Physics 2203, Fall 2012
Modern Physics

- Wednesday, Sept. 19\textsuperscript{th}, 2012:
  Ch. 7: Schrödinger’s equation in one dimension
  --Schrödinger’s Equation.
  --Particle in a box: Standing waves
  --Time Independent Schrödinger Equation
  --Normalization, expectations, etc.
  --Wells

- Friday, Sept. 21\textsuperscript{th}
  --Computer exercise on barriers, room 365
WEEKLY CALENDAR
September 17-21, 2012
DEPARTMENTAL COLLOQUIUM

"Newton’s Gedankenexperiment": Newton and Einstein, gravitation and relativity"

3:40 PM, September 20, 2012
109 Nicholson Hall

George Ford
University of Michigan

Host: Robert O’Connell

• Refreshments served at 3:15 PM in 232 (Library) Nicholson Hall •

This will be an unusual sort of talk. What I will do is tell you a little bit about these two great men, who they were and what they did. My aim will be to give an impression of their place in the history of science and why what they did was important. However, at the same time, I will describe a thought experiment that will illustrate the gravitational theories of the two men.
Quantum Mechanics

Feynman: I think it is safe to say that no one understands quantum mechanics. Do not keep saying to yourself, if you can possible avoid it, “but how can it be like that?” because you will get “down the drain” into a blind alley from which nobody has yet escaped. Nobody knows how it can be like that.
“Those who are not shocked when they first come across quantum mechanics cannot possibly have understood it.”
**Classical Vs. Quantum**

**Classical:** If we know all of the forces acting on a particle we can **calculate exactly** the position and velocity for any time in the future.

\[
\vec{F} = \frac{d\vec{p}}{dt} = m\vec{a} = m\frac{d^2\vec{r}}{dt^2} : \text{ Second order differential equation}
\]

**Quantum Mechanical:** Like classical mechanics we solve a second order differential equation, the **Schrödinger Equation**. But the interpretation is very different. We find the wave function not the position and velocity. The position, velocity, etc. are all probability functions.

\[
1D \rightarrow i\hbar \frac{\partial}{\partial t} \Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + U(x)\Psi: \quad \langle x \rangle = \int \Psi^* x\Psi dx
\]
We can learn a lot about quantum waves by looking at classical waves in 1-D.

\[ \frac{\partial^2 \psi}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 \Psi}{\partial t^2} \]

This is an example of light incident from the left on a piece of glass.

- In Region 1 there is an incident and reflected wave (A), both with the same wavelength.
- In Region 2 there is an incident and reflected wave (B), both with the same wavelength, but shorter than in region 1.
- In Region 3 there is only a transmitted wave, with the same wavelength as region 1, but smaller amplitude.
**Surface water waves:**

A wave incident from the left encounters a region (2) where the depth is much smaller.

- In Region 1 there is an incident and reflected wave (A), both with the same wavelength.
- In Region 2 there is an incident and reflected wave B), both with the same wavelength, but shorter than in region 1.
- In Region 3 there is only a transmitted wave, with the same wavelength as region 1, but smaller amplitude.
**Quantum Waves: Electron Gun**

**Electron gun:**

An electron moves to the right in region 1 with energy E. At A it enters a region (2) where its energy is $E - V_0$ and at B it returns to a region (3) where its energy is E.

- In Regions 1 and 3 the wave length is the same and given by:
  \[ \lambda = \frac{1240eV \cdot nm}{\sqrt{E}} \]

- In Region 2 the wave length is longer and given by:
  \[ \lambda = \frac{1240eV \cdot nm}{\sqrt{E - V_0}} \]

- In Regions 1 & 2 there are incident and reflected waves:

- The amplitude in region 3 is less than in region 1 because of reflection at the barrier:

**Is there any qualitative difference between the classical and quantum waves in these pictures?**
Waves: Classical vs. Quantum

Classical water waves

Shorter wavelength

Region 1  Region 2  Region 3

Classical water waves

Quantum Electron Waves

Longer wavelength

\[ V(x) \]

\[ V_0 \]

\[ B e^{-i k_1 x} \]

\[ D e^{-i k_2 x} \]

\[ A e^{i k_1 x} \]

\[ C e^{i k_2 x} \]

\[ E e^{i k_1 x} \]

\[ |\psi(x)|^2 \]

\[ E > V_0 \]
There is another common property between classical waves and quantum waves: **Continuity!**

The wave function must be continuous at a boundary!

The slope of the wave function must be continuous at a boundary!

Correct!
There is a similarity between Quantum waves (tunneling) and light totally reflected from a surface. If surface A was coated with a perfect reflecting material, then the wave amplitude in regions 2 and 3 would be zero.

When a light wave is totally reflected an exponentially decreasing wave (evanescent wave) penetrates in region 2.

Since 100% of intensity is reflected, the evanescent wave carries no energy!

But if the glass is thin enough, light will come out the other side.

Correct wave function

Thin glass or quantum tunneling

Thick Glass
Confining a particle

Quantum Mechanics is easy!

Elastic collision with wall. All energies allowed

\[ \lambda_n = \frac{2L}{n} \quad n=1, 2, 3, \ldots \]

\[ p = \frac{h}{\lambda} = n \frac{h}{2L} \]

\[ E_n = n^2 \frac{h^2}{8mL^2} \]

Quantum Electrons

Consider waves (electrons) trapped in the center part and let the well be deep.
A reasonable approximation for the uncertainty in $x$ is $L - \Delta x \sim L$.

The uncertainty in momentum $\Delta p_x$ can be determined by going back to the statistical distribution for the standard deviation $\sigma_A$ of the quantity $A$ that has a mean or average value $A_{av}$.

$$\sigma_A = \sqrt{(A^2)_{av} - (A_{av})^2}$$

$$\Delta p_x = \sqrt{(p_x^2)_{av} - (p_{x,av})^2}$$

The particle is moving with equal probability to the right and to the left, so $p_{x,av} = 0$

$$p_x = \frac{nh}{L}$$

$$\Delta p_x = \frac{nh}{L}$$
In 1926 Schrödinger published the quantum mechanical wave equation. It can’t be derived from any previous laws or postulates—just like Newton’s laws.

\[
1D \rightarrow i\hbar \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t)
\]

What motivated him to propose this equation???

He was looking for an equation like

\[
\hat{\mathcal{E}}\Psi = \hat{\mathcal{K}}\Psi + \hat{\mathcal{U}}\Psi: \quad \hat{\mathcal{E}} \text{ is an operator.}
\]

He knew that the wave functions were going to look like \( e^{i(kx-\omega t)} \)

\[
\hat{\mathcal{E}}\Psi = i\hbar \frac{\partial e^{i(kx-\omega t)}}{\partial t} = \hbar \omega \Psi
\]  
\[
\hat{\mathcal{K}}\Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 e^{i(kx-\omega t)}}{\partial x^2} = \frac{\hbar^2 k^2}{2m} \Psi
\]  
\[
\hat{\mathcal{U}}\Psi = U\Psi
\]
Schrödinger’s Equation: \( t \) independent

In 1926 Schrödinger published the quantum mechanical wave equation. It can’t be derived from any previous laws or postulates—just like Newton’s laws.

\[
1D \rightarrow \frac{i\hbar}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t)
\]

If we have a stationary, standing wave state, then

\[
E\psi(x) = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x)\psi(x)
\]

The wave function is \( \Psi(x,t) = \psi(x)e^{-i\omega t} \)

Let’s discuss the properties of these equations and how we use them to explain experimental observations.
Properties of the wave functions

1) **Superposition principle** to form wave packets.

   If \( \Psi_1 \) and \( \Psi_2 \) satisfy Sch. Eqn. prove that
   
   \[
   \Psi(x,t) = a\Psi_1(x,t) + b\Psi_2(x,t) \text{ satisfies Sch. Eqn.}
   \]

2) **Probability** of finding a particle at some position \( P(x)dx \)

   \[
   P(x)dx \equiv |\psi(x)|^2 \, dx : \text{remember } |\Psi(x,t)|^2 = |\psi(x)|^2 |e^{-i\omega t}|^2 = |\psi(x)|^2
   \]

3) The wave function must be **normalized**.

   \[
   \int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1
   \]

4) The probability of finding a particle between any two position –see above

   \[
   P(x_1, x_2) = \int_{x_1}^{x_2} |\psi(x)|^2 \, dx
   \]
Properties of the wave functions

4) The probability of finding a particle between any two position –see above

\[ P(x_1, x_2) = \int_{x_1}^{x_2} |\psi(x)|^2 dx \]

5) We can only speak of the probability of finding the particle at some \( x \). We need to define how to determine \( x_{av} \).

We make a large number of measurements and find the value \( x_1 \) a certain number of time \( n_1 \), \( x_2 \) a number of times \( n_2 \), etc., the definition of average is:

\[ x_{av} = \frac{n_1 x_1 + n_2 x_2 + \cdots}{n_1 + n_2 + \cdots} = \frac{\sum n_i x_i}{\sum n_i} \]

The number of times \( n_i \) that we measure each \( x_i \) is proportional to the probability \( P(x_i)dx \)—so we have in the limit of large \( n \)-

\[ x_{av} \equiv \langle x \rangle = \int_{-\infty}^{+\infty} |\psi(x)|^2 x dx \equiv \int_{-\infty}^{+\infty} \psi^*(x)x \psi(x) dx \equiv \text{Expectation Value} \]
Solution for Constant Potential

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U_0 \psi(x) = E \psi(x)\]

\[-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = (E - U_0) \psi(x)\]

We know that \(\frac{d^2 \psi}{dx^2} = -k^2 \psi(x)\)

so \(k = \sqrt{\frac{2m(E - U_0)}{\hbar^2}}\) \(E > U_0\)

The most general wave function is \(\psi(x) = A \sin kx + B \cos kx\)

You prove that this is the same: \(\psi(x) = A'e^{ikx} + Be^{-ikx}\)

\(\frac{d \psi(x)}{dx} = A'ke^{ikx} - ikBe^{-ikx}\),

\(\frac{d^2 \psi(x)}{dx^2} = -A'k^2e^{ikx} - k^2 Be^{-ikx} = -k^2 \psi(x)\) QED

What happens when \(U_0 > E\)?

\(\frac{d^2 \psi(x)}{dx^2} = -k' \psi(x) \rightarrow k' = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}\)

\(\psi(x) = Ae^{k'x} + Be^{-k'x}\)
Solution for a free particle \( U=0 \)

\[
- \frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U_0 \psi(x) = E \psi(x) \quad \rightarrow \quad - \frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = E \psi(x)
\]

\[
E = \frac{\hbar^2 k^2}{2m} \quad \psi(x) = A'e^{ikx} + Be^{-ikx}
\]

**Time Dependent**

\[
\Psi(x,t) = A'e^{i(kx-\omega t)} + Be^{-i(kx+\omega t)}
\]

How would you describe a wave moving on in the + x direction?

\[
\Psi(x,t) = A'e^{i(kx-\omega t)} \quad P(x) = |\Psi(x,t)|^2 = |A'|^2
\]

The probability of finding the particle is a constant. How do you normalize this??
Standing Waves: Particle in a box

Remember that a standing wave is
\[ Ae^{i(kx-\omega t)} \rightarrow \text{ and } Ae^{-i(kx+\omega t)} \leftarrow \]
\[ \Psi(x,t) = Ae^{-i\omega t} \left[ e^{i(kx)} \pm e^{-i(kx)} \right] \]
\[ \Psi(x,t) = 2Ae^{-i\omega t} \sin kx \]

*The* boundary conditions determine the standing waves and the allowed  \( \lambda \)s
\[ \psi(x) = B \sin kx \] must be zero at  \( x=0 \) and  \( x=L \)

*Giving*  \( kL=n\pi \)

\[ k = \frac{2\pi}{\lambda} = \frac{n\pi}{L} \]
\[ E_n = \frac{(\hbar k)^2}{2m} = \frac{(n\pi\hbar)^2}{2mL^2} \quad n=1,2,... \]
\[ \Delta x \Delta p \geq \frac{\hbar}{2} : \Delta x=L \]
\[ \Delta p \geq \frac{\hbar}{2L} : E_0 = \frac{p^2}{2m} \]
\[ E = \frac{\hbar^2}{8mL^2} : \text{OK} \]
Standing Waves: Particle in a box

\[ \psi(x) = A \sin\left(\frac{n\pi x}{L}\right) \]

\[ |\psi(x)|^2 = A^2 \sin^2\left(\frac{n\pi x}{L}\right) \]

Let us normalize these functions.

\[ |\psi(x)|^2 = \int_0^L A^2 \sin^2\left(\frac{n\pi x}{L}\right) dx = 1 \]

Change variables: \( z = \frac{n\pi x}{L} \)

\[ |\psi(z)|^2 = \frac{LA^2}{n\pi} \int_0^{n\pi} \sin^2(z) dz = 1 \]

\[ \int_0^{n\pi} \sin^2(z) dz = \frac{n\pi}{2} \]

\[ \psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \]
Standing Waves: Particle in a box

\[ \psi(x) = \sqrt{\frac{2}{L}} \sin \left( \frac{n\pi x}{L} \right) \]

\[ \psi^2(x) = \frac{2}{L} \sin^2 \left( \frac{n\pi x}{L} \right) \]

Let's examine the properties of the first excited state, \( n=2 \).

--- Where is the particle most likely to be found?
--- What is the probability of finding the particle between \( x=0.5L \) and \( x=0.51L \)
--- What would be the average result if the position of a particle in this state were measured many times?

Where is the particle most likely to be found?

At \( x= \frac{L}{4} \) and \( \frac{3L}{4} \), \( \psi^2 = \frac{2}{L} \)
Let's examine the properties of the first excited state, n=2.

--- Where is the particle least likely to be found?

--- What is the probability of finding the particle between x=0.5L and x=0.51L

--- What would be the average result if the position of a particle in this state were measured many times?

Where is the particle least likely to be found?

At x=0, \( \frac{L}{2} \), and L: \( \psi^2 = 0 \)
Standing Waves: Particle in a box

\[ \psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \]

\[ \psi^2(x) = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) \]

Let's examine the properties of the first excited state, \( n=2 \).

-- Where is the particle most likely to be found?

--- What is the probability of finding the particle between \( x=0.5L \) and \( x=0.51L \)?

--- What would be the average result if the position of a particle in this state were measured many times?

Probability of finding the particle between \( x=0.50L \) and \( 0.51L \)

\[ P = \int_{0.5}^{0.51} \psi^2(x) \, dx \approx \psi^2(0.5) \Delta x = 0 \]
Standing Waves: Particle in a box

Let's examine the properties of the first excited state, n=2.

--- Where is the particle most likely to be found?
--- What is the probability of finding the particle between x=0.0L and x=0.25L?
--- What would be the average result if the position of a particle in this state were measured many times?

\[
\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \\
\psi^2(x) = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right)
\]

What is the answer?
You do this!
Standing Waves: Particle in a box

\[ \psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \]

\[ \psi^2(x) = \frac{2}{L} \sin^2\left(\frac{n\pi x}{L}\right) \]

Let's examine the properties of the first excited state, \( n=2 \).

--- Where is the particle most likely to be found?
--- What is the probability of finding the particle between \( x=0.0L \) and \( x=0.25L \)?
--- What would be the average result if the position of a particle in this state were measured many times?

\[ \langle x \rangle = \int_{0}^{L} x \frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right) dx: \text{ look at problem 7.33} \]

\[ Just \ look \ at \ the \ plot \ \langle x \rangle = \int_{0}^{L} x \frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right) dx \equiv \frac{L}{2} \]
END