

Confirmed: 2D Final Exam: Thursday 18th March 11:30-2:30 PM WLH 2005

Date	Time	Read	Topic	HW problems for the week	Location
Monday	11:00 am	Ch 5	Quantum Mechanics in 1 Dimension	Ch 5 : 1, 2, 3, 5, 7, 9	WLH 2005
Tuesday	8:00 pm	Ch 5	Quantum Mechanics in 1 Dimension	Ch 5 : 14, 17, 20, 21, 25	WLH 2005
Wednesday	11:00 am	Ch 5	Quantum Mechanics in 1 Dimension	Ch 5 : 30, 33, 34, 39, 40	WLH 2005
Wednesday	3:00 pm	Ch 5	Discussion	-	WLH 2005
Thursday	5:00-6:20 pm	-	Problem Session		Peterson 108
Friday	11:00am	-	Quiz	Ch 5.1 - 5.8	WLH 2005



Physics 2D Lecture Slides
Lecture 22: Feb 24rd

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UCSD Physics

Introducing the Schrodinger Equation

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

- $U(x)$ = characteristic Potential of the system
- Different potential for different forces
- Hence different solutions for the Diff. eqn.
- \rightarrow characteristic wavefunctions for a particular $U(x)$

Schrodinger Wave Equation

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

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

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

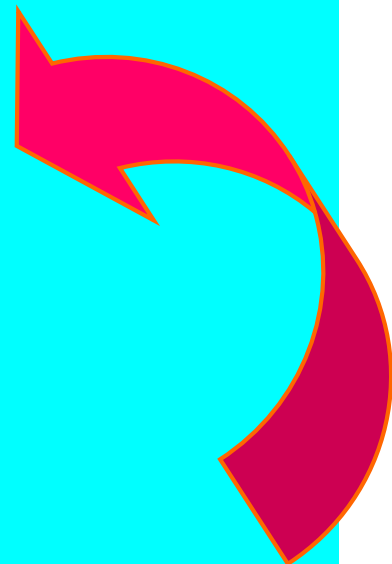
$$\psi(x,0) \xrightarrow{\text{Force (potential)}} \psi(x,t)$$

Evolves the System as a function of space-time

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

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

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:

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

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

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

LHS is a function of x ; RHS is fn of t

x and t are independent variables, hence:

\Rightarrow RHS = LHS = 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 $\psi(x)$

Schrodinger Eqn: Stationary State Form

- Recall → when potential does not depend on time explicitly
 - $U(x,t) = U(x)$ only... we used separation of x,t variables to simplify
 - $\Psi(x,t) = \psi(x) \phi(t)$
 - broke S. Eq. into two: one with x only and another with t only

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

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

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

How to put **Humpty-Dumpty** back together ? e.g to say how to go from an expression of $\psi(x) \rightarrow \Psi(x,t)$ which describes time-evolution of the overall wave function

Schrodinger Eqn: Stationary State Form

Since $\frac{d}{dt} [\ln f(t)] = \frac{1}{f(t)} \frac{df(t)}{dt}$

In $i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t)$, rewrite as $\frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = \frac{E}{i\hbar} = -\frac{iE}{\hbar}$

and integrate both sides w.r.t. time

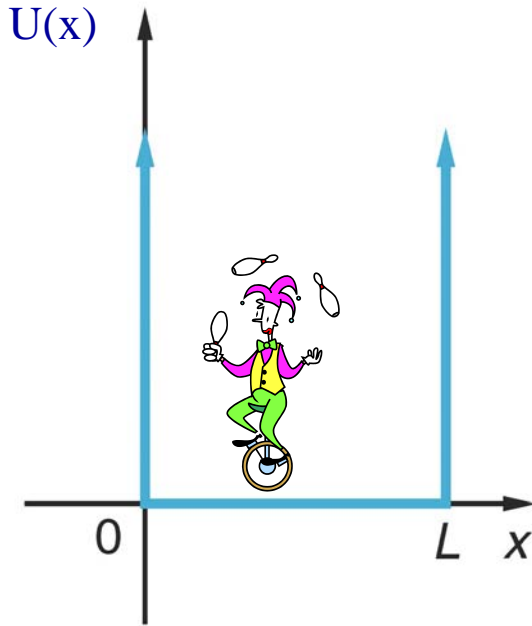
$$\int_{t=0}^{t=t} \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} dt = \int_0^t -\frac{iE}{\hbar} dt \Rightarrow \int_0^t \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} dt = -\frac{iE}{\hbar}$$

$\therefore \ln \phi(t) - \ln \phi(0) = -\frac{iE}{\hbar} t$, now exponentiate both sides

$\Rightarrow \phi(t) = \phi(0) e^{-\frac{iE}{\hbar} t}$; $\phi(0) = \text{constant} = \text{initial condition} = 1$ (e.g)

$\Rightarrow \phi(t) = e^{-\frac{iE}{\hbar} t}$ & Thus $\Psi(x,t) = \psi(x) e^{-\frac{iE}{\hbar} t}$ where $E = \text{energy of system}$

A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

$$U(x,t) = \infty; \quad x \leq 0, \quad x \geq L$$

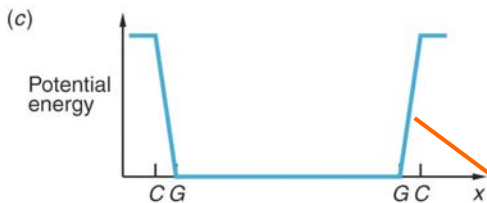
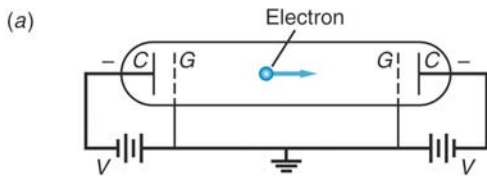
$$U(x,t) = 0; \quad 0 < x < L$$

• Classical Picture:

- Particle dances back and forth
- Constant speed, const KE
- Average $\langle P \rangle = 0$
- 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 ??

Example of a Particle Inside a Box With Infinite Potential



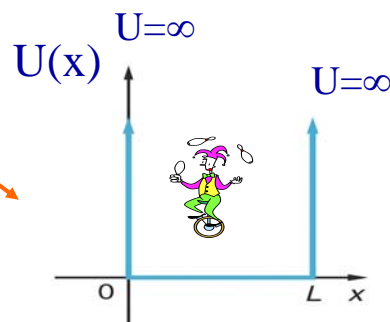
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

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 $V \rightarrow \infty$

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



Ψ(x) for Particle Inside 1D Box with Infinite Potential Walls

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

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

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

or $\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$ \leftarrow figure out what $\psi(x)$ 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

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

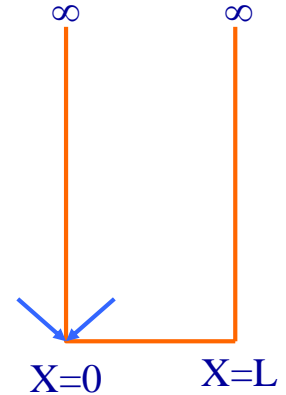
$$\therefore \psi(x=0) = B = 0 \quad (\text{Continuity condition at } x=0)$$

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

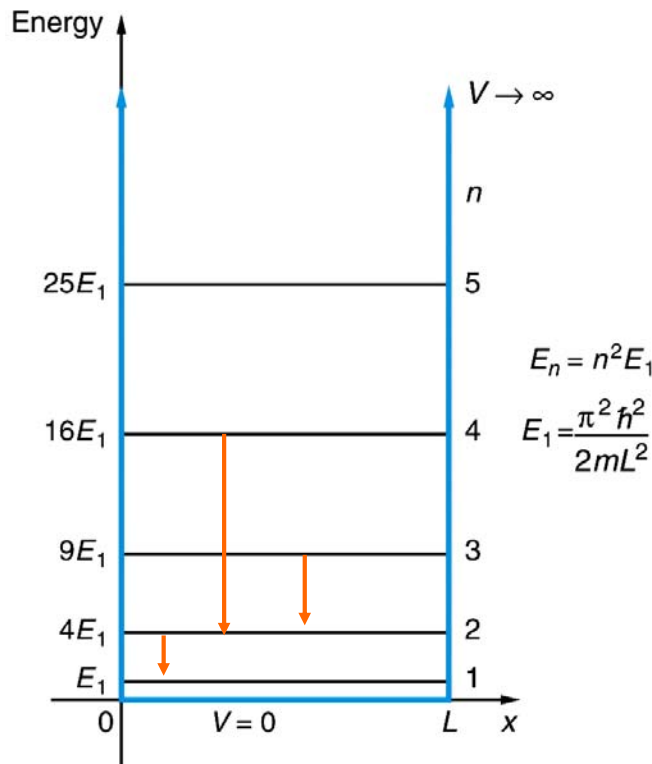
$$\Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}, n = 1, 2, 3, \dots \infty$$

So what does this say about Energy E ? : $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ Quantized (not Continuous)!

Why can't the particle exist Outside the box ?
 \rightarrow E Conservation



Quantized Energy levels of Particle in a Box



What About the Wave Function Normalization ?

The particle's Energy and Wavefunction are determined by a number n
 We will call $n \rightarrow$ Quantum Number , just like in Bohr's Hydrogen atom
 What about the wave functions corresponding to each of these energy states?

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

$$= 0 \quad \text{for } x \leq 0, x \geq L$$

Normalized Condition :

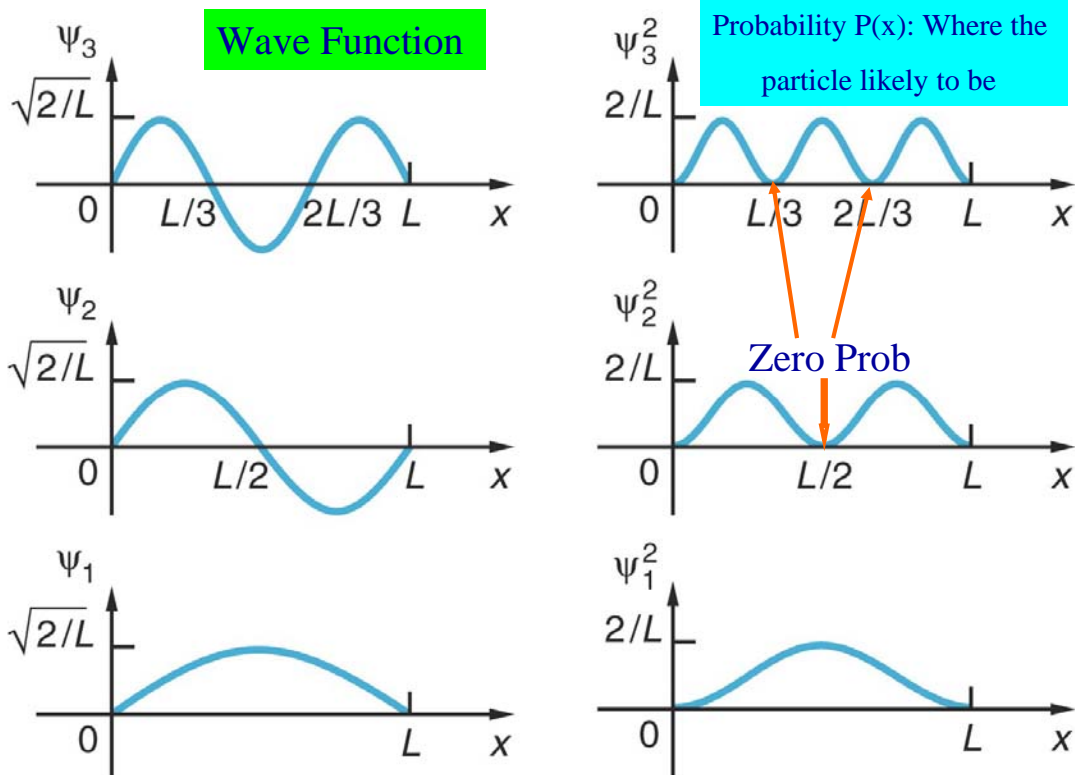
$$1 = \int_0^L \psi_n^* \psi_n dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \quad \text{Use } 2\sin^2\theta = 1 - 2\cos 2\theta$$

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

$$1 = \frac{A^2}{2} L \Rightarrow A = \sqrt{\frac{2}{L}}$$

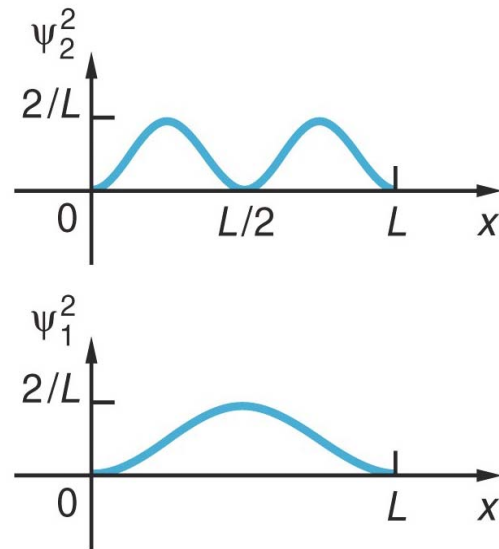
$$\text{So } \psi_n = \sqrt{\frac{2}{L}} \sin(kx) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad \dots \text{What does this look like?}$$

Wave Functions : Shapes Depend on Quantum # n



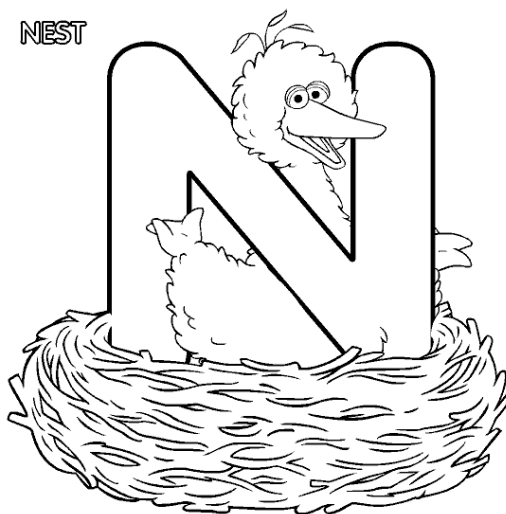
Where in The World is Carmen San Diego?

- 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 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 $P\left(\frac{L}{4} \leq x \leq \frac{3L}{4}\right)$?

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

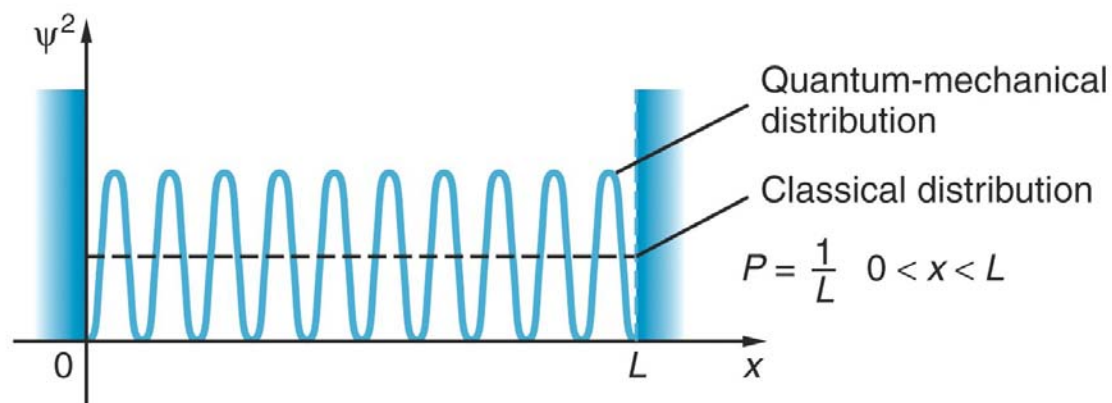
$$P = \frac{1}{L} \left[\frac{L}{2} - \right] \left[\frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi} \left(\sin \frac{2\pi}{L} \cdot \frac{3L}{4} - \sin \frac{2\pi}{L} \cdot \frac{L}{4} \right)$$

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

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

\Rightarrow Substantial difference between Classical & Quantum predictions

When The Classical & Quantum Pictures Merge: $n \rightarrow \infty$



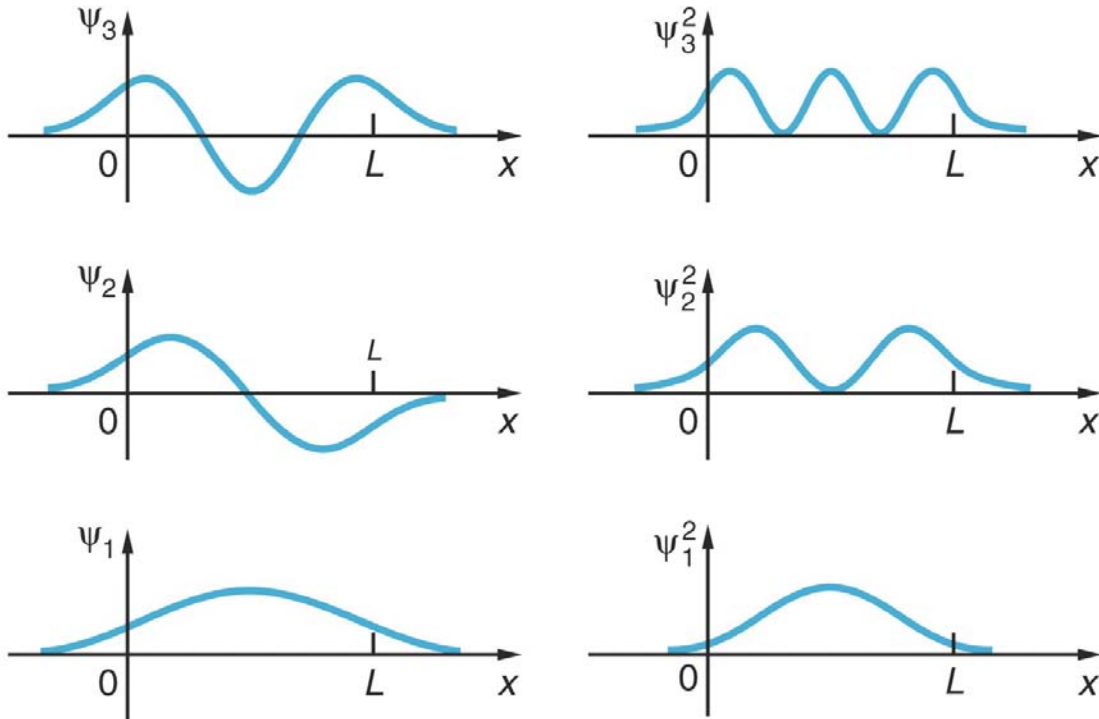
But one issue is irreconcilable:

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

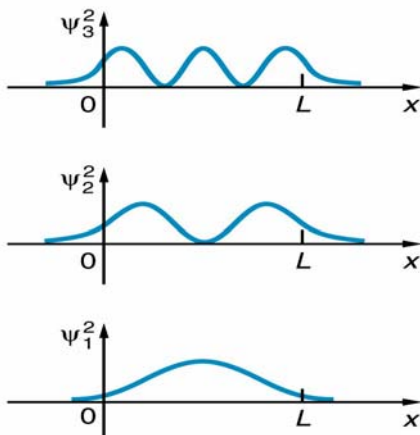
This is a consequence of the Uncertainty Principle

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

Finite Potential 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 $\Delta t \approx \hbar / \Delta E$

ΔE = Energy particle needs to borrow to

Get outside $\Delta E = U - E + KE$

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)

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

If $U \gg E \Rightarrow$ Tiny penetration

If $U \rightarrow \infty \Rightarrow \delta \rightarrow 0$

Finite Potential Well: Particle can Burrow Outside Box

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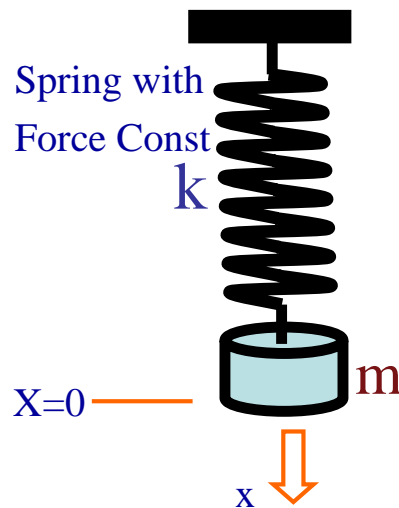
$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m(L + 2\delta)^2}, n = 1, 2, 3, 4, \dots$$

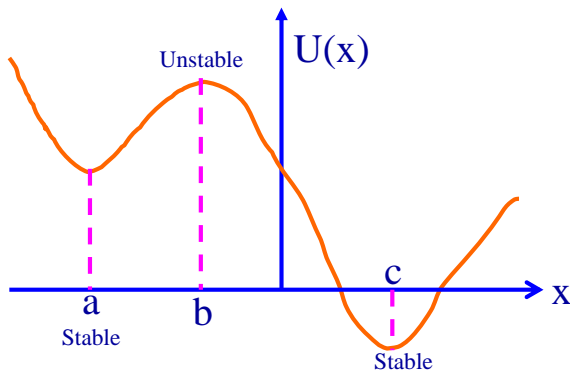
When $E=U$ then solutions blow up

\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





Stable Equilibrium: General Form :

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

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

Motion of a Classical Oscillator (ideal)

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

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

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

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

Max. KE at $x=0$, KE=0 at $x=\pm A$

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

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

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

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

look at the Curvature:

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

Quantum Picture: Harmonic Oscillator

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

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

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

$$\Rightarrow \frac{d^2\psi(x)}{dx^2} = \frac{2m}{\hbar^2} \left(E - \frac{1}{2}m\omega^2x^2 \right) \psi(x) = 0 \quad \text{What } \psi(x) \text{ solves this?}$$

Two guesses about the simplest Wavefunction:

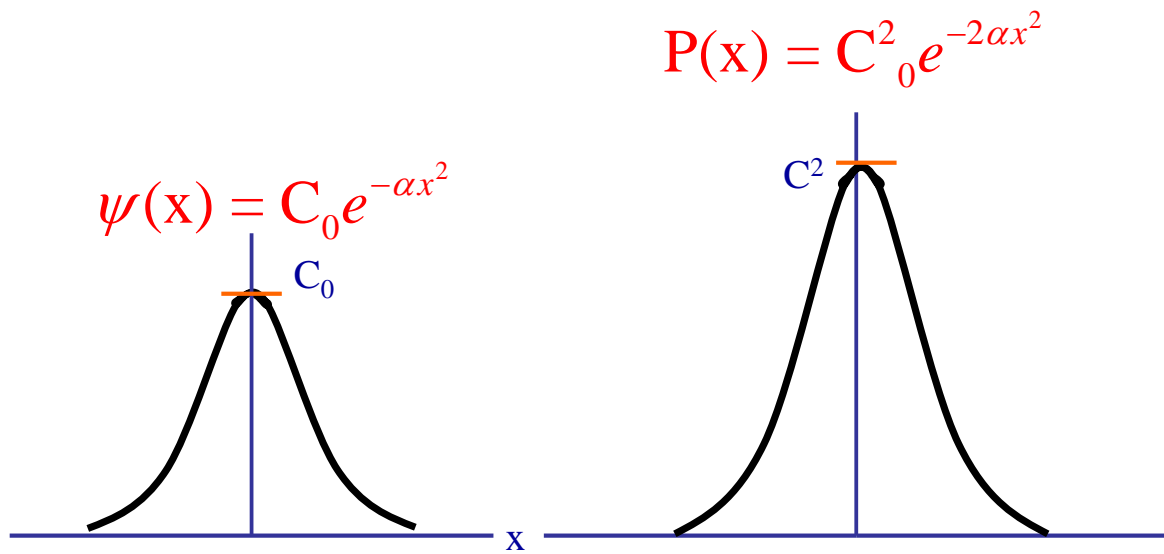
1. $\psi(x)$ should be symmetric about x 2. $\psi(x) \rightarrow 0$ as $x \rightarrow \infty$

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

My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator



How to Get C_0 & α ?? ... Try plugging in the wave-function into the time-independent Schr. Eqn.