Physics 2D Lecture Slides
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Where Do Wave Functions Come From ?

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

U(x) = characteristic Potential of the system

Factorization Condition For Wave Function Leads to:

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

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

What is the Constant E ? How to Interpret it ?

Consider the free particle situation :

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

$U(x,t) = 0$

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

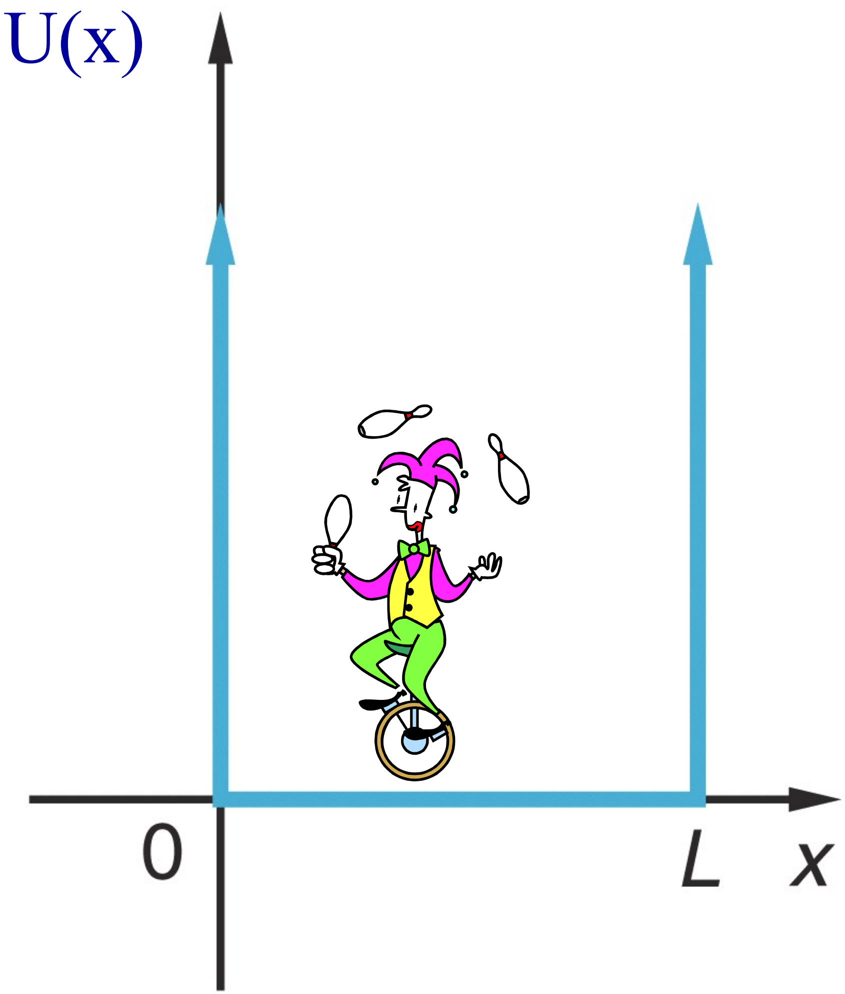
$$\frac{-\hbar^2}{2m}\frac{d^2(Ae^{(ikx)})}{dx^2}+0=E\ Ae^{(ikx)} \Rightarrow E=\frac{\hbar^2k^2}{2m}=\frac{p^2}{2m}=\text{(NR Energy)}$$

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

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

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 <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 ??

Ψ(x) for Particle Inside 1D Box with Infinite Potential Walls

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 ψ(x) 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)

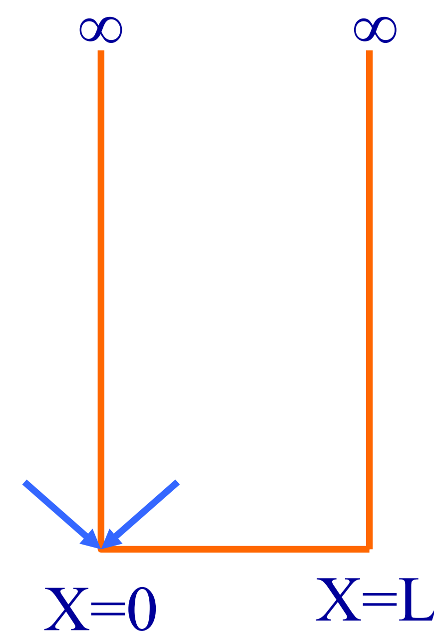
& $\psi(x=L) = 0 \Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

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

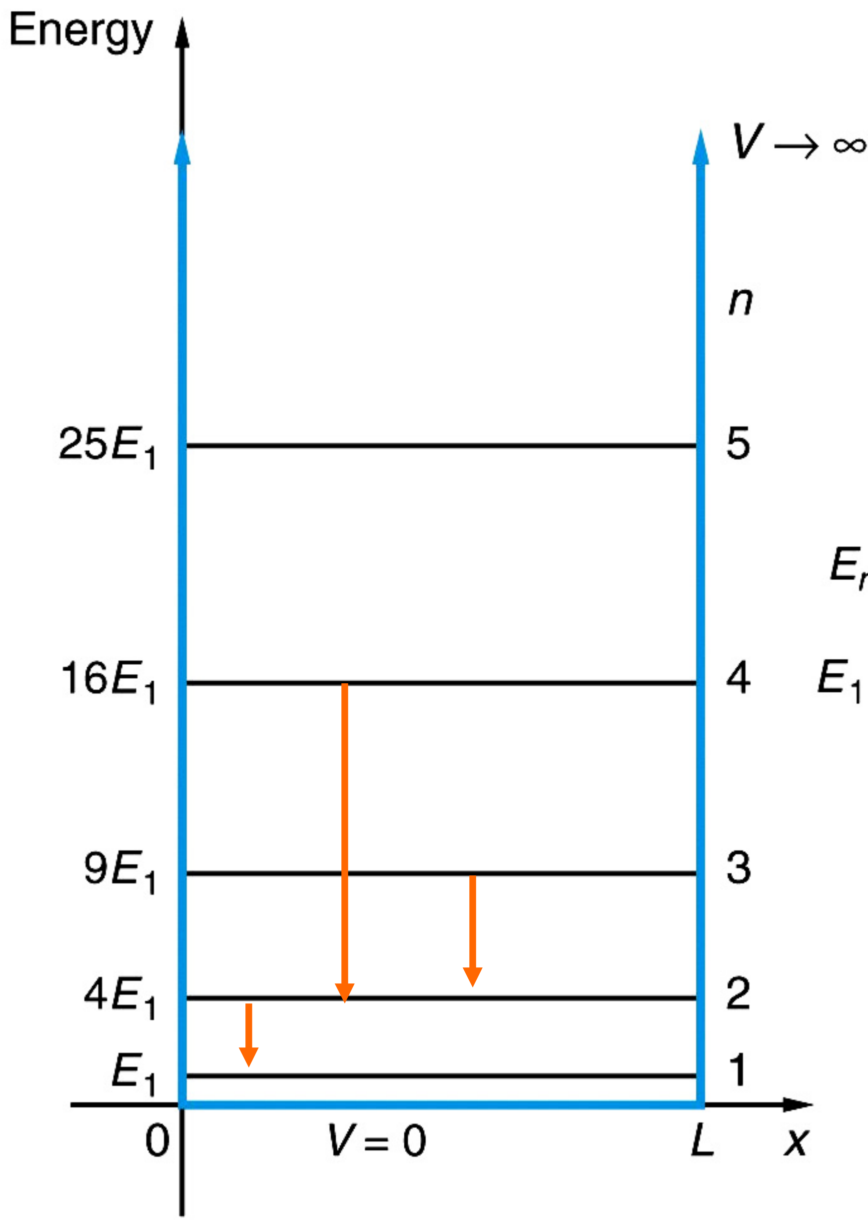
So what does this say about Energy E ? : $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ Quantized (not Continuous)!

Why can't the particle exist Outside the box ?

→ E Conservation



Quantized Energy levels of Particle in a Box



$$E_n = n^2 E_1$$

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2}$$

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 :

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

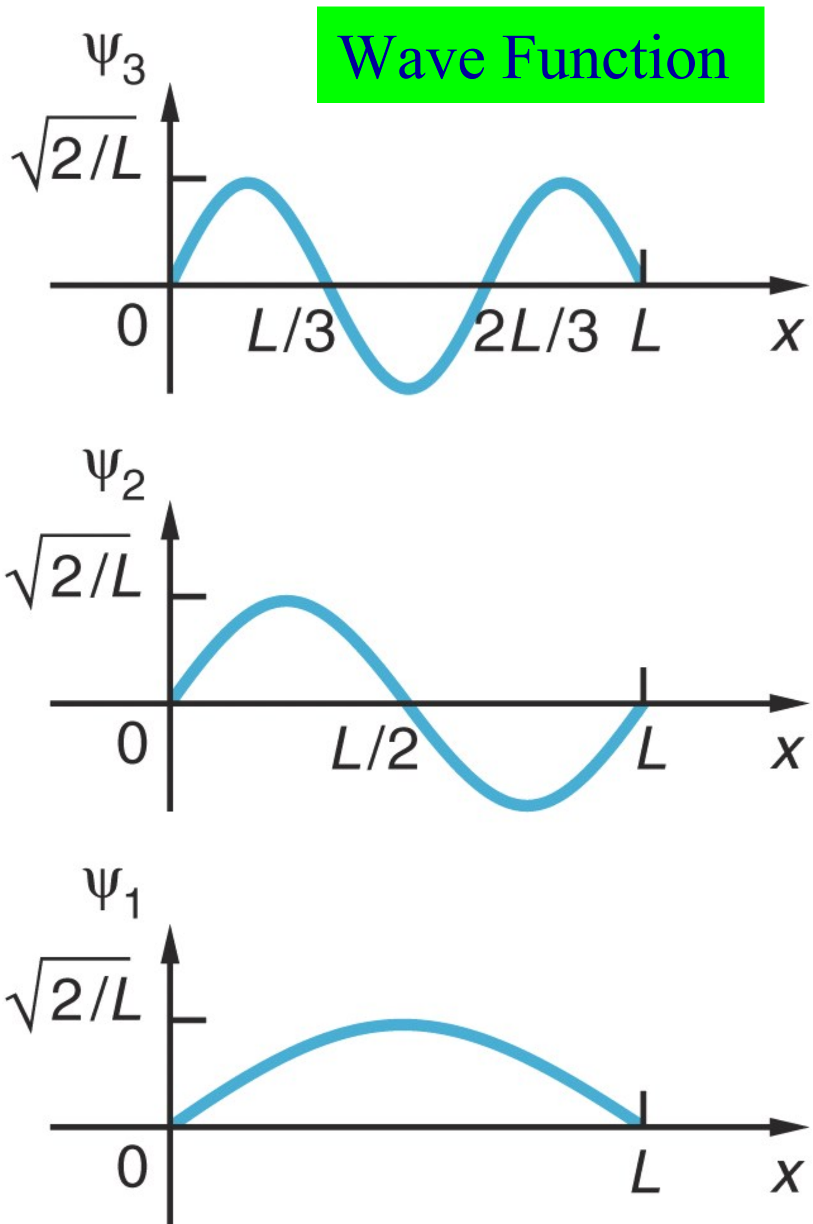
Use $2\mathrm{Sin}^2\theta = 1 - 2Cos2\theta$

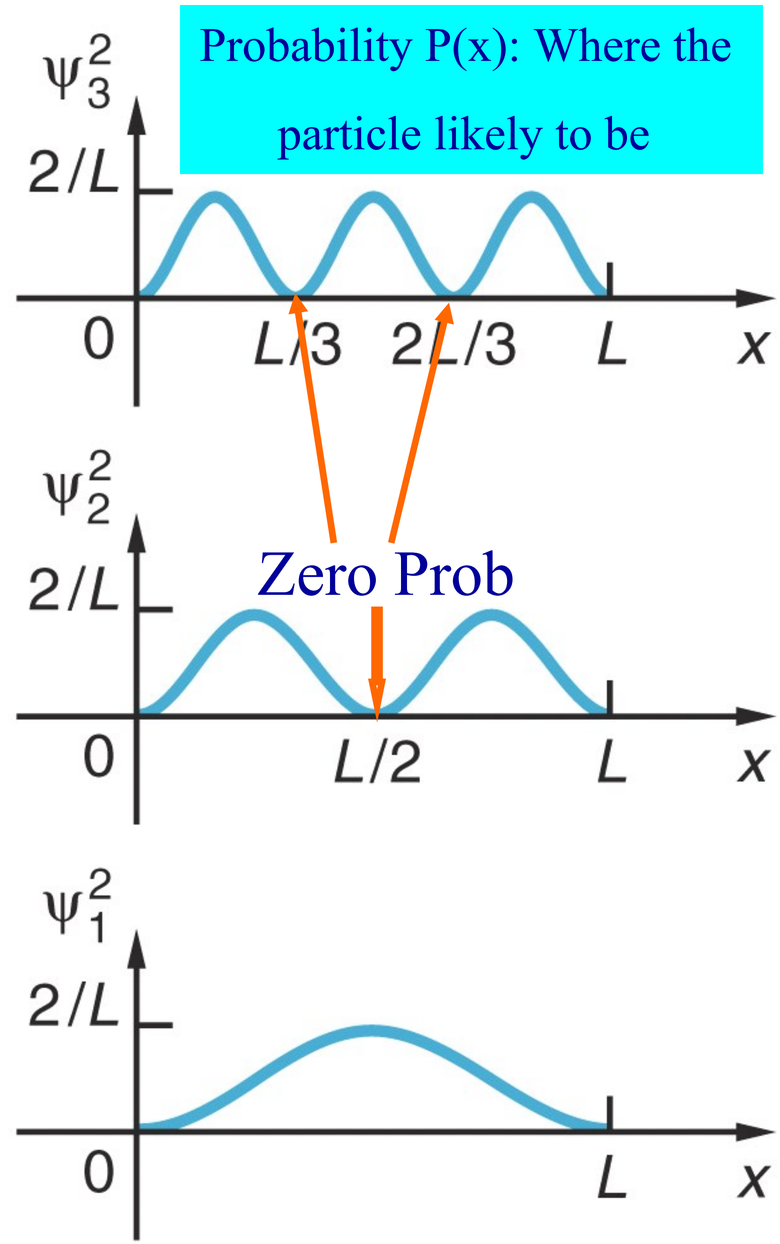
$$1 = \frac{A^2}{2}\int_0^L \left(1 - \cos(\frac{2n\pi x}{L})\right)$$ and since $\int \cos\,\theta = \sin\theta$

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

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

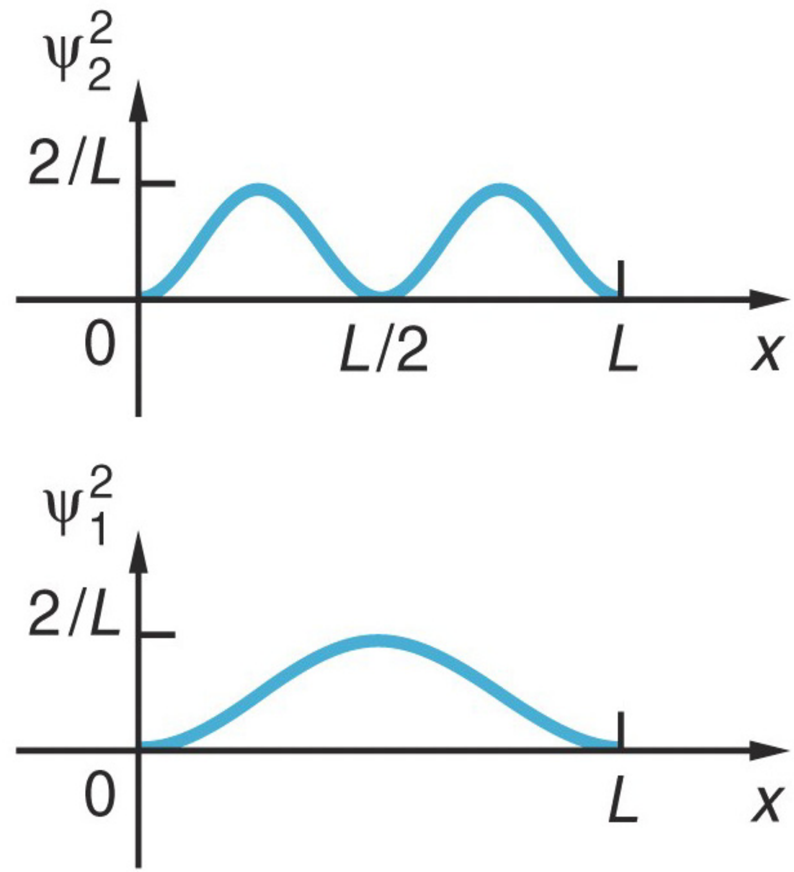
Wave Functions : Shapes Depend on Quantum # n





Where in The World is Carmen San Diego?

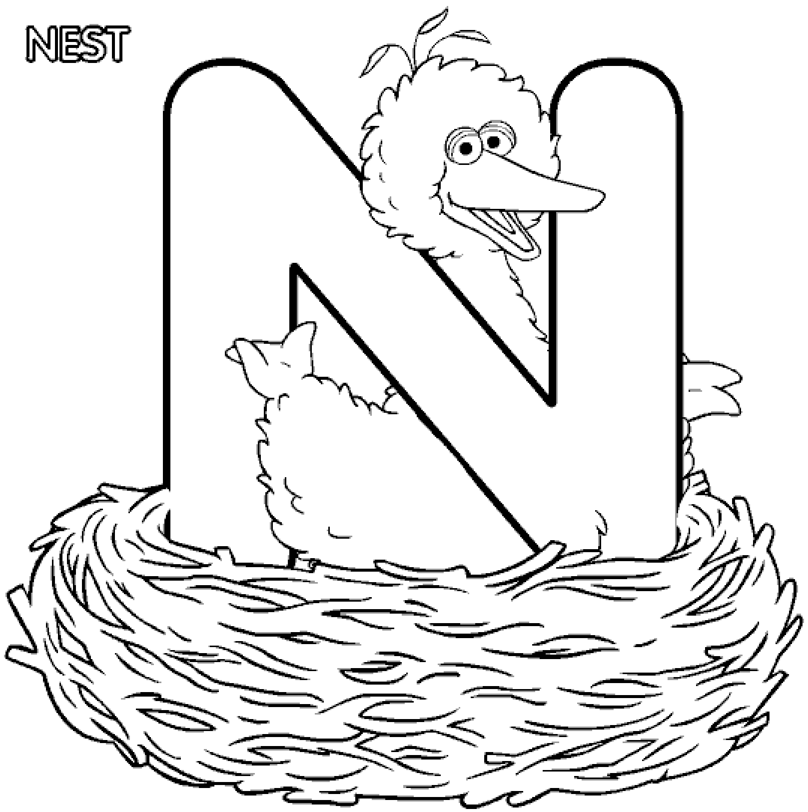
- We can only guess the probability of finding the particle somewhere in x
  - For n=1 (ground state) particle most likely at x = L/2
  - For n=2 (first excited state) particle most likely at L/4, 3L/4
    - Prob. Vanishes at x = L/2 & L
      - How does the particle get from just before x=L/2 to just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



Classically, where is the particle most Likely to be : Equal prob of being anywhere inside the Box

NOT SO says Quantum Mechanics!

What Was Sesame Street Trying to Teach you !



This <u>particle in the box</u> 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 $P\left(\frac{L}{4} \le x \le \frac{3L}{4}\right)$?

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

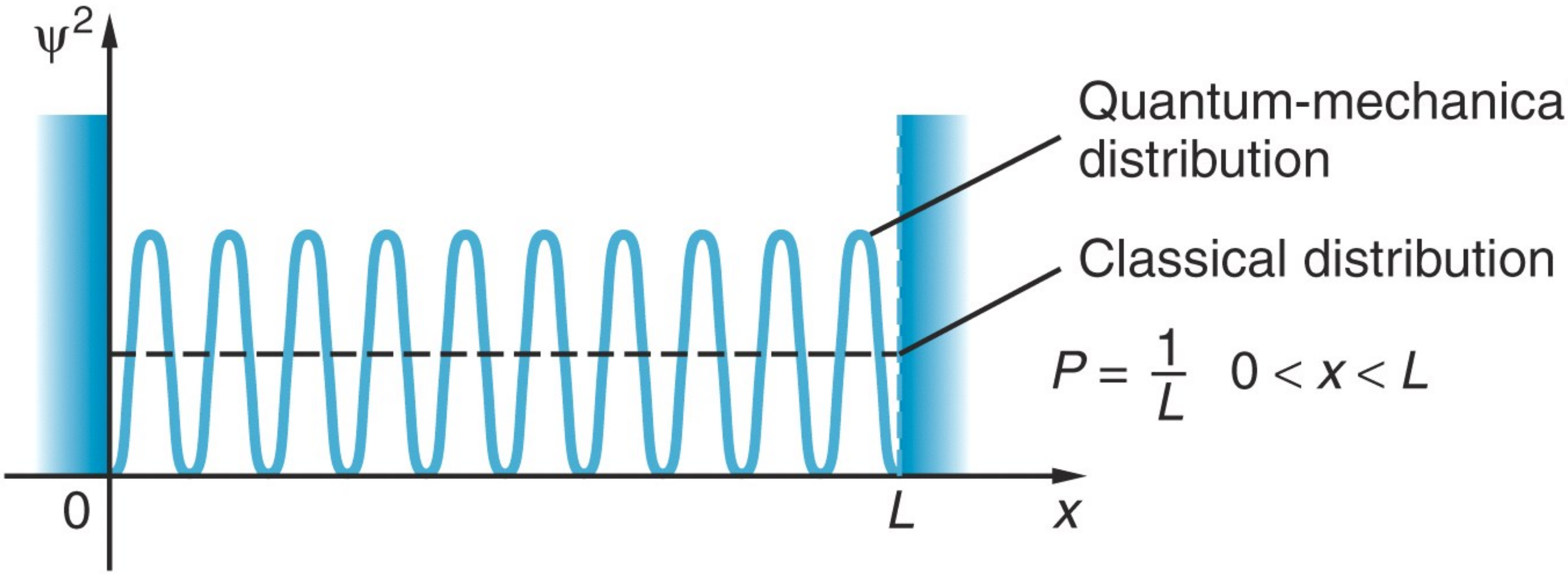
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin\frac{2\pi}{L}\cdot\frac{3L}{4} - \sin\frac{2\pi}{L}\cdot\frac{L}{4}\right)$$

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

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

$\Rightarrow$ Substantial difference between Classical & Quantum predictions

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



But one issue is irreconcilable:

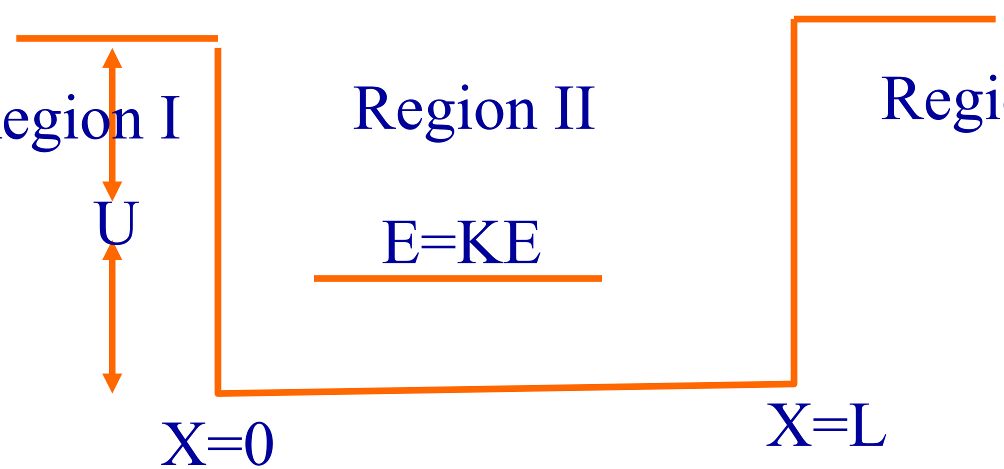
Quantum Mechanically the particle can not have $E = 0$

This is a consequence of the Uncertainty Principle

The particle moves around with KE inversely proportional to the Length Of the 1D Box

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

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

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

$$=\alpha^2\psi(x);\ \alpha=\sqrt{\frac{2\mathrm{m(U\text{-}E)}}{\hbar^2}}$$

$\Rightarrow$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)

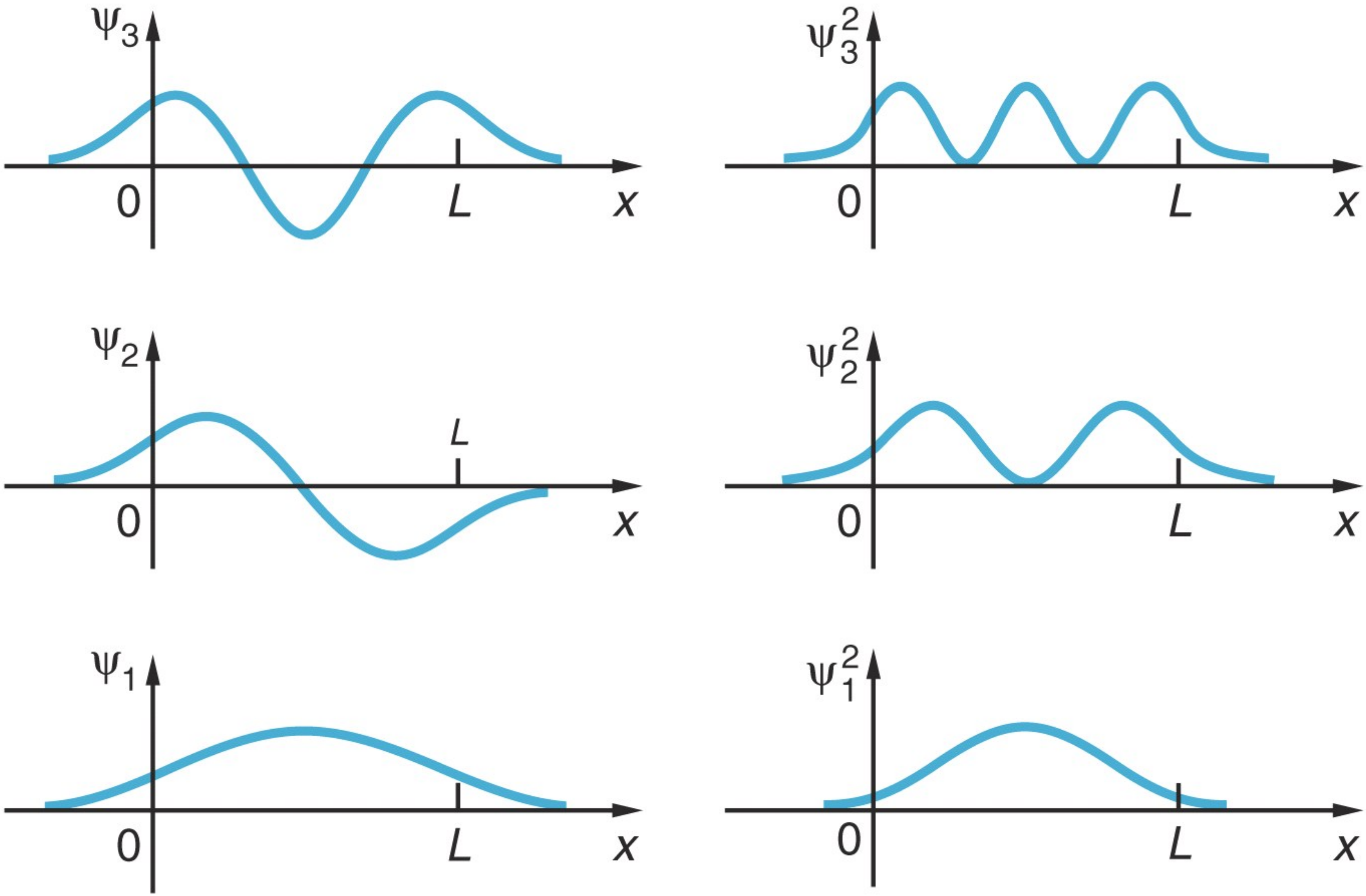
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

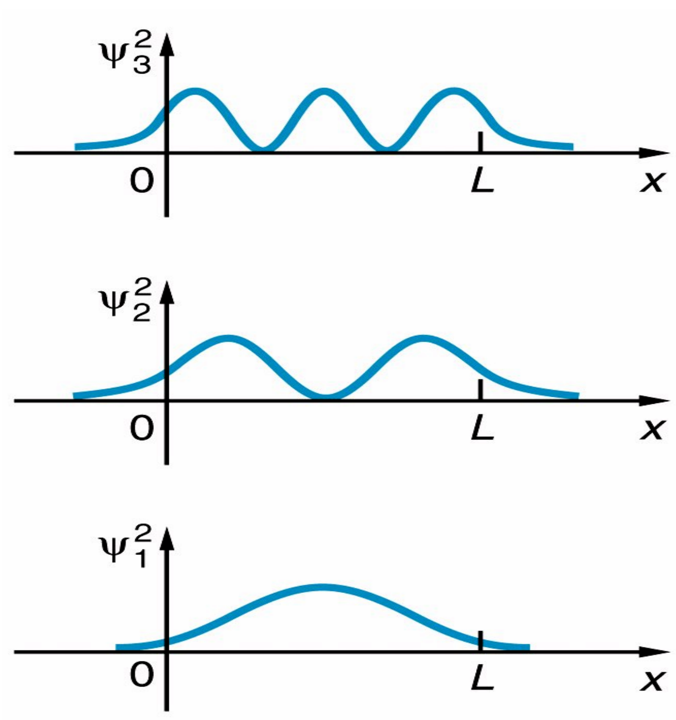
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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 $\Delta E = U\text{-}E + KE$

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)

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

If $U >> E \Rightarrow$ Tiny penetration

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

Finite Potential Well: Particle can Burrow Outside Box

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

If U>>E $\Rightarrow$ Tiny penetration

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

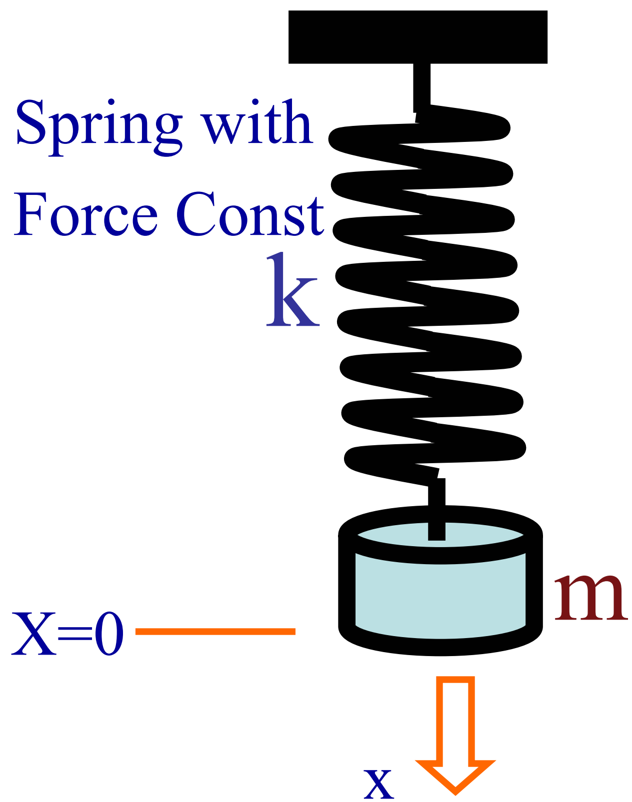
$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4...$$

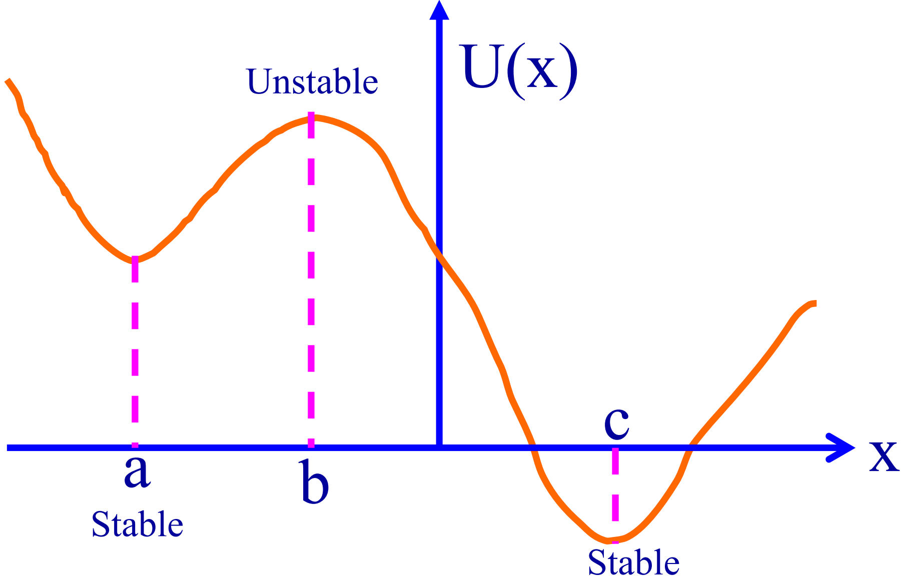
When E=U then solutions blow up

$\Rightarrow$ 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 equilibirium position, motion confined between x=0 & x=A

$U(x) = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2; \omega = \sqrt{\frac{k}{m}} = Ang.\ Freq$

$E = \frac{1}{2}kA^2 \Rightarrow$ Changing A changes E

E can take any value & if $A \to 0$, $E \to 0$

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 $U(x)=\frac{1}{2}m\omega^2x^2$

Time Dependent Schrodinger Eqn: $\boxed{\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x}+\frac{1}{2}m\omega^2x^2\psi(x)=E\ \psi(x)}$

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

Two guesses about the simplest Wavefunction:

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

$+\ \psi(x)$ should be continuous & $\frac{d\psi(x)}{dx}$ = continuous

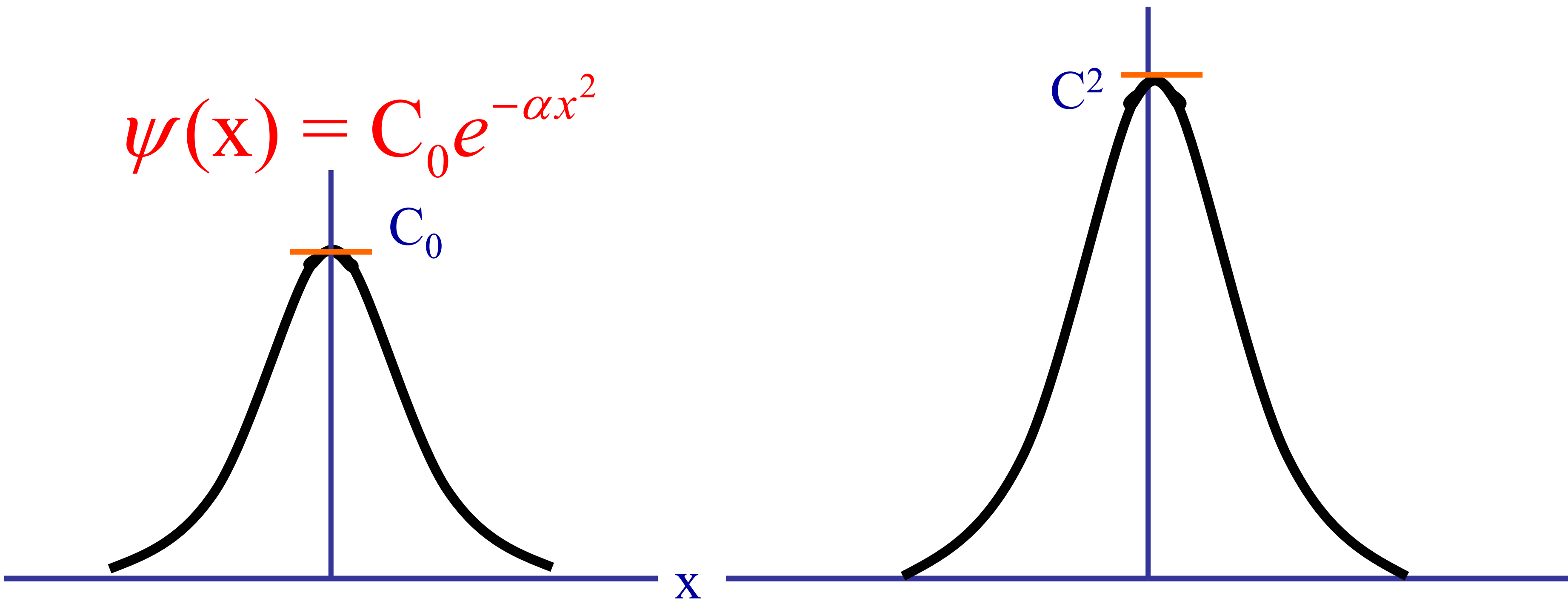
My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

$$\psi(x) = C_0 e^{-\alpha x^2}$$

$$P(x) = C^2{}_0 e^{-2\alpha x^2}$$



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

Time Independent Sch. Eqn & The Harmonic Oscillator

Master Equation is : $\frac{\partial^2\psi(x)}{\partial x^2} = \frac{2m}{\hbar^2}[\frac{1}{2}m\omega^2x^2 - E]\psi(x)$

Since $\psi(x) = C_0 e^{-\alpha x^2}$, $\frac{d\psi(x)}{dx} = C_0(-2\alpha x)e^{-\alpha x^2}$,

$$\frac{d^2\psi(x)}{dx^2} = C_0\frac{d(-2\alpha x)}{dx}e^{-\alpha x^2} + C_0(-2\alpha x)^2 e^{-\alpha x^2} = C_0[4\alpha^2x^2 - 2\alpha]e^{-\alpha x^2}$$

$$\Rightarrow C_0[\boxed{4\alpha^2x^2} - \boxed{2\alpha}]e^{-\alpha x^2} = \frac{2m}{\hbar^2}[\boxed{\frac{1}{2}m\omega^2x^2} - E]C_0e^{-\alpha x^2}$$

Match the coeff of x^2 and the Constant terms on LHS & RHS

$$\Rightarrow 4\alpha^2 = \frac{2m}{\hbar^2}\frac{1}{2}m\omega^2 \text{ or } \alpha = \frac{m\omega}{2\hbar}$$

& the other match gives $2\alpha = \frac{2m}{\hbar^2}E$, substituing $\alpha \Rightarrow$

$$\boxed{E = \frac{1}{2}\hbar\omega = hf \quad \text{!!!!......(Planck's Oscillators)}}$$

What about C_0? We learn about that from the Normalization cond.

SHO: Normalization Condition

$$\int_{-\infty}^{+\infty} |\psi_0(x)|^2\, dx = 1 = \int_{-\infty}^{+\infty} C_0^2 e^{\frac{-m\omega x^2}{\hbar}}\, dx$$

Since $\int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$ (dont memorize this)

Identifying $a = \frac{m\omega}{\hbar}$ and using the identity above

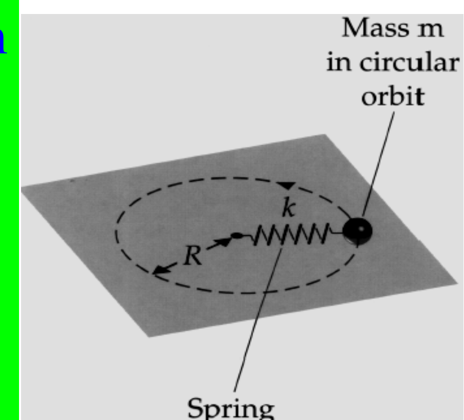
$$\Rightarrow \qquad C_0 = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}}$$

Hence the Complete NORMALIZED wave function is :

$$\boxed{\psi_0(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} e^{\frac{-m\omega x^2}{2\hbar}}}$$ Ground State Wavefunction

has energy E = hf

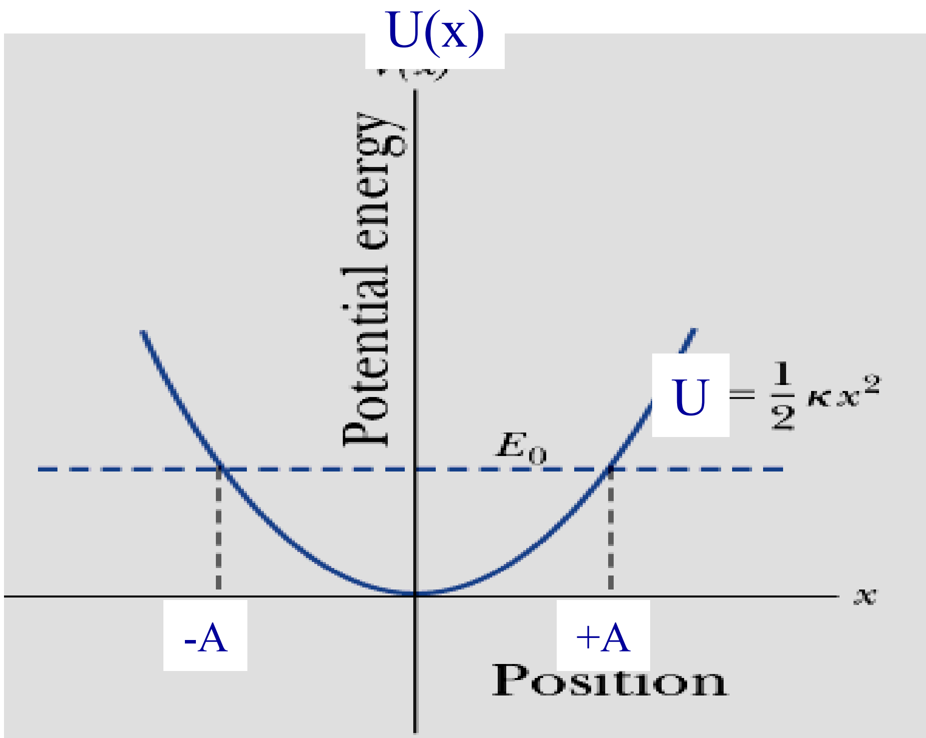
Planck's Oscillators were electrons tied by the "spring" of the mutually attractive Coulomb Force

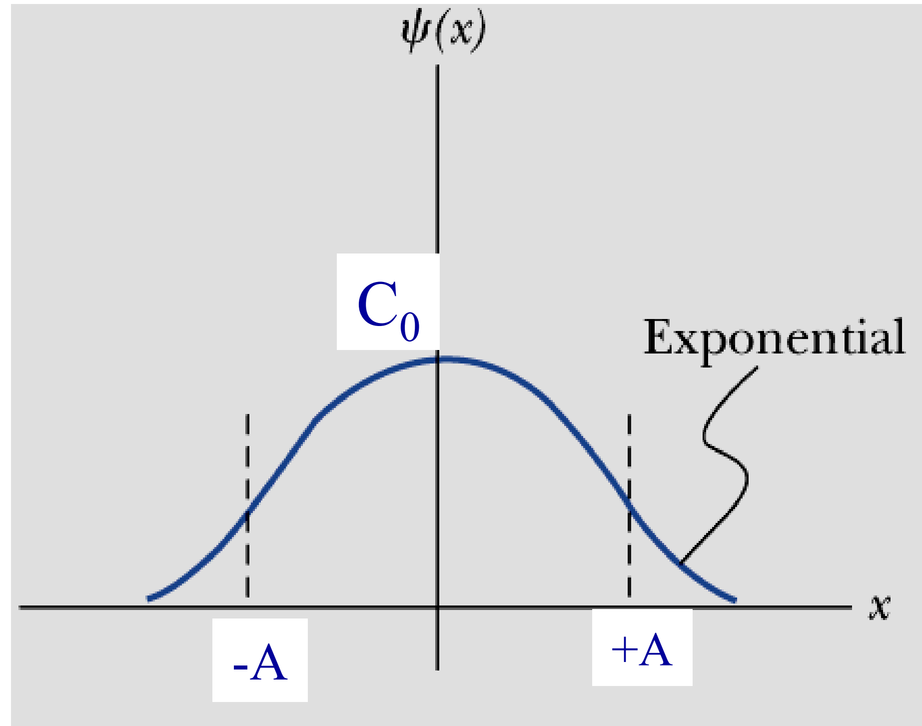


Quantum Oscillator In Pictures

$E = KE + U(x) > 0$ for n=0

Quantum Mechanical Prob for particle
To live outside classical turning points
Is finite !





Classically particle most likely to be at the turning point (velocity=0)
Quantum Mechanically , particle most likely to be at $x=x_0$ for n=0

Classical & Quantum Pictures of SHO compared

- Limits of classical vibration : Turning Points (do on Board)
- Quantum Probability for particle outside classical turning points $P(|x|>A) = 16\%$!!
  - Do it on the board (see Example problems in book)

Excited States of The Quantum Oscillator

$$\psi_n(x) = C_n H_n(x)\, e^{-\frac{m\omega x^2}{2\hbar}}\ ;$$

$H_n(x) =$ Hermite Polynomials

with

$H_0(x)=1$

$H_1(x)=2x$

$H_2(x)=4x^2-2$

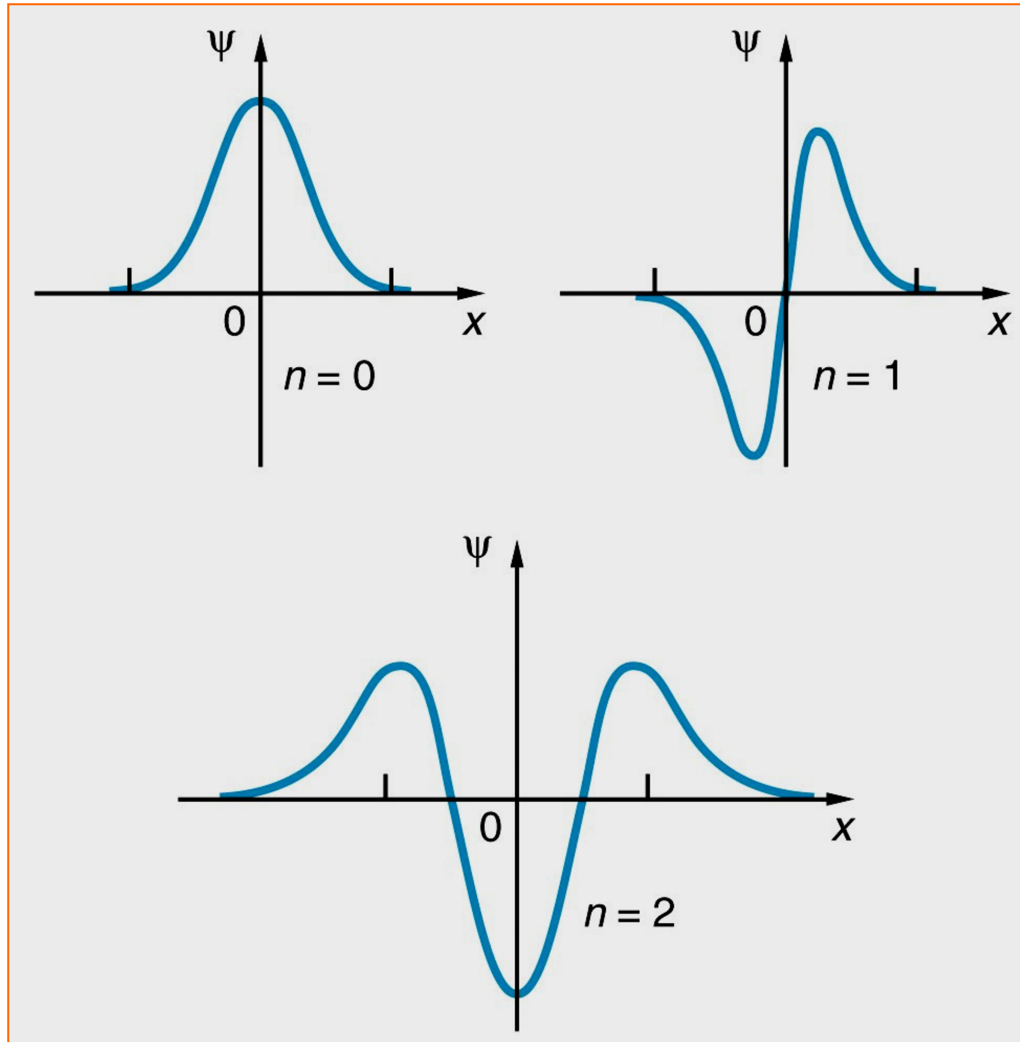
$H_3(x)=8x^3-12x$

$$H_n(x)=(-1)^n e^{x^2}\frac{d^n e^{-x^2}}{dx^n}$$

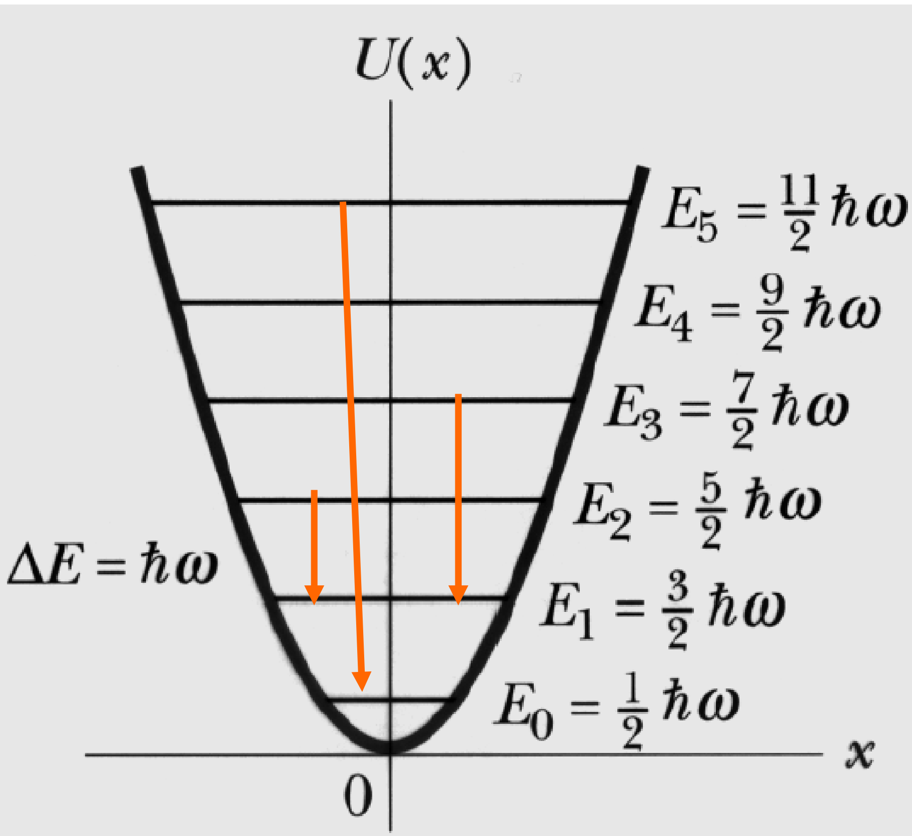
and

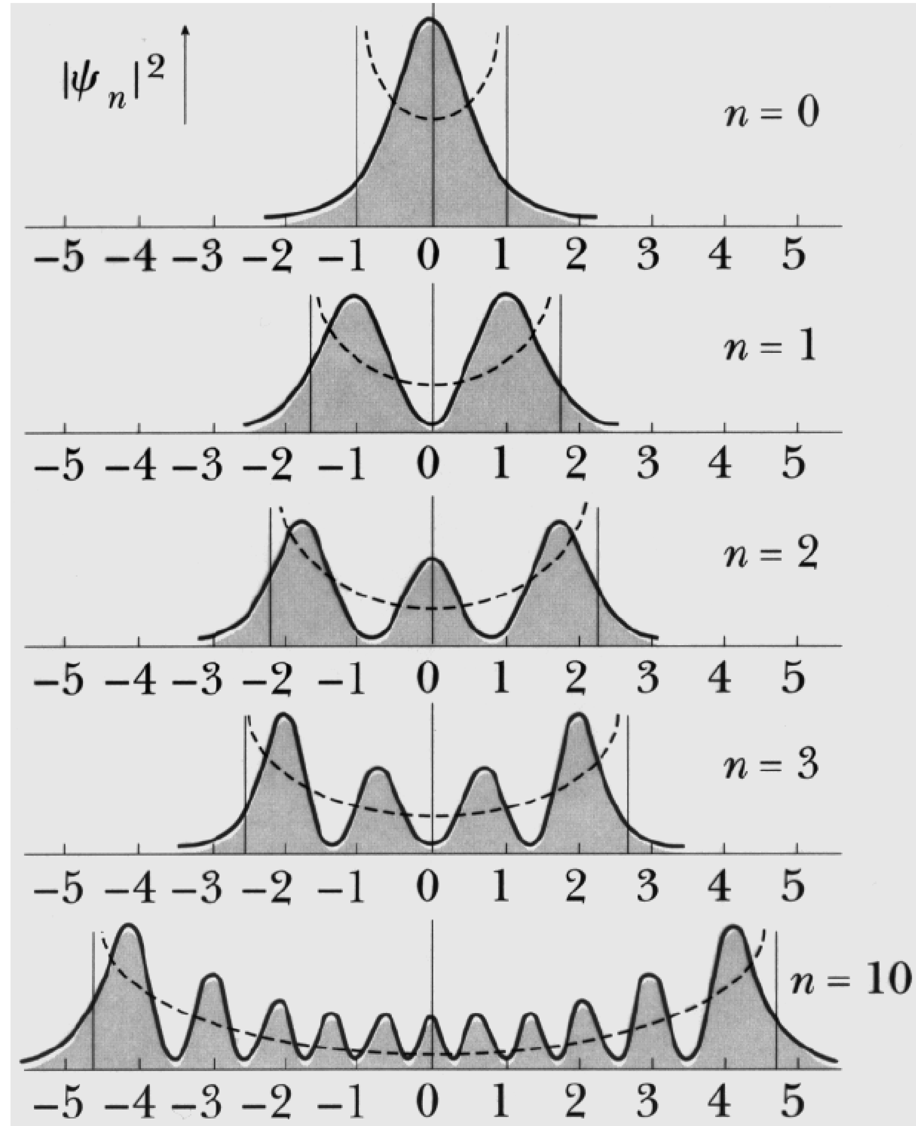
$$E_n = (n+\frac{1}{2})\hbar\omega = (n+\frac{1}{2})hf$$

Again n=0,1,2,3...∞ Quantum #



Excited States of The Quantum Oscillator





Ground State Energy >0 always

Measurement Expectation: Statistics Lesson

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

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

For a general Fn f(x)

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

Sharpness of A Distr:

Scatter around average

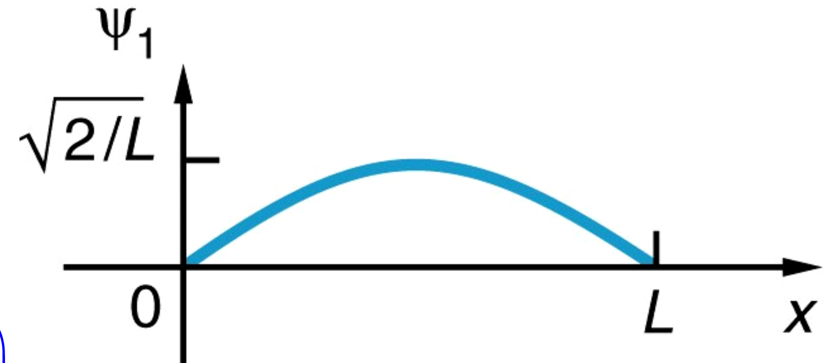
$$\sigma = \sqrt{\frac{\sum (\mathrm{x_i} - \bar{x})^2}{N}}$$

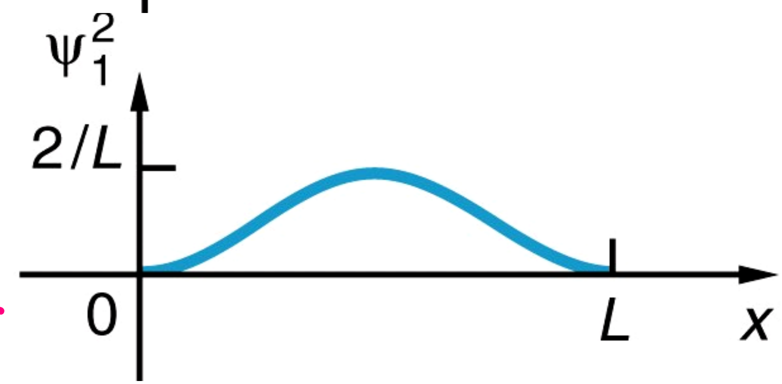
$$\sigma = \sqrt{(\overline{x^2}) - (\bar{x})^2}$$

$\sigma =$ small $\rightarrow$ Sharp distr.

Uncertainty $\Delta X = \sigma$

Particle in the Box, n=1, <x> & Δx ?





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

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

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

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

$$\Rightarrow \langle x\rangle=\frac{2L}{2\pi^2}\left[\int_0^{\pi}\theta d\theta - \int_0^{\pi}\theta\cos 2\theta d\theta\right]$$ use $\int udv=uv-\int$

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

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

and $\Delta X=\sqrt{\langle x^2\rangle-\langle x\rangle^2}=\sqrt{\frac{L^2}{3}-\frac{L^2}{2\pi^2}-\frac{L^2}{4}}=.18L$

ΔX= 20% of L, Particle not sharply confined in Box