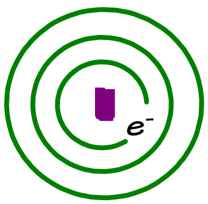
Physics 123, April 3, 2013

- Exam 2 looms large   Apr. 11, Dewey 1101, 0800
- Up to start of Bohr's model of atom (Apr. 1 lecture)
- With all the crazy optics stuff . . .

  Can use Both Sides of an 8.5 × 11 inch Sheet for notes + Formulas

  I will provide a formula sheet as well
- More on material coverage in email soon . . .

  But it will cover from end of Exam 1 material to start of Bohr Model



Bohr model

- e^- in circular orbits
- e^- held in atom via Coulomb attraction
- Single e^-
- e^- exists in discrete stable orbits
- photons emitted as e^- jumps between orbits
- Photon energy corresponds to difference in energy between the two Energy levels

quantized circular orbits

$n = 1, 2, 3 \ldots$

$$r_n = \frac{n^2 \hbar^2}{k Z e^2 m}$$

with quantized energies

$$E_{n_{\text{TOTAL}}} = -\frac{m k^2 Z^2 e^4}{2 n^2 h^2}$$

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er ... last class I forgot to mention something important

Bohr's model works!!

For single e^- atoms Bohr's model reproduces fairly well the experimentally determined discrete atomic spectra!

Not perfect ... revisions made

e.g., allow nucleus to move + have e^- orbit center-of-mass

elliptical orbits

⋮

- Bohr model gets people to take Rutherford's nuclear atom seriously
  relates quanta of light and quantization of Atomic Energy levels
- Generally a decent starting place for intuition

But

- Fails to describe spectra of larger atoms
- Treats e^- classically (can think of de Broglie motivating the quantization ... But this mixes wave + particle for e^-)
- Fails to describe detailed structure ("Fine" structure, Zeeman Splitting ... etc.)

Successful model of atom must come from a theory that treats e^- as wave from the ground up $\to$ quantum Mechanics

Particles & waves leads to a strange new world

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Recall from waves + Fourier analysis

A Can describe waves in position or spatial frequency

x $\qquad$ $k = 2\pi/\lambda$

If wave is narrow in x, require higher frequency components

B Can describe waves in time or temporal frequency

t $\qquad$ $\omega = 2\pi/T$

If wave is narrow in t, require higher frequency components

C

So, for all waves $\quad \underbrace{\Delta x}_{\text{width in position space}} \underbrace{\Delta k}_{\text{width in frequency space}} \sim 1$ and $\Delta t \Delta \omega \sim 1$

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De Broglie $\rightsquigarrow p = \frac{h}{\lambda} = h\frac{k}{2\pi} = \hbar k \rightsquigarrow \Delta k = \frac{\Delta p}{\hbar}$

h-bar $\equiv \frac{h}{2\pi}$

$\Delta x \Delta k \sim 1 \longrightarrow \Delta x \frac{\Delta p}{\hbar} \sim 1 \longrightarrow \Delta x \Delta p \sim \hbar$

$E = h\nu = \hbar\omega \longrightarrow \Delta\omega = \frac{\Delta E}{\hbar}$

$\Delta t \Delta\omega \sim 1 \longrightarrow \Delta t \frac{\Delta E}{\hbar} \sim 1 \longrightarrow \Delta t \Delta E \sim \hbar$

Two forms of
Heisenberg's Uncertainty Principle

In world of Newton and Particles 'R Particles:

Know (Position
Momentum
Forces) → Know the future

Universe is deterministic!

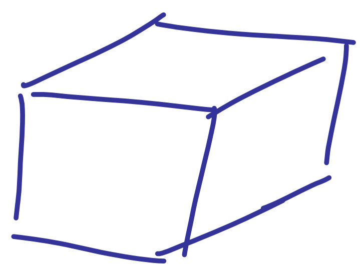
Not so in world of Particles 'R Waves

The better I determine the position
the less well I know the momentum
+ vice versa

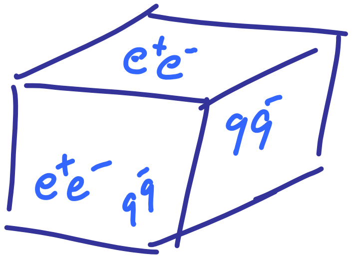
Inherent Uncertainty!

Mourn the loss of Deterministic universe !
Rejoice in the new freedom !

The uncertainty Principle
opens up Harry Potterish possibilities



a box of
Empty space
vacuum



a box of Empty space

vacuum

consider this bit of empty space over a very short time

Energy over that time is very uncertain

Can have fluctuations in the energy → Particle-Antiparticle pairs

Virtual particles, fleeting existance

The vacuum is a seething mess of virtual particles 

Quantum Mechanics

[recall $\vec{F} = -\vec{\nabla} V$]

Need a wave equation that allows us to calculate the motion of a particle under the influence of a force (Moving in a "potential")

Why not use $\nabla^2 \psi = \frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2}$?

This is for free traveling wave (No force)

Also need consistency w/ $E = h\nu$, $p = h/\lambda$

Want:

- consistency w/ $E = h\nu$, $p = h/\lambda$
- Energy conservation including potential
  $$E = \frac{p^2}{2m} + V$$
- Linear in $\psi(x,t)$ in order to satisfy superposition

(11)

(A)
$$E = h\nu = \hbar\omega$$
$$p = h/\lambda = k\hbar$$

(B)
$$E = \frac{p^2}{2m} + V$$

(C)
$$\hbar\omega = \frac{k^2\hbar^2}{2m} + V$$

Let's assume particle is a 1-d wave, Amplitude = 1

(D)
$$\psi(x,t) = e^{i(kx-\omega t)}$$

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

Mult by i/i

1-d nonrelativistic time-dependent Schrödinger equation

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

Two of the Big players in the early development of QM

Werner Karl Heisenberg

(1901 - 1976)

Nobel Prize in physics - 1932
for "the creation of quantum Mechanics"
(Max Born, Pascual Jordan - co-workers)

Matrix formulation

Erwin Rudolf Josef Alexander Schrödinger

(1887 - 1961) Austria

1933 Nobel Prize in physics

1926 - Paper on wave Mechanics of Matter
Annalen der Physik

"For discovery of new and productive forms of atomic theory"

Wave equation formulation

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

What do you do with this?

Put in the physical situation $V(x,t)$

Solve for $\psi(x,t)$ and Energy

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Will do examples shortly
but let me carry on for a bit with more background/theory

Can imagine it is useful to consider static situations

let $V(x,t) \longrightarrow V(x)$ Potential is CONSTANT in time

$\psi(x,t) \longrightarrow \psi(x)\psi(t)$ Assume space + time dependence are separable

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

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

$\div$ by $\psi(x)\psi(t)$

$$\underbrace{-i\hbar \frac{1}{\psi(t)} \frac{\partial \psi(t)}{\partial t}}_{\text{Function of } t \text{ only}} = \underbrace{\frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)}_{\text{Function of } x \text{ only}}$$

Equality only holds for all x and t if both sides are equal to same constant $\rightsquigarrow$ choose it to be E

A

$$\underbrace{-i\hbar \frac{1}{\psi(t)} \frac{\partial \psi(t)}{\partial t} = E}$$

one soln of this is

$$\psi(t) = e^{-i\frac{E}{\hbar}t}$$

And B $\frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) = E$

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for our 1d wave $\psi(x,t) = e^{i(kx-\omega t)} = \psi(x)\,\psi(t) = e^{ikx}\,e^{-i\omega t}$

recall $E = \hbar\omega$

$$\boxed{\psi(x,t) = \psi(x)\, e^{-i\frac{E}{\hbar}t}}$$

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = E$$

Time independent 1d nonrelativistic Schrödinger eqn

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\,\psi(x) = E\,\psi(x)}$$

Woohoo! We got wave equations . . .

But what's waving?

What is $\psi(x,t)$? it is complex (i.e., has $i = \sqrt{-1}$ in it as opposed to being complicated)

So association of ψ w/ real world is NOT obvious

Max Born - 1926 - Born interpretation

Square of ψ represents the probability density for the particle/wave

Born's postulate : at time t, $\psi^*_{(x,t)}\,\psi_{(x,t)}\,dx = |\psi^2_{(x,t)}|\,dx$ gives the probability of finding the particle between x and $x+dx$

Normalize $\psi_{(x,t)}$ so that the total probability is 1

$$\int_{-\infty}^{\infty} |\psi^2_{(x,t)}|\,dx = 1$$

The particle must be somewhere

in 3d ... $\int |\psi^2_{(\vec{r},t)}|\,dV = 1$ ...

Are we having fun yet? Need to do a couple of examples

Example: 1d Free particle

$V(x) = 0$ for all x

(A)

Time ind. Schr. eqn $\quad -\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\,\psi(x)$

$V(x) \to 0$

Try $\psi(x,t) = e^{i(kx - \frac{E}{\hbar}t)} = e^{ikx}\, e^{-i\frac{E}{\hbar}t}$ as a solution

$\psi(x) = e^{ikx} \qquad \frac{\hbar^2 k^2}{2m} e^{ikx} = E\, e^{ikx}$ works if $k = \sqrt{\frac{2mE}{\hbar^2}}$

$\psi(x,t)$ here is a wave traveling in $+x$ direction

$\psi(x) = e^{-ikx}$ also a soln ... $k = \sqrt{\frac{2ME}{\hbar^2}}$

$\psi(x,t)$ here is a wave traveling in $-x$ direction

So, general Solution

$$\psi(x) = Ae^{ikx} + Be^{-ikx}$$

where $k^2 = 2ME/\hbar^2$

or equivalently

$$\psi(x) = A'\sin(kx) + B'\cos(kx)$$

$$k^2 = \frac{2ME}{\hbar^2}$$

(You will find that it is easiest to solve different types of problems using one form or the other)

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$$\frac{e^{i\theta}+e^{-i\theta}}{2}$$

recall Euler's Formula

$$e^{i\theta} = \cos\theta + i\sin\theta$$

$$\frac{e^{i\theta}-e^{-i\theta}}{2}$$

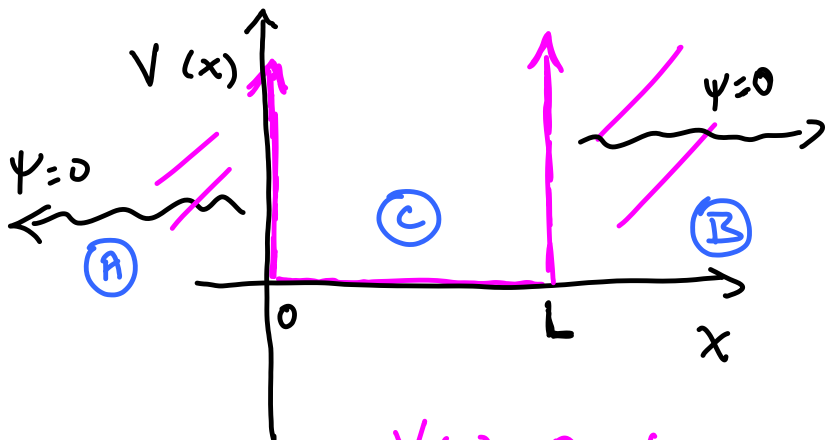
$$A'\sin kx + B'\cos kx$$

$$\frac{A'}{2}\left(e^{ikx}-e^{-ikx}\right) + \frac{B'}{2}\left(e^{ikx}+e^{-ikx}\right)$$

$$\underbrace{\left(\frac{A'}{2}+\frac{B'}{2}\right)}_{\equiv A}e^{ikx} + \underbrace{\left(\frac{B'}{2}-\frac{A'}{2}\right)}_{\equiv B}e^{-ikx}$$

1-d Particle in a box

infinite square well potential



$V(x) = 0$ for $0<x<L$

$V(x) = \infty$ for $x<0$, $L<x$

as $V \to \infty$ Schr eqn makes no sense
so $\psi = 0$ there

for $0<x<L$ $V(x) = 0$
particle is free
inside the Box

$$\psi(x) = A \sin kx + B \cos kx$$

Use Boundry conditions to constrain Solution :

- at $x = 0$, $\psi(x) = 0$ $\quad$ $\underbrace{0 = A \sin kx + B \cos kx} \Rightarrow B = 0$ $\quad$ $\psi(x) = A \sin kx$

- at $x = L$, $\psi(x) = 0$ $\quad$ $0 = A \sin kL$

$$kL = n\pi \qquad n = 1, 2, 3 \cdots$$

$n=0$ not considered because for $n = 0$ Either $k = 0$ or $L = 0$ $\quad$ $\psi(x) = 0$ $\quad$ No box

$$\psi(x) = A \sin\left(\frac{n\pi}{L} x\right) \qquad n = 1, 2, 3 \cdots$$

in region $0 < x < L$

(12) $k = \dfrac{n\pi}{L}$ So, (13) $E_n = \dfrac{n^2 \pi^2 \hbar^2}{L^2 \, 2m}$ where $n = 1, 2, 3 \cdots$ (23)

energy is quantized! You'll find this is always true in attractive potentials

as in wanting to bind or capture

$$E_1 = \underbrace{\frac{\pi^2 \hbar^2}{L^2 \, 2m}}_{} \qquad E_2 = \frac{4\pi^2 \hbar^2}{L^2 \, 2m} \qquad \cdots\cdots$$

This is the lowest energy allowed
Note that it is NOT zero as we would have in classical physics

Determine A by using normalization to probability of 1

(A)

$$\int \psi^*_{(x)} \psi(x) = 1 \longrightarrow \int_0^L A^2 \sin^2(kx)\, dx = 1$$

$$A^2 \underbrace{\int_0^L \sin^2(kx)\, dx}_{= \frac{L}{2}} = 1$$

Done in Giancoli ex 38-6 p. 1032

$$A = \sqrt{\frac{2}{L}}$$

1d ∞ square well Wave function

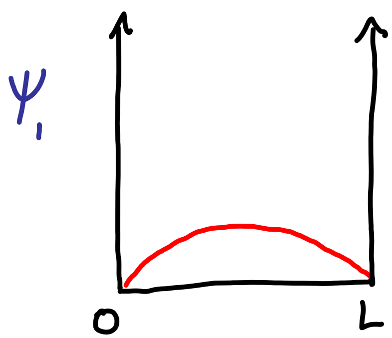
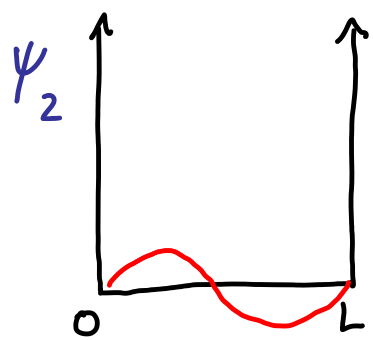
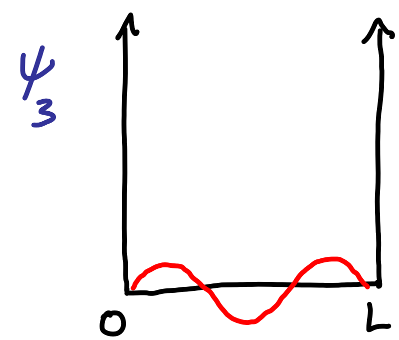
$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \quad \text{for } n = 1, 2, 3 \cdots \quad \text{in} \quad 0 < x < L$$

What does the wavefunction look like?

$kL = n\pi$

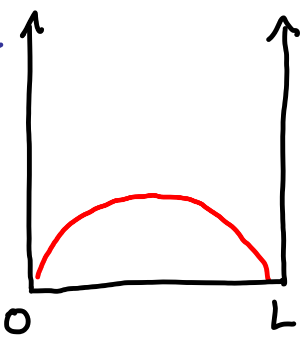
$\frac{2\pi}{\lambda} L = n\pi$

$\lambda = \frac{2L}{n}$

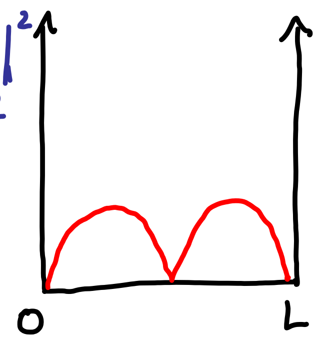
$n=1$	$n=2$	$n=3$	
			$\cdots$
$\lambda = 2L$	$\lambda = L$	$\lambda = \frac{2L}{3}$	
$\psi_1 = \sqrt{\frac{2}{L}} \sin \frac{\pi}{L} x$	$\psi_2 = \sqrt{\frac{2}{L}} \sin \frac{2\pi}{L} x$	$\psi_3 = \sqrt{\frac{2}{L}} \sin \frac{3\pi}{L} x$	$\cdots$
A	B	C	

What is the probability density for seeing particle at position x 26

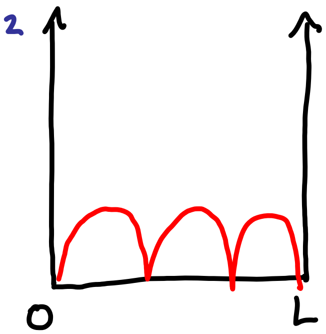
$n=1$ $|\psi_1|^2$



$n=2$ $|\psi_2|^2$



$n=3$ $|\psi_3|^2$



...

$\lambda = 2L$ $\qquad$ $\lambda = L$ $\qquad$ $\lambda = \frac{2L}{3}$

$$|\psi_1|^2 = \frac{2}{L}\sin^2\frac{\pi}{L}x \qquad |\psi_2|^2 = \frac{2}{L}\sin^2\frac{2\pi}{L}x \qquad |\psi_3|^2 = \frac{2}{L}\sin^2\frac{3\pi}{L}x \qquad \ldots$$

A $\qquad$ B $\qquad$ C