Mathematics of Quantum Mechanics on Thin Structures

Evans Harrell
Georgia Tech
www.math.gatech.edu/~harrell

Marrakech
May, 2008

© 2008 by Evans M. Harrell II
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

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

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

\[ =: H \Psi, \]

\[ H = H^* \]
The Schrödinger equation

Why is it reasonable to expect the quantity

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

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 $x_0 \to 0$ and set $f_\epsilon(0) := \frac{\int_{|x|=\epsilon} f(x) dS}{|\partial B_\epsilon|}$.

$$\frac{d}{d\epsilon} f_\epsilon(0) := \frac{|\partial B_\epsilon| \left( \int_{|x|=\epsilon} e_r \cdot \nabla f(x) dS + \int_{|x|=\epsilon} f(x) \sigma dS \right) - \int_{|x|=\epsilon} f(x) dS \int_{|x|=\epsilon} \sigma dS}{|\partial B_\epsilon|^2}$$
How does $f(x_0)$ relate to averages of $f(x)$ at nearby positions?

Let $x_0 \to 0$ and set $f_\epsilon(0) := \frac{\int_{|x|=\epsilon} f(x) dS}{|\partial B_\epsilon|}$.

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

Therefore

$$\frac{d}{d\epsilon} f_\epsilon(0) = \frac{\int_{|x|=\epsilon} n \cdot \nabla f(x) dS}{|\partial B_\epsilon|} = \frac{\int_{|x|\leq\epsilon} \nabla^2 f(x) dV}{|\partial B_\epsilon|}$$
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 isotropic averaging of a state function over a small neighborhood, the Schrödinger operator

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

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

- $1 \text{ nm} = 10^{-9} \text{ m}$. The “nanoscale” refers to 1-100+ nm.
- “Mesoscopic.”: 1nm is about 10 hydrogen radii.
- Laboratories by 1990
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
- 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 online.
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.
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 $\Omega$. The coefficients in $H$ and the boundary of $\Omega$ may not be very nice, so we can begin by asking how $H$ acts on functions $\varphi \in C^\infty_c(\Omega)$, the set of infinitely smooth functions that vanish in a neighborhood of $\partial \Omega$. 

*The weak form of a differential operator*
The weak form of a differential operator

Defining an inner product as

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

we can choose to analyze the functionals $\psi, \varphi \in C_0^\infty \rightarrow \langle \psi, H\varphi \rangle$ rather than directly calculating $H\varphi$. For instance, we can integrate by parts and get a functional requiring fewer derivatives on $\varphi$: In the case of the Laplacian,

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

\[ \varphi, \psi \rightarrow \langle \varphi, A \psi \rangle \]
The weak form of a differential operator

Because of the polarization identity,

\[ \langle \psi, H\varphi \rangle = \frac{1}{4} \left( \langle \psi + \varphi, H(\psi + \varphi) \rangle - \langle \psi - \varphi, H(\psi - \varphi) \rangle + \right. \]

\[ + i \langle \psi + i\varphi, H(\psi + i\varphi) \rangle - i \langle \psi - i\varphi, H(\psi - i\varphi) \rangle \], \]

it is often sufficient to understand the quadratic functional \( \varphi \to \langle \varphi, H\varphi \rangle \).
Thus for the Laplacian, it suffices to understand the *Dirichlet form*, which in quantum mechanics is the *kinetic energy* associated with a state $\varphi$.

\[ T(\varphi) := \langle \varphi, -\Delta \varphi \rangle = \int_{\Omega} |\nabla \varphi(x)|^2 dV. \]
Thin structures and local geometry

Thin domain of fixed width
variable \( r = \) distance from edge

Energy form in separated variables:

\[
\int_D \left| \nabla_\parallel \xi \right|^2 d^{d+1}x + \int_D \left| \xi_r \right|^2 d^{d+1}x
\]
Energy form in separated variables:

\[ \int_{D} |\nabla_{\parallel} \xi|^{2} d^{d+1}x + \int_{D} |\xi_{r}|^{2} d^{d+1}x \]

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

\[ \int_D |\nabla \parallel \zeta \parallel^2 d^{d+1} x + \int_D |\zeta_r|^2 d^{d+1} x \]

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

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

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

to find

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

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

When the final term is integrated by parts, we get

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

\[ q(x) := -\frac{1}{4} \left( \frac{\rho_r}{\rho} \right)^2 + \frac{1}{2} \frac{\rho_{rr}}{\rho}. \]
Effective potential

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

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

\[ q(x) = \frac{1}{4} \left( \sum_{j=1}^{d} \kappa_j \right)^2 - \frac{1}{2} \sum_{j=1}^{d} \kappa_j^2. \]
Hint: Two helpful formulae.

\[ \frac{\partial p}{\partial r} = \pm \rho \sum k_j \]

\[ \frac{\partial}{\partial r} \sum k_j = \sum k_j^2 \]
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

\[ \int_{0}^{\delta} |\zeta_r|^2 \rho dr = \int_{0}^{\delta} \left( |(\sqrt{\rho} \zeta)_r|^2 + \frac{1}{4} \left( \frac{\rho_r}{\rho} \right)^2 |\zeta|^2 \rho + \frac{\rho}{2} \left( \frac{1}{\rho} \right)_r (\rho |\zeta|^2)_r \right) dr. \]

When the final term is integrated by parts, we get

\[ \int_{D} |\nabla \parallel \zeta|^2 d^{d+1}x + \int_{D} q(x) |\zeta|^2 d^{d+1}x \]

\[ \int_{\Omega} \left( \int_{0}^{\delta} |(\sqrt{\rho} \zeta)_r|^2 dr \right) dV_{\Omega}. \]
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

\[- \nabla_{\parallel}^2 + q(x) = -\Delta_{\Omega} + q(x)\]

\[q(x) = \frac{1}{4} \left( \sum_{j=1}^{d} \kappa_j \right)^2 - \frac{1}{2} \sum_{j=1}^{d} \kappa_j^2\]
Discuss the specific dimensions of $d=1,2,3$. Consider other thin-domain problems involving the 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.
Let \( x \) be a Cartesian position and \( p \) the corresponding momentum (classically, \( p = m v \)). Then Heisenberg’s \textit{canonical commutation relation} reads:

\[
x p - p x = i \hbar,
\]

where Planck’s constant is

\[
\hbar = 1.0545716\ldots \times 10^{-34} \text{ J} \cdot \text{s}
\]

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 \( p = mx \)
- 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: \( H(p, x) = \frac{|p|^2}{2m} + V(x) \)
  - Kinetic energy of relativistic particle: \( c|p| \)
x p - p x = iℏ,

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?
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 $L^2(\mathbb{R})$: $x\varphi$ is the operator multiplying $\varphi$ by $x$, while $p \to -i\frac{\partial}{\partial x}$.

Then by the chain rule
\[ p \times \varphi = (px)\varphi + x \times p \varphi, \] so
\[ x \times p \varphi - p \times \varphi = -(px)\varphi = i. \]
Quantum mechanics

Variables $x_\alpha$ and $p_\alpha$ cannot be measured simultaneously. $xp - px = i$. 
Classical vs. quantum mechanics

Quantum mechanics

- Variables $x_\alpha$ and $p_\alpha$ cannot be measured simultaneously. $xp-px = i$.
- A pure state is determined by a vector in Hilbert space, usually $L^2(\Omega)$.
Quantum mechanics

- Variables $x_{\alpha}$ and $p_{\alpha}$ cannot 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 $p_{\alpha}$ where it occurs to $-i \frac{\delta}{\delta x_{\alpha}}$. 

Classical vs. quantum mechanics
Every “observable” is modeled by a self-adjoint operator $\langle A \phi, \psi \rangle = \langle \phi, A\psi \rangle$ on a Hilbert space. (Complete, normed, linear space. Usually $L^2(\Omega)$, $\langle f, g \rangle := \int_{\Omega} f(x)\overline{g(x)}dV$.)

The possible measurements are $\text{sp}(A)$
- 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: $E(f(A)) = \langle (A) \psi, \psi \rangle$
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 $x$.

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

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

\[ H\psi = \frac{-\hbar^2}{2m} \nabla^2 \psi + V(x)\psi \]
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.
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