

# *4E : The Quantum Universe*

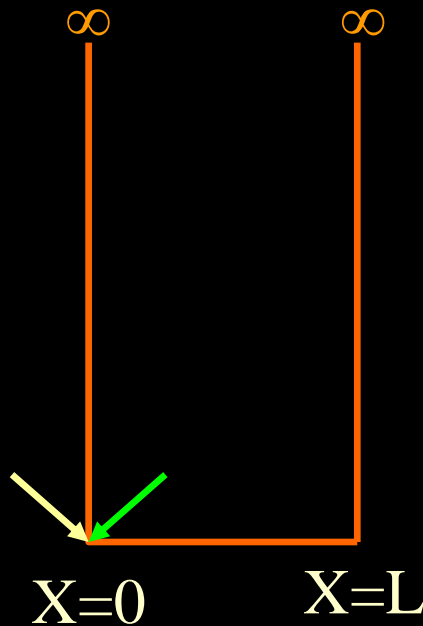


Lecture 14, April 21

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# $\Psi(x)$ 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  $x = 0$ )

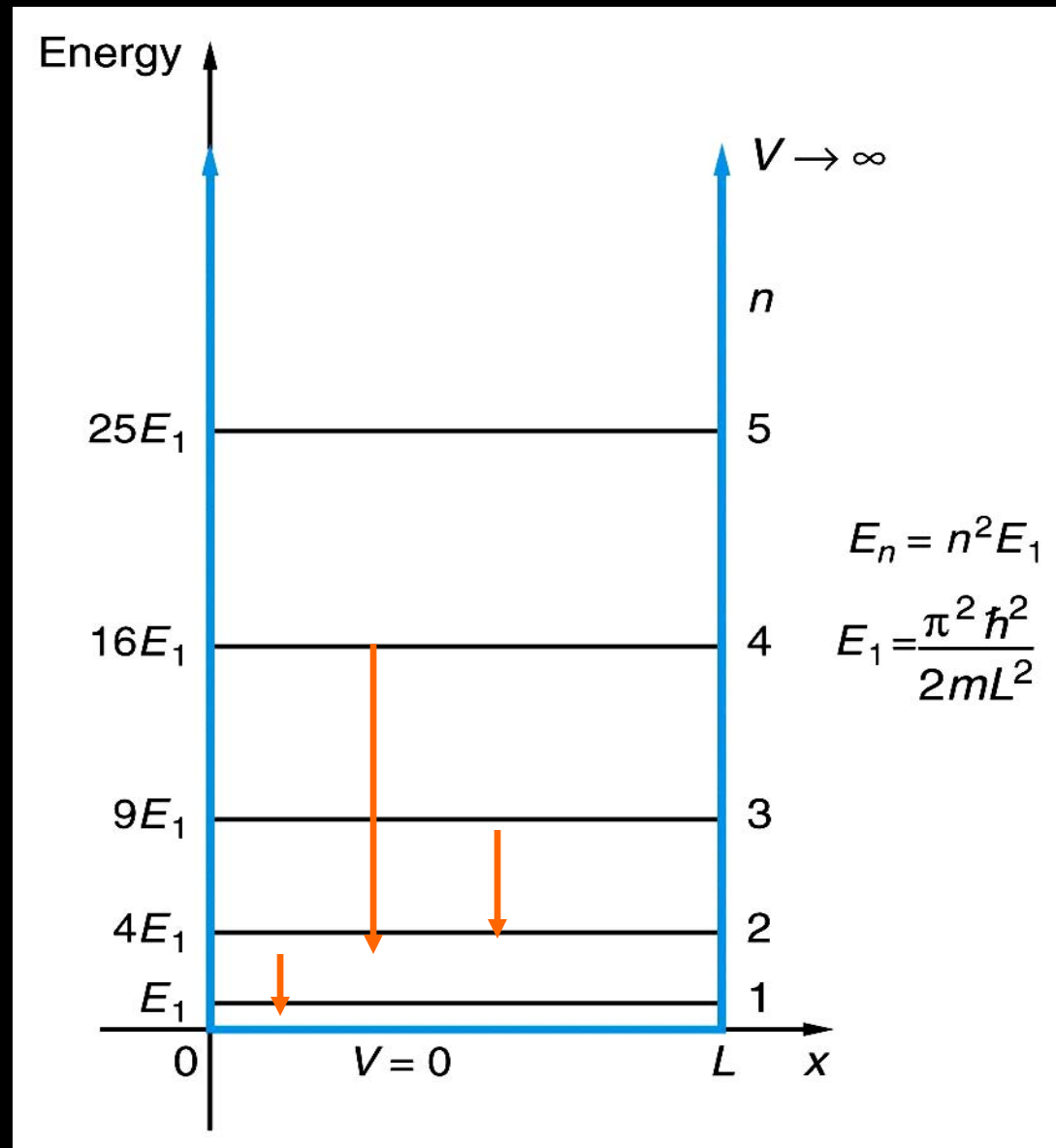
&  $\psi(x = L) = 0 \Rightarrow A \sin kL = 0$  (Continuity condition at  $x = L$ )

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

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

Quantized (not Continuous)!

# 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?

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

Normalized Condition :

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

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

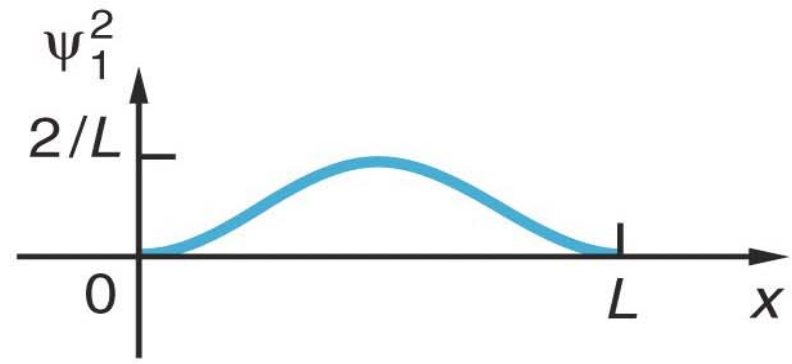
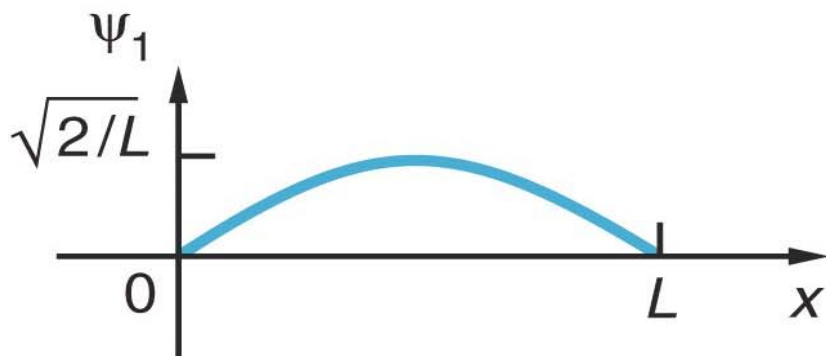
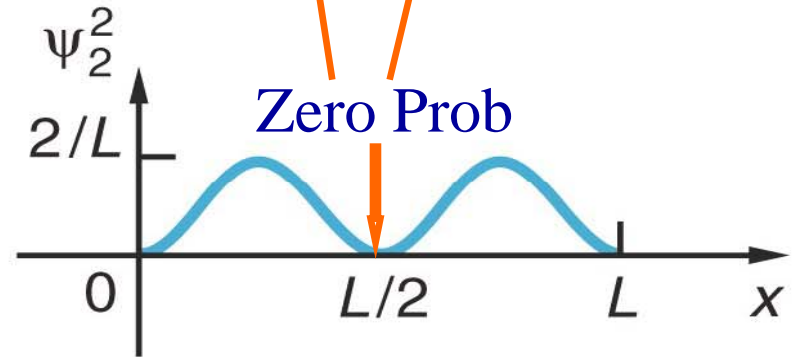
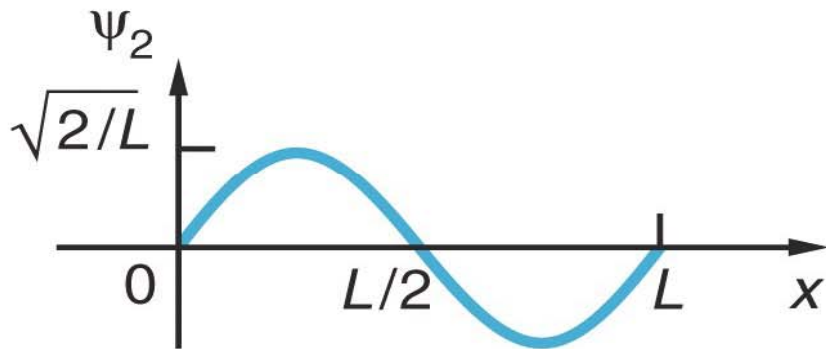
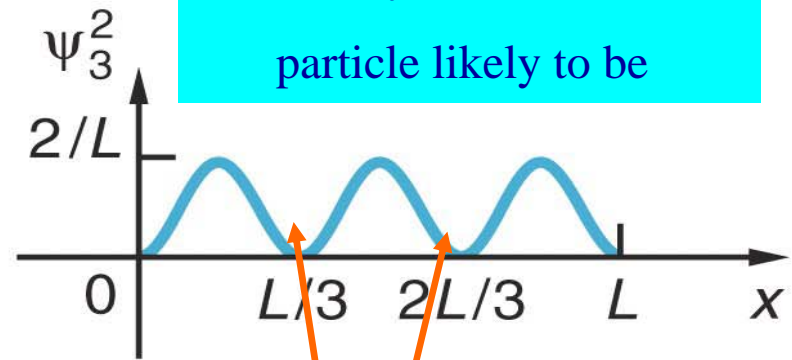
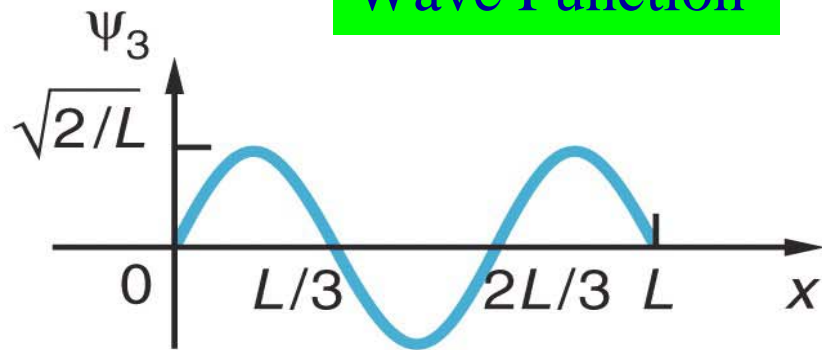
$$1 = \frac{A^2}{2} L \Rightarrow A = \sqrt{\frac{2}{L}}$$

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

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

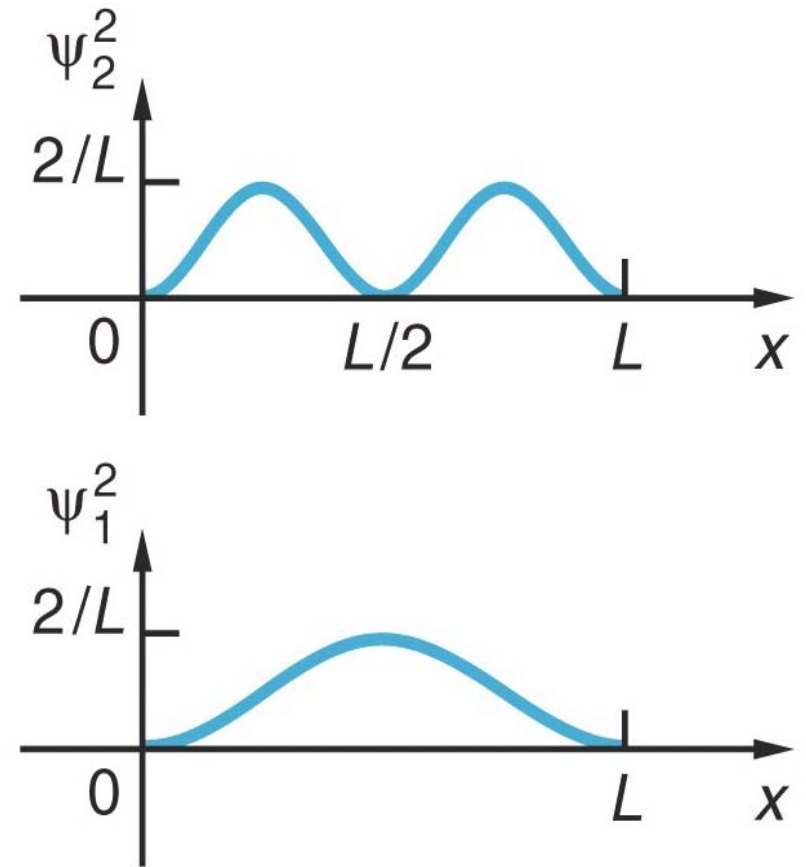
Wave Function

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



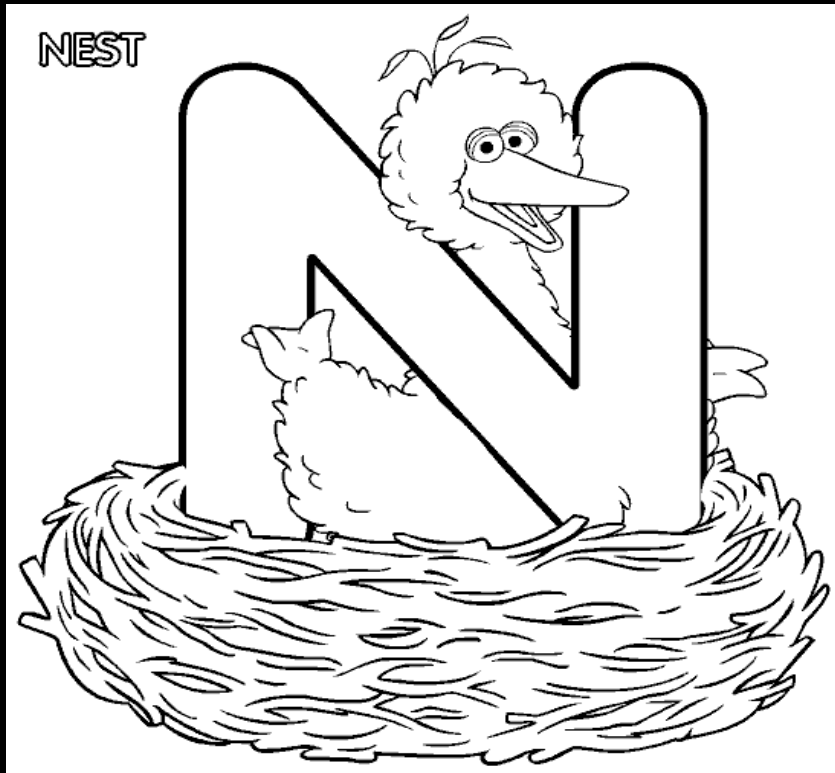
## Where in The World is Carmen San Diego?

- 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

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

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

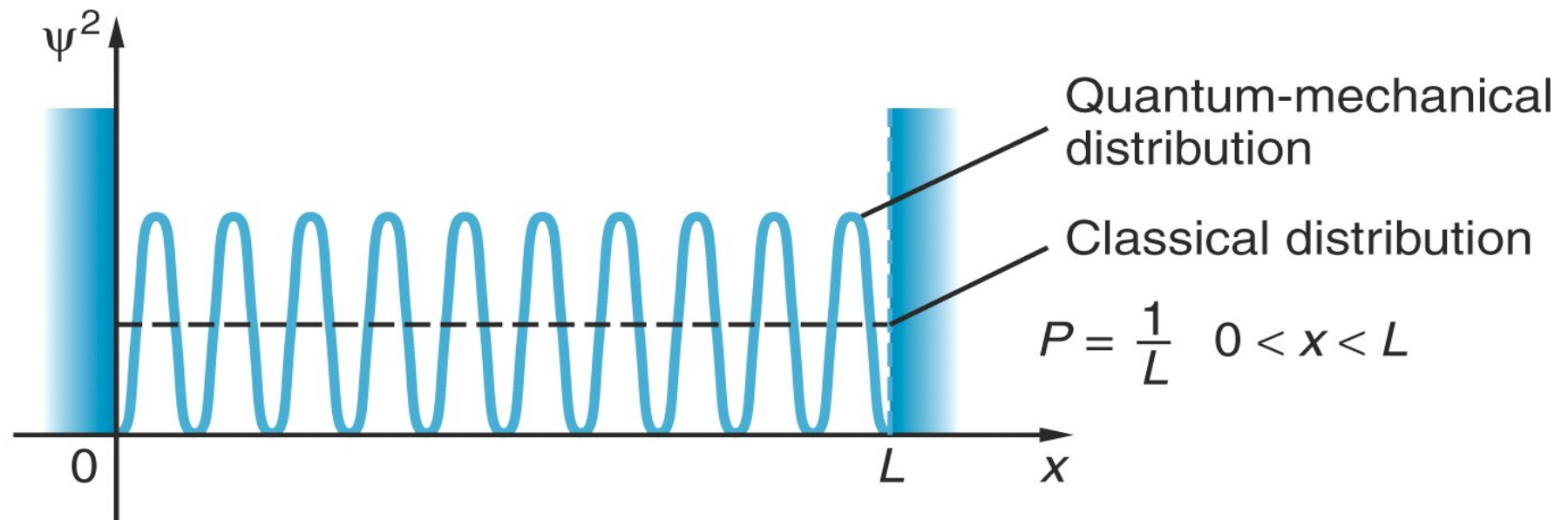
$$P = \frac{1}{L} \left[ \frac{L}{2} - \right] \left[ \frac{L}{2\pi} \sin \frac{2\pi x}{L} \right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi} \left( \sin \frac{2\pi}{L} \cdot \frac{3L}{4} - \sin \frac{2\pi}{L} \cdot \frac{L}{4} \right)$$

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

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:

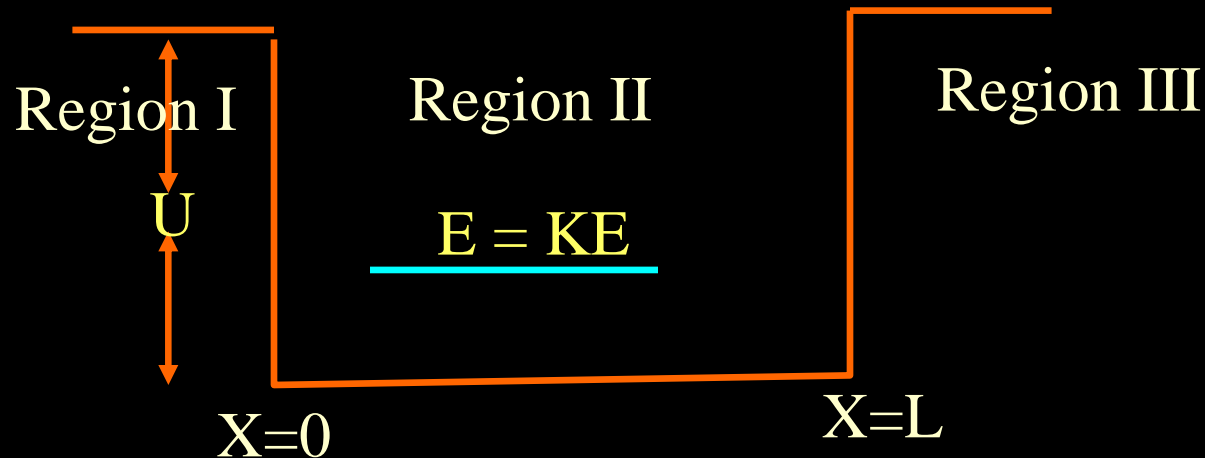
Quantum Mechanically the particle can not have  $E = 0$

This is a 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 a 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  $\Delta E \cdot \Delta t \leq h/2\pi$

Particle can leak out of the Box of finite potential  $P(|x| > L) \neq 0$

# Finite Potential Well

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

$\Rightarrow$  General Solutions :  $\psi(x) = Ae^{+\alpha x} + Be^{-\alpha x}$

Require finiteness of  $\psi(x)$

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

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

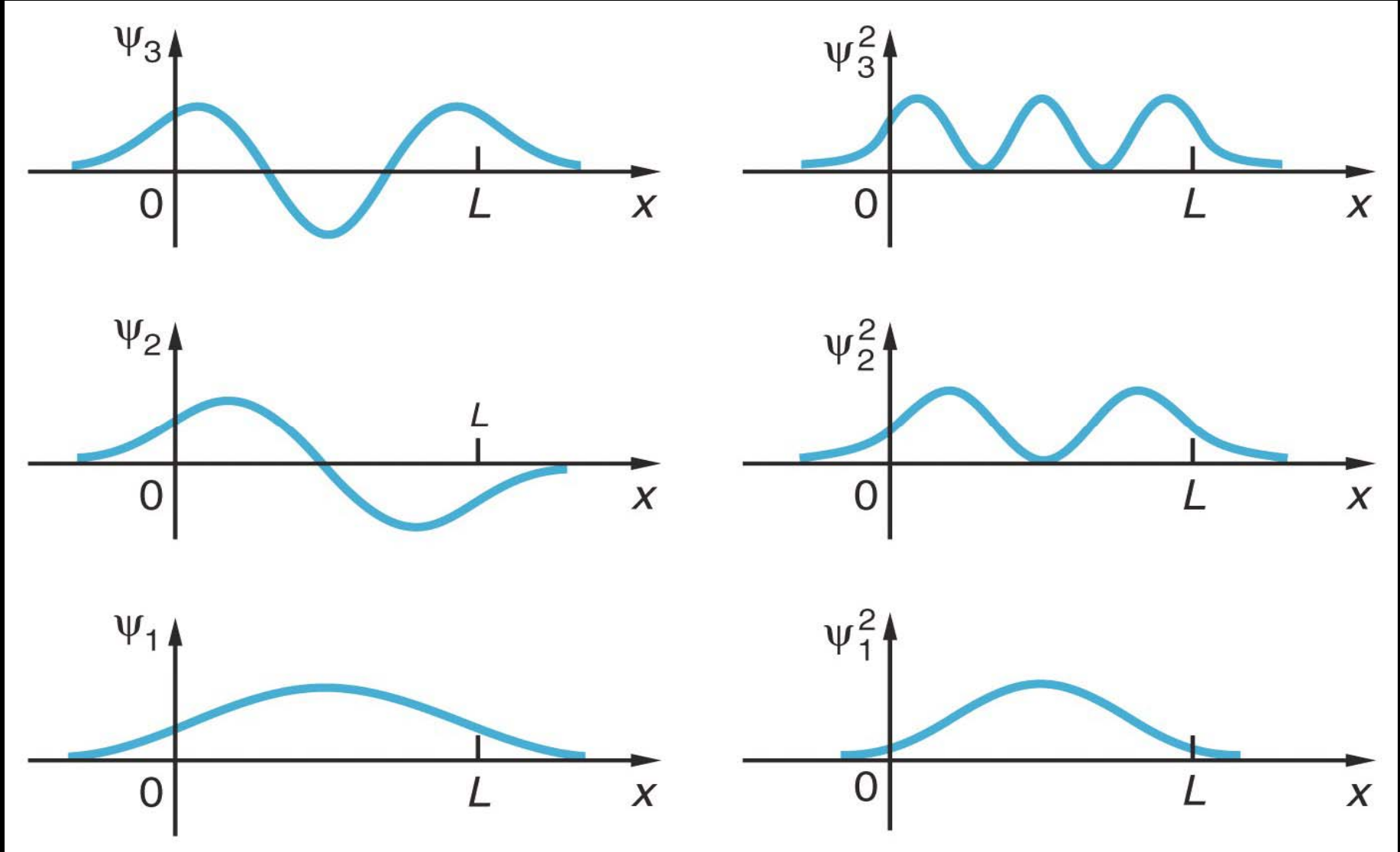
Again, coefficients A & B come from matching conditions at the edge of the walls ( $x = 0, L$ )

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

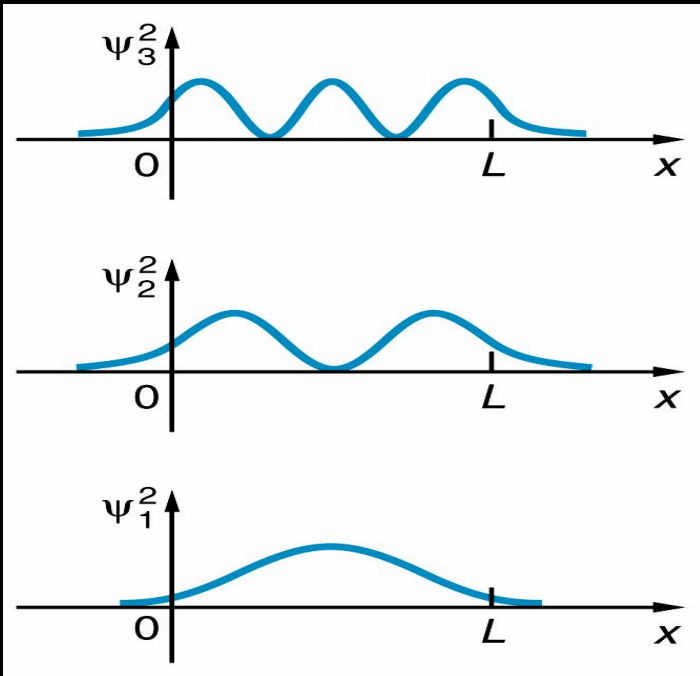
Further require Continuity of  $\psi(x)$  and  $\frac{d\psi(x)}{dx}$

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  $\Delta t \approx \hbar / \Delta E$

$\Delta E =$  Energy particle needs to borrow to

Get outside  $\Delta E = U - E + KE$

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)

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

If  $U \gg E \Rightarrow$  Tiny penetration

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

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

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

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"

# Measurement Expectation: Statistics Lesson

- Ensemble & probable outcome of a single measurement or the average outcome of a large # of measurements

$$\langle x \rangle = \frac{n_1 x_1 + n_2 x_2 + n_3 x_3 + \dots + n_i x_i}{n_1 + n_2 + n_3 + \dots + n_i} = \frac{\sum_{i=1}^n n_i x_i}{N} = \frac{\int_{-\infty}^{\infty} x P(x) dx}{\int_{-\infty}^{\infty} P(x) dx}$$

For a general Fn  $f(x)$

$$\langle f(x) \rangle = \frac{\sum_{i=1}^n n_i f(x_i)}{N} = \frac{\int_{-\infty}^{\infty} \psi^*(x) f(x) \psi(x) dx}{\int_{-\infty}^{\infty} P(x) dx}$$

Sharpness of A Distr:

Scatter around average

$$\sigma = \sqrt{\frac{\sum (x_i - \bar{x})^2}{N}}$$

$$\sigma = \sqrt{(\overline{x^2}) - (\bar{x})^2}$$

$\sigma = \text{small} \rightarrow \text{Sharp distr.}$

Uncertainty  $\Delta X = \sigma$

# Particle in the Box, $n=1$ , find $\langle x \rangle$ & $\Delta x$ ?

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right)$$

$$\langle x \rangle = \int_{-\infty}^{\infty} \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) x \sqrt{\frac{2}{L}} \sin\left(\frac{\pi}{L}x\right) dx$$

$$= \frac{2}{L} \int_0^L x \sin^2\left(\frac{\pi}{L}x\right) dx \quad , \text{ change variable } \theta = \left(\frac{\pi}{L}x\right)$$

$$\Rightarrow \langle x \rangle = \frac{2}{L\pi^2} \int_0^{\pi} \theta \sin^2\theta \quad , \text{ use } \sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$$

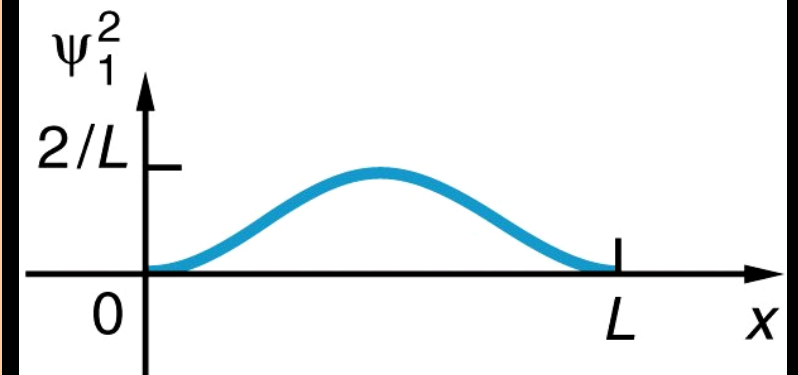
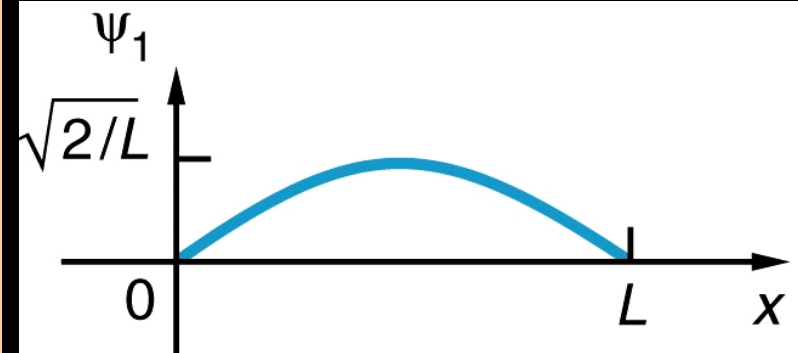
$$\Rightarrow \langle x \rangle = \frac{2L}{2\pi^2} \left[ \int_0^{\pi} \theta d\theta - \int_0^{\pi} \theta \cos 2\theta d\theta \right] \quad \text{use } \int u dv = uv - \int v du$$

$$\Rightarrow \langle x \rangle = \frac{L}{\pi^2} \left( \frac{\pi^2}{2} \right) = \frac{L}{2} \quad (\text{same result as from graphing } \psi^2(x))$$

$$\text{Similarly } \langle x^2 \rangle = \int_0^L x^2 \sin^2\left(\frac{\pi}{L}x\right) dx = \frac{L^2}{3} - \frac{L^2}{2\pi^2}$$

$$\text{and } \Delta X = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{L^2}{3} - \frac{L^2}{2\pi^2} - \frac{L^2}{4}} = 0.18L$$

$\Delta X = 20\%$  of  $L$ , Particle not sharply confined in Box



## Expectation Values & Operators: More Formally

- **Observable:** Any particle property that can be measured
  - X,P, KE, E or some combination of them,e,g:  $x^2$
  - How to calculate the probable value of these quantities for a QM state ?
- **Operator:** Associates an **operator** with each observable
  - Using these Operators, one calculates the average value of that Observable
  - The Operator acts on the Wavefunction (Operand) & extracts info about the Observable in a straightforward way → gets Expectation value for that observable

$$\langle Q \rangle = \int_{-\infty}^{+\infty} \Psi^*(x,t) [\hat{Q}] \Psi(x,t) dx$$

$Q$  is the observable,  $[\hat{Q}]$  is the operator

&  $\langle Q \rangle$  is the Expectation value

Examples:

$$[\mathbf{X}] = x, \quad [\mathbf{P}] = \frac{\hbar}{i} \frac{d}{dx}$$
$$[\mathbf{K}] = \frac{[\mathbf{P}]^2}{2m} = \frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}, \quad [\mathbf{E}] = i\hbar \frac{\partial}{\partial t}$$

**Table 5.2 Common Observables and Associated Operators**

<b>Observable</b>	<b>Symbol</b>	<b>Associated Operator</b>
position	$x$	$x$
momentum	$p$	$\frac{\hbar}{i} \frac{\partial}{\partial x}$
potential energy	$U$	$U(x)$
kinetic energy	$K$	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}$
hamiltonian	$H$	$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x)$
total energy	$E$	$i\hbar \frac{\partial}{\partial t}$

# Operators $\rightarrow$ Information Extractors

$$[p] \text{ or } \hat{p} = \frac{\hbar}{i} \frac{d}{dx} \quad \text{Momentum Operator}$$

gives the value of average momentum in the following way:

$$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^*(x) [p] \psi(x) dx = \int_{-\infty}^{+\infty} \psi^*(x) \left( \frac{\hbar}{i} \right) \frac{d\psi}{dx} dx$$

Similarly :

$$[K] \text{ or } \hat{K} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \text{ gives the value of average KE}$$

$$\langle K \rangle = \int_{-\infty}^{+\infty} \psi^*(x) [K] \psi(x) dx = \int_{-\infty}^{+\infty} \psi^*(x) \left( -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} \right) dx$$

Similarly

$$\langle U \rangle = \int_{-\infty}^{+\infty} \psi^*(x) [U(x)] \psi(x) dx \quad : \text{ plug in the } U(x) \text{ fn for that case}$$

$$\text{and } \langle E \rangle = \int_{-\infty}^{+\infty} \psi^*(x) [K + U(x)] \psi(x) dx = \int_{-\infty}^{+\infty} \psi^*(x) \left( -\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} + U(x) \right) dx$$

**Hamiltonian Operator**  $[H] = [K] + [U]$

**The Energy Operator**  $[E] = i\hbar \frac{\partial}{\partial t}$  informs you of the average energy

Plug & play form

## *[H] & [E] Operators*



- [H] is a function of  $x$
- [E] is a function of  $t$  .....they are really different operators
- But they produce identical results when applied to any solution of the time-dependent Schrodinger Eq.
  
- $[H]\Psi(x,t) = [E] \Psi(x,t)$

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

- Think of S. Eq as an expression for Energy conservation for a Quantum system

## Where do Operators come from ? A touchy-feely answer

*Example : [p]* The momentum Extractor (operator):

Consider as an example: Free Particle Wavefunction

$$\Psi(x,t) = Ae^{i(kx-wt)} \quad ; \quad k = \frac{2\pi}{\lambda}, \lambda = \frac{h}{p} \Rightarrow k = \frac{p}{\hbar}$$

*rewrite*  $\Psi(x,t) = Ae^{i(\frac{p}{\hbar}x-wt)}$  ;  $\frac{\partial \Psi(x,t)}{\partial x} = i \frac{p}{\hbar} Ae^{i(\frac{p}{\hbar}x-wt)} = i \frac{p}{\hbar} \Psi(x,t)$

$$\Rightarrow \left[ \frac{\hbar}{i} \frac{\partial}{\partial x} \right] \Psi(x,t) = p \Psi(x,t)$$

So it is not unreasonable to associate  $[p] = \left[ \frac{\hbar}{i} \frac{\partial}{\partial x} \right]$  with observable p

## Example : Average Momentum of particle in box

- Given the symmetry of the 1D box, we argued last time that  $\langle p \rangle = 0$   
: now some inglorious math to prove it !
  - Be lazy, when you can get away with a symmetry argument to solve a problem..do it & avoid the evil integration & algebra.....but be sure!

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right) \quad \& \quad \psi_n^*(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x\right)$$

$$\langle p \rangle = \int_{-\infty}^{+\infty} \psi^* [p] \psi dx = \int_{-\infty}^{\infty} \psi^* \left[ \frac{\hbar}{i} \frac{d}{dx} \right] \psi dx$$

$$\langle p \rangle = \frac{\hbar}{i} \frac{2}{L} \frac{n\pi}{L} \int_{-\infty}^{\infty} \sin\left(\frac{n\pi}{L}x\right) \cos\left(\frac{n\pi}{L}x\right) dx$$

$$\text{Since } \int \sin ax \cos ax dx = \frac{1}{2a} \sin^2 ax \quad \dots \text{here } a = \frac{n\pi}{L}$$

$$\Rightarrow \langle p \rangle = \frac{\hbar}{iL} \left[ \sin^2\left(\frac{n\pi}{L}x\right) \right]_{x=0}^{x=L} = 0 \text{ since } \sin^2(0) = \sin^2(n\pi) = 0$$

We knew THAT before doing any math !

Quiz 1: What is the  $\langle p \rangle$  for the Quantum Oscillator in its symmetric ground state

Quiz 2: What is the  $\langle p \rangle$  for the Quantum Oscillator in its asymmetric first excited state

*But what about the  $\langle KE \rangle$  of the Particle in Box ?*

$\langle p \rangle = 0$  so what about expectation value of  $K = \frac{p^2}{2m}$  ?

$\langle K \rangle = 0$  because  $\langle p \rangle = 0$ ; clearly not, since we showed  $E = KE \neq 0$

Why ? What gives ?

Because  $p_n = \pm \sqrt{2mE_n} = \pm \frac{n\pi\hbar}{L}$ ; "±" is the key!

The AVERAGE  $p = 0$ , since particle is moving back & forth

$\langle KE \rangle = \langle \frac{p^2}{2m} \rangle \neq 0$ ; not  $\frac{\langle p^2 \rangle}{2m}$  !

Be careful when being "lazy"

Quiz: what about  $\langle KE \rangle$  of a quantum Oscillator?

Does similar logic apply??

## Schrodinger Eqn: Stationary State Form

$$P(x,t) = \Psi^* \Psi = \psi^*(x) e^{+\frac{iE}{\hbar}t} \psi(x) e^{-\frac{iE}{\hbar}t} = \psi^*(x) \psi(x) e^{\frac{iE}{\hbar}t - \frac{iE}{\hbar}t} = |\psi(x)|^2$$

In such cases, P(x,t) is **INDEPENDENT** of time.

These are called "stationary" states because Prob is independent of time

Examples : Particle in a box (why?)

: Quantum Oscillator (why?)

Total energy of the system depends on the spatial orientation of the system : characteristic of the potential situation !