

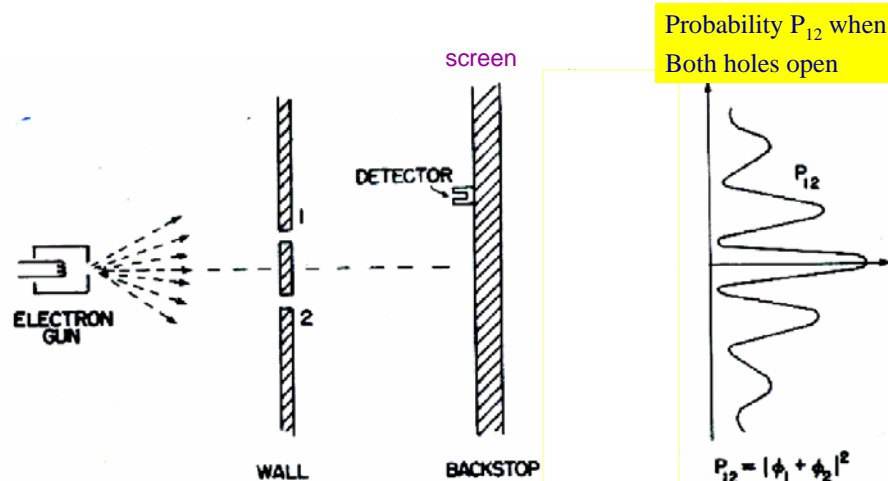


Physics 2D Lecture Slides

Lecture 20: Feb 15th 2005

Vivek Sharma
UCSD Physics

An Experiment With (indestructible) Electrons



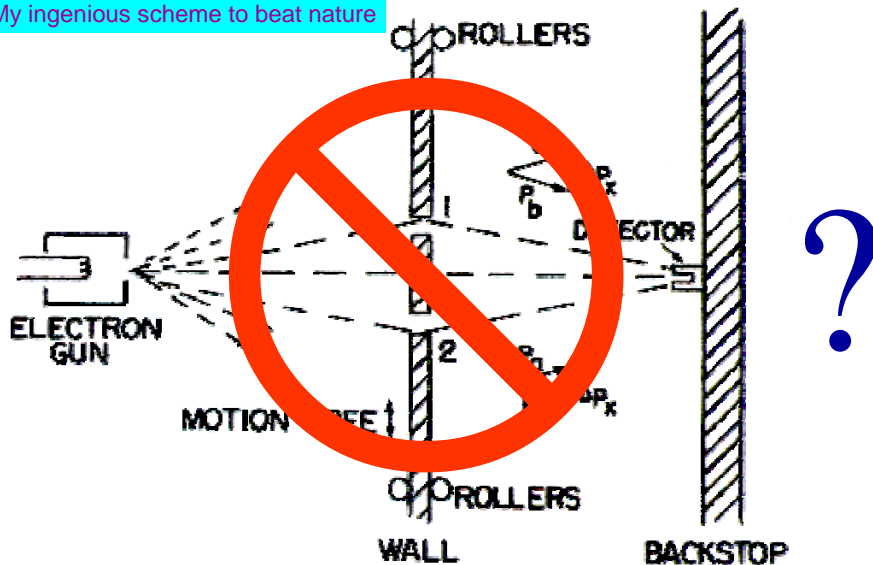
$$P_{12} \neq P_1 + P_2$$

Is There No Way to Beat The Uncertainty Principle?

- How about NOT watching the electrons!
- Let's be a bit crafty !!
- Since this is a *thought* experiment → ideal conditions
- Make up a contraption which does not violate any law
 - Mount the wall on rollers, put a lot of *grease* → frictionless
 - Wall will move when electron hits it
 - Watch recoil of the wall containing the slits when the electron hits it
 - By watching whether wall moved up or down I can tell
 - Electron went thru hole # 1
 - Electron went thru hole #2
- Will my ingenious plot succeed? After all I am so smart!

Measuring The Recoil of The Wall → Not Watching Electron !

My ingenious scheme to beat nature



Losing Out To Uncertainty Principle

- To measure the RECOIL of the wall \Rightarrow
 - must know the initial momentum of the wall before electron hit it
 - Final momentum after electron hits the wall
 - Calculate vector sum = recoil
- Uncertainty principle :
 - To do this \Rightarrow must know momentum at all times exactly so $\Delta P = 0 \rightarrow$ knowledge of wall location is imprecise, $\Delta X = \infty$ [so can not know the position of wall exactly]
 - If don't know the wall location, **then dont know where the holes were**
 - Holes will be in different place for every electron that goes thru
 - \rightarrow The center of interference pattern will have different (random) location (interference pattern) for each electron
 - Such random shift is just enough to *smear out the I. pattern* so that no interference is observed !
- Uncertainty Principle Protects Quantum Mechanics !

Summary

- Probability of an event in an ideal experiment is given by the square of the absolute value of a complex number Ψ which is call probability amplitude
 - $P = \text{probability}$
 - $\Psi = \text{probability amplitude,}$
 - $P = |\Psi|^2$
- When an even can occur in several alternative ways, the probability amplitude for the event is the sum of the probability amplitudes for each way considered separately. There is interference:
 - $\Psi = \Psi_1 + \Psi_2$
 - $P = |\Psi_1 + \Psi_2|^2$
- If an experiment is performed which is capable of determining whether one or other alternative is actually taken, the probability of the event is the sum of probabilities for each alternative. The interference is lost: $P = P_1 + P_2$

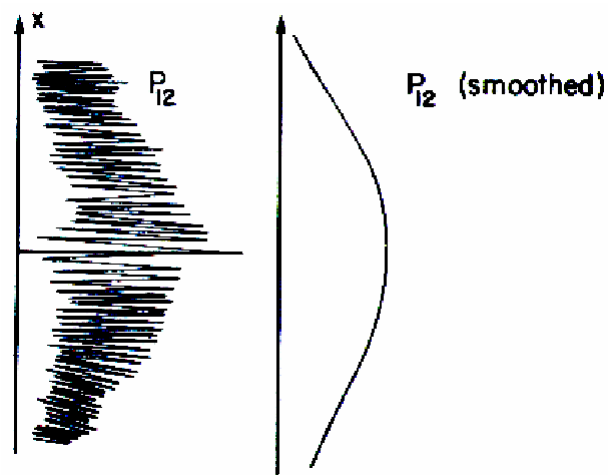
The Lesson Learnt From These Experiments

- In trying to determine which slit the particle went through, we are examining particle-like behavior
- In examining the interference pattern of electron, we are using wave like behavior of electron

Bohr's Principle of Complementarity:

It is not possible to simultaneously determine physical observables in terms of both particles and waves

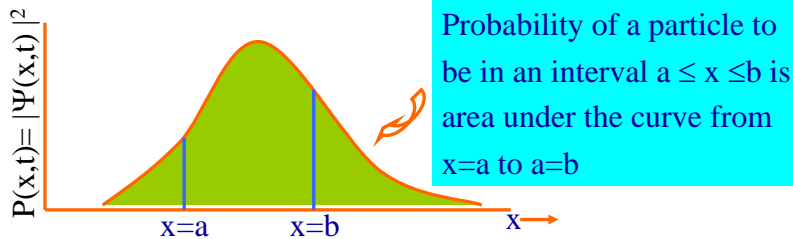
The Bullet Vs The Electron: Each Behaves the Same Way



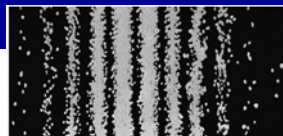
Quantum Mechanics of Subatomic Particles

- 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 $\Psi(x,y,z,t)$
- Ψ 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



- 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



Ψ: The Wave function Of A Particle

- The particle must be some where

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

- Any Ψ satisfying this condition is **NORMALIZED**
- Prob of finding particle in finite interval

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

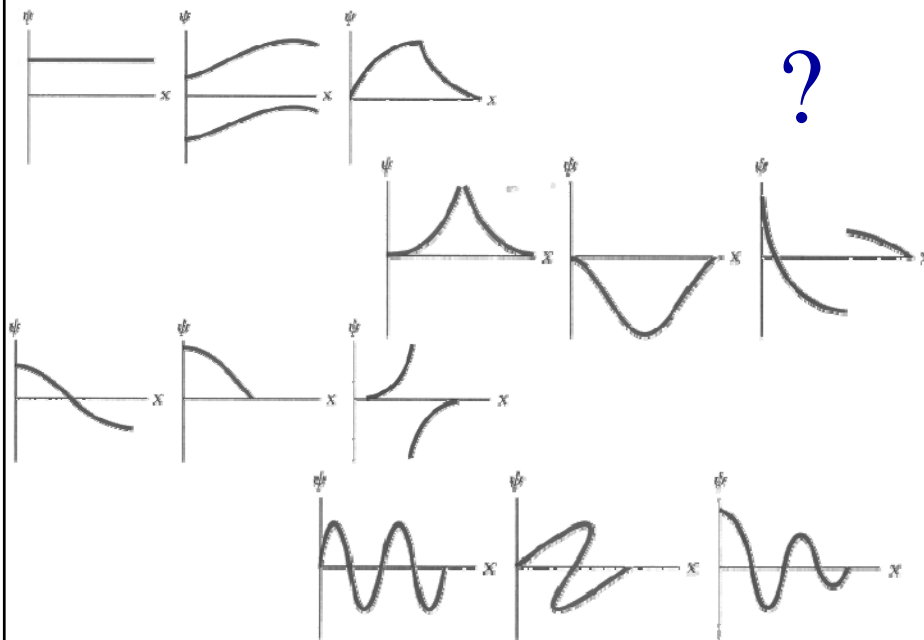
- Fundamental aim of Quantum Mechanics
 - Given the wavefunction at some instant (say t=0) find Ψ at some subsequent time t
 - Ψ(x,t=0) → Ψ(x,t) ...evolution
 - Think of a probabilistic view of particle's "newtonian trajectory"
 - We are replacing Newton's 2nd law for subatomic systems

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

- Ψ must be finite
- Ψ must be continuous fn of x,t
- Ψ must be single-valued
- Ψ must be smooth fn → $\frac{d\psi}{dx}$ must be continuous

WHY ?

Bad (Mathematical) Wave Functions Of a Physical System : You Decide Why



A Simple Wave Function : Free Particle

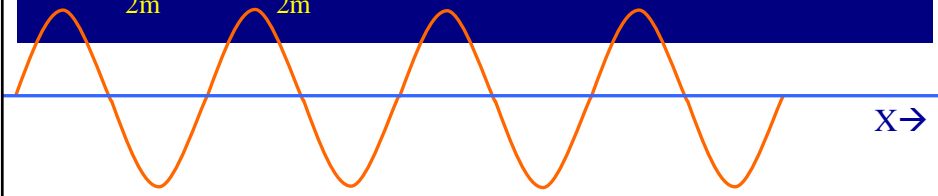
- Imagine a free particle of mass m , momentum p and $K=p^2/2m$
- Under no force, no attractive or repulsive potential to influence it
- Particle is where it wants : can be any where $[-\infty \leq x \leq +\infty]$
 - Has No relationship, no mortgage, no quiz, no final exam...its essentially a **bum!**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

• $\Psi(x,t) = A e^{i(kx - \omega t)} = A(\cos(kx - \omega t) + i \sin(kx - \omega t))$
 $k = \frac{p}{\hbar}; \quad \omega = \frac{E}{\hbar}$

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:

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

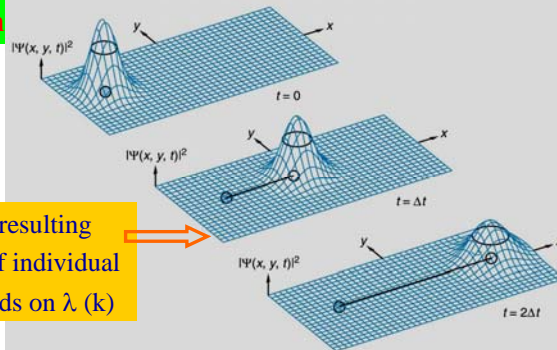
$$\Psi(x,t) = \int_{-\infty}^{+\infty} a(k) e^{i(kx - \omega t)} dk$$

Wave Packet initially localized in ΔX , Δt 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 ?

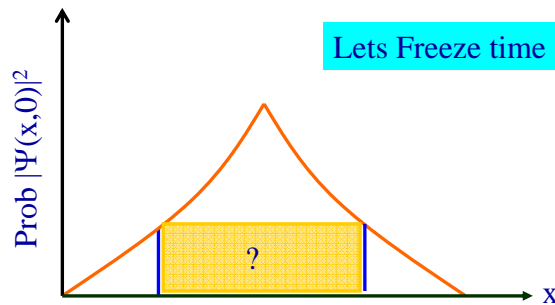
A real particle must be somewhere: Probability of finding

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

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

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

Where is the particle within a certain location $x \pm \Delta x$



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

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

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

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

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

Schrodinger Wave Equation

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

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

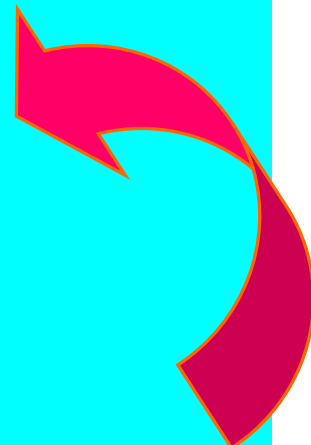
Schrodinger Equation is a Dynamical Equation much like Newton's Equation $\vec{F} = m \vec{a}$

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

Evolves the System as a function of space-time
The Schrodinger Eq. propagates 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 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 :

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

$$U(x,t) = 0$$

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

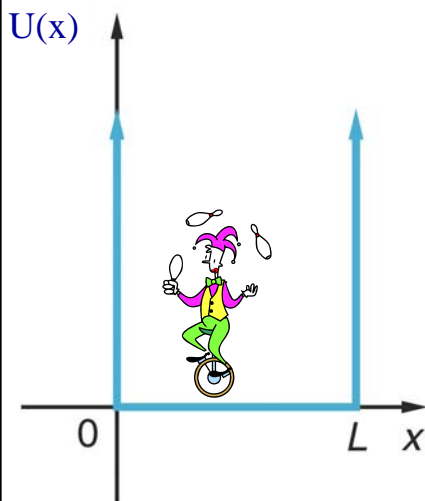
$$\frac{-\hbar^2}{2m} \frac{d^2(Ae^{ikx})}{dx^2} + 0 = E Ae^{ikx} \Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} = (\text{NR Energy})$$

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 $\psi(x)$

A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

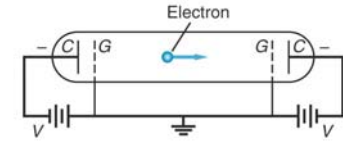
$$U(x,t) = \infty; x \leq 0, x \geq L$$


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


- 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) 

(b) 

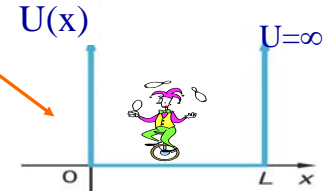
(c) 

(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



$U(x)$

$U = \infty$

x

0 L

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

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

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

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

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

In General the solution is $\psi(x) = A \sin kx + B \cos kx$ (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

$$\Rightarrow \text{At } x=0 \Rightarrow \psi(x=0)=0 \quad \& \quad \text{At } x=L \Rightarrow \psi(x=L)=0$$

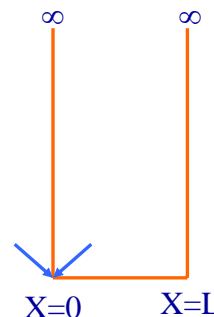
$$\therefore \psi(x=0)=B=0 \quad (\text{Continuity condition at } x=0)$$

$$\& \quad \psi(x=L)=0 \Rightarrow A \sin kL = 0 \quad (\text{Continuity condition at } x=L)$$

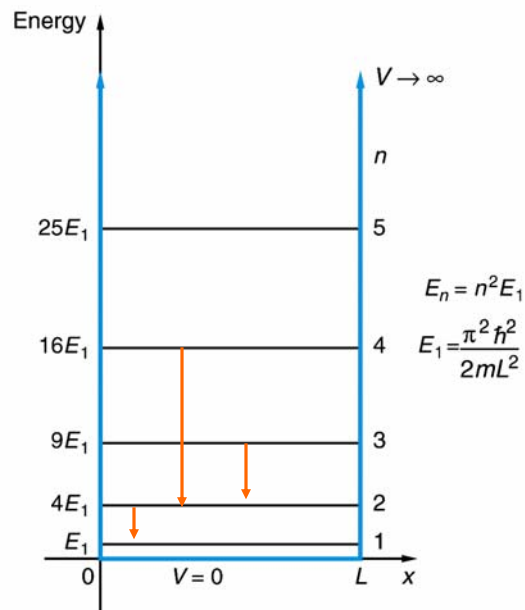
$$\Rightarrow kL = n\pi \Rightarrow k = \frac{n\pi}{L}, n=1,2,3,\dots,\infty$$

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

Why can't the particle exist Outside the box ?
 \rightarrow 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?

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

$$= 0 \quad \text{for } x \geq 0, x \geq L$$

Normalized Condition :

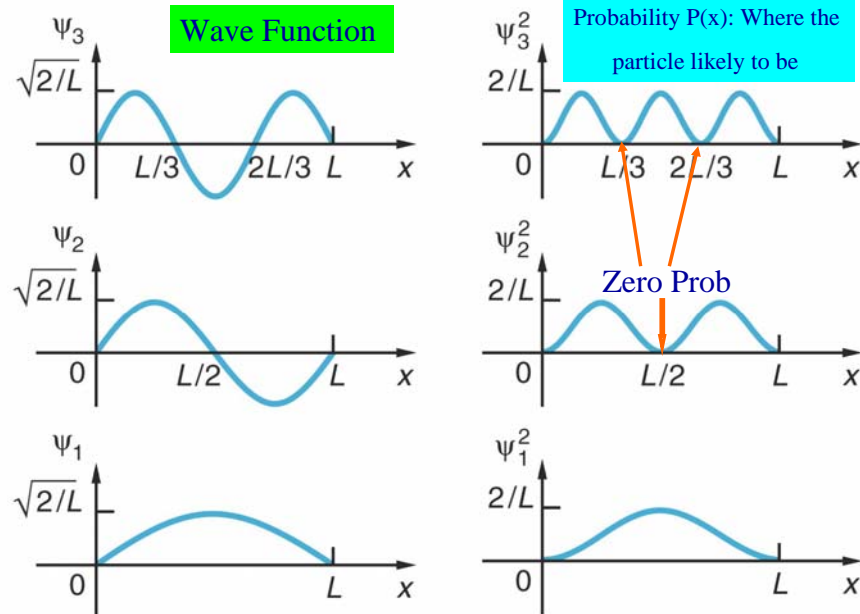
$$1 = \int_0^L \psi_n^* \psi_n dx = A^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx \quad \text{Use } 2\sin^2\theta = 1 - 2\cos 2\theta$$

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

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

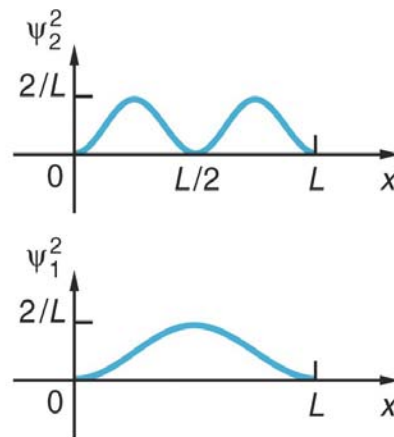
$$\text{So } \psi_n = \sqrt{\frac{2}{L}} \sin(kx) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad \dots \text{What does this look like?}$$

Wave Functions : Shapes Depend on Quantum # n



Where in The World is Carmen San Diego?

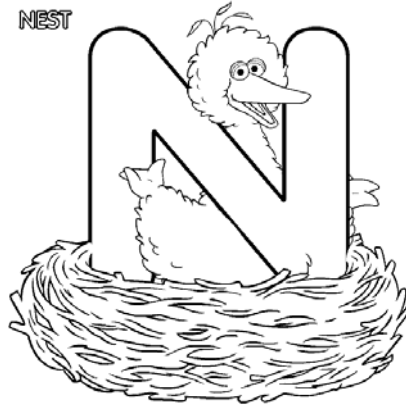
- We can only guess the probability of finding the particle somewhere in x
 - For $n=1$ (ground state) particle most likely at $x = L/2$
 - For $n=2$ (first excited state) particle most likely at $L/4, 3L/4$
 - Prob. Vanishes at $x = L/2$ & L
 - How does the particle get from just before $x=L/2$ to just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

NEST



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

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

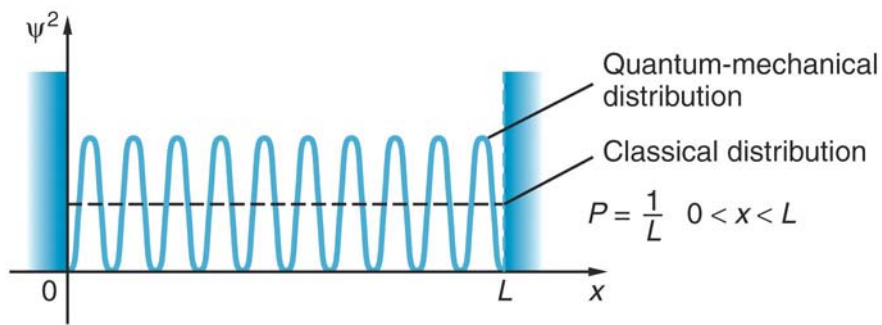
$$P = \frac{1}{L} \left[\frac{L}{2} - \left[\frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{L/4}^{3L/4} \right] = \frac{1}{2} - \frac{1}{2\pi} \left(\sin \frac{2\pi}{L} \cdot \frac{3L}{4} - \sin \frac{2\pi}{L} \cdot \frac{L}{4} \right)$$

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

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

\Rightarrow Substantial difference between Classical & Quantum predictions

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



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