4E : The Quantum Universe

Lecture 13, April 20

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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

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

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:

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

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

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) $\Rightarrow$

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

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

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

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

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

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

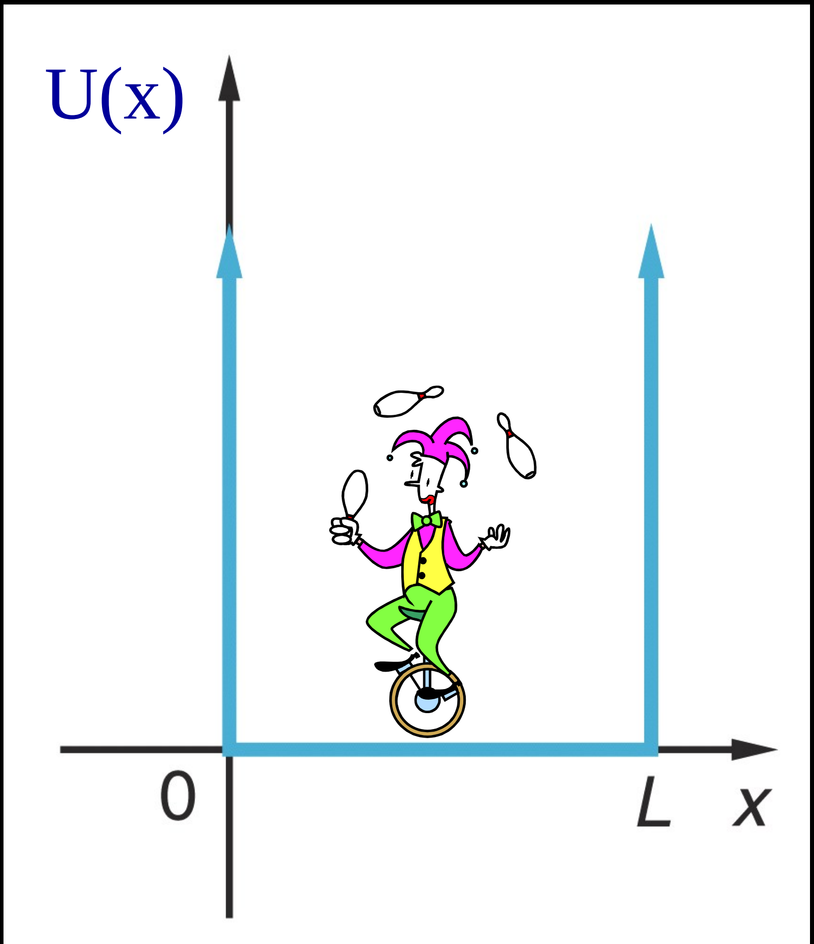
$$\int_{t=0}^{t=t}\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial \mathrm{t}}dt = \int_0^t -\frac{iE}{\hbar}dt \Rightarrow \int_0^t \frac{1}{\phi(t)}\frac{\mathrm{d}\phi(t)}{\mathrm{dt}}dt = -\frac{iE}{\hbar}$$

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

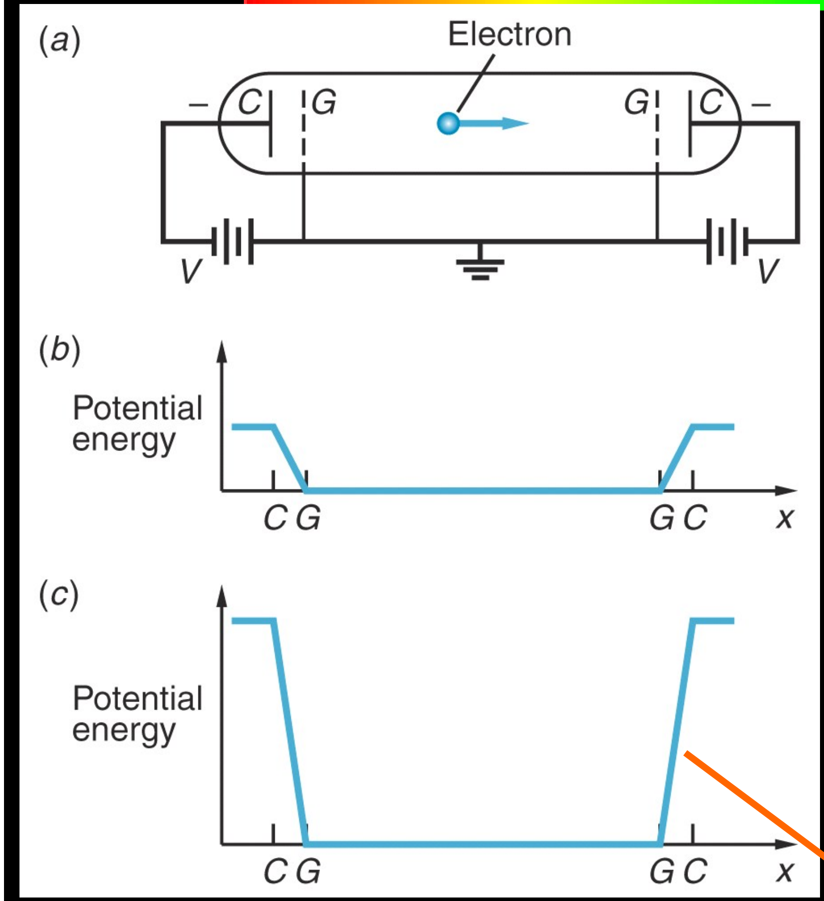
$U(x,t) = \infty; \; x \leq 0, \; x \geq L$

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

- 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



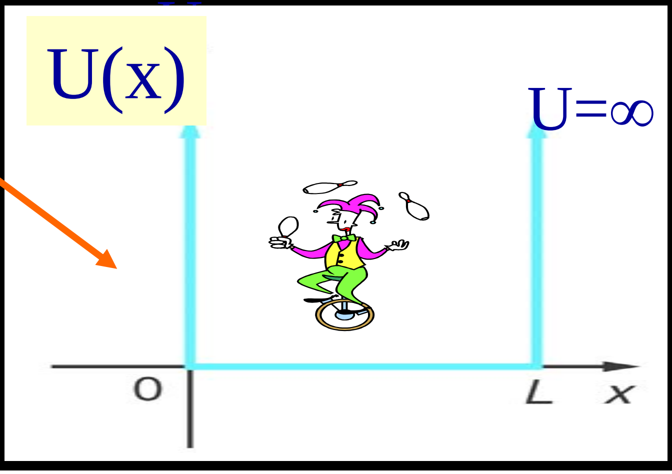
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

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 $V \to \infty$

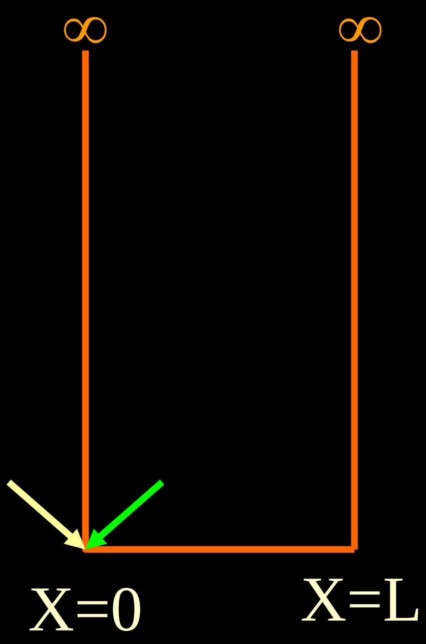
(d) The straight infinite walls are an approximation of such a situation



$\Psi(x)$ 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 ⇒ U=0 or constant (same thing)

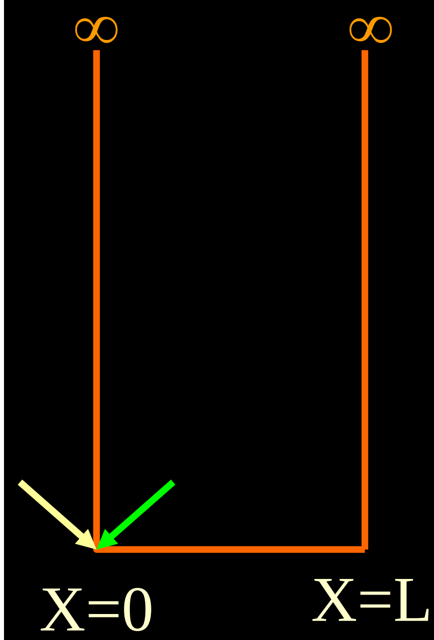
$$\Rightarrow \boxed{\frac{-\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + 0\ \psi(x) = E\ \psi(x)}$$

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

$$or\ \boxed{\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0}$$

⇐ figure out what ψ(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

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

$\therefore\ \psi(x=0) = B = 0$ (Continuity condition at x =0)

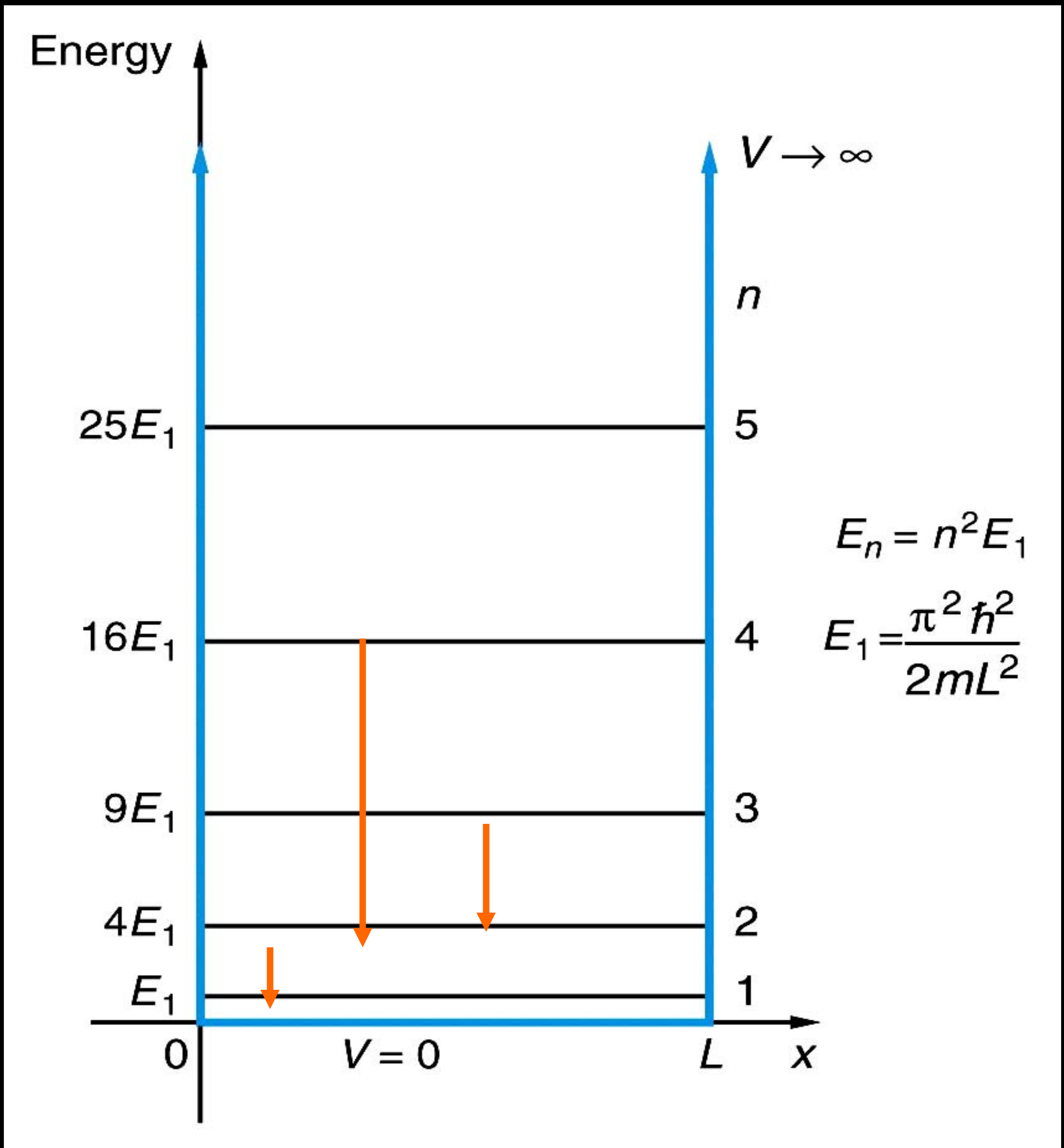
& $\boxed{\psi(x=L)=0 \Rightarrow \text{A Sin kL = 0}}$ (Continuity condition at x =L)

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

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

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?

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

Normalized Condition :

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

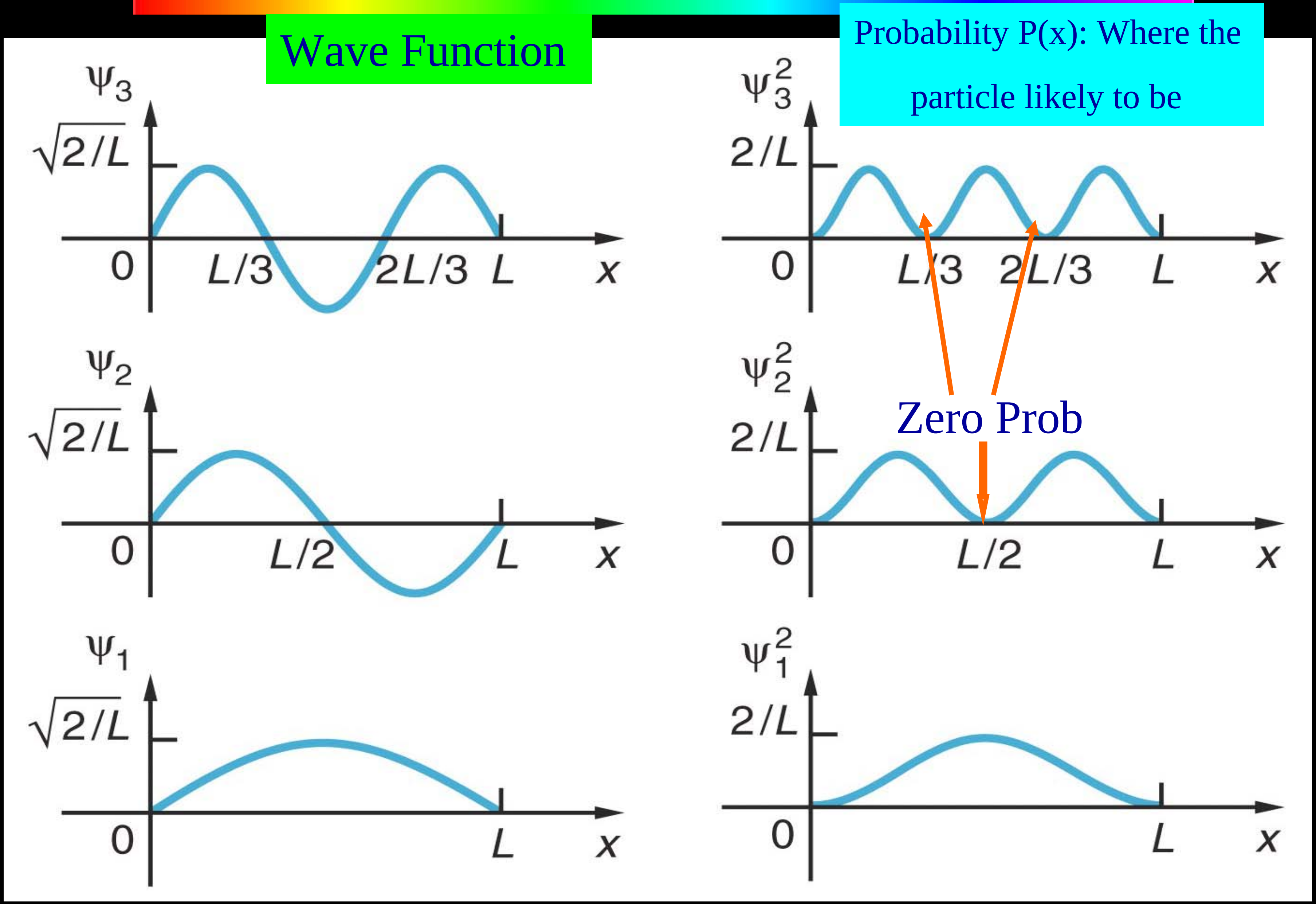
Use $2\mathrm{Sin}^2\theta = 1 - 2Cos2\theta$

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

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

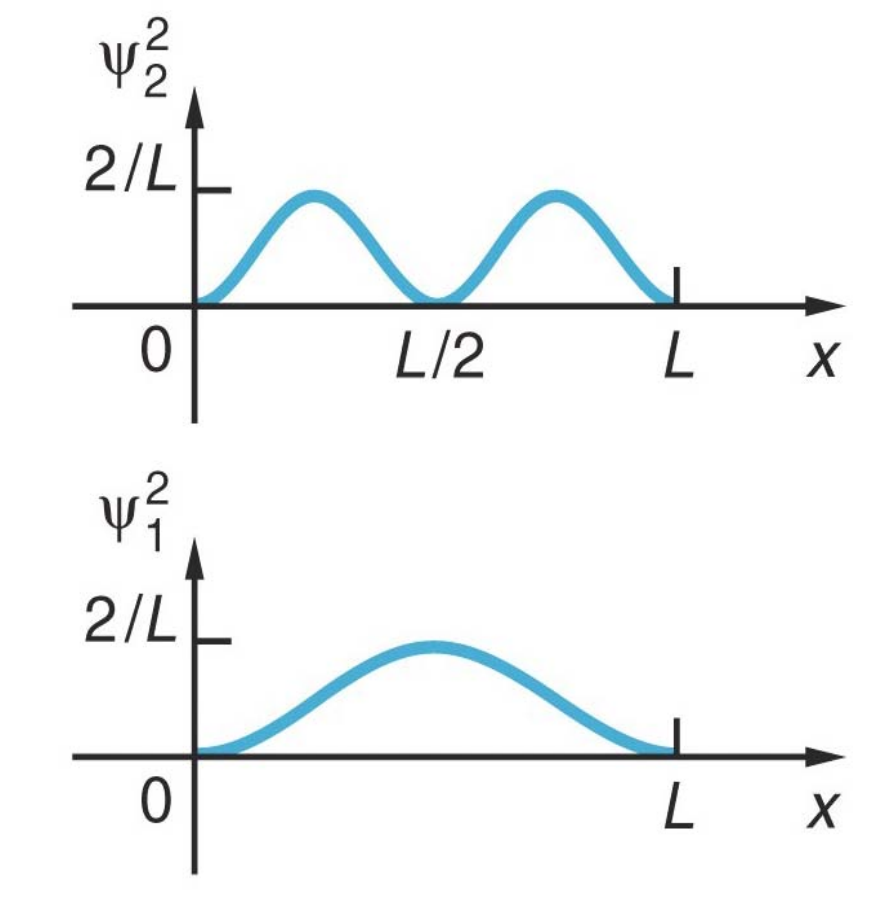
So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$ ...What does this look like?

Wave Functions : Shapes Depend on Quantum # n



Where in The World is Carmen San Diego?

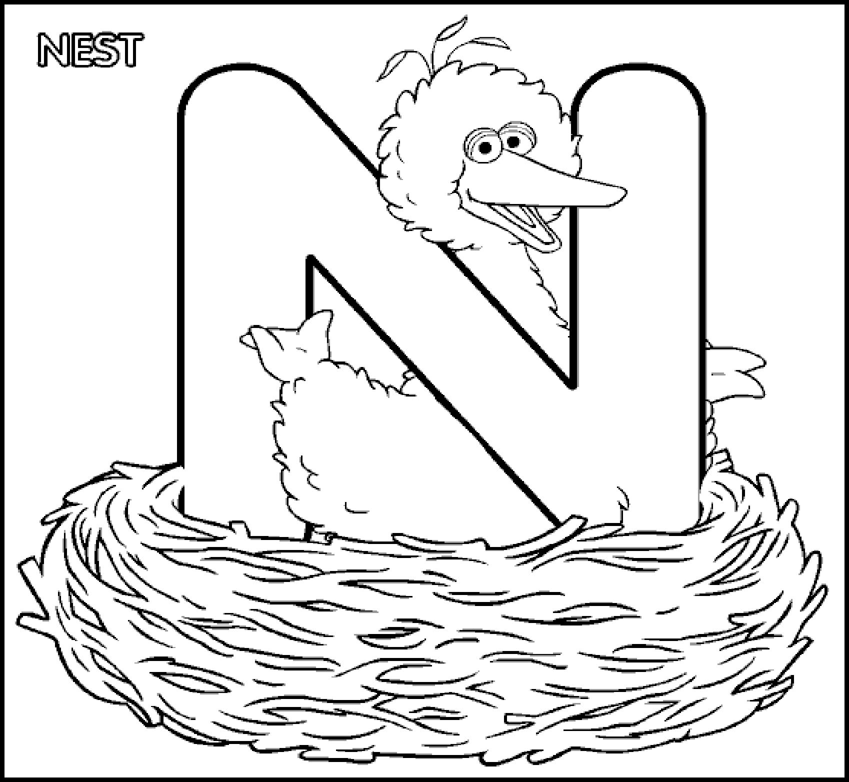
- We can only guess the probability of finding the particle somewhere in x
  - For n=1 (ground state) particle most likely at x = L/2
  - For n=2 (first excited state) particle most likely at L/4, 3L/4
    - Prob. Vanishes at x = L/2 & L
      - How does the particle get from just before x=L/2 to just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

The QM Prob. of Finding Particle in Some Region in Space

Consider n =1 state of the particle

Ask : What is P $(\frac{L}{4} \le x \le \frac{3L}{4})$?

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

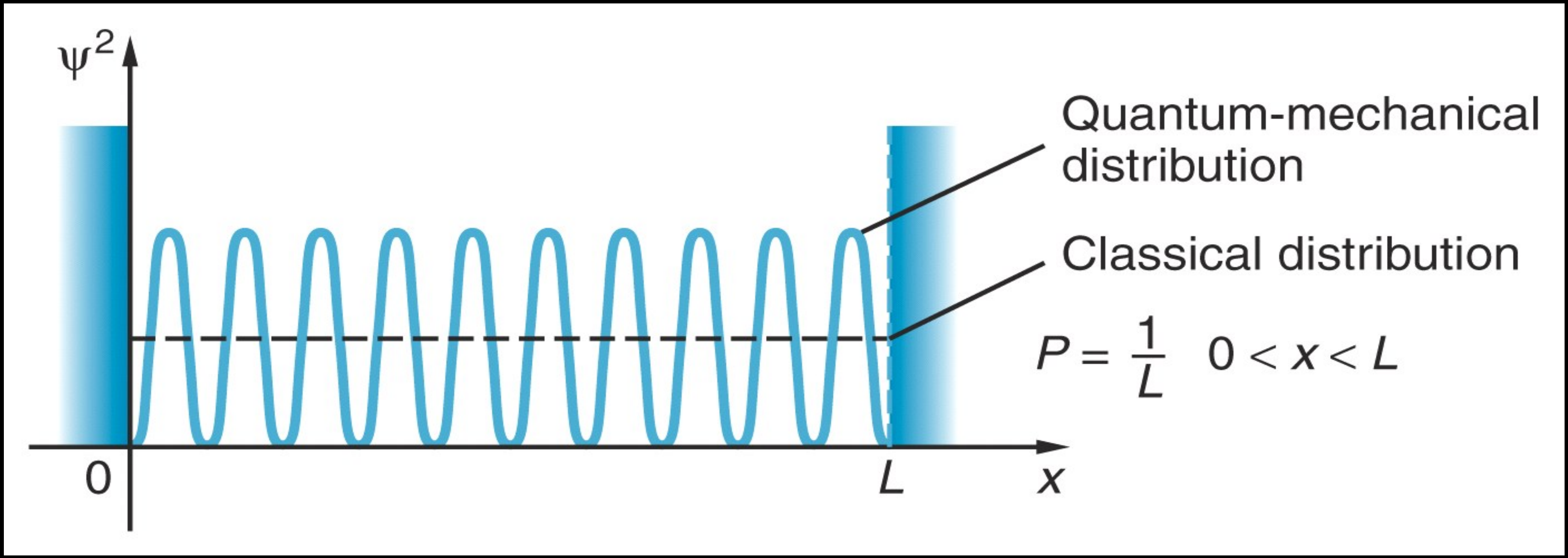
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi} \sin \frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin \frac{2\pi}{L} . \frac{3L}{4} - \sin \frac{2\pi}{L} . \frac{L}{4}\right)$$

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

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:

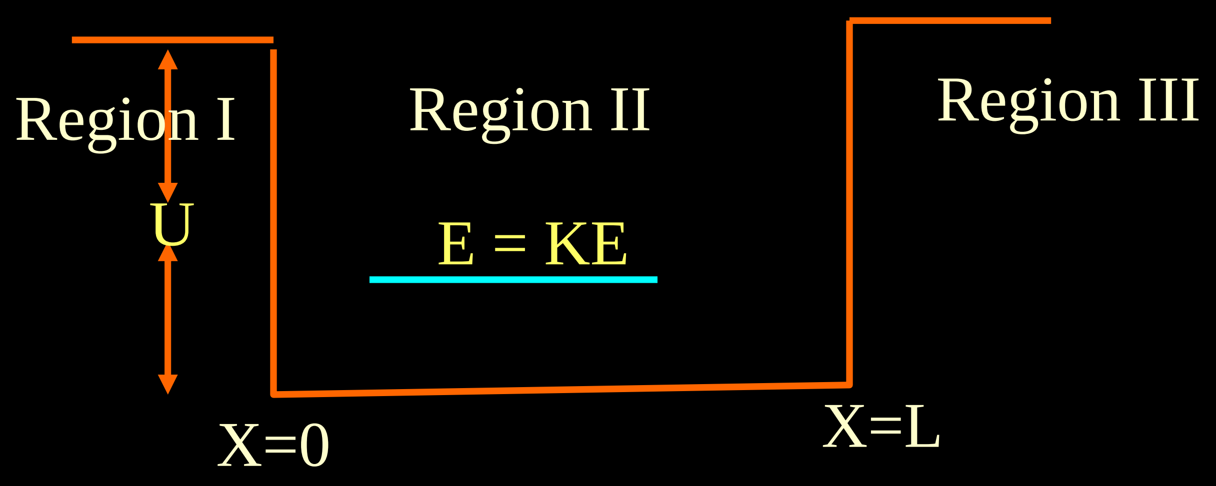
Quantum Mechanically the particle can not have E = 0

This is a direct 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 : $\boxed{\psi(x)=Ae^{+\alpha x}+Be^{-\alpha x}}$

Require finiteness of $\psi(x)$

$\Rightarrow \psi(x)=Ae^{+\alpha x}$ .....x<0 (region I)

$\psi(x)=Ae^{-\alpha x}$ .....x>L (region III)

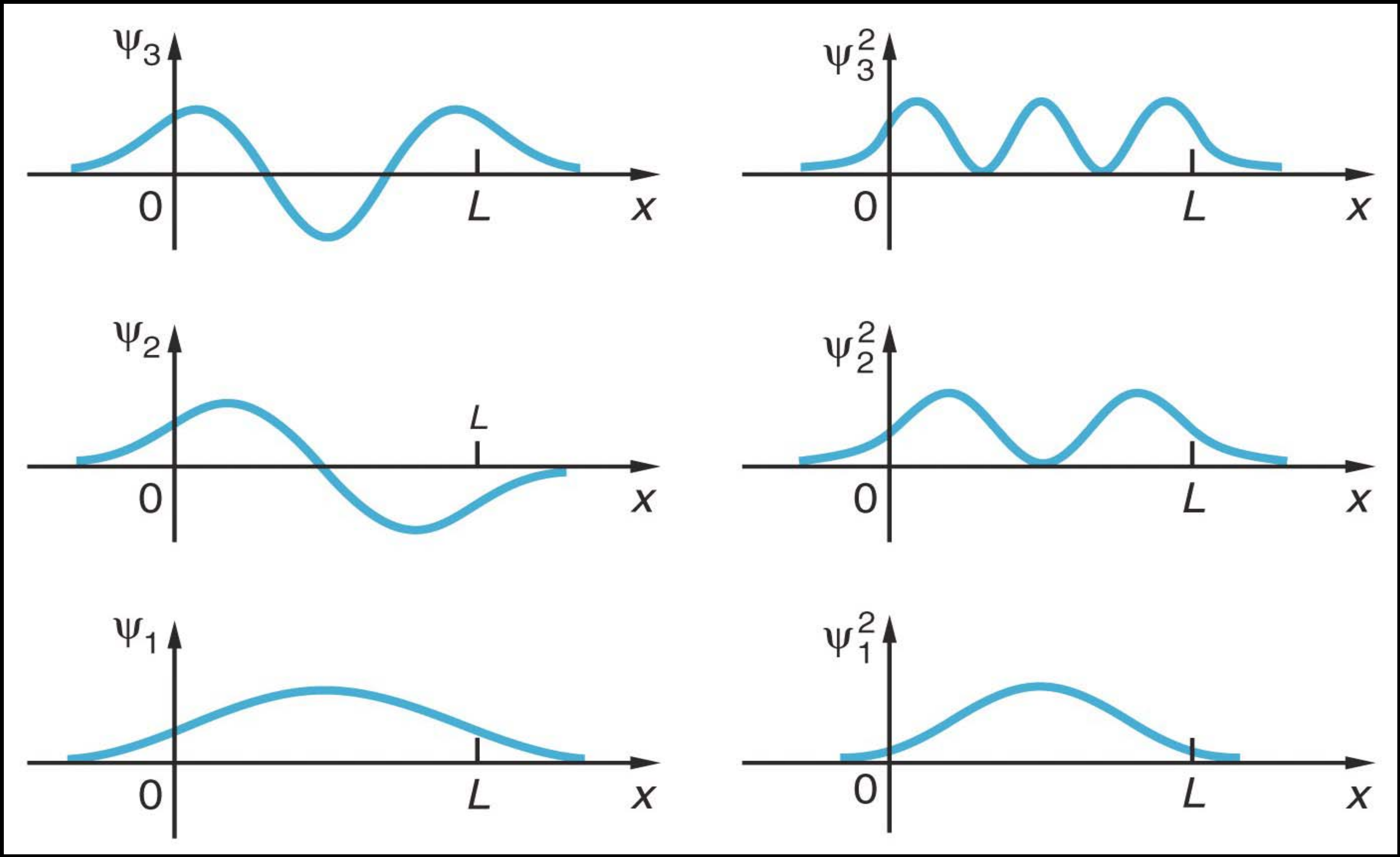
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

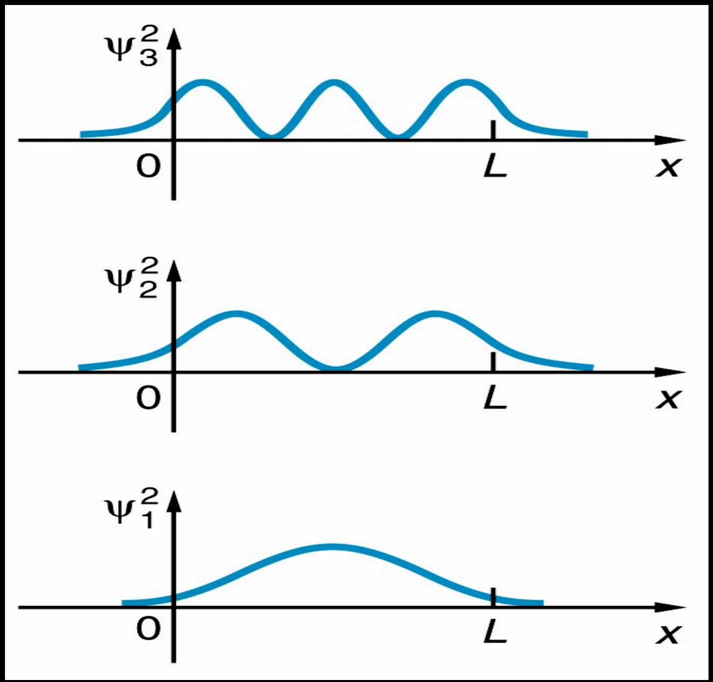
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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

If U>>E $\Rightarrow$ Tiny penetration

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