Physics 2D Lecture Slides
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Factorization Condition For Wave Function Leads to:

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

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

What is the Constant E ? How to Interpret it ?

Back to a Free particle :

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

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

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

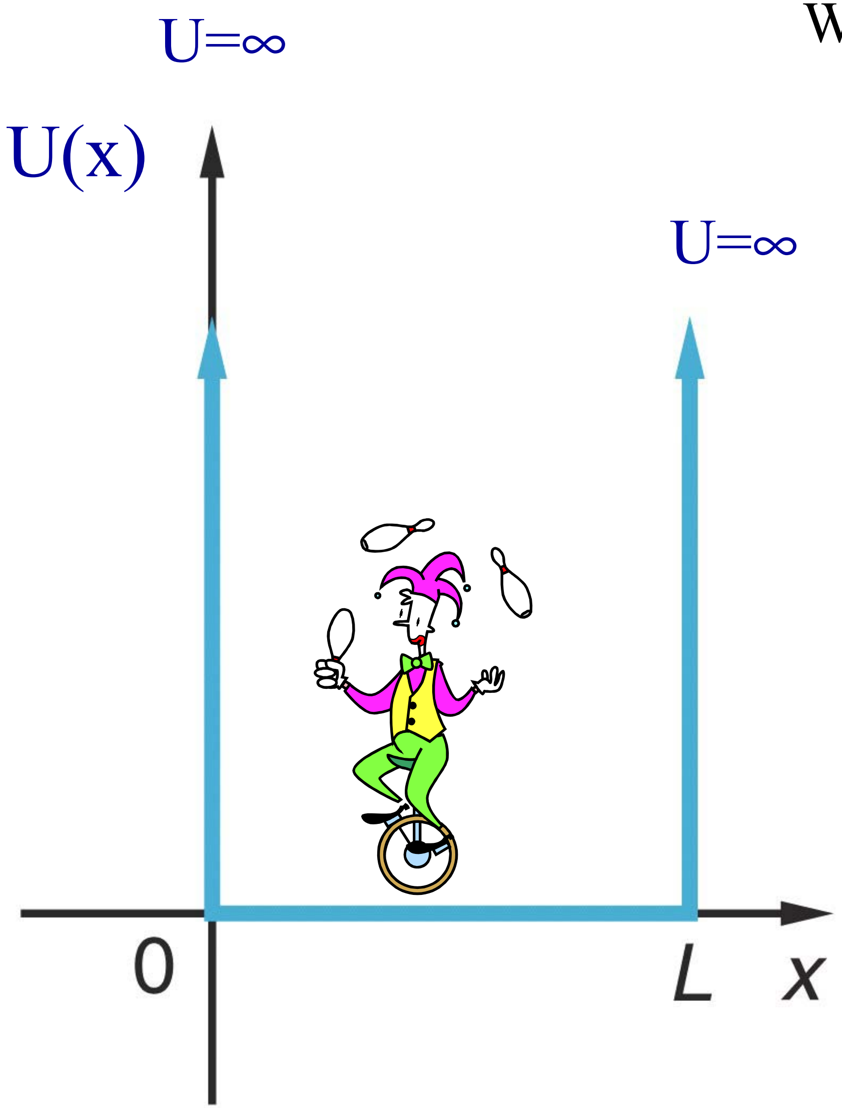
$$\frac{-\hbar^2}{2m}\frac{d^2(Ae^{(ikx)})}{dx^2}+0=E\ Ae^{(ikx)}\ \ \Rightarrow E=\frac{\hbar^2k^2}{2m}=\frac{p^2}{2m}=\text{(NR Energy)}$$

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

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

Probability is static in time t, character of wave function depends on $\psi(x)$

A More Interesting Potential : Particle In a Box (like an atom)



Write the Form of Potential: Infinite Wall

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

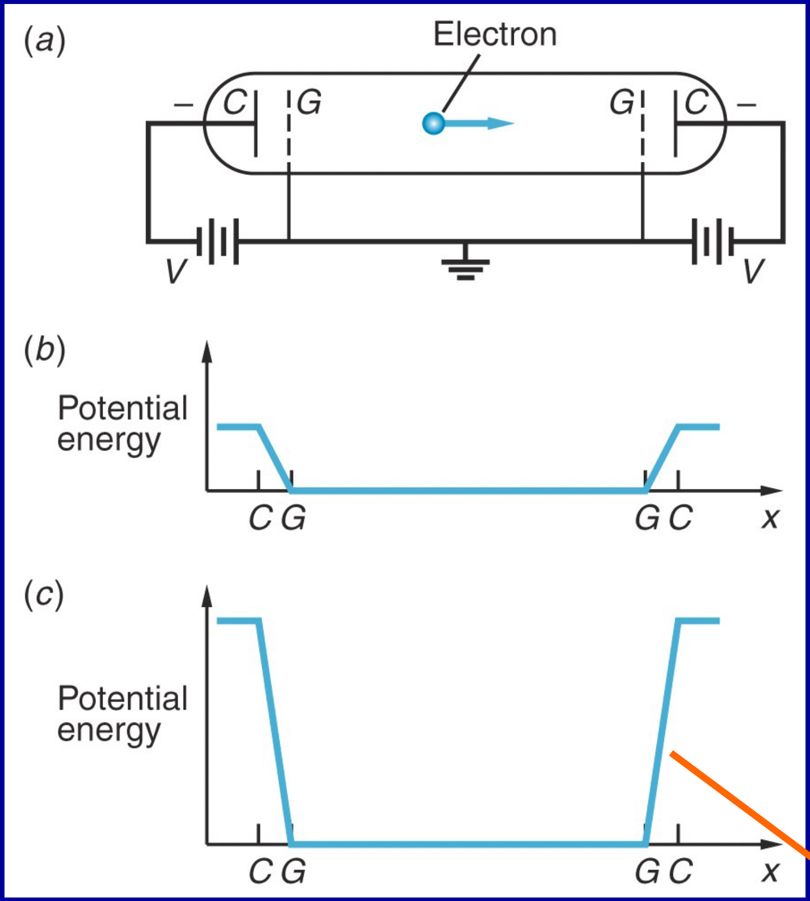
$U(x,t) = 0\ \ ;\ \ 0 > X > L$

Classical Picture:

- Particle dances back and forth
- Constant speed, const KE
- Average <P> = 0
- No restriction on energy value
  - $E = K + U = K + 0 = P^2/2m$
- 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



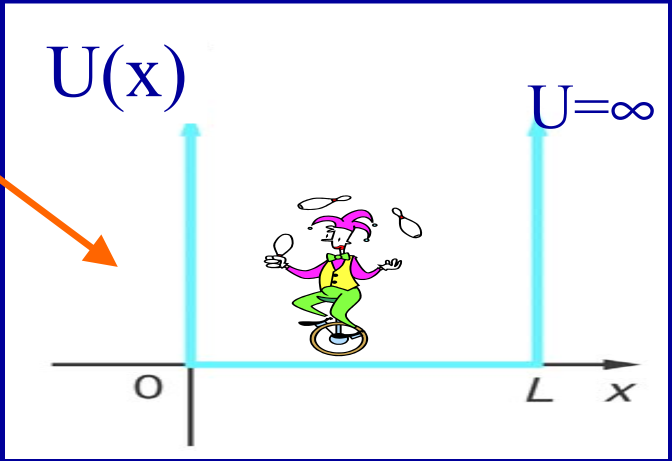
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

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→∞

(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)

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

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

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

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

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 ?

$\boxed{\text{Apply BOUNDARY Conditions on the Physical Wavefunction}}$

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

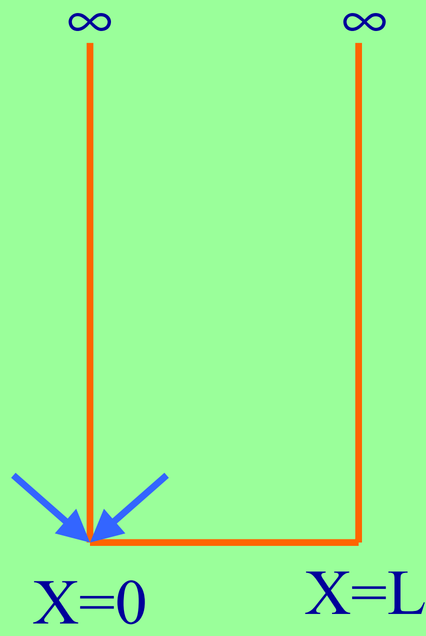
So match the wavefunction just outside box to the wavefunction value just inside the box

$\Rightarrow$ 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)

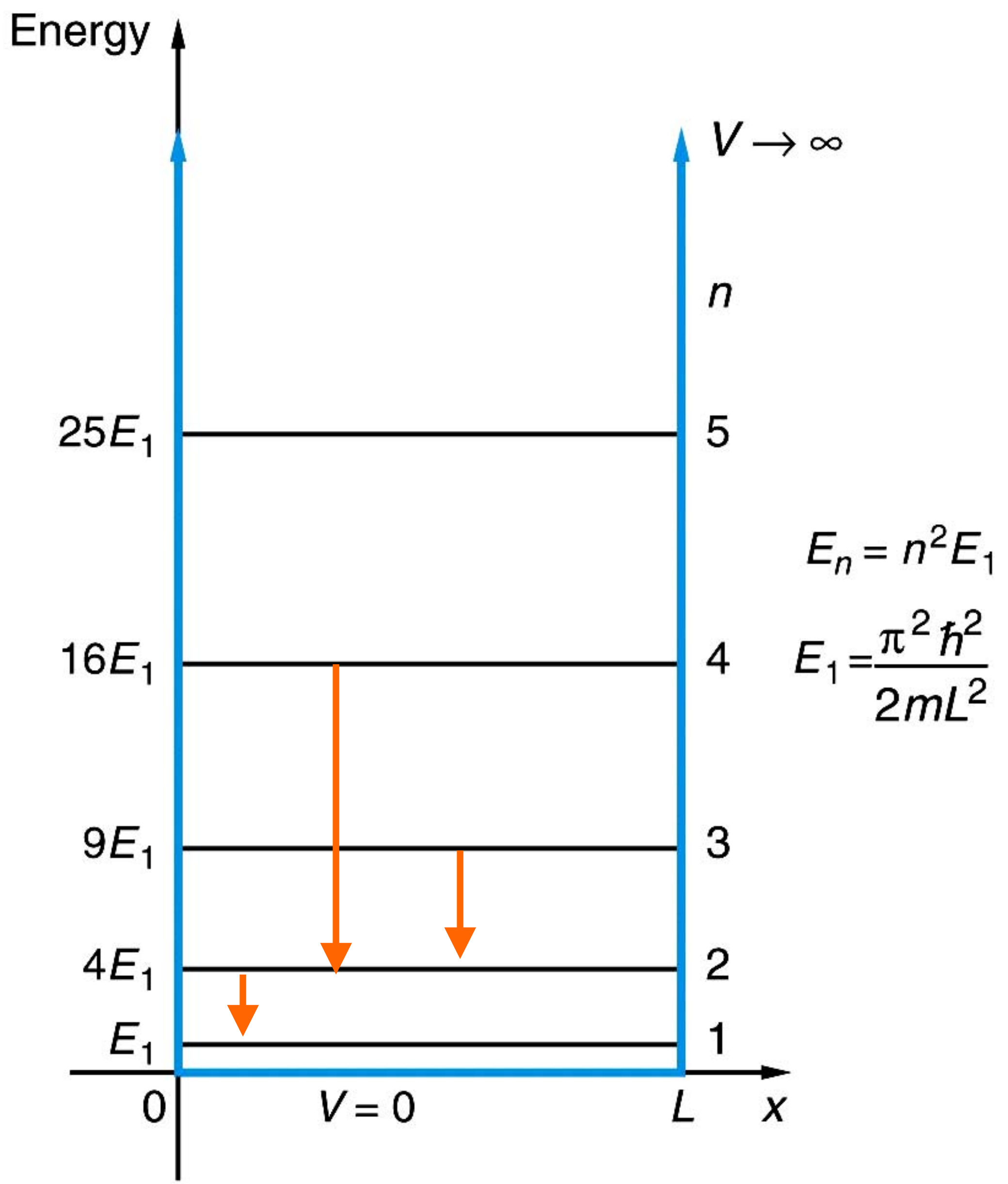
& $\psi(x=L) = 0 \Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

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



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

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?

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

Normalized Condition :

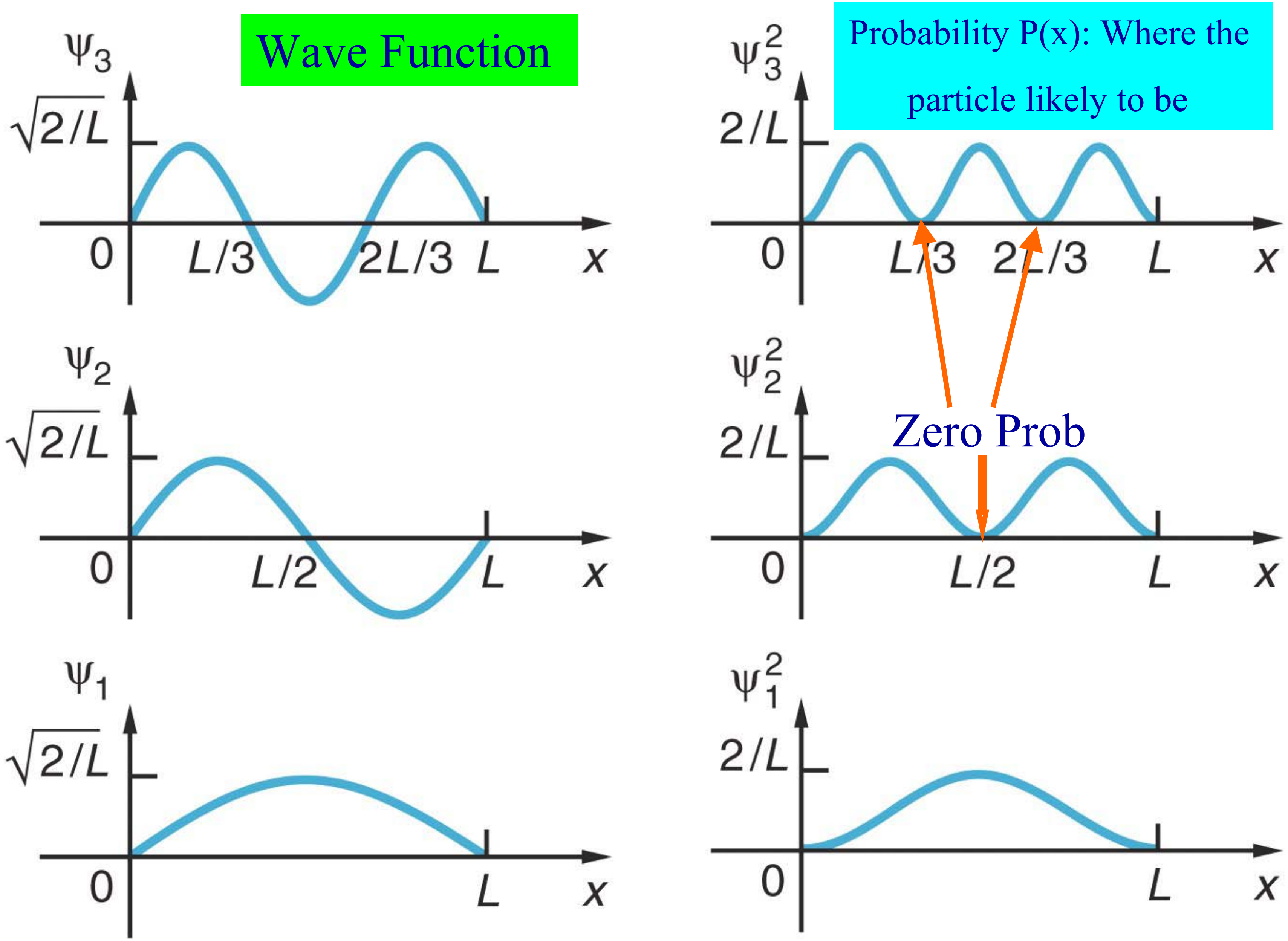
$$1 = \int_0^L \psi_n^* \psi_n dx = A^2 \int_0^L Sin^2(\frac{n\pi x}{L}) \qquad \boxed{\text{Use } 2\text{Sin}^2\theta = 1 - 2Cos2\theta}$$

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

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

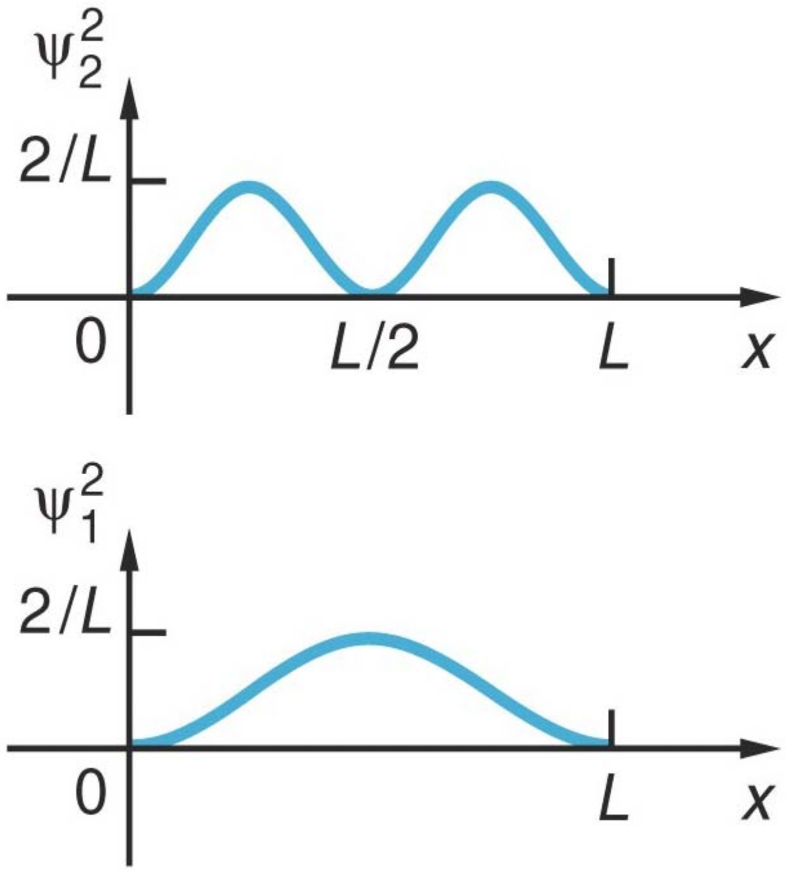
So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ ...What does this look like?

Wave Functions : Shapes Depend on Quantum # n



Where in The World is Carmen San Diego?

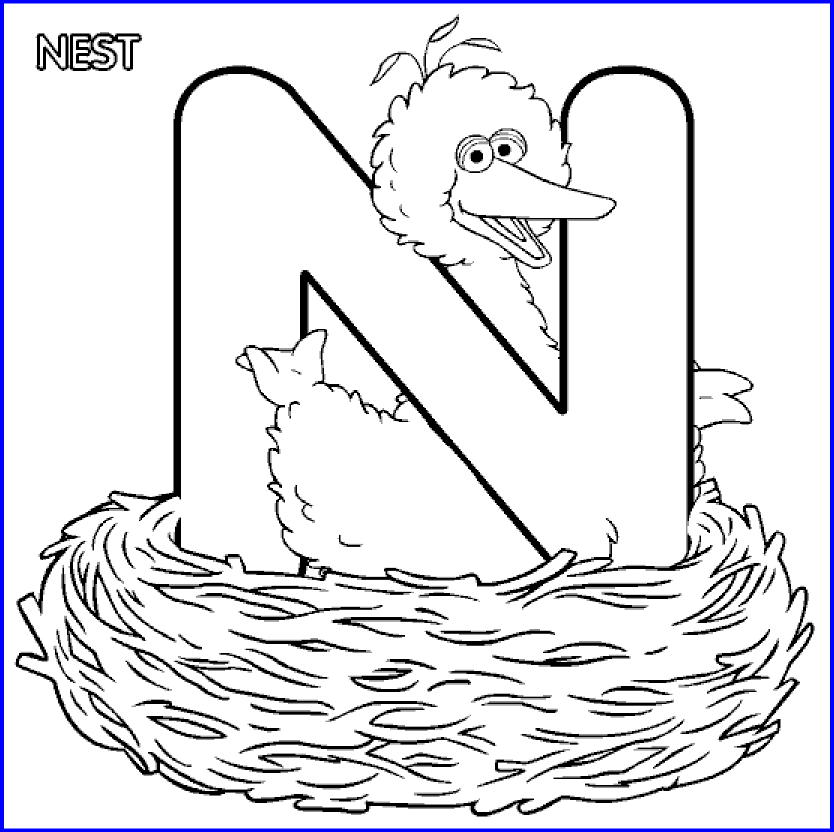
- We can only guess the probability of finding the particle somewhere in x
  - For n=1 (ground state) particle most likely at x = L/2
  - For n=2 (first excited state) particle most likely at L/4, 3L/4
    - Prob. Vanishes at x = L/2 & L
      - How does the particle get from just before x=L/2 to just 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

$\boxed{n}$

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

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

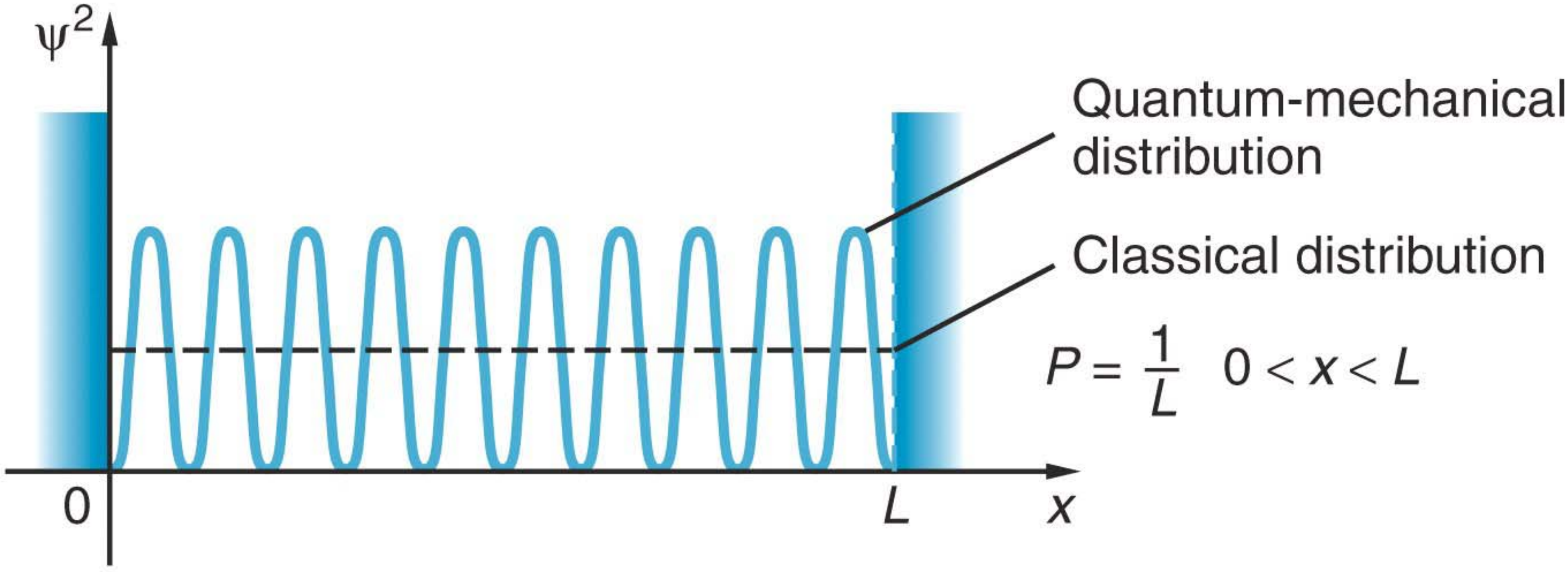
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi} \sin \frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin \frac{2\pi}{L} \cdot \frac{3L}{4} - \sin \frac{2\pi}{L} \cdot \frac{L}{4}\right)$$

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

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:

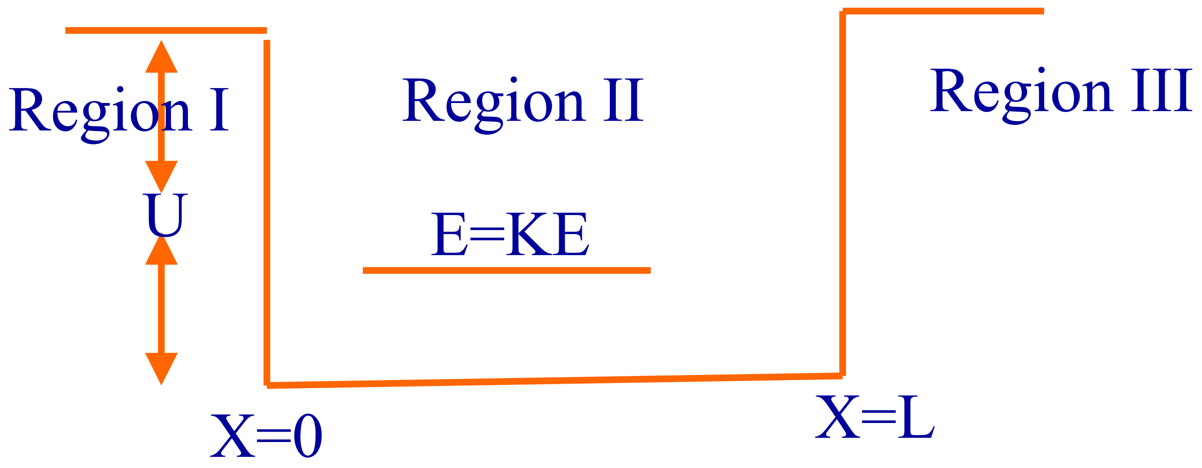
Quantum Mechanically the particle can not have E = 0

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

Schrodinger Eq :

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

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

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

$\Rightarrow$ 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)

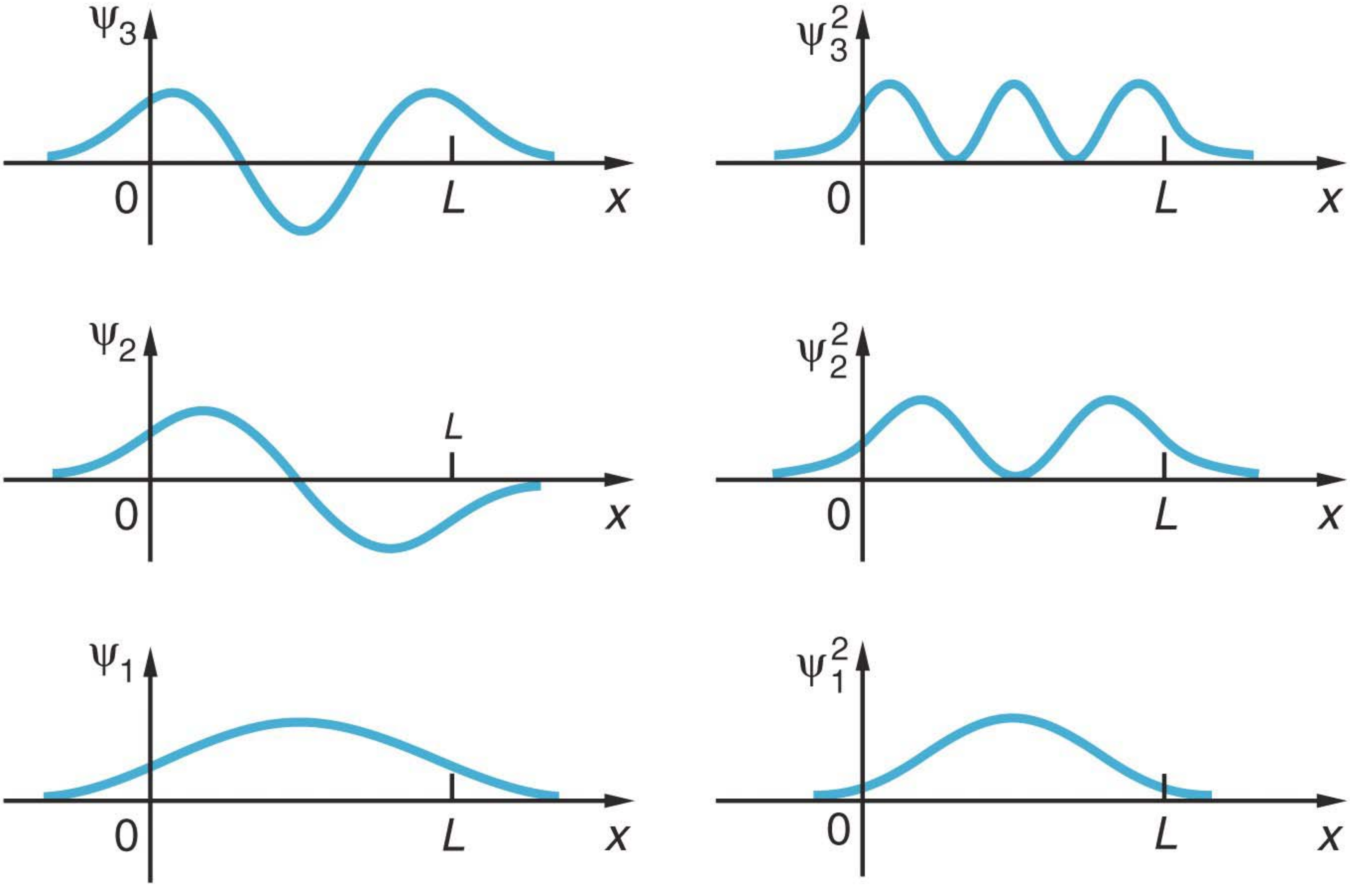
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

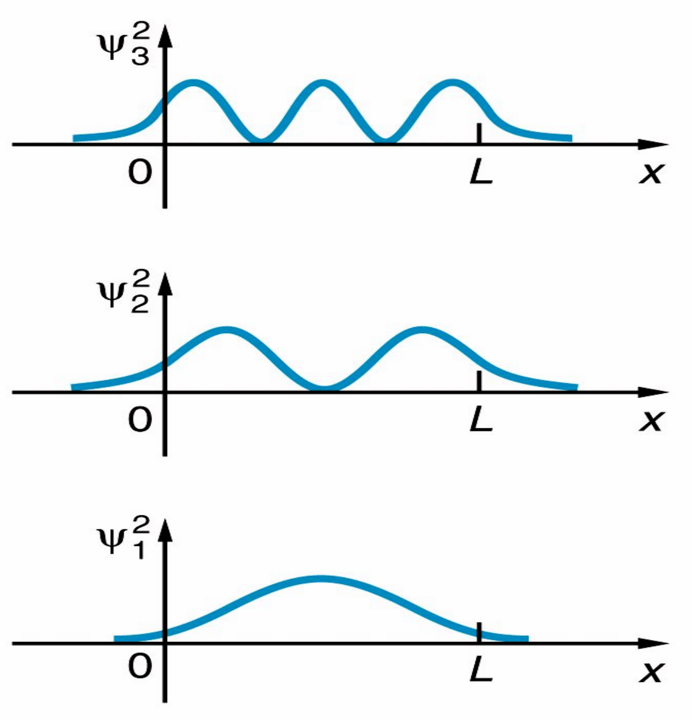
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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

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 $\rightarrow \infty \Rightarrow \delta \rightarrow 0$

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

If U>>E $\Rightarrow$ Tiny penetration

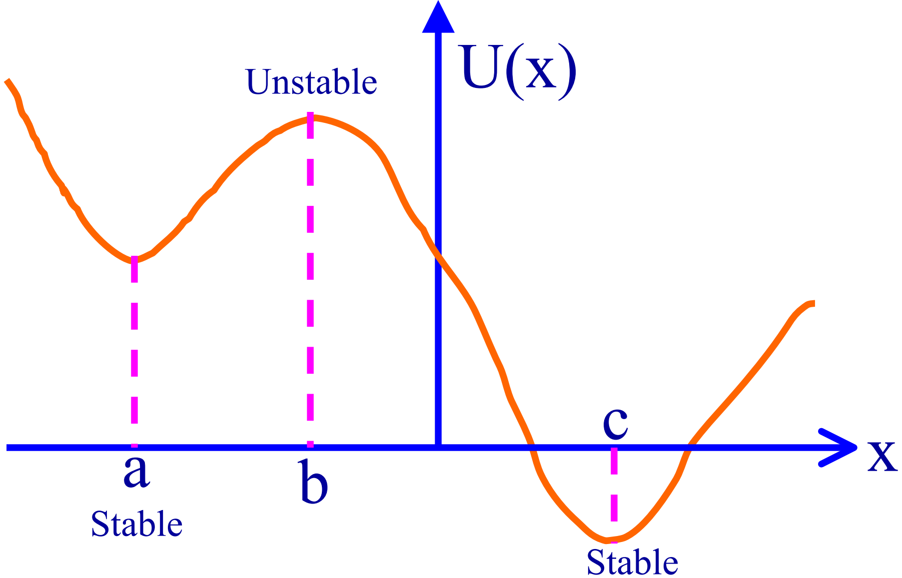
If U $\rightarrow \infty \Rightarrow \delta \rightarrow 0$

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

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"



Particle of mass m within a potential U(x)

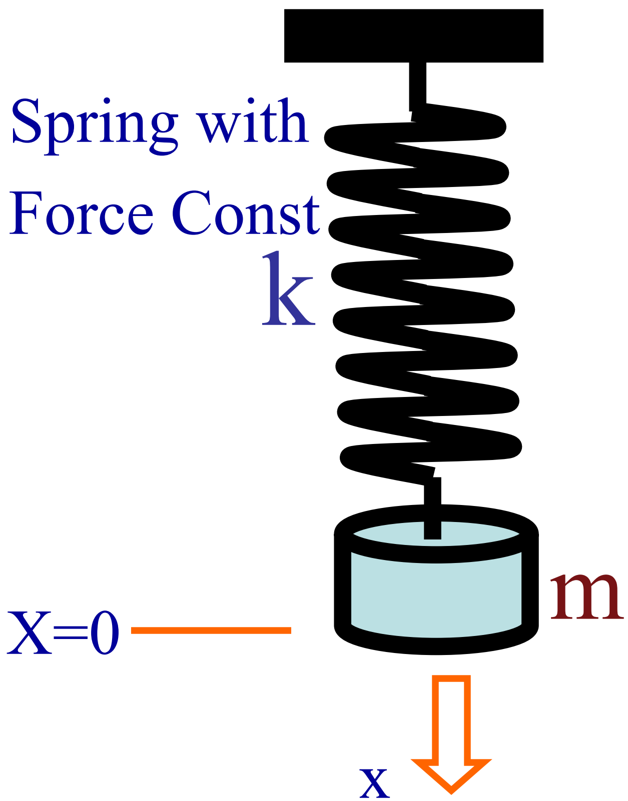
$$\vec{F}(x) = -\frac{dU(x)}{dx}$$

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

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

look at the Curvature:

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



Stable Equilibrium: General Form :

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

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

$\boxed{\text{Motion of a Classical Oscillator (ideal)}}$

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= $\pm$ A

Quantum Picture: Harmonic Oscillator

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

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

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

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

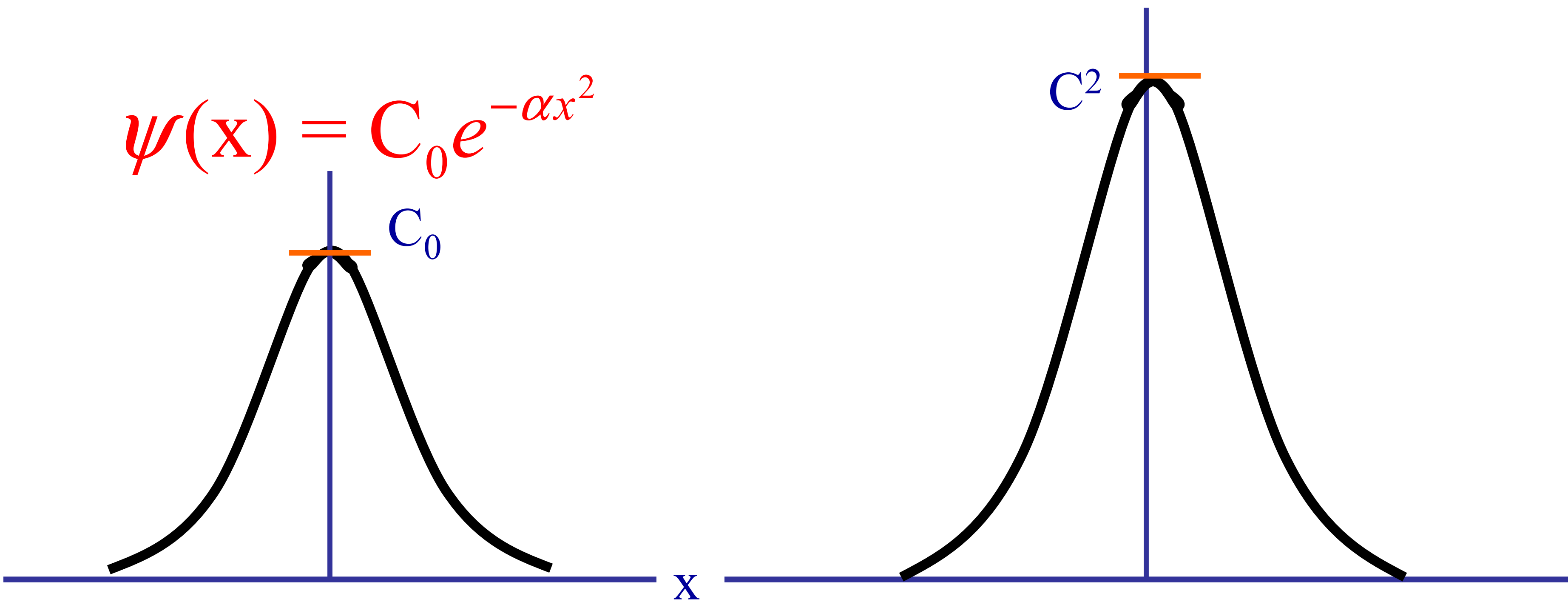
My guess: $\psi(\mathrm{x}) = \mathrm{C}_0 e^{-\alpha x^2}$; Need to find C_0 & α:

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

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

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



How to Get C_0 & α ?? …Try plugging in the Wavefunction into Time-Independent Schr. Eqn.