The Final Exam is on Wednesday 10th Dec 2003
at 11:30 am in WLH 2005

Be (T)here !!
Where Do Wave Functions Come From?

- Are solutions of the time-dependent Schrödinger Differential Equation (inspired by Wave Equation seen in 2C)
  \[
  -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x,t)}{\partial x^2} + U(x)\Psi(x,t) = i\hbar \frac{\partial \Psi(x,t)}{\partial t}
  \]

- Given a potential \( U(x) \)\) → particle under certain force
  \[
  F(x) = -\frac{\partial U(x)}{\partial x}
  \]

Schrodinger had an interesting life!
Schrodinger Wave Equation

Wavefunction $\psi$ which is a sol. of the Sch. Equation embodies all modern physics experienced/learnt so far:

$$E=hf, \quad p=\frac{\hbar}{\lambda}, \quad \Delta x.\Delta p \sim \hbar, \quad \Delta E.\Delta t \sim \hbar, \quad \text{quantization etc}$$

Schrodinger Equation is a Dynamical Equation much like Newton's Equation $\vec{F}=m\vec{a}$

$$\psi(x,0) \rightarrow \text{Force (potential)} \rightarrow \psi(x,t)$$

Evolves the System as a function of space-time

The Schrodinger Eq. propagates the system forward & backward in time:

$$\psi(x,\delta t) = \psi(x,0) + \left[\frac{d\psi}{dt}\right]_{t=0} \delta t$$

Where does it come from ?? ..."First Principles"..no real derivation exists
Time Independent Sch. Equation

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

Sometimes (depending on the character of the Potential \(U(x,t)\))

The Wave function is factorizable: can be broken up

\(\Psi(x,t) = \psi(x) \phi(t)\)

*Example*: Plane Wave \(\Psi(x,t) = e^{i(kx - \omega t)} = e^{i(kx)} e^{-i(\omega t)}\)

In such cases, use separation of variables to get:

\[-\frac{\hbar^2}{2m} \phi(t) \frac{\partial^2 \psi(x)}{\partial x^2} + U(x)\psi(x)\phi(t) = i\hbar \psi(x) \frac{\partial \phi(t)}{\partial t}\]

Divide Throughout by \(\Psi(x,t) = \psi(x)\phi(t)\)

\[\Rightarrow \quad \frac{-\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + U(x) = i\hbar \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t}\]

LHS is a function of \(x\); RHS is fn of \(t\)

\(x\) and \(t\) are independent variables, hence:

\[\Rightarrow \quad \text{RHS} = \text{LHS} = \text{Constant} = E\]
Factorization Condition For Wave Function Leads to:

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

\[i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t)\]

What is the Constant E? How to Interpret it?

Back to a Free particle:

\[\Psi(x,t) = Ae^{ikx}e^{-i\omega t}, \quad \psi(x) = Ae^{ikx}\]

\[U(x,t) = 0\]

Plug it into the Time Independent Schrodinger Equation (TISE) \(\Rightarrow\)

\[-\frac{\hbar^2}{2m} \frac{d^2 (Ae^{ikx})}{dx^2} + 0 = E Ae^{ikx} \Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} = (\text{NR Energy})\]

Stationary states of the free particle: \(\Psi(x,t) = \psi(x)e^{-i\omega t}\)

\[\Rightarrow |\Psi(x,t)|^2 = |\psi(x)|^2\]

Probability is static in time t, character of wave function depends on \(\psi(x)\)
A More Interesting Potential: Particle In a Box

Write the Form of Potential: Infinite Wall

\[ U(x,t) = \infty; \ x \leq 0, \ x \geq L \]
\[ U(x,t) = 0 \ ; \ 0 < X < L \]

- Classical Picture:
  - Particle dances back and forth
  - Constant speed, const KE
  - Average \(<P> = 0\)
  - No restriction on energy value
    - \( E = K + U = K + 0 \)
  - Particle can not exist outside box
    - Can’t get out because needs to borrow infinite energy to overcome potential of wall

What happens when the joker is subatomic in size??
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential. However in the regions between each C & G is a repelling electric field whose strength depends on the magnitude of V.

(b) If V is small, then electron’s potential energy vs x has low sloping “walls”.

(c) If V is large, the “walls” become very high & steep, becoming infinitely high for $V \to \infty$.

(d) The straight infinite walls are an approximation of such a situation.

$$U(x)$$
\[ \Psi(x) \text{ for Particle Inside 1D Box with Infinite Potential Walls} \]

Inside the box, no force \( \Rightarrow U=0 \) or constant (same thing)

\[
\Rightarrow \left\{-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + 0\right\} \psi(x) = E \psi(x)
\]

\[
\Rightarrow \frac{d^2\psi(x)}{dx^2} = -k^2\psi(x) ; \quad k^2 = \frac{2mE}{\hbar^2}
\]

or

\[
\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0 \quad \Leftarrow \text{figure out what } \psi(x) \text{ solves this diff eq.}
\]

In General the solution is \( \psi(x) = A \sin kx + B \cos kx \) (A,B are constants)

Need to figure out values of A, B : How to do that ?

**Apply BOUNDARY Conditions on the Physical Wavefunction**

We said \( \psi(x) \) must be continuous everywhere

So match the wavefunction just outside box to the wavefunction value just inside the box

\[
\Rightarrow \text{At } x = 0 \Rightarrow \psi(x = 0) = 0 \quad \& \quad \text{At } x = L \Rightarrow \psi(x = L) = 0
\]

\[
\Rightarrow \psi(x = 0) = B = 0 \quad (\text{Continuity condition at } x =0)
\]

\[
\& \psi(x = L) = 0 \Rightarrow A \sin kL = 0 \quad (\text{Continuity condition at } x =L)
\]

\[
\Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}, n = 1, 2, 3, \ldots \infty
\]

So what does this say about Energy \( E \) ?

\[
E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \quad \text{Quantized (not Continuous)!}
\]

**Why can’t the particle exist Outside the box ?**

\[ \Rightarrow E \text{ Conservation} \]

\[ X=0 \quad X=L \]
Quantized Energy levels of Particle in a Box

\[ E_n = n^2 E_1 \]

\[ E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \]
The particle's Energy and Wavefunction are determined by a number \( n \)

We will call \( n \rightarrow \text{Quantum Number} \), just like in Bohr's Hydrogen atom

What about the wave functions corresponding to each of these energy states?

\[
\psi_n = A \sin(kx) = A \sin\left(\frac{n\pi x}{L}\right) \quad \text{for} \quad 0 < x < L
\]

\[
= 0 \quad \text{for} \quad x \geq 0, \ x \geq L
\]

Normalized Condition:

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

Use \( 2 \sin^2 \theta = 1 - 2 \cos 2\theta \)

\[
1 = \frac{A^2}{2} \int_0^L \left(1 - \cos\left(\frac{2n\pi x}{L}\right)\right) \quad \text{and since} \quad \int \cos \theta = \sin \theta
\]

\[
1 = \frac{A^2}{2} L \quad \Rightarrow \quad A = \sqrt{\frac{2}{L}}
\]

So \( \psi_n = \sqrt{\frac{2}{L}} \sin(kx) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \) ...What does this look like?
Wave Functions: Shapes Depend on Quantum # \( n \)

Wave Function

Probability \( P(x) \): Where the particle likely to be

Zero Prob
Where in The World is Carmen San Diego?

- We can only guess the probability of finding the particle somewhere in \( x \)
  - For \( n=1 \) (ground state) particle most likely at \( x = L/2 \)
  - For \( n=2 \) (first excited state) particle most likely at \( L/4, 3L/4 \)
- Prob. Vanishes at \( x = L/2 \) & \( L \)
  - How does the particle get from just before \( x=L/2 \) to just after?
    » QUIT thinking this way, particles don’t have trajectories
    » Just probabilities of being somewhere

Classically, where is the particle most Likely to be: Equal prob of being anywhere inside the Box
NOT SO says Quantum Mechanics!
Remember Sesame Street?

This particle in the box is brought to you by the letter n.

Its the Big Boss Quantum Number.
How to Calculate the QM prob of Finding Particle in Some region in Space

Consider \( n = 1 \) state of the particle

Ask : What is \( P \left( \frac{L}{4} \leq x \leq \frac{3L}{4} \right) \)?

\[
P = \int_{\frac{L}{4}}^{\frac{3L}{4}} \left| \psi_1 \right|^2 dx = \frac{2}{L} \int_{\frac{L}{4}}^{\frac{3L}{4}} \sin^2 \frac{\pi x}{L} \; dx = \left( \frac{2}{L} \right) \frac{1}{2} \int_{\frac{L}{4}}^{\frac{3L}{4}} (1 - \cos \frac{2\pi x}{L}) dx
\]

\[
P = \frac{1}{L} \left[ \frac{L}{2} - \right] \left[ \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{\frac{L}{4}}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi} \left( \sin \frac{2\pi}{L} \cdot \frac{3L}{4} - \sin \frac{2\pi}{L} \cdot \frac{L}{4} \right)
\]

\[
P = \frac{1}{2} - \frac{1}{2\pi} (-1 - 1) = 0.818 \Rightarrow 81.8\%
\]

Classically \( \Rightarrow 50\% \) (equal prob over half the box size)

\( \Rightarrow \) Substantial difference between Classical & Quantum predictions
But one issue is irreconcilable:

Quantum Mechanically the particle can not have $E = 0$

This is a consequence of the Uncertainty Principle

The particle moves around with KE inversely proportional to the Length Of the 1D Box
Finite Potential Barrier

- There are no Infinite Potentials in the real world
  - Imagine the cost of a battery with infinite potential diff
    - Will cost infinite $ sum + not available at Radio Shack
- Imagine a realistic potential: Large $U$ compared to $KE$ but not infinite

Classical Picture: A bound particle (no escape) in $0 < x < L$
Quantum Mechanical Picture: Use $\Delta E \cdot \Delta t \leq \hbar/2\pi$
Particle can leak out of the Box of finite potential $P(|x| > L) \neq 0$
Finite Potential Well

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

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

\[ = \alpha^2 \psi(x); \quad \alpha = \sqrt{\frac{2m(U-E)}{\hbar^2}} \]

\[ \Rightarrow \text{General Solutions: } \psi(x) = Ae^{\alpha x} + Be^{-\alpha x} \]

Require finiteness of \( \psi(x) \)

\[ \Rightarrow \psi(x) = Ae^{\alpha x} \quad \text{...} x < 0 \quad \text{(region I)} \]

\[ \psi(x) = Ae^{-\alpha x} \quad \text{...} x > L \quad \text{(region III)} \]

Again, coefficients A & B come from matching conditions at the edge of the walls (x = 0, L)

But note that wave fn at \( \psi(x) \) at (x = 0, L) \( \neq 0 \) !! (why?)

Further require Continuity of \( \psi(x) \) and \( \frac{d\psi(x)}{dx} \)

These lead to rather different wave functions
Finite Potential Well: Particle can Burrow Outside Box
Finite Potential Well: Particle can Burrow Outside Box

Particle can be outside the box but only for a time $\Delta t \approx \frac{\hbar}{\Delta E}$

$\Delta E = \text{Energy particle needs to borrow to Get outside} = U - E + KE$

The Cinderella act (of violating E Conservation cant last very long

Particle must hurry back (cant be caught with its hand inside the cookie-jar)

Penetration Length $\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U-E)}}$

If $U \gg E \Rightarrow$ Tiny penetration

If $U \rightarrow \infty \Rightarrow \delta \rightarrow 0$
Finite Potential Well: Particle can Burrow Outside Box

Penetration Length $\delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m(U-E)}}$

If $U >> E$ $\Rightarrow$ Tiny penetration
If $U \to \infty \Rightarrow \delta \to 0$

$E_n = \frac{n^2 \pi^2 \hbar^2}{2m(L + 2\delta)^2}, n = 1, 2, 3, 4...$

When $E=U$ then solutions blow up
$\Rightarrow$ Limits to number of bound states ($E_n < U$)
When $E>U$, particle is not bound and can get either reflected or transmitted across the potential "barrier"
Simple Harmonic Oscillator: Quantum and Classical

Spring with Force Const $k$

$m$ at $x=0$
Particle of mass m within a potential $U(x)$

$$\bar{F}(x) = -\frac{dU(x)}{dx}$$

$$\bar{F}(x=a) = -\left.\frac{dU(x)}{dx}\right|_{x=a} = 0,$$

$$\bar{F}(x=b) = 0, \quad \bar{F}(x=c) = 0 \quad \text{...But...}$$

look at the Curvature:

$$\frac{\partial^2 U}{\partial x^2} > 0 \quad \text{(stable)}, \quad \frac{\partial^2 U}{\partial x^2} < 0 \quad \text{(unstable)}$$

**Stable Equilibrium: General Form:**

$$U(x) = U(a) + \frac{1}{2}k(x-a)^2$$

Rescale $\Rightarrow U(x) = \frac{1}{2}k(x-a)^2$

**Motion of a Classical Oscillator (ideal)**

Ball originally displaced from its equilibrium position, motion confined between $x=0$ & $x=A$

$$U(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2x^2; \quad \omega = \sqrt{\frac{k}{m}} = \text{Ang. Freq}$$

$$E = \frac{1}{2}kA^2 \Rightarrow \text{Changing } A \text{ changes } E$$

$E$ can take any value & if $A \to 0$, $E \to 0$

Max. KE at $x = 0$, KE $= 0$ at $x = \pm A$
Quantum Picture: Harmonic Oscillator

Find the Ground state Wave Function \( \psi(x) \)

Find the Ground state Energy \( E \) when \( U(x) = \frac{1}{2} m \omega^2 x^2 \)

Time Dependent Schrodinger Eqn:
\[
\frac{-\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + \frac{1}{2} m \omega^2 x^2 \psi(x) = E \psi(x)
\]

\[
\Rightarrow \frac{d^2 \psi(x)}{dx^2} = \frac{2m}{\hbar^2} \left( E - \frac{1}{2} m \omega^2 x^2 \right) \psi(x) = 0
\]

What \( \psi(x) \) solves this?

Two guesses about the simplest Wavefunction:
1. \( \psi(x) \) should be symmetric about \( x \)
2. \( \psi(x) \rightarrow 0 \) as \( x \rightarrow \infty \)

\( \psi(x) \) should be continuous & \( \frac{d\psi(x)}{dx} \) = continuous

My guess: \( \psi(x) = C_0 e^{-\alpha x^2} \); Need to find \( C_0 \) & \( \alpha \):
Quantum Picture: Harmonic Oscillator

$P(x) = C_0^2 e^{-2\alpha x^2}$

$\psi(x) = C_0 e^{-\alpha x^2}$

How to get $C_0$ & $\alpha$??...Try plugging in the wave-function into the time-independent Schröd. Eqn.