Physics 2D Lecture Slides
Lecture 21: Feb 16th 2005

Vivek Sharma
UCSD Physics

Normalization Condition: Particle Must be Somewhere

Example: $\psi(x,0) = Ce^{-\left|\frac{x}{x_0}\right|}$, C & x_0 are constants

This is a symmetric wavefunction with diminishing amplitude

The Amplitude is maximum at x =0 $\Rightarrow$ Probability is max too

Normalization Condition: How to figure out C ?

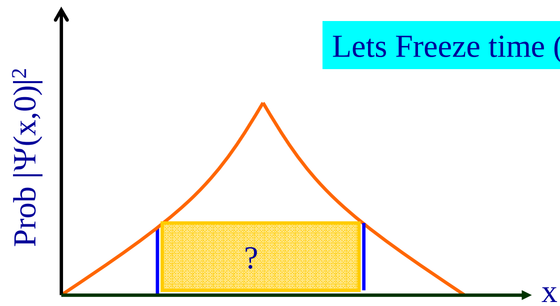
A real particle must be somewhere: Probability of finding

particle is finite $P(-\infty \leq x \leq +\infty) = \int_{-\infty}^{+\infty} |\psi(x,0)|^2 dx = \int_{-\infty}^{+\infty} C^2 e^{-2\left|\frac{x}{x_0}\right|} dx = 1$

$$\Rightarrow 1 = 2C^2 \int_0^\infty e^{-2\left|\frac{x}{x_0}\right|} dx = 2C^2 \left[\frac{x_0}{2}\right] = C^2 x_0$$

$$\Rightarrow \boxed{\psi(x,0) = \frac{1}{\sqrt{x_0}} e^{-\left|\frac{x}{x_0}\right|}}$$

Where is the particle within a certain location x ± Δx



$$P(-x_0 \le x \le +x_0) = \int_{-x_0}^{+x_0} |\psi(x,0)|^2 dx = \int_{-x_0}^{+x_0} C^2 e^{-2\left|\frac{x}{x_0}\right|} dx$$

$$= 2C^2\left[\frac{x_0}{2}\right]\left[1-e^{-2}\right] = \left[1-e^{-2}\right] = 0.865 \Rightarrow 87\%$$

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
  - $F(x) = -\dfrac{\partial U(x)}{\partial x}$

Schrodinger had an interesting life

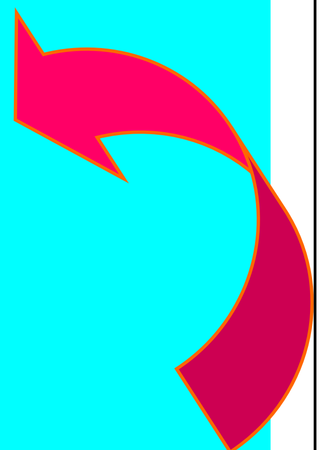
Schrodinger Wave Equation

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

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

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

$$\psi(x,0) \;\to\; \overrightarrow{\text{Force}}\,(\text{potential}) \;\to\; \psi(x,t)$$



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 seperation of variables to get :

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

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

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

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:

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

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

What is the Constant E ? How to Interpret it ?

Back to a Free particle :

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

$U(x,t)=0$

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

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

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

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

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

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

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

Schrodinger Eqn: Stationary State Form

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

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

and integrate both sides w.r.t. time

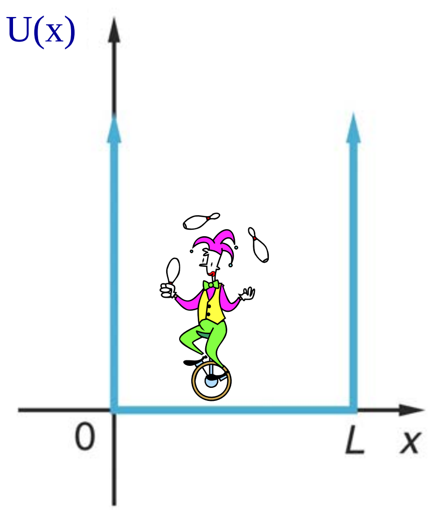
$$\int_{\mathrm{t}=0}^{t=t}\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial \mathrm{t}}dt = \int_0^t -\frac{iE}{\hbar}dt \Rightarrow \int_0^t \frac{1}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{dt}}dt = -\frac{iE}{\hbar}$$

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

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

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

A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

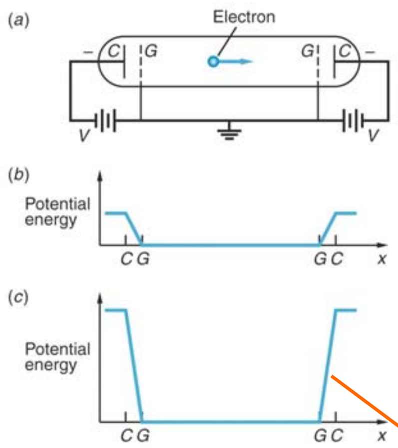
$U(x,t) = \infty$; $x \le 0$, $x \ge L$

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

- Classical Picture:
  - •Particle dances back and forth
  - •Constant speed, const KE
  - •Average <P> = 0
  - •No restriction on energy value
    - • E=K+U = K+0
  - •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



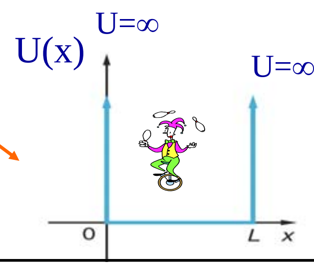
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

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)

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

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

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

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)

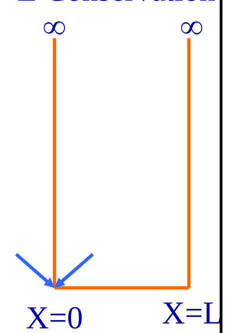
& $\psi(x=L) = 0 \Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

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

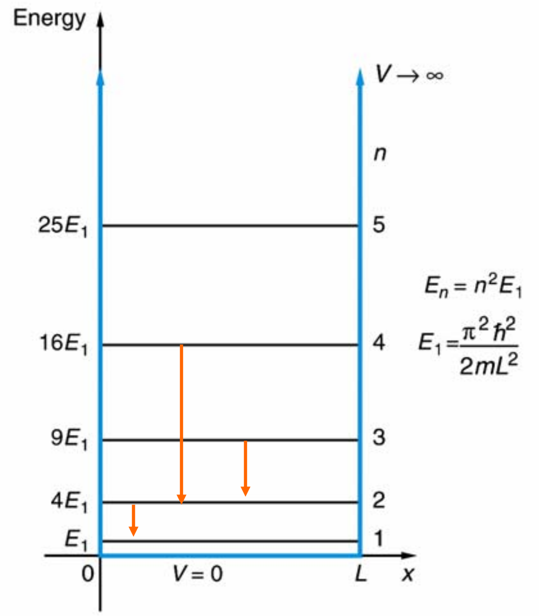
So what does this say about Energy E ? : $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ Quantized (not Continuous)!

Why can't the particle exist Outside the box ?

→ E Conservation



Quantized Energy levels of Particle in a Box



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 :

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

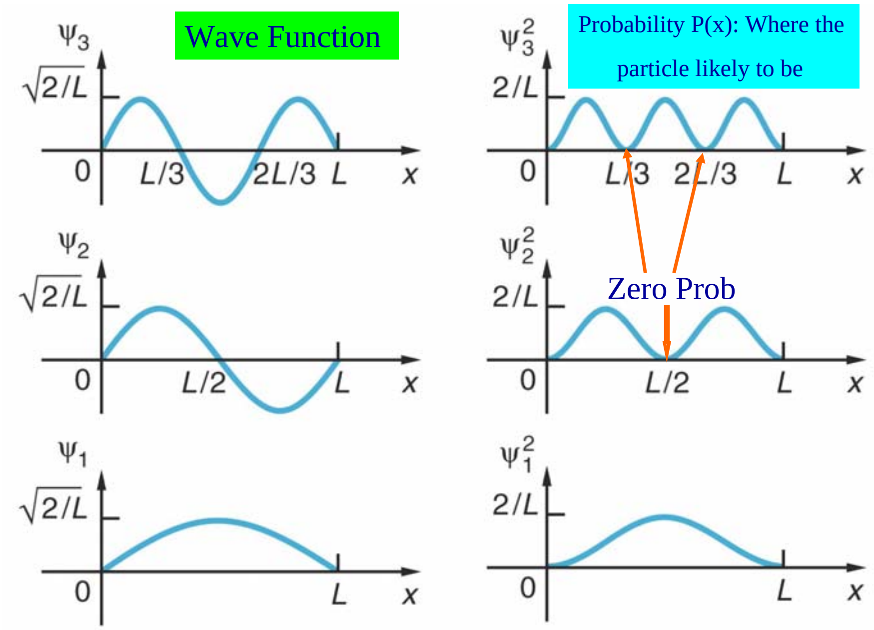
Use $2\text{Sin}^2\theta = 1 - 2Cos2\theta$

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

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

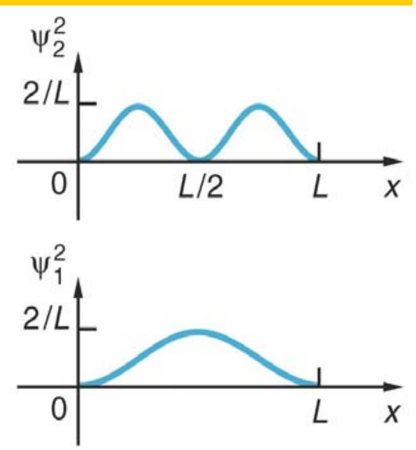
So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ ...What does this look like?

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

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

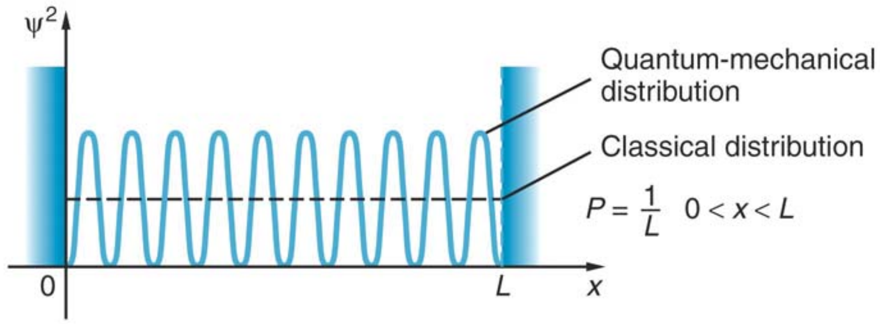
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin\frac{2\pi}{L}.\frac{3L}{4} - \sin\frac{2\pi}{L}.\frac{L}{4}\right)$$

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

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:

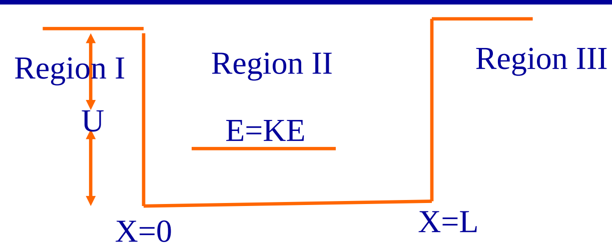
Quantum Mechanically the particle can not have E = 0

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)

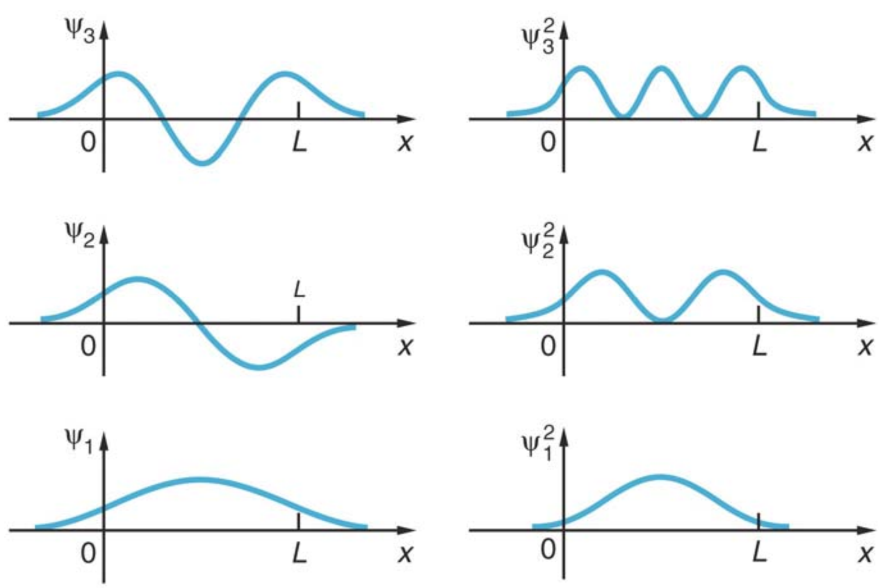
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

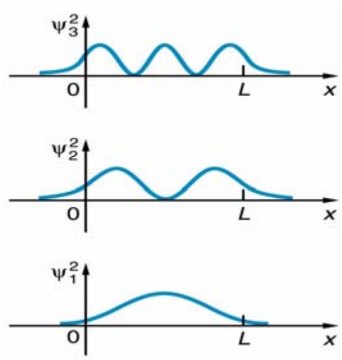
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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)

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

If U>>E $\Rightarrow$ Tiny penetration

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

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If U>>E $\Rightarrow$ Tiny penetration

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

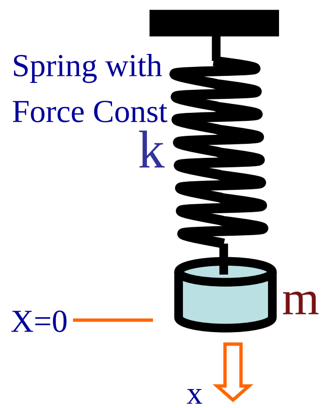
$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4...$$

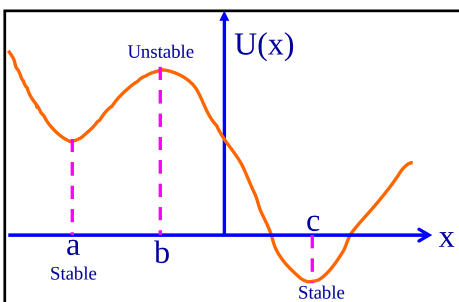
When E=U then solutions blow up

$\Rightarrow$ 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





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 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 $A \rightarrow 0$, $E \rightarrow 0$

Max. KE at x = 0, KE= 0 at x= ± 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: $\frac{-\hbar^2}{2m}\frac{\partial^2 \psi(x)}{\partial^2 x} + \frac{1}{2} m\omega^2 x^2 \psi(x) = E\ \psi(x)$

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

Two guesses about the simplest Wavefunction:

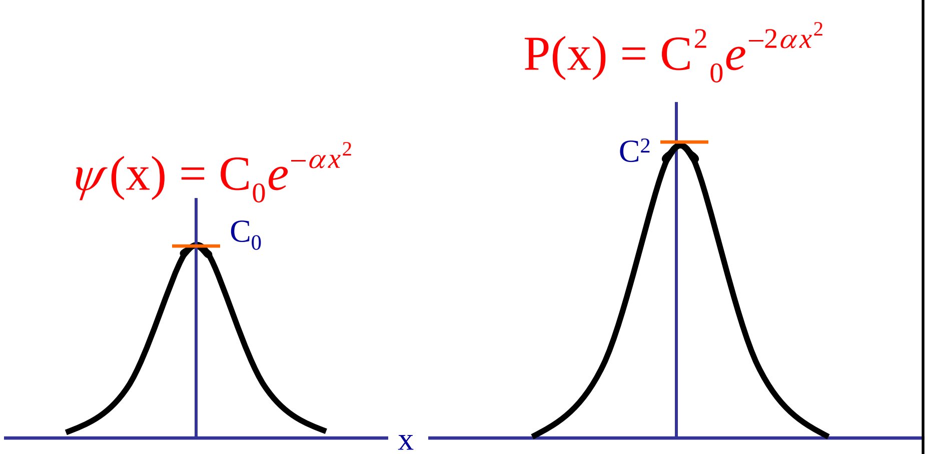
1. $\psi(x)$ should be symmetric about x 2. $\psi(x) \to 0$ as $x \to \infty$

+ $\psi(x)$ 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



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