Physics 2D Lecture Slides
Feb 26

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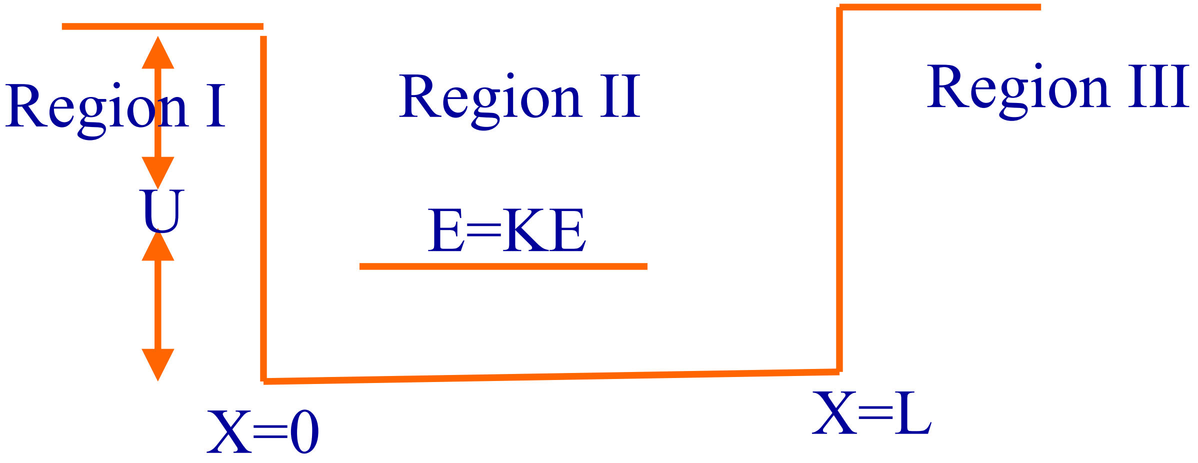
Finite Potential Barrier

- 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

Schrodinger Eq :

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

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

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

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

Require finiteness of $\psi(x)$

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

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

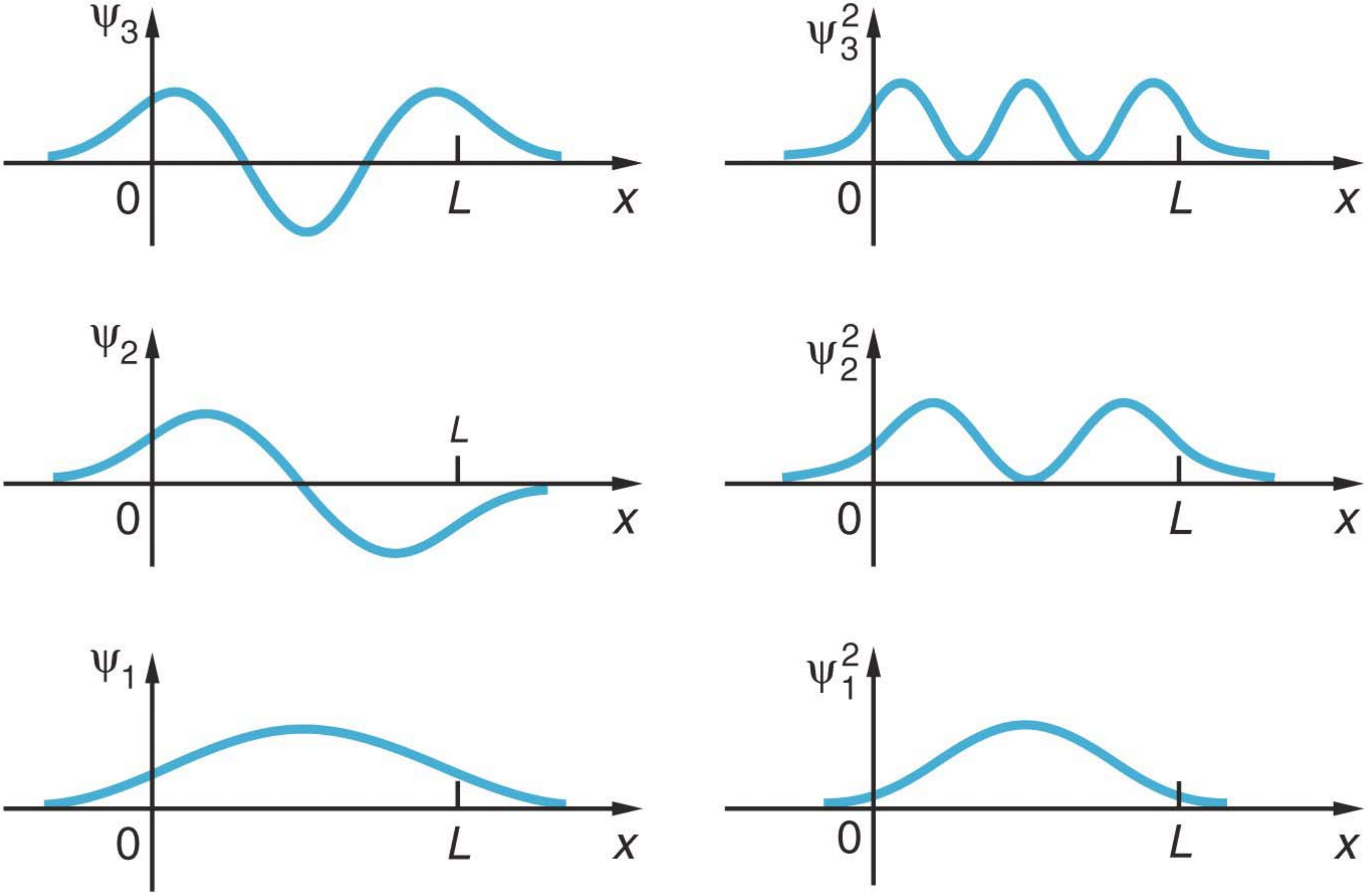
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

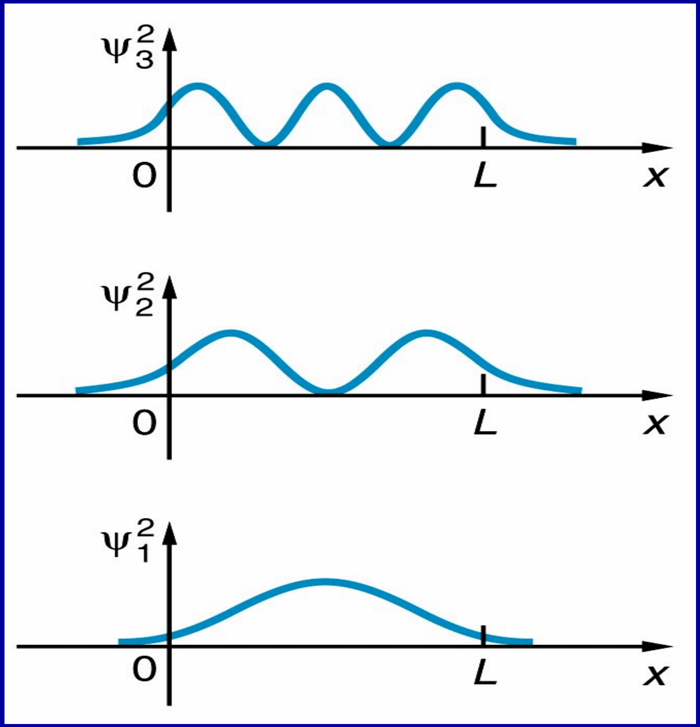
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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 $\Delta E = U - E + KE$

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)

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

$$\text{If } U >> E \Rightarrow \text{ Tiny penetration}$$

$$\text{If } U \to \infty \Rightarrow \delta \to 0$$

Finite Potential Well: Particle can Burrow Outside Box

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

If U>>E $\Rightarrow$ Tiny penetration

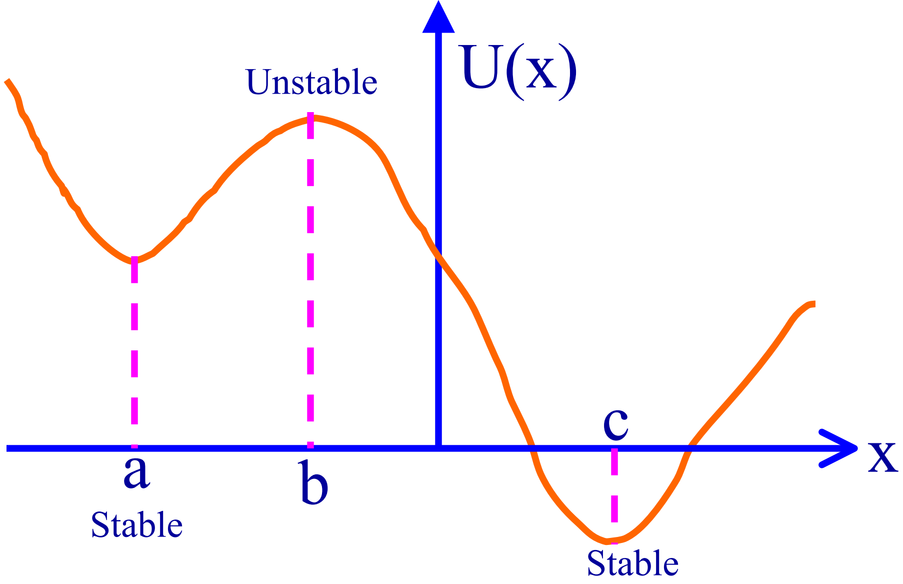
If U $\rightarrow \infty \Rightarrow \delta \rightarrow 0$

$$\text{E}_\text{n} = \frac{\text{n}^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4\ldots$$

When E=U then solutions blow up

$\Rightarrow$ Limits to number of bound states($\text{E}_\text{n} < U$)

When E>U, particle is not bound and can get either reflected or transmitted across the potential "barrier"



Particle of mass m within a potential U(x)

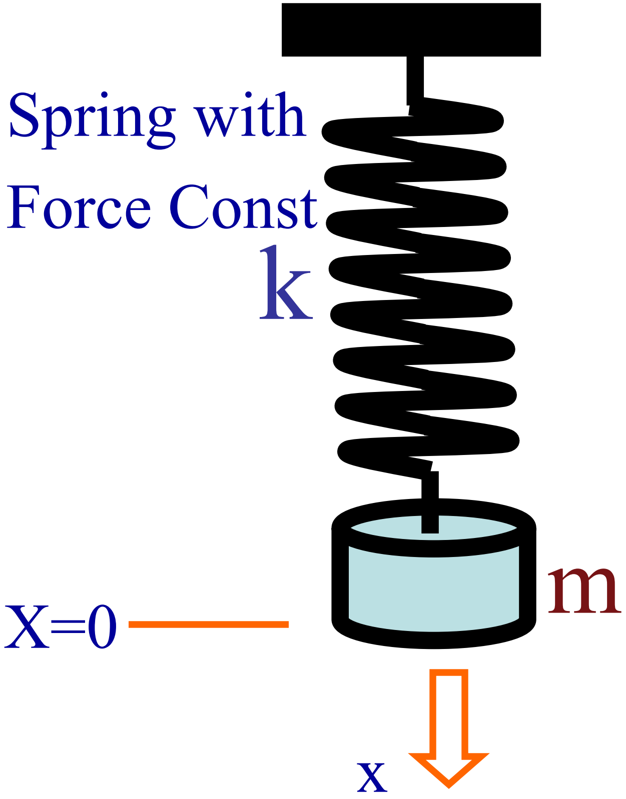
$$\vec{F}(x) = -\frac{dU(x)}{dx}$$

$$\vec{F}(x=a) = -\left.\frac{dU(x)}{dx}\right| = 0,$$

$\vec{F}(x=b) = 0$, $\vec{F}(x=c)=0$ ...But...

look at the Curvature:

$\frac{\partial^2 U}{\partial x^2} > 0$ (stable), $\frac{\partial^2 U}{\partial x^2} < 0$ (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

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

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

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

Max. KE at x = 0, KE= 0 at x= ± A

Quantum Picture: Harmonic Oscillator

Find the Ground state Wave Function $\psi(\mathrm{x})$

Find the Ground state Energy E when $\mathrm{U(x)}=\frac{1}{2}m\omega^2x^2$

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

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

Two guesses about the simplest Wavefunction:

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

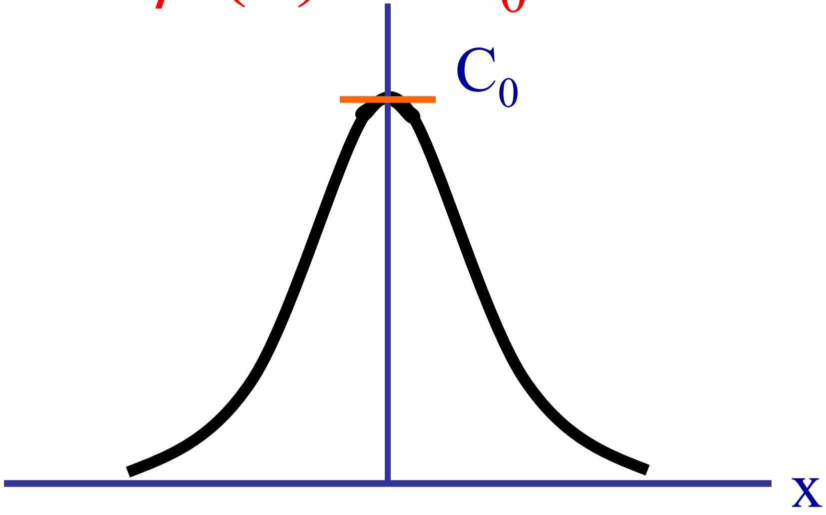
\+ $\psi(\mathrm{x})$ should be continuous & $\frac{d\psi(\mathrm{x})}{dx}$ = continuous

My guess: $\psi(\mathrm{x}) = \mathrm{C}_0 e^{-\alpha x^2}$; Need to find C_0 & α:

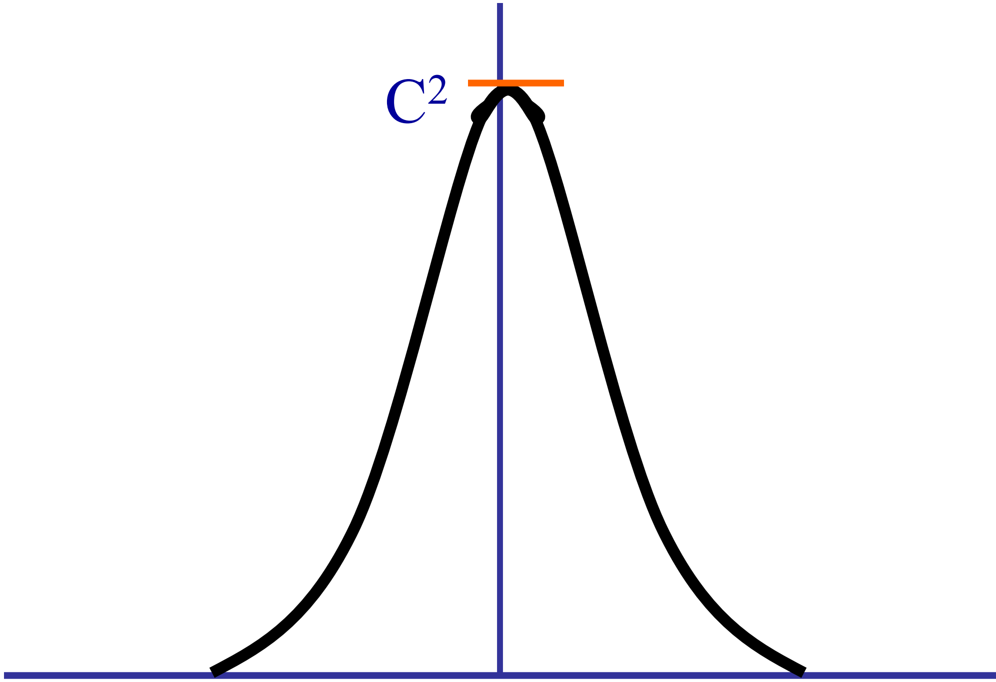
What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

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



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



How to Get C_0 & α ?? …Try plugging in the Wavefunction into Time-Independent Schr. Eqn.

Time Independent Sch. Eqn & The Harmonic Oscillator

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

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

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

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

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

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

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

$\boxed{E = \frac{1}{2}\hbar\omega = hf}$!!!!....same as in last quiz (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)

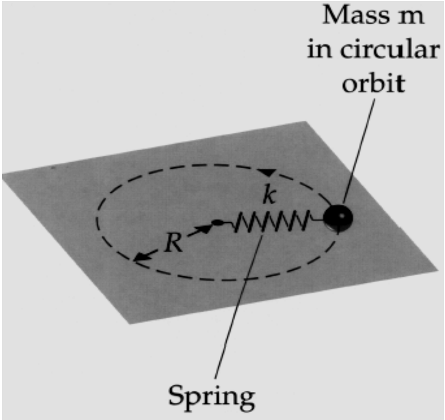
Identifying $a = \frac{m\omega}{\hbar}$ and using the identity above

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

Hence the Complete NORMALIZED wave function is :

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

has energy E = hf

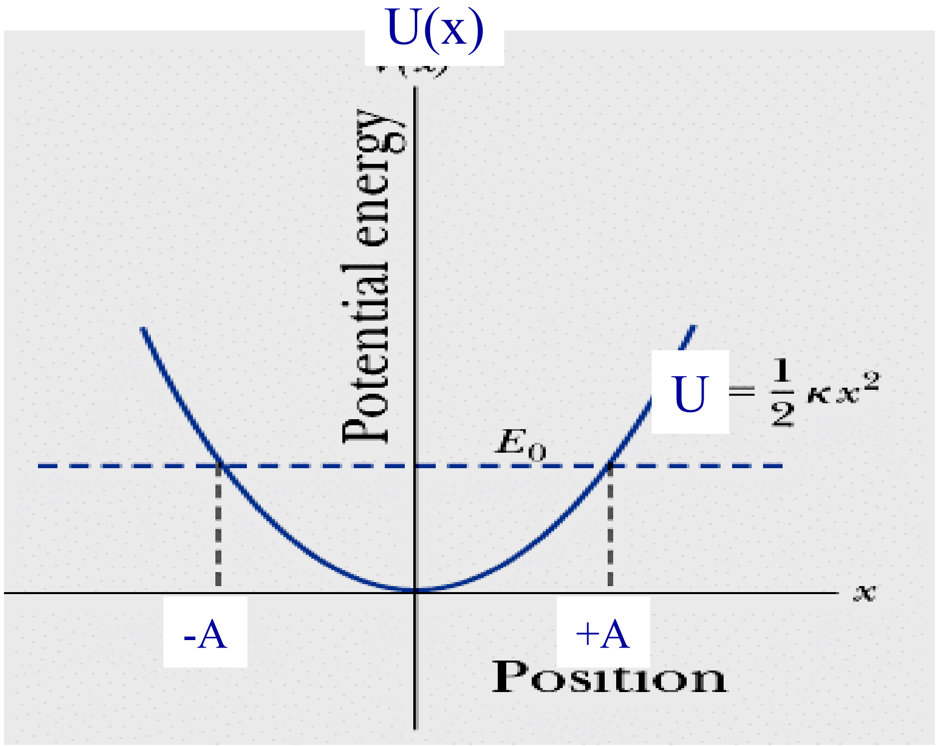


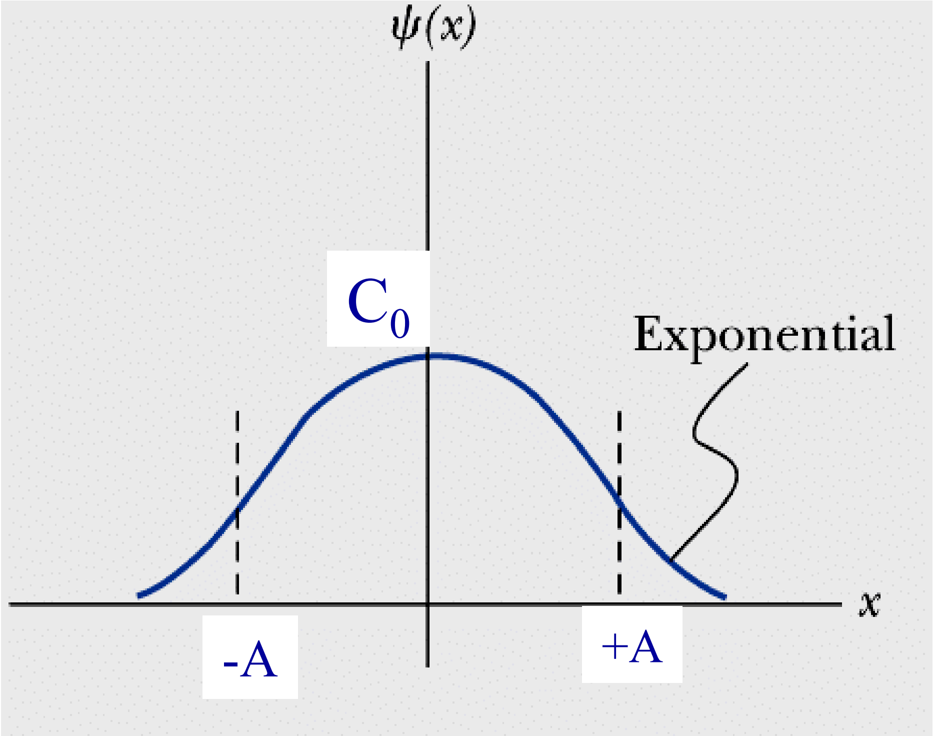
Planck's Oscillators were electrons tied by the "spring" of the mutually attractive Coulomb Force

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

$H_0(x)=1$

$H_1(x)=2x$

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

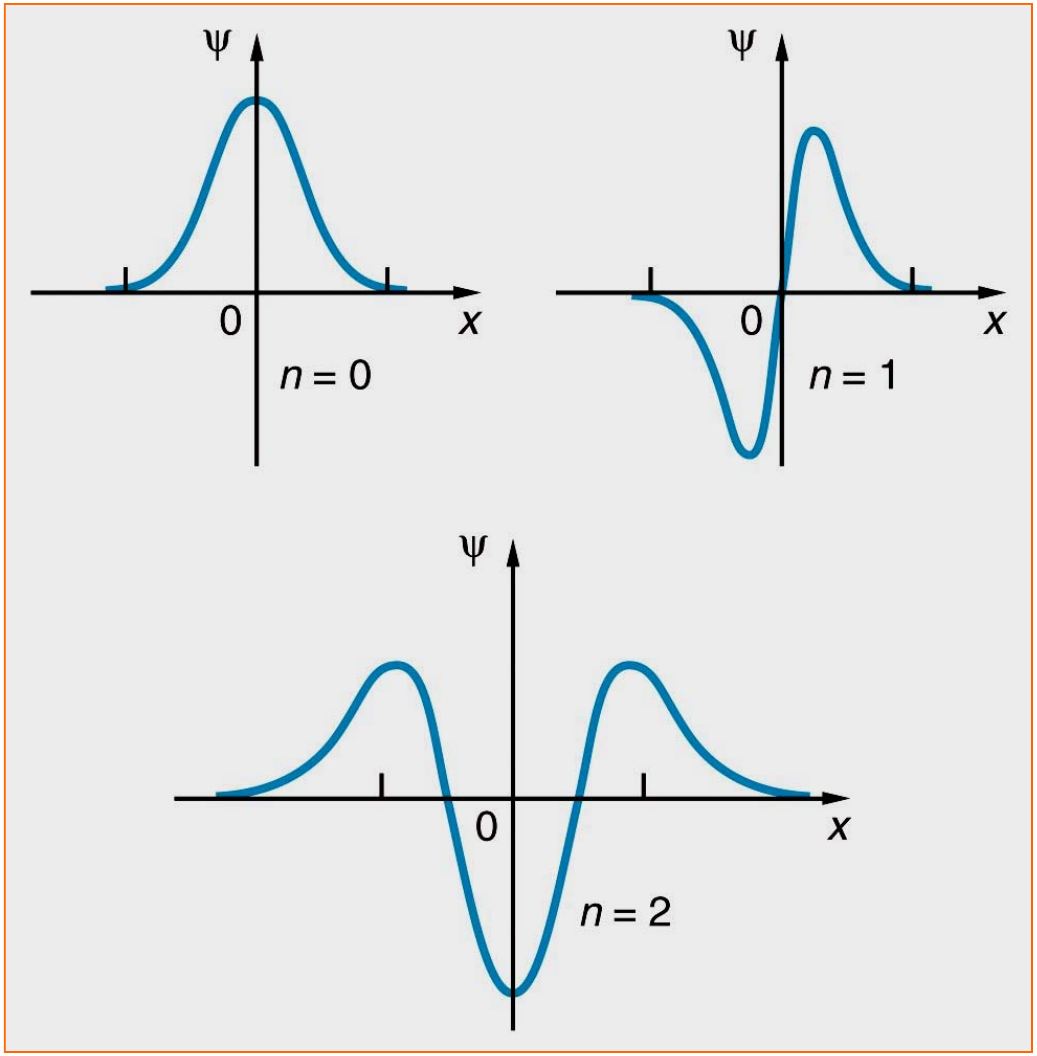
$H_3(x)=8x^3-12x$

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

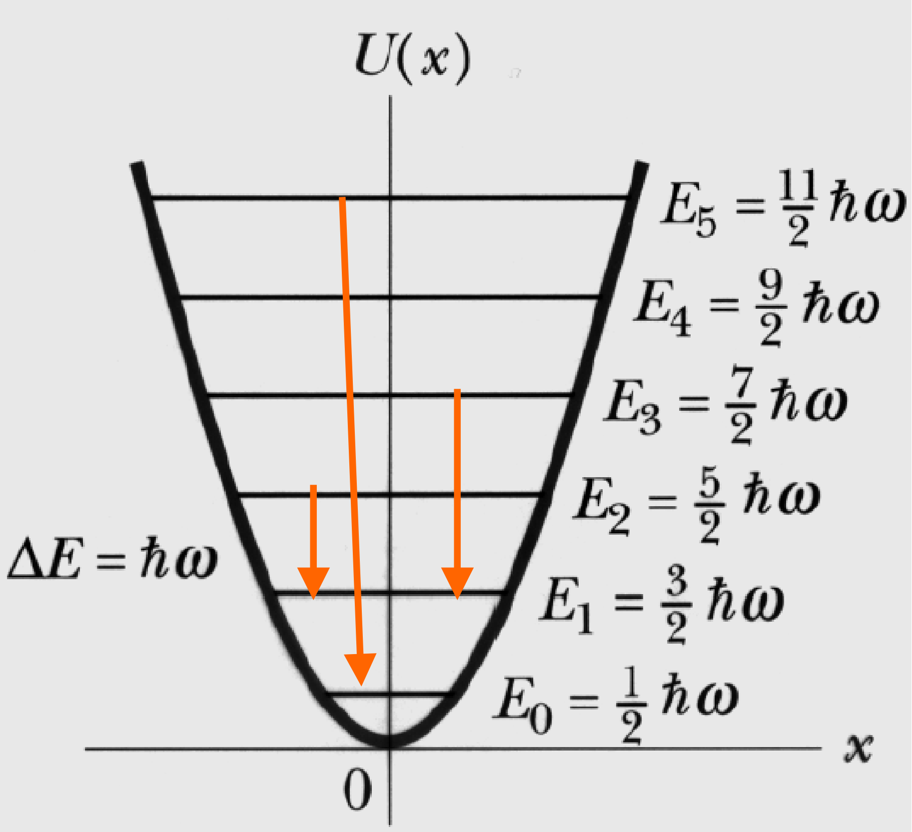
and

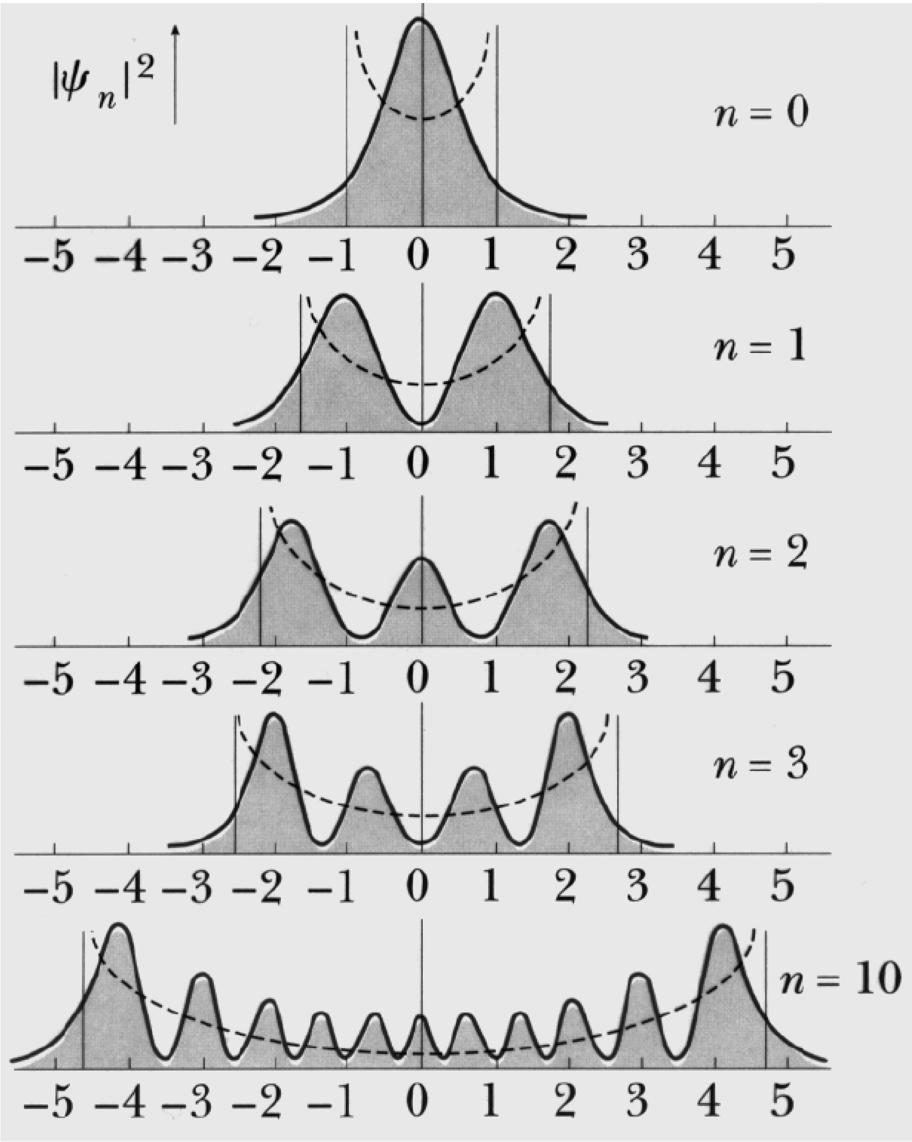
$$\boxed{E_n = (n+\frac{1}{2})\hbar\omega = (n+\frac{1}{2})hf}$$

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

$$< x >= \frac{n_1x_1 + n_2x_2 + n_3x_3 + \ldots .n_ix_i}{n_1 + n_2 + n_3 + \ldots n_i} = \frac{\sum_{i=1}^{n} n_ix_i}{N} = \frac{\int_{-\infty}^{\infty} xP(x)dx}{\int_{-\infty}^{\infty} P(x)dx}$$

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

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

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

σ = small → Sharp distr.

Uncertainty $\Delta X = \sigma$

Particle in the Box, n=1, <x> & Δx ?

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

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

$$=\frac{2}{\mathrm{L}}\int_{0}^{L}x\sin^2\left(\frac{\pi}{L}x\right)dx \quad \text{, change variable } \theta=\left(\frac{\pi}{L}x\right)$$

$$\Rightarrow <\mathrm{x}>=\frac{2}{\mathrm{L}\pi^2}\int_{0}^{\pi}\theta\sin^2\theta \quad \text{, use } \sin^2\theta=\frac{1}{2}(1-\cos 2\theta)$$

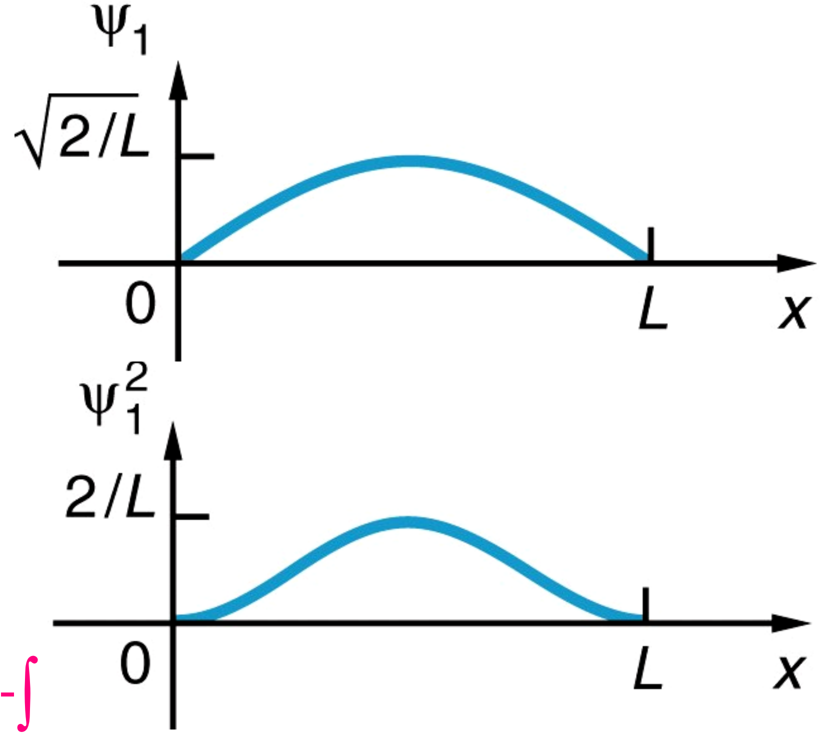
$$\Rightarrow <\mathrm{x}>=\frac{2\mathrm{L}}{2\pi^2}\left[\int_{0}^{\pi}\theta d\theta\ -\ \int_{0}^{\pi}\theta\cos 2\theta d\theta\right] \quad \text{use } \int \mathrm{udv=uv-}\int$$

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

$$\text{Similarly } <\mathrm{x}^2>=\int_{0}^{\mathrm{L}}\mathrm{x}^2\sin^2\left(\frac{\pi}{L}x\right)dx=\frac{L^2}{3}-\frac{L^2}{2\pi^2}$$

$$\text{and } \Delta\mathrm{X}=\sqrt{<\mathrm{x}^2>-<x>^2}=\sqrt{\frac{L^2}{3}-\frac{L^2}{2\pi^2}-\frac{L^2}{4}}=.18L$$

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



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 in a straightforward way→ gets Expectation value for that observable

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

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

& $<Q>$ is the Expectation value

Examples: $[X] = x$, $\qquad [P] = \frac{\hbar}{i}\frac{d}{dx}$

$$[K] = \frac{[P]^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \qquad [E] = i\hbar\frac{\partial}{\partial t}$$

Table 5.2 Common Observables and Associated Operators

Observable	Symbol	Associated Operator
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	$i\hbar\frac{\partial}{\partial t}$