

# *4E : The Quantum Universe*



Lecture 12, April 19

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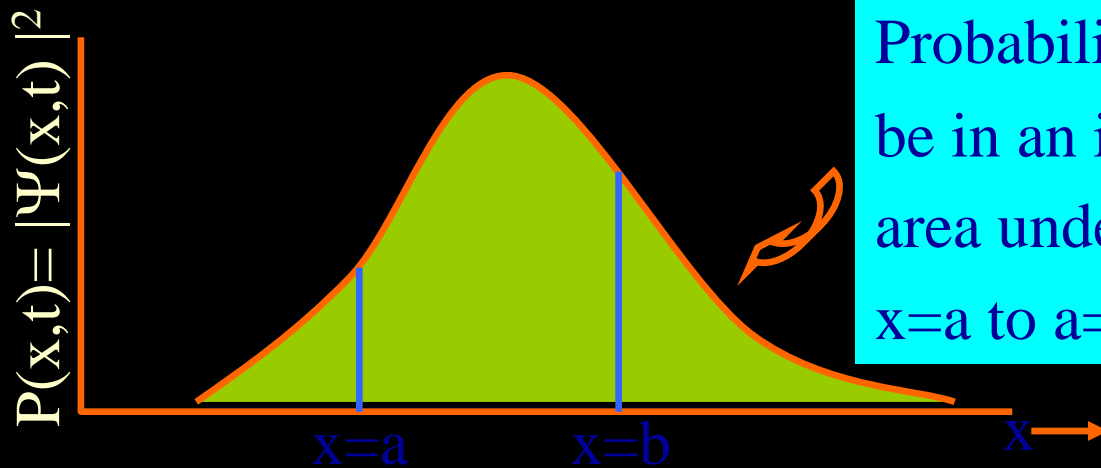
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## *Quantum Mechanics of Subatomic Particles*



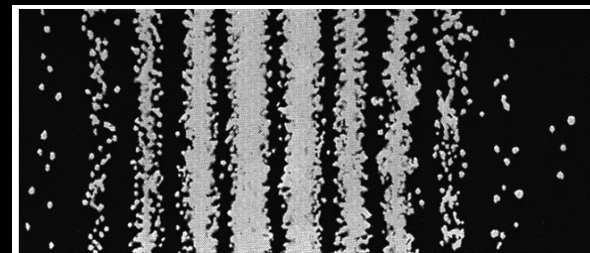
- Act of Observation destroys the system (No watching!)
- If can't watch then all conversations can only be in terms of Probability P
- Every particle under the influence of a force is described by a Complex wave function  $\Psi(x,y,z,t)$
- $\Psi$  is the ultimate DNA of particle: contains all info about the particle under the force (in a potential e.g Hydrogen )
- Probability of per unit volume of finding the particle at some point  $(x,y,z)$  and time  $t$  is given by
  - $P(x,y,z,t) = \Psi(x,y,z,t) \cdot \Psi^*(x,y,z,t) = |\Psi(x,y,z,t)|^2$
- When there are more than one path to reach a final location then the probability of the event is
  - $\Psi = \Psi_1 + \Psi_2$
  - $P = |\Psi^* \Psi| = |\Psi_1|^2 + |\Psi_2|^2 + 2 |\Psi_1| |\Psi_2| \cos\phi$

## Wave Function of "Stuff" & Probability Density



Probability of a particle to be in an interval  $a \leq x \leq b$  is area under the curve from  $x=a$  to  $x=b$

- Although not possible to specify with certainty the location of particle, its possible to assign probability  $P(x)dx$  of finding particle between  $x$  and  $x+dx$
- $P(x) dx = |\Psi(x,t)|^2 dx$
- E.g intensity distribution in light diffraction pattern is a measure of the probability that a photon will strike a given point within the pattern



# $\Psi$ : The Wave function Of A Particle

- The particle must be some where

$$\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = 1$$

- Any  $\Psi$  satisfying this condition is NORMALIZED
- Prob of finding particle in finite interval

$$P(a \leq x \leq b) = \int_a^b \psi^*(x,t) \psi(x,t) dx$$

- Fundamental aim of Quantum Mechanics
  - Given the wavefunction at some instant (say  $t=0$ ) find  $\Psi$  at some subsequent time  $t$
  - $\Psi(x,t=0) \rightarrow \Psi(x,t)$  ...evolution
  - Think of a probabilistic view of particle's "newtonian trajectory"
    - We are replacing Newton's 2<sup>nd</sup> law for subatomic systems

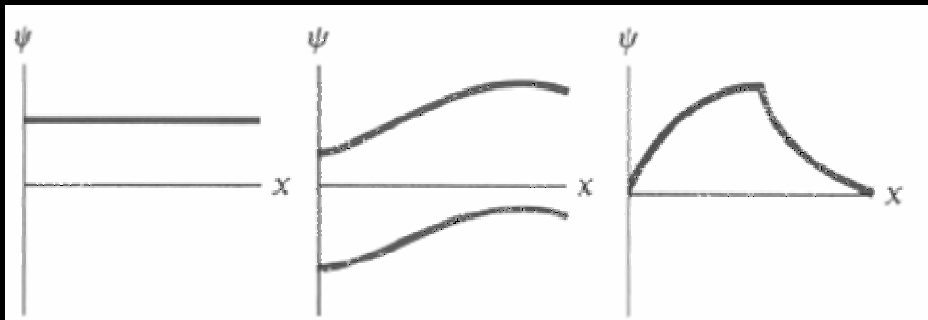
The Wave Function is a mathematical function that describes a physical object  $\rightarrow$  Wave function must have some rigorous properties :

- $\Psi$  must be finite
- $\Psi$  must be continuous fn of  $x,t$
- $\Psi$  must be single-valued
- $\Psi$  must be smooth fn  $\rightarrow$

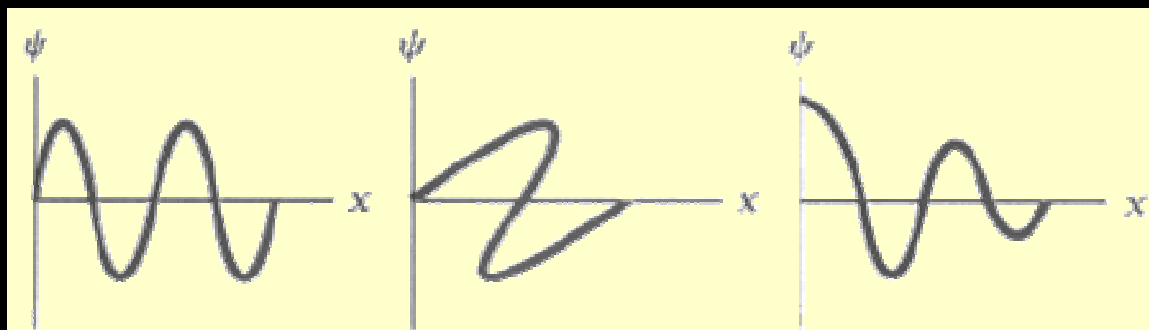
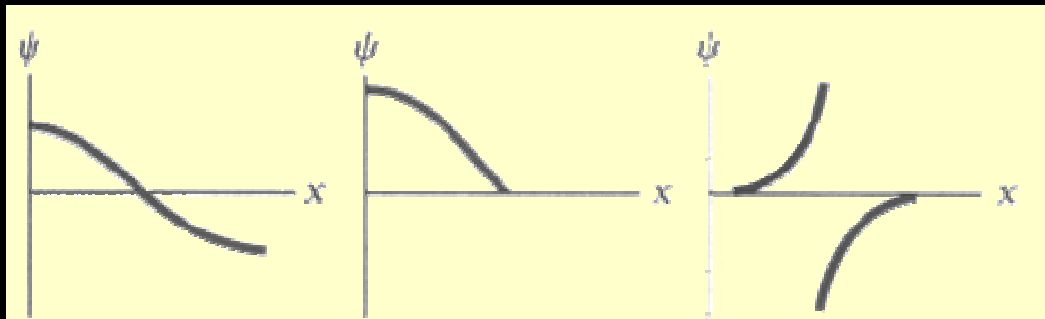
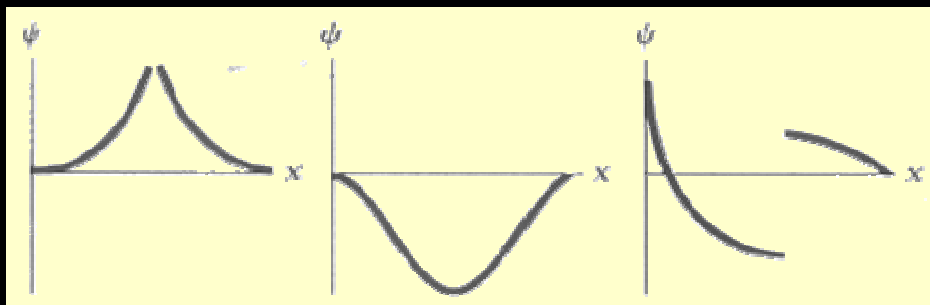
$$\frac{d\psi}{dx} \text{ must be continuous}$$

# WHY ?

# Bad Wave Functions Of Physical Systems : You Decide Why



?



## A Simple Wave Function : Free Particle

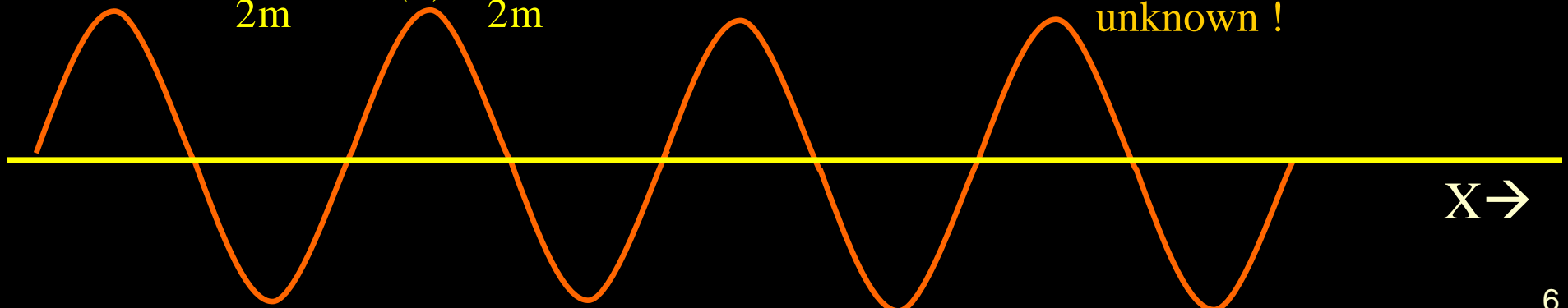
- Imagine a free particle of mass  $m$  , momentum  $p$  and  $K=p^2/2m$
- Under no force , no attractive or repulsive potential to influence it
- Particle is where it wants : can be any where  $[-\infty \leq x \leq +\infty]$ 
  - Has No relationship, no mortgage , no quiz, no final exam...its essentially a **bum** !
  - how to describe a **quantum mechanical bum** ?
    - $\Psi(x,t)= Ae^{i(kx-\omega t)} = A(\text{Cos}(kx-\omega t)+ i \sin (kx-\omega t))$

$$k = \frac{p}{\hbar}; \quad \omega = \frac{E}{\hbar}$$

For non-relativistic particles

$$E = \frac{p^2}{2m} \Rightarrow \omega(k) = \frac{\hbar k^2}{2m}$$

Has definite momentum  
and energy but location  
unknown !



# Wave Function of Different Kind of Free Particle : Wave Packet

Sum of Plane Waves:

$$\Psi(x,0) = \int_{-\infty}^{+\infty} a(k)e^{ikx} dk$$

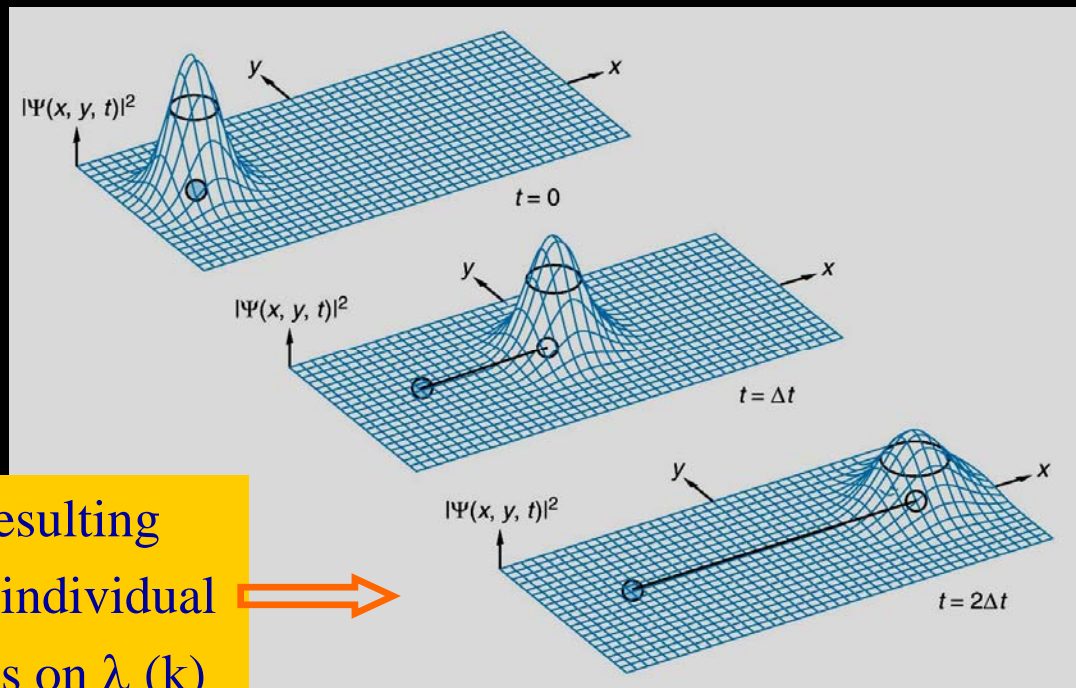
$$\Psi(x,t) = \int_{-\infty}^{+\infty} a(k)e^{i(kx-\omega t)} dk$$

Wave Packet initially localized in  $\Delta X$ ,  $\Delta t$  undergoes dispersion

The more you know now,  
The less you will know later  
Why ?

Spreading is due to DISPERSION resulting from the fact that phase velocity of individual waves making up the packet depends on  $\lambda$  (k)

Combine many free waves to create a localized wave packet (group)



## Normalization Condition: Particle Must be Somewhere

Example:  $\psi(x,0) = Ce^{-\frac{|x|}{x_0}}$ , 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 ?**

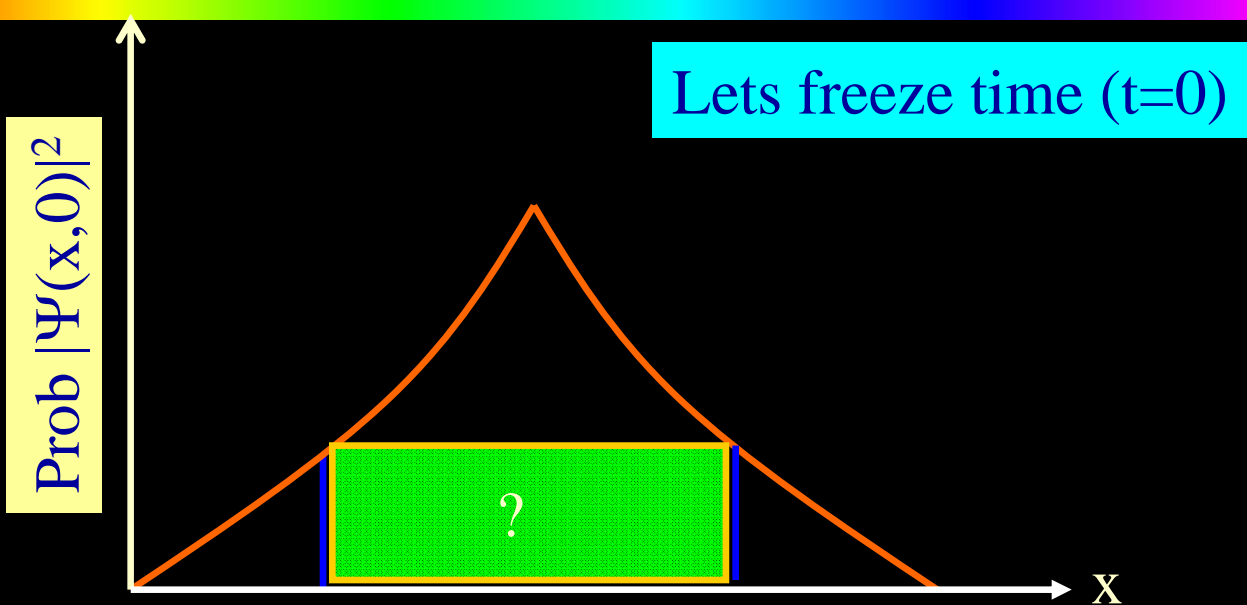
A real particle must be somewhere: Probability of finding particle is finite

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

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

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

# Probability of finding particle within a certain location $x \pm \Delta x$



$$P(-x_0 \leq x \leq +x_0) = \int_{-x_0}^{+x_0} |\psi(x, 0)|^2 dx = \int_{-x_0}^{+x_0} C^2 e^{-2\left|\frac{x}{x_0}\right|} dx$$
$$= 2C^2 \left[ \frac{x_0}{2} \right] [1 - e^{-2}] = [1 - e^{-2}] = 0.865 \Rightarrow 87\%$$

## 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  $U(x) \rightarrow$  particle under certain force

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

Schrodinger had an interesting life



# *Introducing the Schrodinger Equation*

Consider for simplicity just a one-dimensional system

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

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

# Schrodinger Equation in 1, 2, 3 dimensional systems

## 1-dimension

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

## 2-dimension

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

## 3-dimension

$$-\frac{\hbar^2}{2m} \left[ \frac{\partial^2 \Psi(x,y,z,t)}{\partial x^2} + \frac{\partial^2 \Psi(x,y,z,t)}{\partial y^2} + \frac{\partial^2 \Psi(x,y,z,t)}{\partial z^2} \right] + U(x,y,z)\Psi(x,y,z,t) = i\hbar \frac{\partial \Psi(x,y,z,t)}{\partial t}$$

# Schrodinger Wave Equation in Quantum Mechanics

Wavefunction  $\psi$  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 S. 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 :

$\Rightarrow \text{RHS} = \text{LHS} = \text{Constant} = E$

## 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

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

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

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

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

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

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

and integrate both sides w.r.t. time

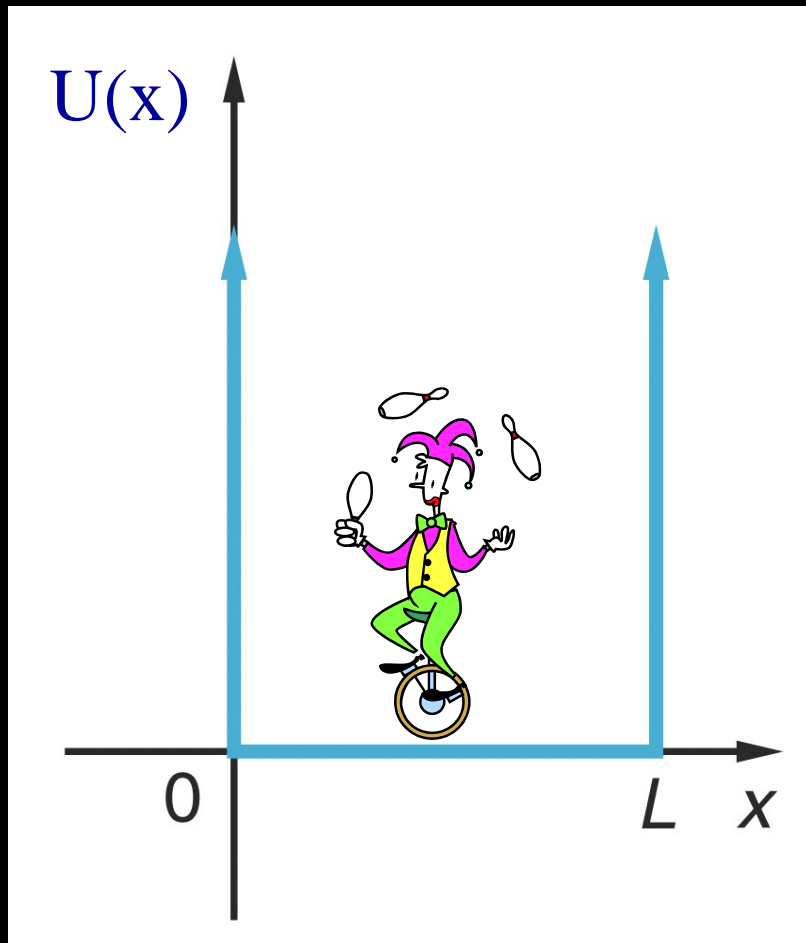
$$\int_{t=0}^{t=t} \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} dt = \int_0^t -\frac{iE}{\hbar} dt \Rightarrow \int_0^t \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} dt = -\frac{iE}{\hbar}$$

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

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

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

## A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

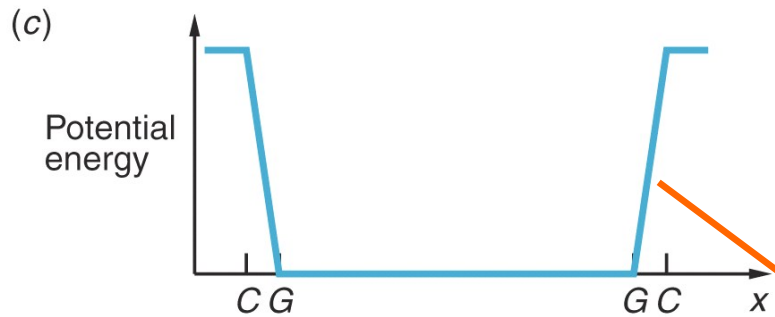
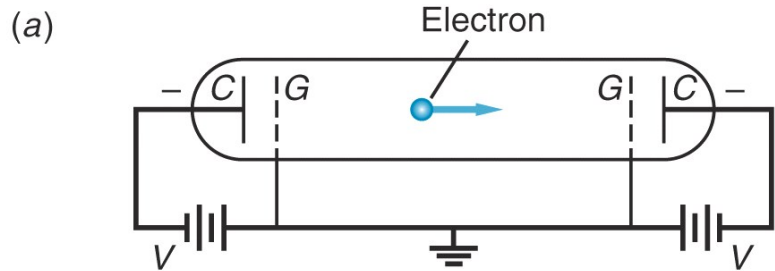
$$U(x,t) = \infty; \quad x \leq 0, \quad x \geq L$$

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

- 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



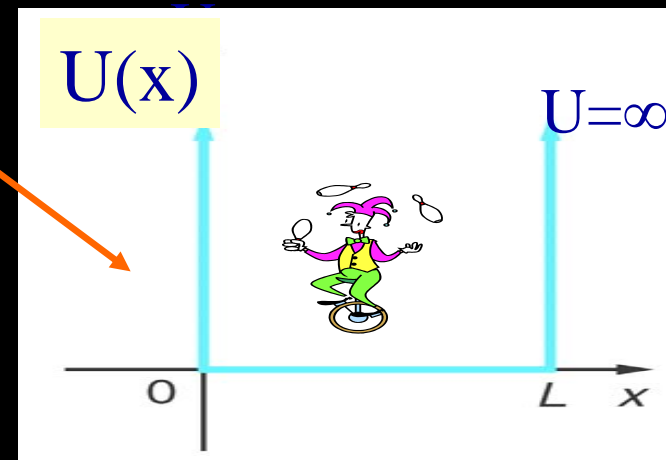
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

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"

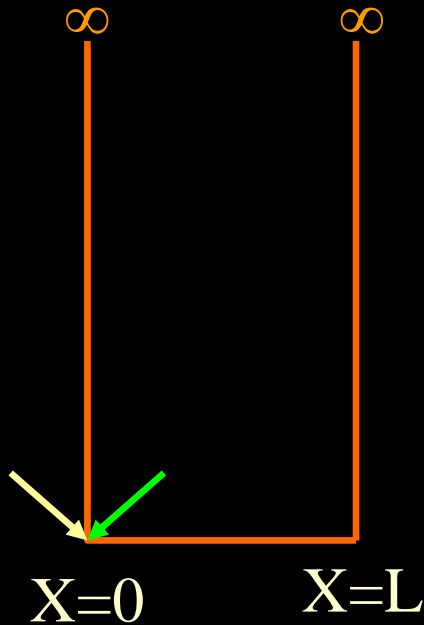
(c) If V is large, the "walls" become very high & steep becoming infinitely high for  $V \rightarrow \infty$

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



# $\Psi(x)$ for Particle Inside 1D Box with Infinite Potential Walls

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



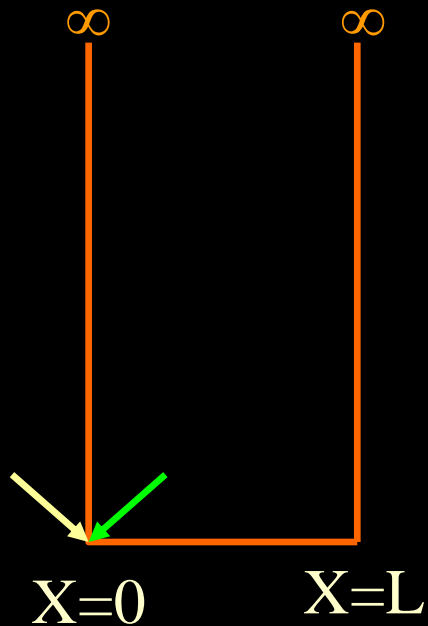
Inside the box, no force  $\Rightarrow U=0$  or constant (same thing)

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

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

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

## $\Psi(x)$ for Particle Inside 1D Box with Infinite Potential Walls



Need to figure out values of A, B : How to do that ?

Apply BOUNDARY Conditions on the Wavefunction

Since  $\psi(x)$  must be continuous everywhere

$\Rightarrow$  match the wavefunction just outside box with 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  $x = L$ )

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

So what does this say about Energy E ? :  $E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$

Quantized (not Continuous)!



## What About the Wave Function Normalization ?

The particle's Energy and Wavefunction are determined by a number **n**

We will call **n** → Quantum Number , just like in Bohr's Hydrogen atom

What about the wave functions corresponding to each of these energy states?

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

Normalized Condition :

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

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

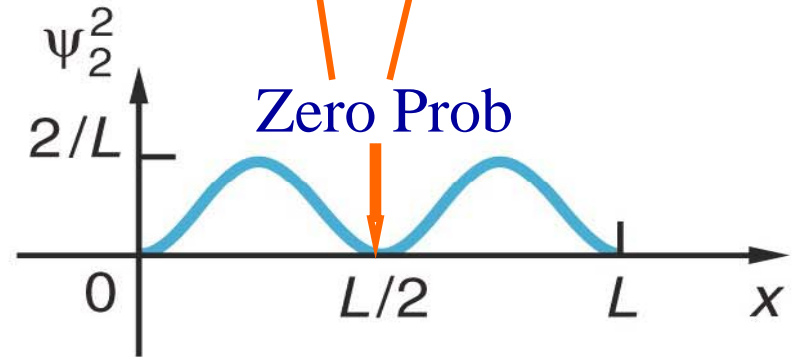
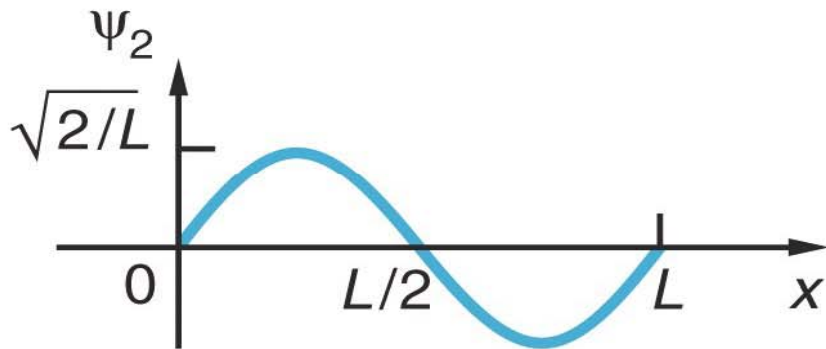
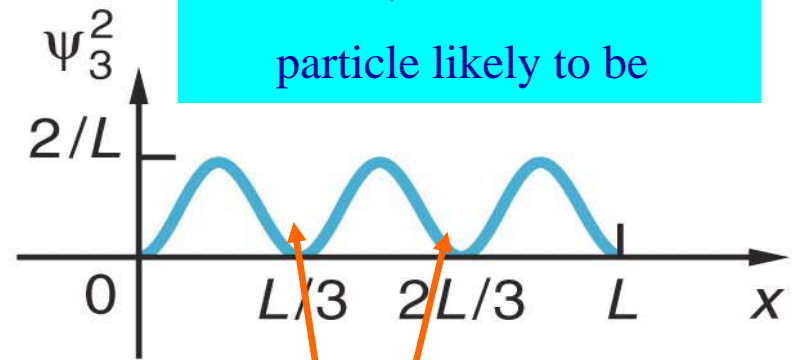
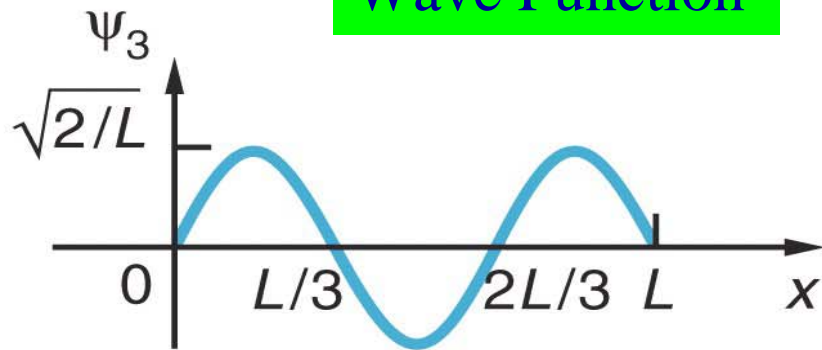
$$1 = \frac{A^2}{2} L \Rightarrow A = \sqrt{\frac{2}{L}}$$

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

# Wave Functions : Shapes Depend on Quantum # $n$

Wave Function

Probability  $P(x)$ : Where the particle likely to be



Zero Prob

