Physics 2D Lecture Slides
Nov 18

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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 <u>interesting</u> life !

Schrodinger Wave Equation

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

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

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

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

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

$$\Psi\left(\mathrm{x,t}\right)=\psi(x)\ \phi(t)$$

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

In such cases, use seperation of variables to get :

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

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

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

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:

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

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

What is the Constant E ? How to Interpret it ?

Back to a Free particle :

$\Psi(\text{x,t})=\ \text{A}e^{\text{ikx}}e^{\text{-i}\omega\text{t}},\ \psi(\text{x})=\text{A}e^{\text{ikx}}$

$\text{U(x,t)} = 0$

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

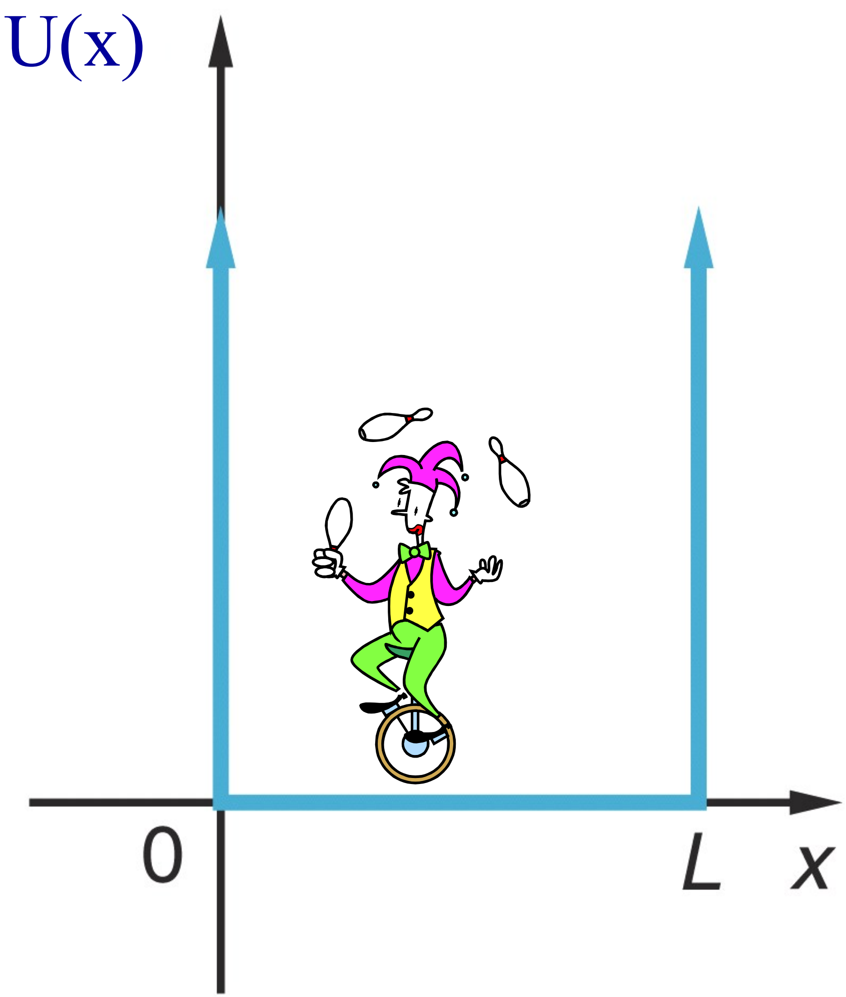
$$\frac{-\hbar^2}{2m}\frac{d^2(Ae^{(ikx)})}{dx^2}+0=E\ Ae^{(ikx)}\quad\Rightarrow E=\frac{\hbar^2k^2}{2m}=\frac{p^2}{2m}=\text{(NR Energy)}$$

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

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

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

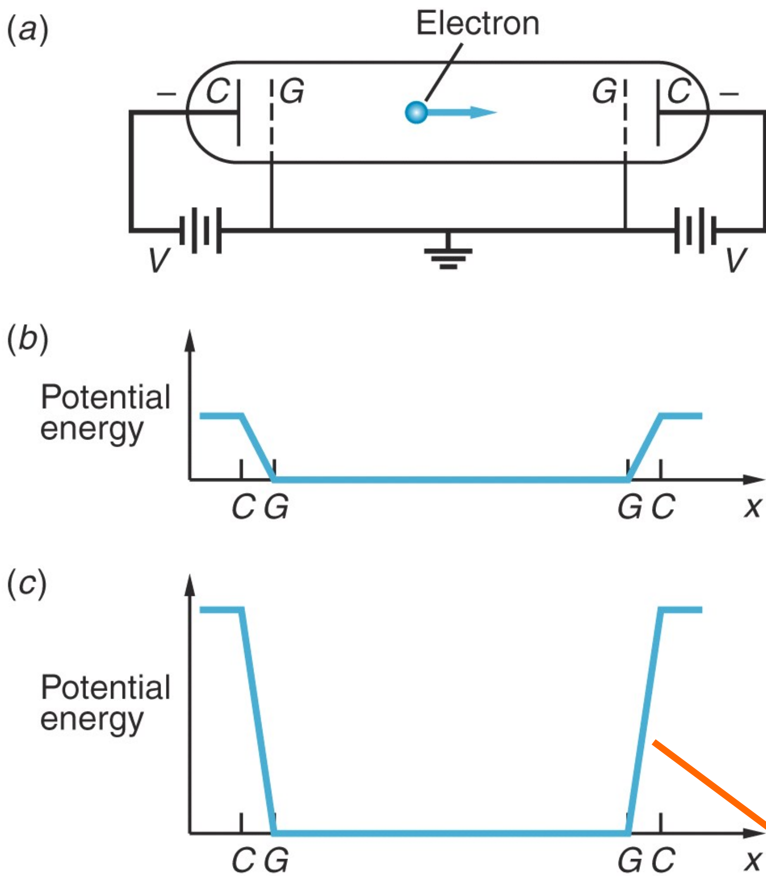
$$U(x,t) = \infty; \quad x \le 0, \quad x \ge L$$

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

- 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



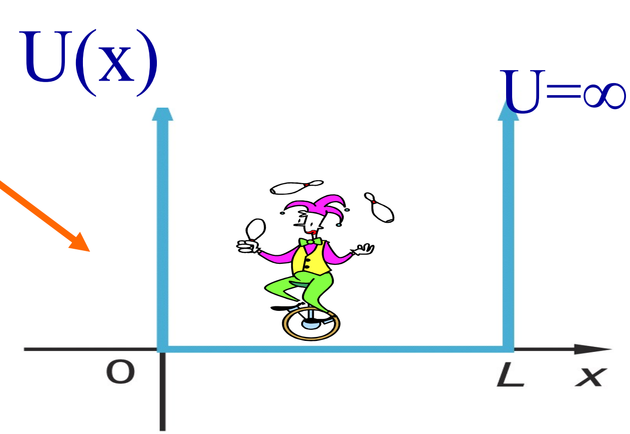
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

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)

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

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

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)

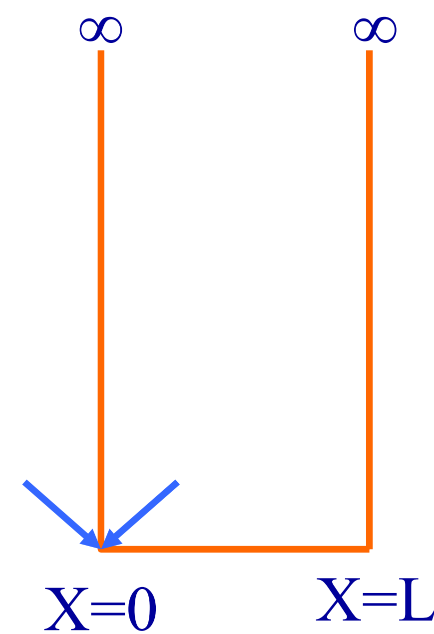
& $\psi(x=L) = 0 \Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

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

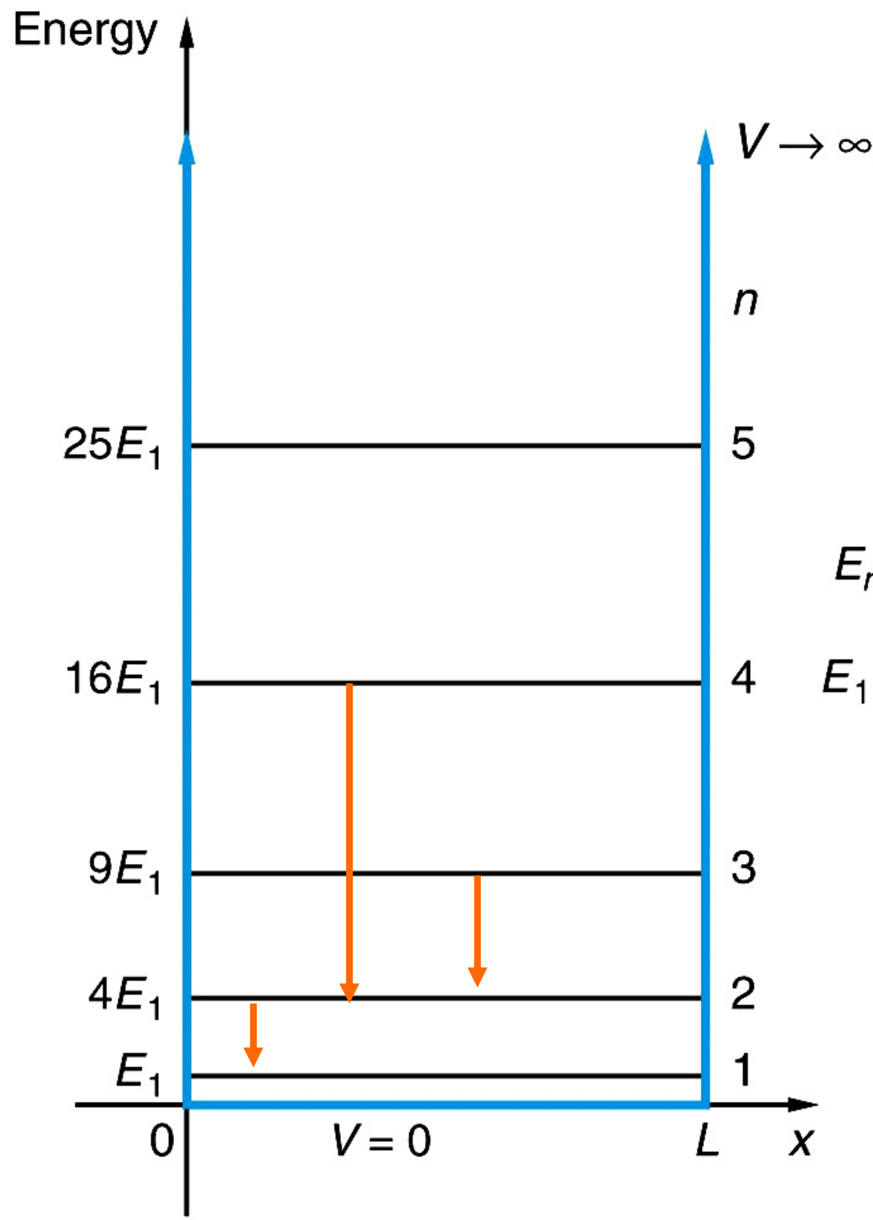
So what does this say about Energy E ? : $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ Quantized (not Continuous)!

Why can't the particle exist Outside the box ?

→ E Conservation



Quantized Energy levels of Particle in a Box



$$E_n = n^2 E_1$$

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

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 :

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

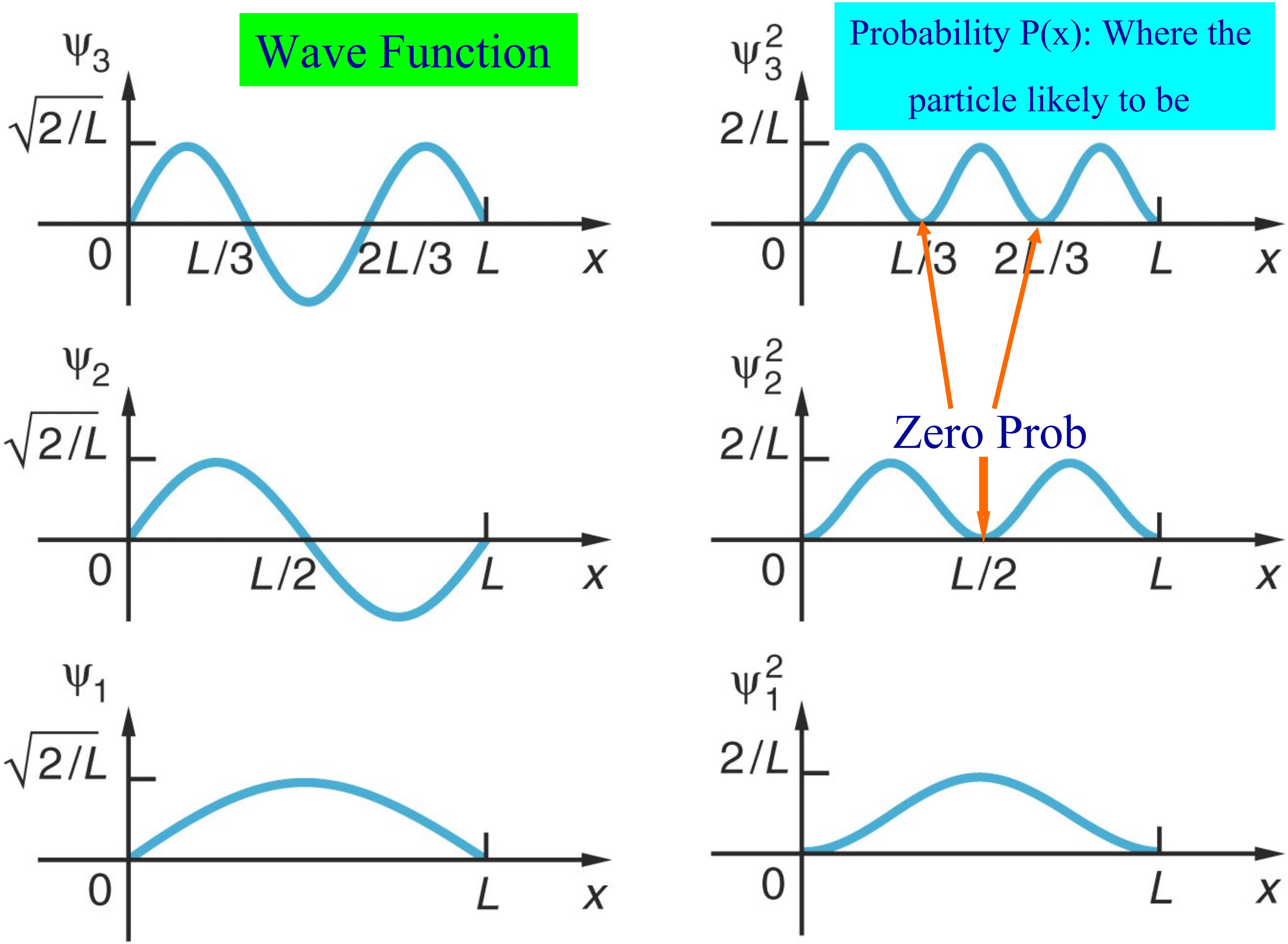
Use $2\text{Sin}^2\theta = 1 - 2Cos2\theta$

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

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

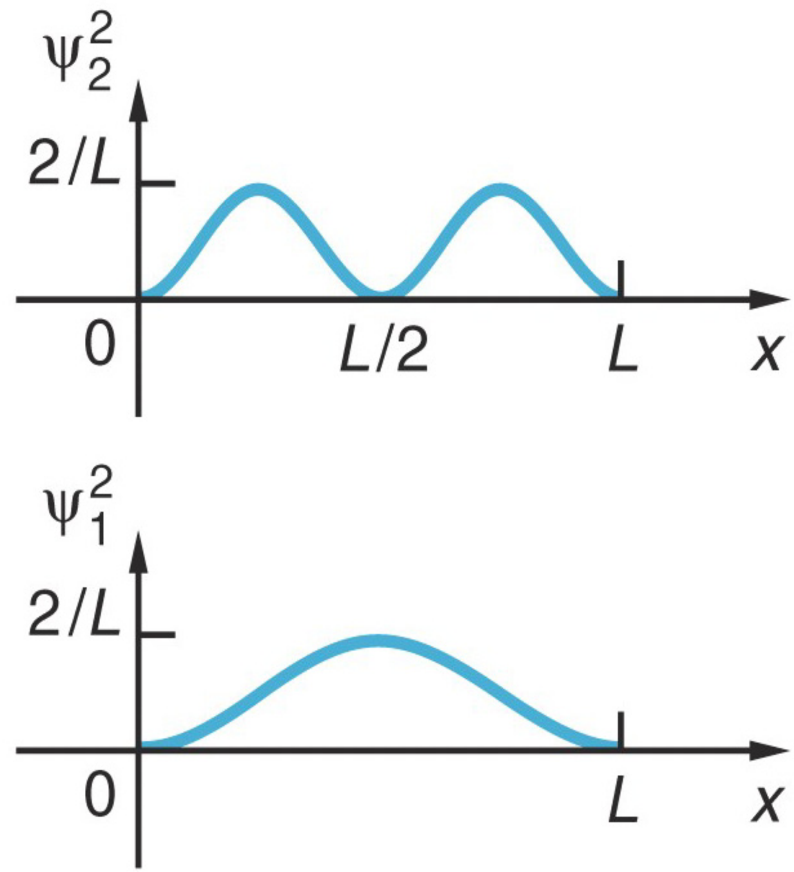
So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ ...What does this look like?

Wave Functions : Shapes Depend on Quantum # n



Where in The World is Carmen San Diego?

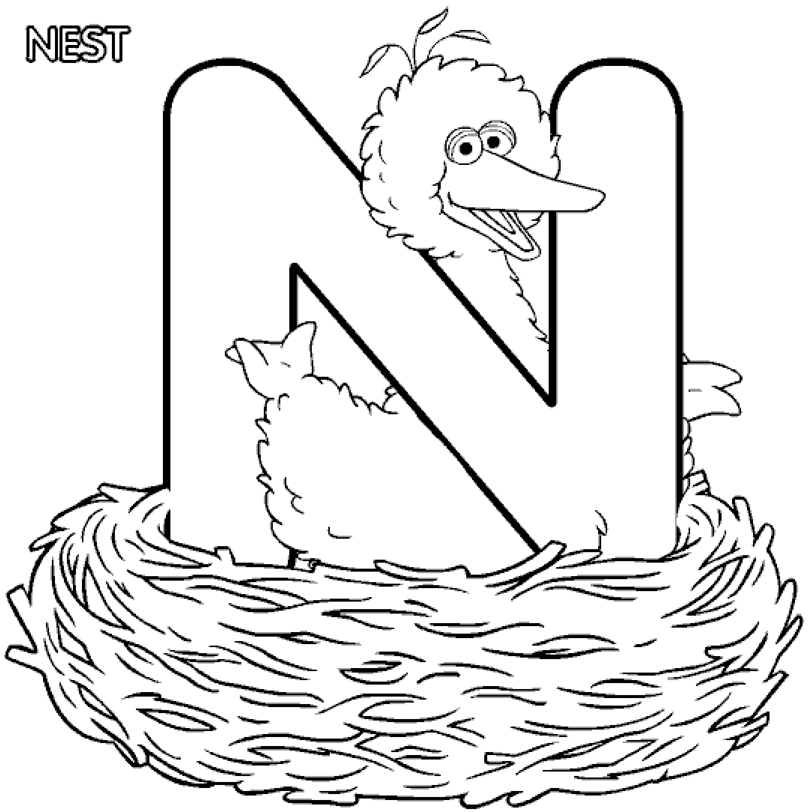
- We can only guess the probability of finding the particle somewhere in x
  - For n=1 (ground state) particle most likely at x = L/2
  - For n=2 (first excited state) particle most likely at L/4, 3L/4
    - Prob. Vanishes at x = L/2 & L
      - How does the particle get from just before x=L/2 to just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



Classically, where is 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 $P\left(\frac{L}{4} \le x \le \frac{3L}{4}\right)$?

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

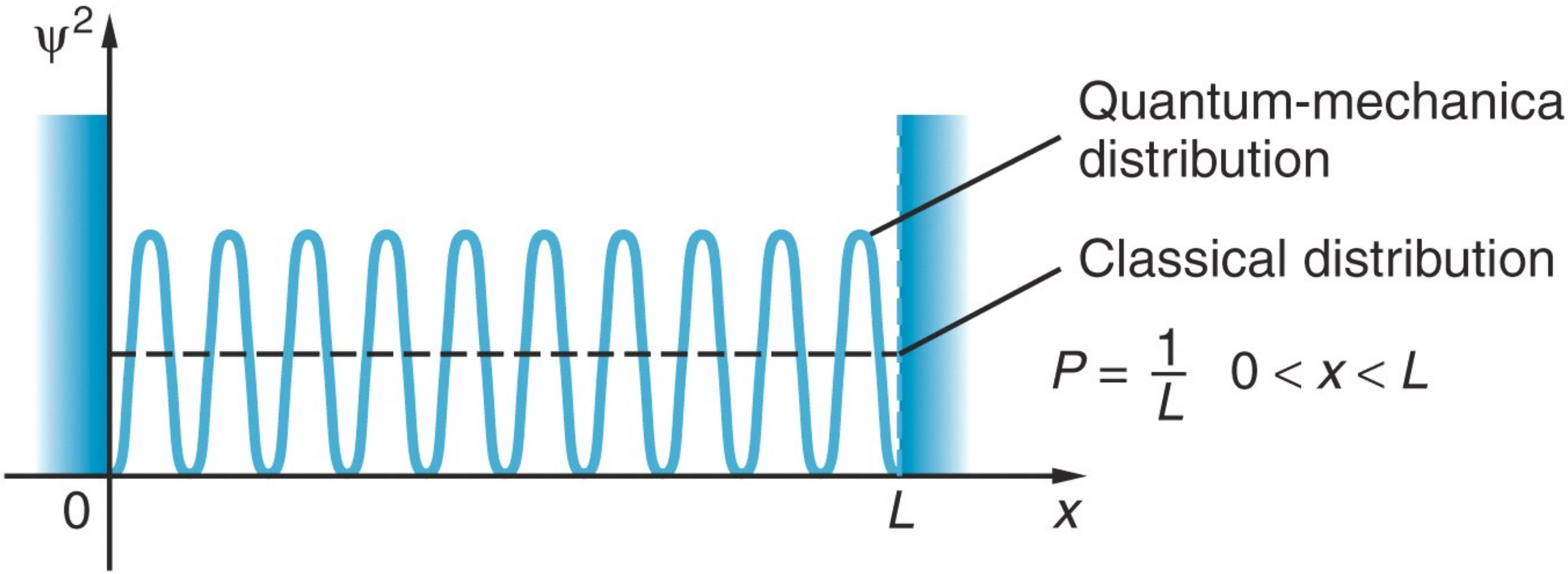
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin\frac{2\pi}{L}.\frac{3L}{4} - \sin\frac{2\pi}{L}.\frac{L}{4}\right)$$

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

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

$\Rightarrow$ Substantial difference between Classical & Quantum predictions

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



But one issue is irreconcilable:

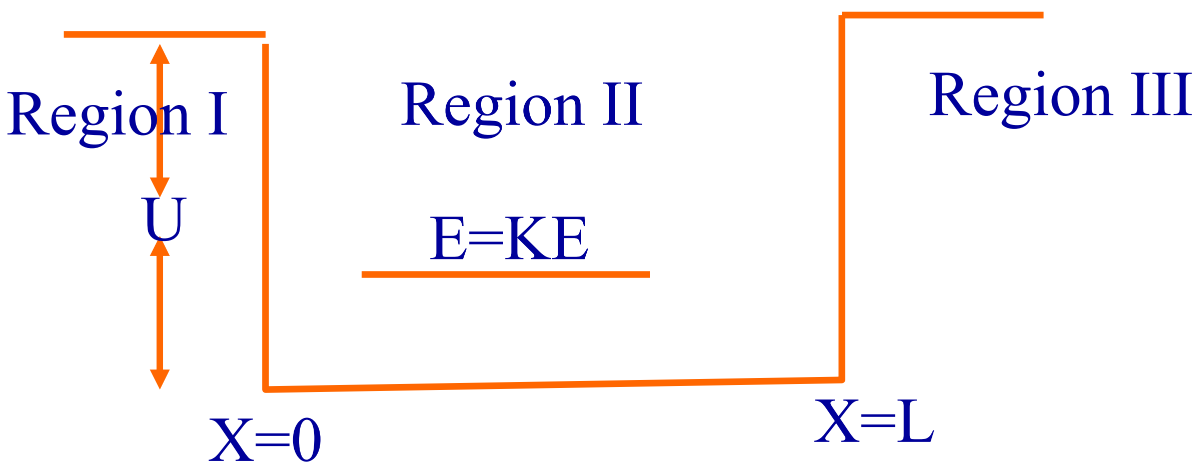
Quantum Mechanically the particle can not have $E = 0$

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 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

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

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

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

$\Rightarrow$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)

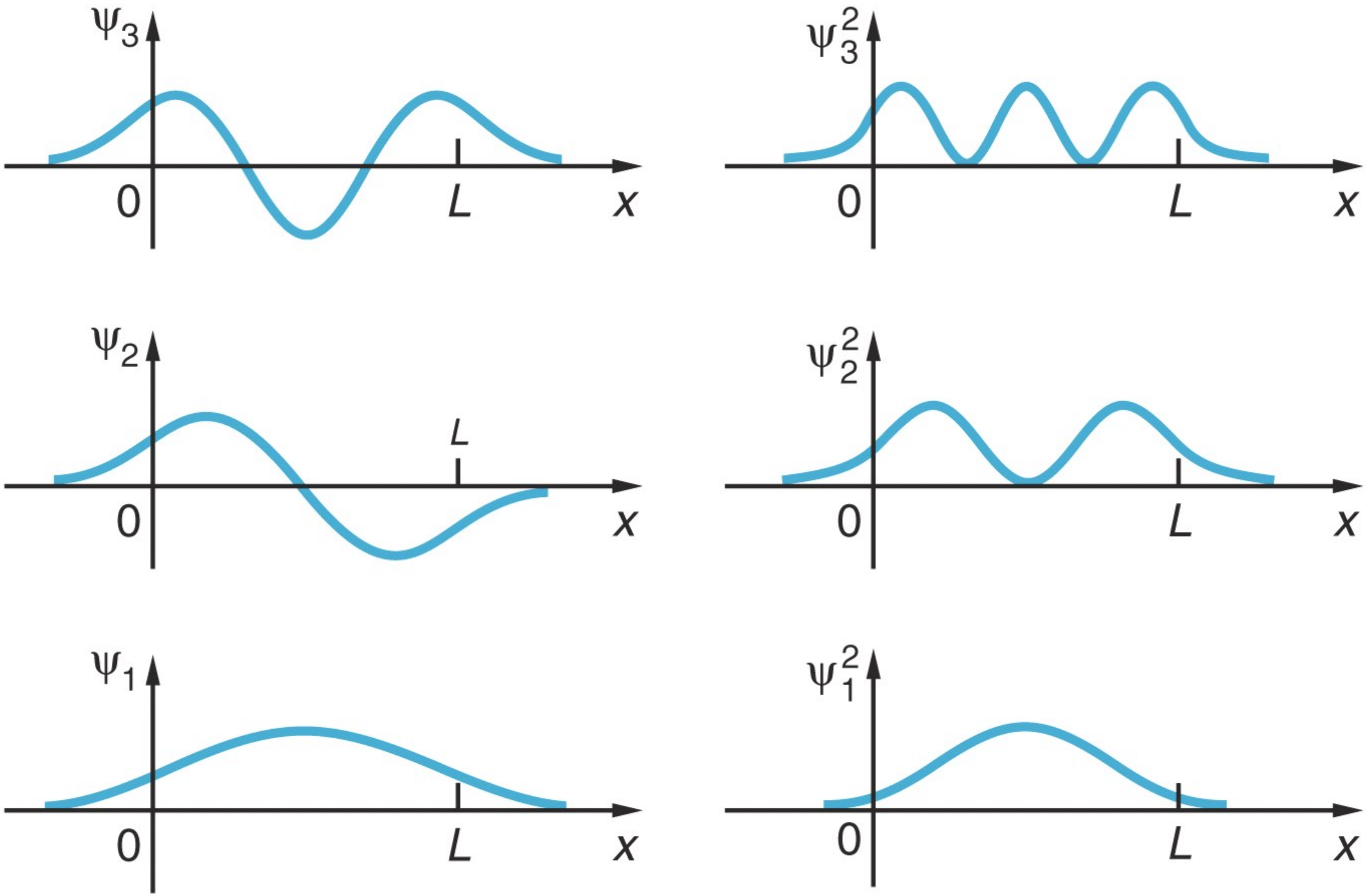
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

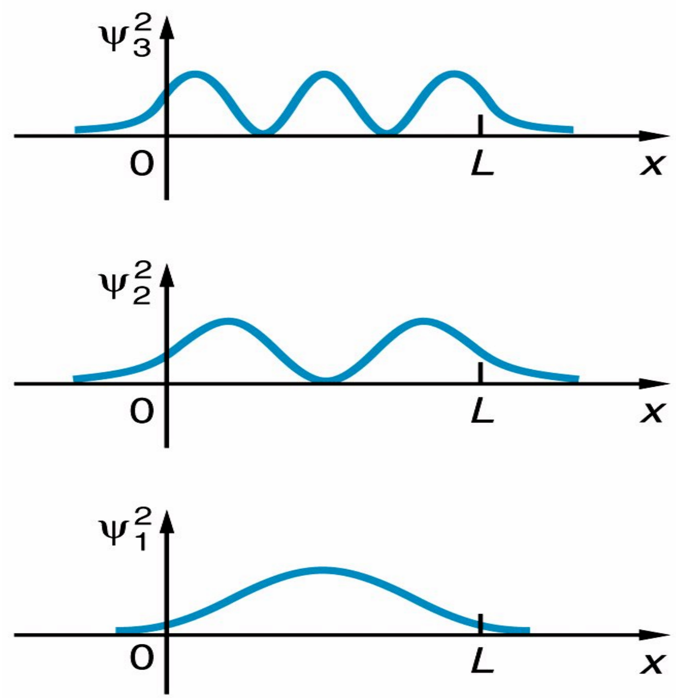
Further require Continuity of $\psi(x)$ and $\dfrac{d\psi(x)}{dx}$

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 $\Delta E = U\text{-}E + KE$

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)

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

If $U >> E \Rightarrow$ Tiny penetration

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

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 $U \to \infty \Rightarrow \delta \to 0$

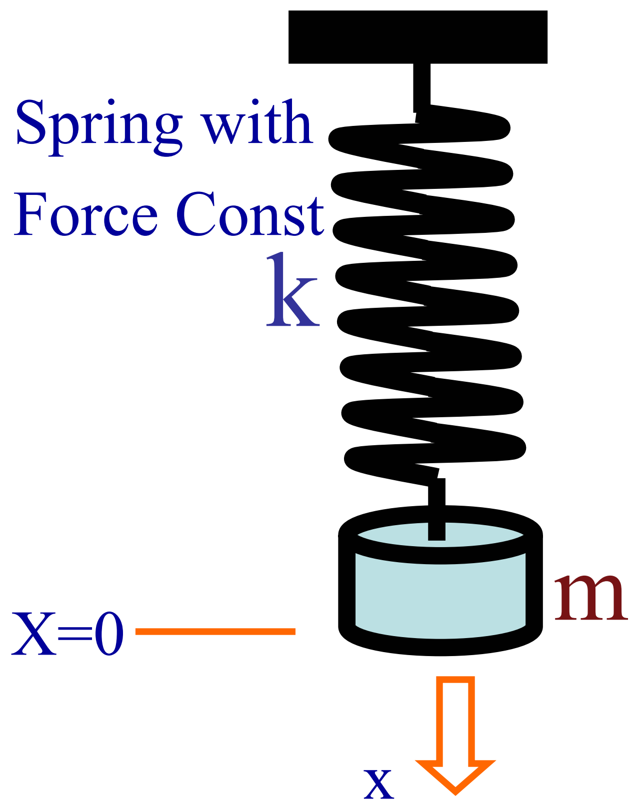
$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4...$$

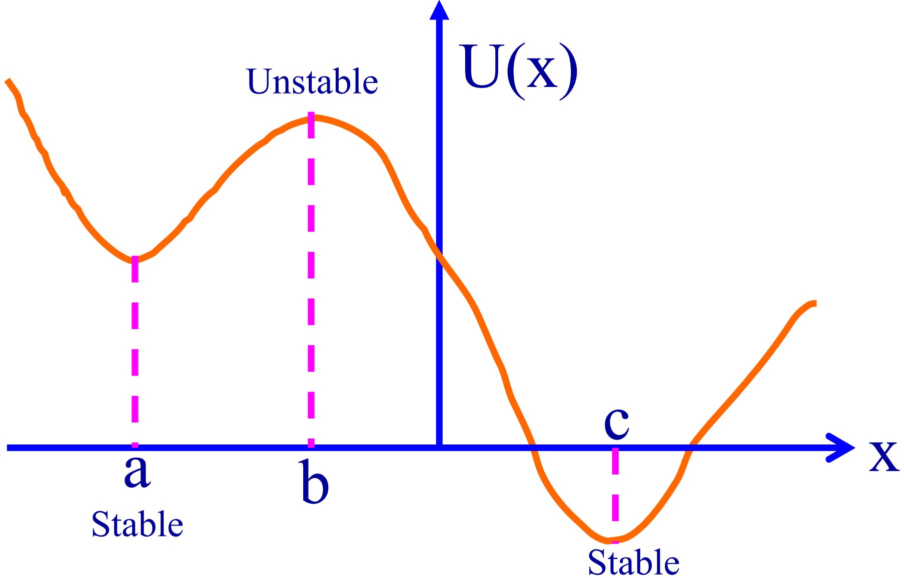
When E=U then solutions blow up

$\Rightarrow$ 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





Particle of mass m within a potential U(x)

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

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

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

look at the Curvature:

$\dfrac{\partial^2 U}{\partial x^2} > 0$ (stable), $\dfrac{\partial^2 U}{\partial x^2} < 0$ (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 equilibirium position, motion confined between x=0 & x=A

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

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

Quantum Picture: Harmonic Oscillator

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

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

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

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

Two guesses about the simplest Wavefunction:

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

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

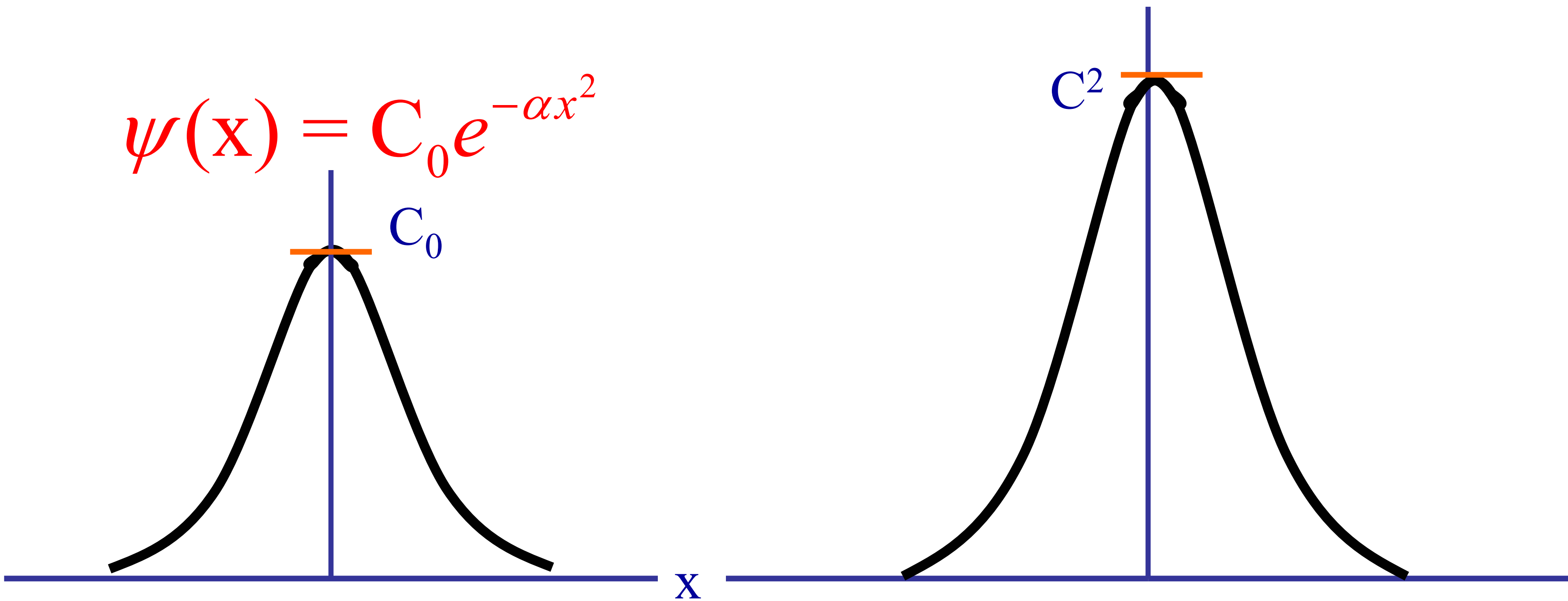
My guess: $\psi(\mathrm{x}) = \mathrm{C}_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

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

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



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