi \rangle := \int_\Omega \psi(\mathbf{x})\overline{\varphi(\mathbf{x})}dV,$$

we can choose to analyze the functionals $\psi, \varphi \in C_c^\infty \to \langle \psi, H\varphi \rangle$ rather than directly calculating $H\varphi$. For instance, we can integrate by parts and get a functional requiring fewer derivatives on φ: In the case of the Laplacian,

$$\langle \psi, -\Delta\varphi \rangle = \int_\Omega \nabla\psi \cdot \nabla\overline{\varphi(\mathbf{x})}dV.$$

The weak form of a differential operator

If you have a sufficiently representative set of test functions you can fully understand a linear operator in terms of its associated *quadratic form*,

$$\varphi,\psi \quad \to \quad \langle\varphi, A\,\psi\rangle$$

The weak form of a differential operator

Because of the *polarization identity*,

$$\langle \psi, H\varphi \rangle = \frac{1}{4}\big(\langle \psi + \varphi, H(\psi + \varphi) \rangle - \langle \psi - \varphi, H(\psi - \varphi) \rangle +$$

$$+ i \langle \psi + i\varphi, H(\psi + i\varphi) \rangle - i \langle \psi - i\varphi, H(\psi - i\varphi) \rangle \big),$$

it is often sufficient to understand the quadratic functional $\varphi \to \langle \varphi, H\varphi \rangle$.

The weak form of a differential operator

Thus for the Laplacian, it suffices to understand the *Dirichlet form*, which in quantum mechanics is the *kinetic energy* associated with a state φ.

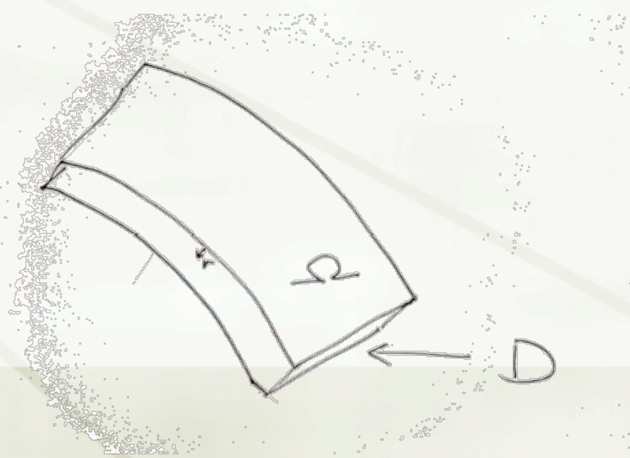
$$T(\varphi) := \langle \varphi, -\Delta\varphi \rangle = \int_\Omega |\nabla\varphi(\mathbf{x})|^2 dV.$$

Thin structures and local geometry

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:

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

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

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

and rewrite the second term (only) in coordinates $(r, \hat{x})$, where $\hat{x}$ are some coordinates on Ω.

$$\int_D |\zeta_r|^2 d^{d+1}x = \int_\Omega \left(\int_0^\delta |\zeta_r|^2 \rho(\mathbf{x}) dr \right) dV_\Omega$$

The trick of *conjugation*.

Write the test function as

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

and use the product rule in the form

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

to find

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

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When the final term is integrated by parts, we get

$$\int_D \left|\nabla_{\|}\zeta\right|^2 d^{d+1}x + \int_D q(\mathbf{x}) \left|\zeta\right|^2 d^{d+1}x + \int_\Omega \left(\int_0^\delta \left|(\sqrt{\rho}\zeta)_r\right|^2 dr \right) dV_\Omega.$$

Effective potential

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

Effective potential

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

Exercise: As $\delta \to 0$, the effective potential tends to:

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

Hint: Two helpful formulae.

$$\frac{\partial \rho}{\partial r} = \pm \rho \sum \kappa_j$$

$$\frac{\partial}{\partial r} \sum \kappa_j = \mp \sum \kappa_j^2$$

The trick of *conjugation*.

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

When the final term is integrated by parts, we get

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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.

Thin-domain Schrödinger operator

$$-\nabla_{||}^2 + q(\mathbf{x}) = -\Delta_\Omega + q(\mathbf{x})$$

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

Discussion break

- Think about specific dimensions d=1,2,3.
- Other thin-domain problems involving Laplacian. What do we expect about the effective potential?

A second look at quantum mechanics

- The weirdness of physics can be modeled by treating "observables" as belonging to a noncommutative algebra.

A second look at quantum mechanics

- Let x be a Cartesian position and p the corresponding momentum (classically, p = m v). Then Heisenberg's **canonical commutation relation** reads:
  - $x\,p - p\,x = i\hbar$, where Planck's constant is

    $\hbar = 1.0545716\ldots \times 10^{-34}$ J·s
  - In "atomic units" we set $\hbar = 1$.

Classical vs. quantum mechanics

- Classical mechanics
  - Variables x and p can be measured simultaneously. xp=px, and in fact $p = m\dot{x}$
  - A pure state is determined by a point in phase space (**x**,**p**)
  - The future is determined by the present state and the Hamiltonian energy H(p,x)
    - One non-relativistic particle: $H(\mathbf{p},\mathbf{x}) = \frac{|\mathbf{p}|^2}{2m} + V(\mathbf{x})$
    - Kinetic energy of relativistic particle: c|**p**|

Canonical commutation

- $x\,p - p\,x = i\hbar$,
- Heisenberg thought that p and x could be represented as square matrices, since the algebra of matrices M^{nn} is not commutative, but this is impossible!
- QUIZ: Why?

Canonical commutation

- $x\,p - p\,x = i$,
- The argument against Heisenberg fails if it is not possible to calculate a trace. The usual way to represent the CCR is with p and x operators on $L^2(R)$: $x\,\varphi$ is the operator multiplying φ by x, while $p \to -i\ \partial/\partial x$.
- Then by the chain rule

$$p\,x\,\varphi = (px)\varphi + x\,p\,\varphi, \text{ so}$$

$$x\,p\,\varphi - p\,x\,\varphi = -(px)\varphi = i\,.$$

Classical vs. quantum mechanics

- Quantum mechanics
  - Variables x_α and p_α can*not* be measured simultaneously. $xp-px = i$.

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Classical vs. quantum mechanics

- Quantum mechanics
  - Variables x_α and p_α can*not* be measured simultaneously. $xp-px = i$.
  - A pure state is determined by a vector in Hilbert space, usually $L^2(\Omega)$.
  - The future is determined by the present state and the Hamiltonian energy $H(p,x)$ via the Schrödinger equation $i\psi_t = H\,\psi$
    - *Change* p_α *where it occurs to* $-i\,\partial/\partial x_\alpha$.

The postulates of quantum theory

- Every “observable” is modeled by a self-adjoint operator $<A \phi, \psi> = <\phi, A\psi>$ on a Hilbert space. (Complete, normed, linear space. Usually $L^2(\Omega)$, $\langle f, g\rangle := \int_\Omega f(\mathbf{x})\overline{g(\mathbf{x})}dV$.)
- The possible measurements are sp(A)
  - If A has discrete eigenvalues, it is “quantized.”
- The state of the system is defined by a vector that has been normalized:

$$\|\psi\|^2 = \langle \psi, \psi \rangle = 1$$

- Expectation values: $E(f(A)) =<(A)\,\psi, \psi>$

The postulates of quantum theory

- How do things change in time?
  - There is a Hamiltonian operator, corresponding to the total energy: H, which is a function of momentum **p** and position **x**.
  -

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi.$$

$$\psi(t) = e^{-iHt}\psi(0)$$

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

Not at all weird

- Solving for the wave function.
- A well-defined initial value problem for a PDE:

$$u_t = H\,u, \text{ where } H = H^*$$

- The solution operator is a unitary group in Hilbert space

Coming attractions

- The spectrum – eigenvalues and other good things.
  - The spectral theorem
  - The rôle of the eigenvalues in physics
- Some good examples
- Some good techniques
  - variational methods
  - perturbation theory
  - algebraic methods