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

Quiz 7 will cover Sections 5.1-5.6
Do HW problems from these sections

Physics 2D Lecture Slides
Lecture 23: Feb 25rd

Vivek Sharma
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.
- → characteristic wavefunctions for a particular U(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
    - Ψ(x,t) = ψ(x) ϕ(t)
    - broke S. Eq. into two: one with x only and another with t only

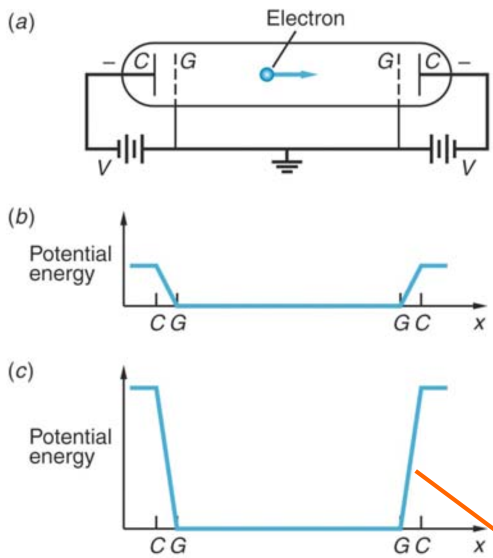
$$\frac{-\hbar^2}{2\text{m}}\frac{\partial^2\psi(x)}{\partial^2 x}+U(x)\psi(x)=E\ \ \psi(x)$$

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

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

How to put Humpty-Dumpty back together ? e.g to say how to go from an expression of ψ(x)→Ψ(x,t) which describes time-evolution of the overall wave function

Example of a Particle Inside a Box With Infinite Potential



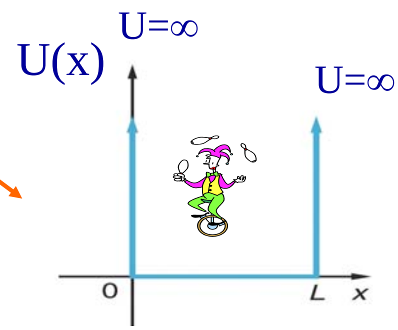
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

However in the regions between each C & G is a repelling electric field whose strength depends on the magnitude of V

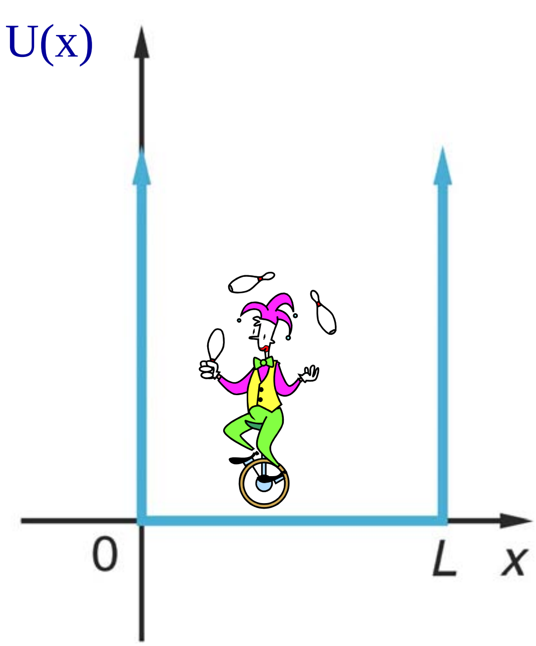
(b) If V is small, then electron's potential energy vs x has low sloping "walls"

(c) If V is large, the "walls"become very high & steep becoming infinitely high for V→∞

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



A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

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

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

- 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 ??

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

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

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

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

or $\boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0}$ $\Leftarrow$ figure out what ψ(x) solves this diff eq.

In General the solution is $\psi(x) = A\ sinkx + B\ coskx$ (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

$\Rightarrow$ At x = 0 $\Rightarrow \psi(x=0) = 0$ & At x = L $\Rightarrow \psi(x=L) = 0$

$\therefore\ \psi(x=0) = B = 0$ (Continuity condition at x =0)

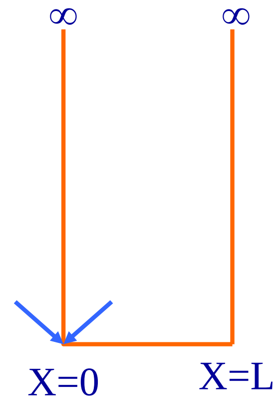
& $\psi(x=L) = 0 \Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

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

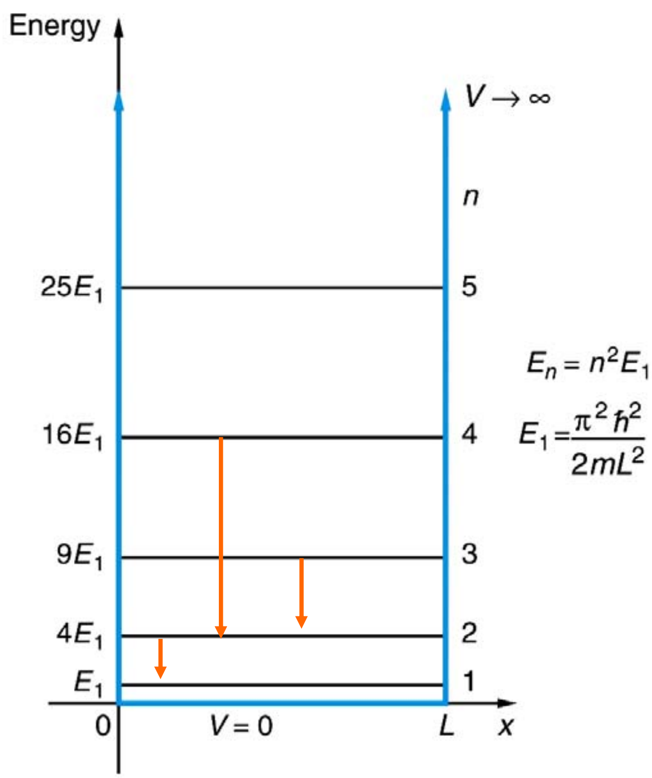
So what does this say about Energy E ? : $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ Quantized (not Continuous)!

Why can't the particle exist Outside the box ?

→ 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?

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

Normalized Condition :

$$1 = \int_0^L \psi_n^* \psi_n dx = A^2 \int_0^L Sin^2(\frac{n\pi x}{L})$$

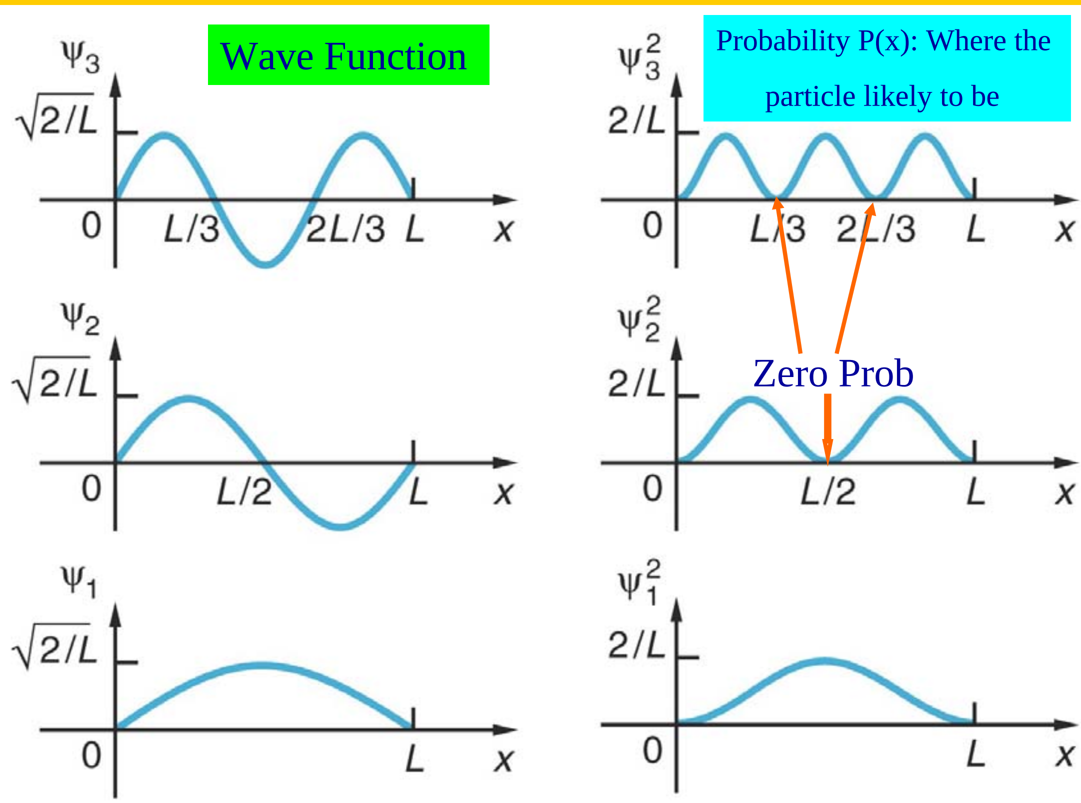
Use $2Sin^2\theta = 1 - 2Cos2\theta$

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

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

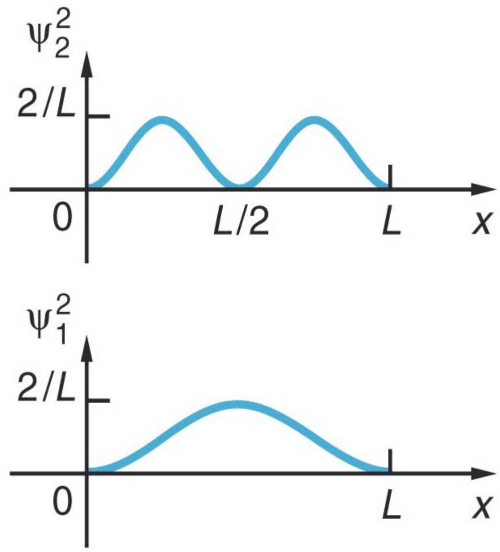
So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ ...What does this look like?

Wave Functions : Shapes Depend on Quantum # n



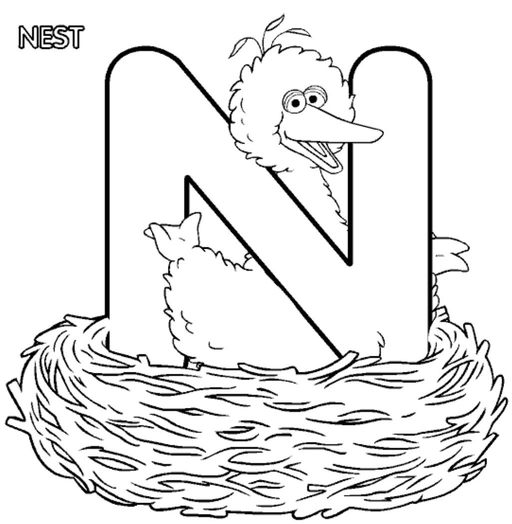
Where in The World is Carmen San Diego?

- 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 $(\frac{L}{4} \le x \le \frac{3L}{4})$?

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

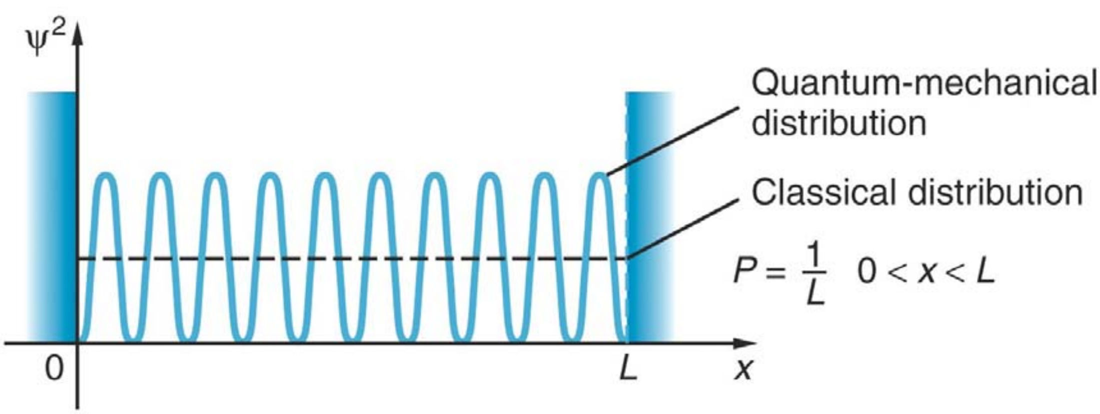
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin\frac{2\pi}{L}.\frac{3L}{4} - \sin\frac{2\pi}{L}.\frac{L}{4}\right)$$

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

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

$\Rightarrow$ Substantial difference between Classical & Quantum predictions

When The Classical & Quantum Pictures Merge: n→∞



But one issue is irreconcilable:

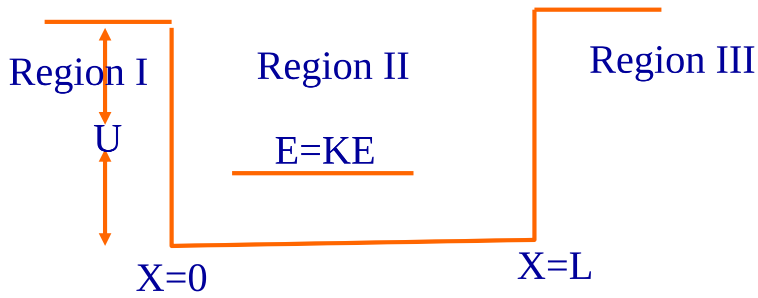
Quantum Mechanically the particle can not have E = 0

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 as 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 $\Delta E.\Delta t \leq h/2\pi$

Particle can leak out of the Box of finite potential $P(|x|>L) \neq 0$

Finite Potential Well

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

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

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

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

Require finiteness of $\psi(x)$

$\Rightarrow \psi(x) = Ae^{+\alpha x}$ .....x<0 (region I)

$\psi(x) = Ae^{-\alpha x}$ .....x>L (region III)

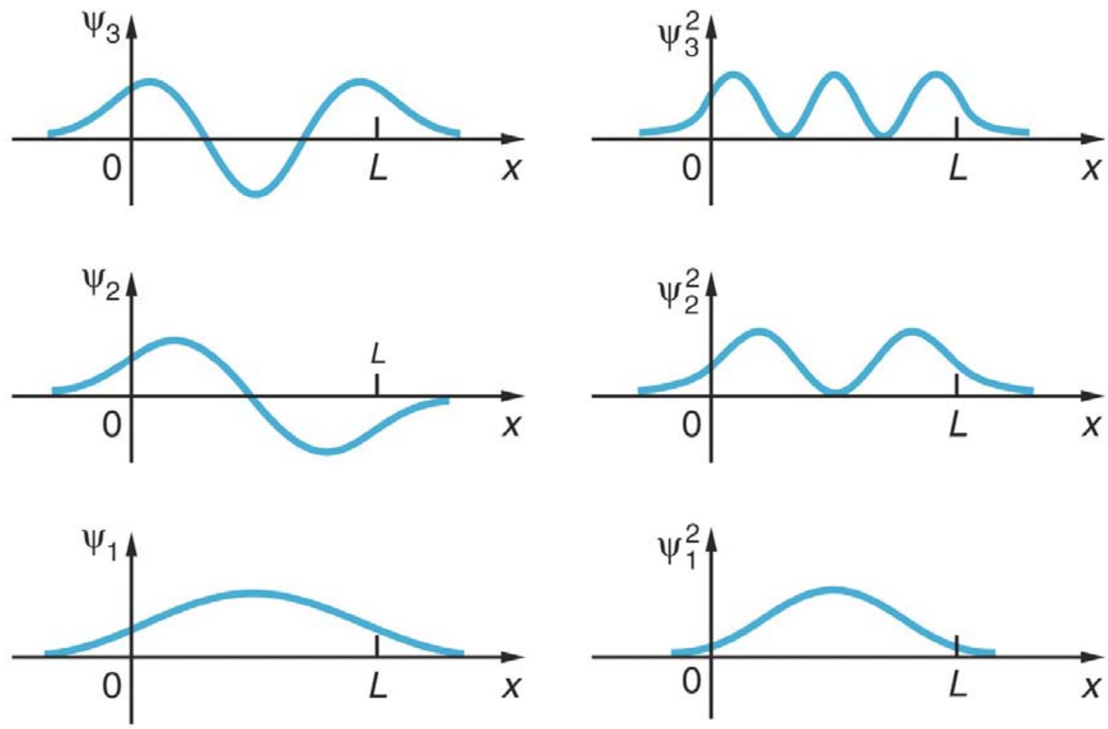
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

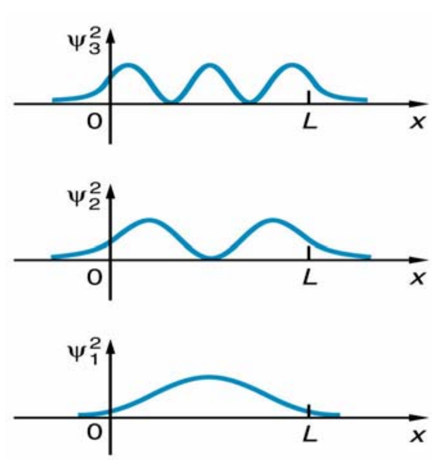
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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 $\Delta t \approx h/\Delta E$

ΔE = Energy particle needs to borrow to Get outside ΔE = 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>>E $\Rightarrow$ Tiny penetration

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

Finite Potential Well: Particle can Burrow Outside Box

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If U>>E $\Rightarrow$ Tiny penetration

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

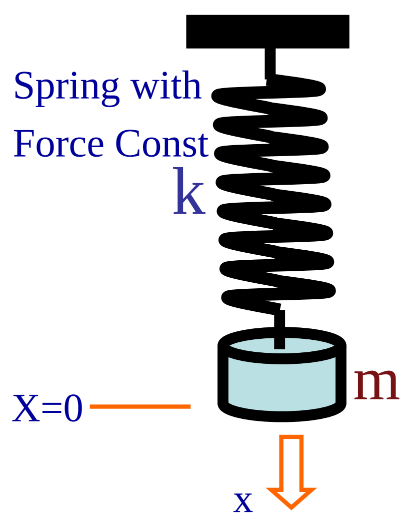
$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4...$$

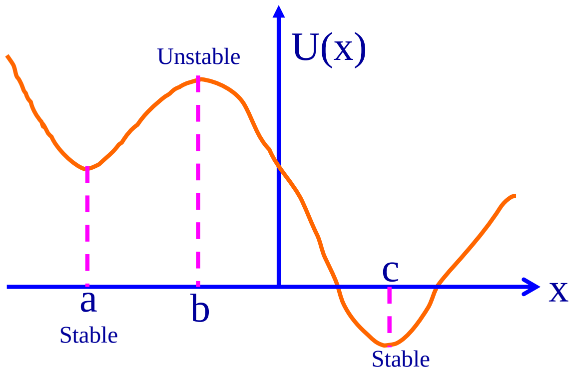
When E=U then solutions blow up

$\Rightarrow$ 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





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

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

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

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

Max. KE at x = 0, KE= 0 at x= ± A

Particle of mass m within a potential U(x)

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

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

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

look at the Curvature:

$\frac{\partial^2 U}{\partial x^2} > 0$ (stable), $\frac{\partial^2 U}{\partial x^2} < 0$ (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: $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x} + \frac{1}{2}m\omega^2x^2\psi(x) = E\ \psi(x)$

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

What $\psi(x)$ solves this?

Two guesses about the simplest Wavefunction:

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

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

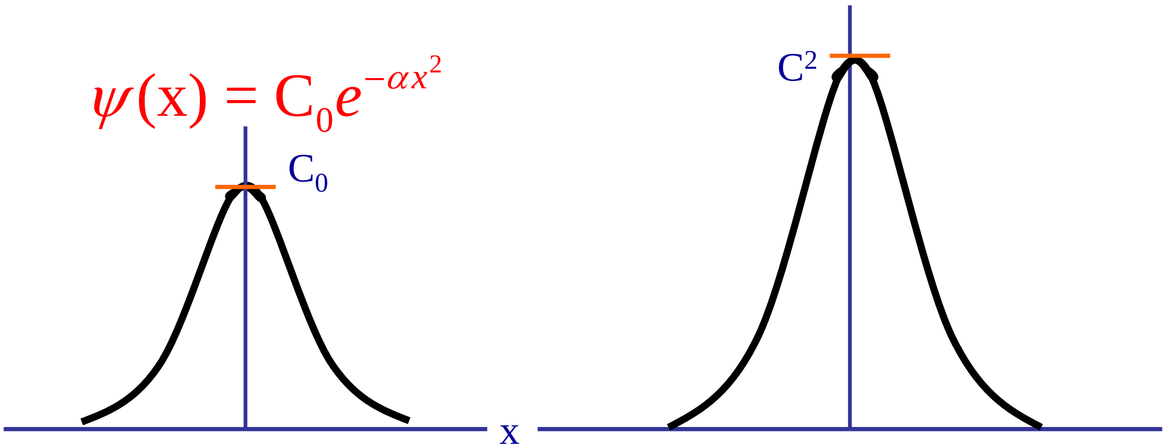
My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

$$P(x) = C^2{}_0 e^{-2\alpha x^2}$$

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



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