Physics 2D Lecture Slides
Lecture 22: Feb 22nd 2005

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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.
- → characteristic wavefunctions for a particular U(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

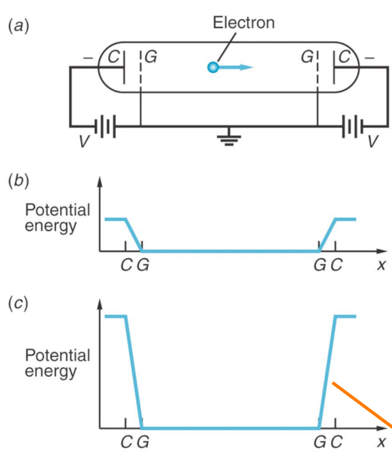
$$\frac{-\hbar^2}{2\text{m}}\frac{\partial^2\psi(x)}{\partial^2 x} + U(x)\psi(x) = E\;\psi(x)$$

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

$$\Psi(x,t) = \psi(x)\phi(t)$$

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

Example of a Particle Inside a Box With Infinite Potential



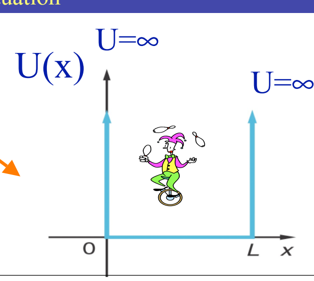
(a) Electron placed between 2 set of electrodes C & grids G experiences no force in the region between grids, which are held at Ground Potential

However in the regions between each C & G is a repelling electric field whose strength depends on the magnitude of V

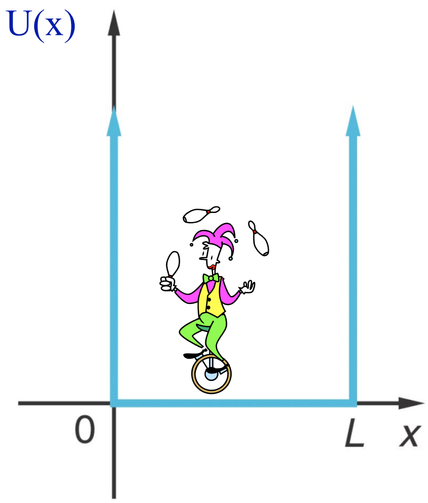
(b) If V is small, then electron's potential energy vs x has low sloping "walls"

(c) If V is large, the "walls"become very high & steep becoming infinitely high for $V\rightarrow\infty$

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



A More Interesting Potential : Particle In a Box



Write the Form of Potential: Infinite Wall

$U(x,t) = \infty; \ x \le 0, \ x \ge L$

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

- 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 ??

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

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

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

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

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

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)

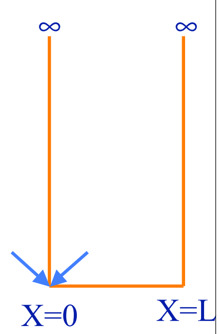
& $\psi(x=L) = 0 \Rightarrow$ A Sin kL = 0 (Continuity condition at x =L)

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

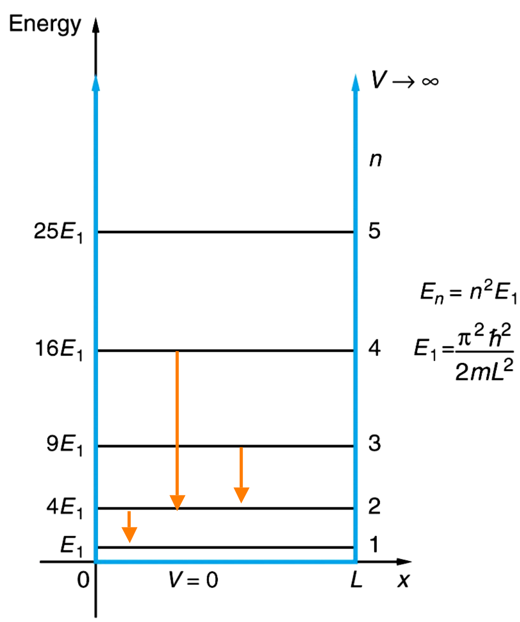
So what does this say about Energy E ? : $\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}}$ Quantized (not Continuous)!

Why can't the particle exist Outside the box ?

→ E Conservation



Quantized Energy levels of Particle in a Box



What About the Wave Function Normalization ?

The particle's Energy and Wavefunction are determined by a number n

We will call n → 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 :

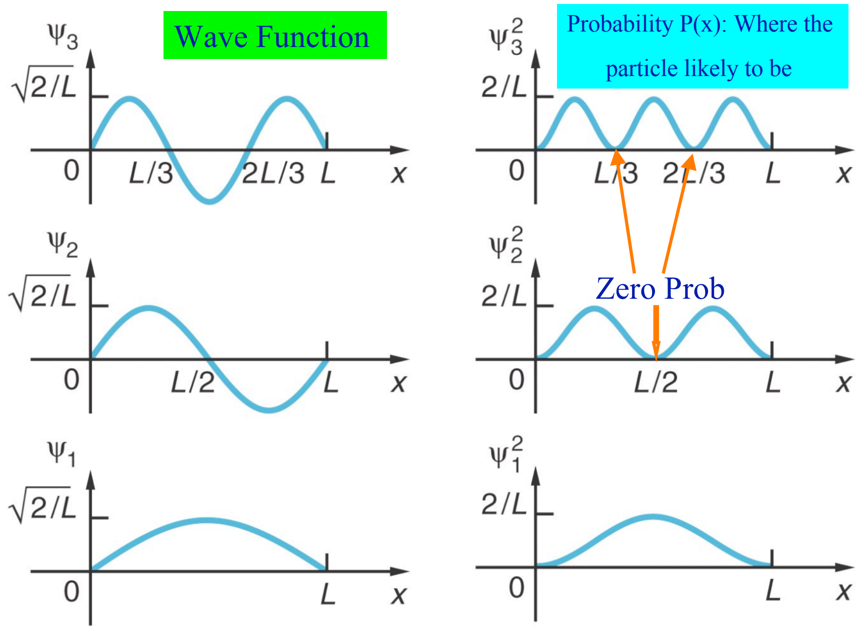
$$1 = \int_0^L \psi_n^* \psi_n dx = A^2 \int_0^L Sin^2(\frac{n\pi x}{L}) \qquad \boxed{\text{Use } 2\text{Sin}^2\theta = 1 - 2Cos2\theta}$$

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

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

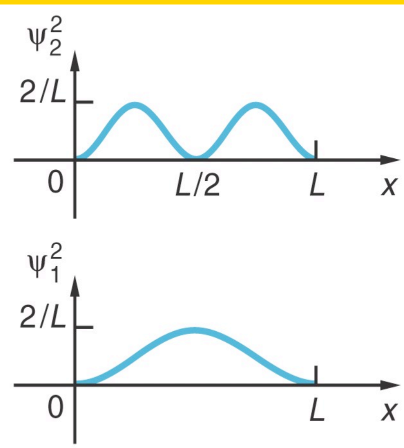
So $\psi_n = \sqrt{\frac{2}{L}}\sin(kx) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$ ...What does this look like?

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

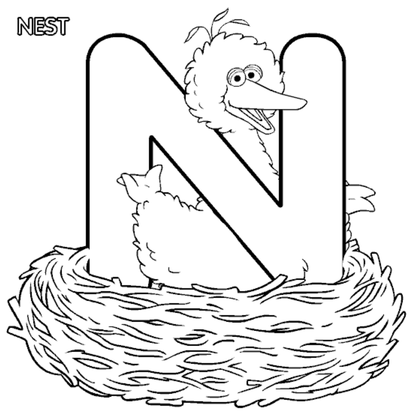


Classically, where is particle most likely to be ?

Equal prob. of being anywhere inside the Box

<u>NOT SO says Quantum Mechanics!</u>

Remember Sesame Street ?



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

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

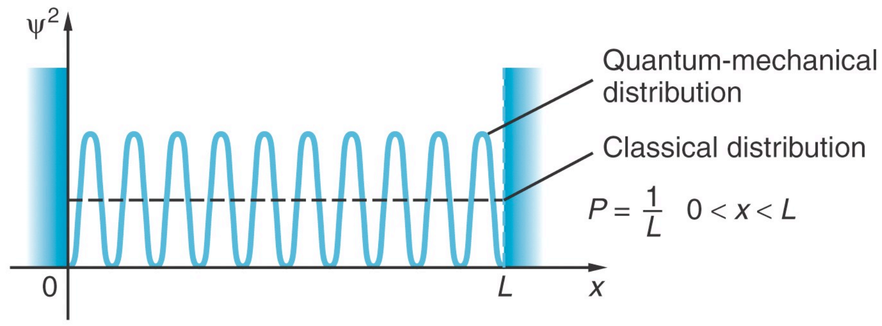
$$P = \frac{1}{L}\left[\frac{L}{2} - \right]\left[\frac{L}{2\pi} \sin \frac{2\pi x}{L}\right]_{L/4}^{3L/4} = \frac{1}{2} - \frac{1}{2\pi}\left(\sin \frac{2\pi}{L} . \frac{3L}{4} - \sin \frac{2\pi}{L} . \frac{L}{4}\right)$$

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

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:

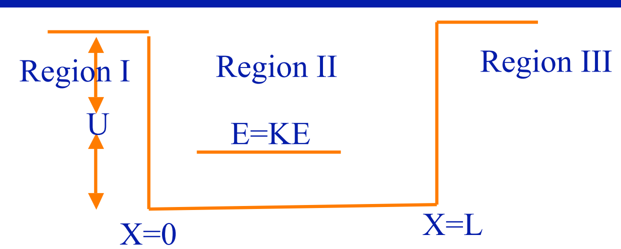
Quantum Mechanically the particle can not have E = 0

This is a 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

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

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

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

$\Rightarrow$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)

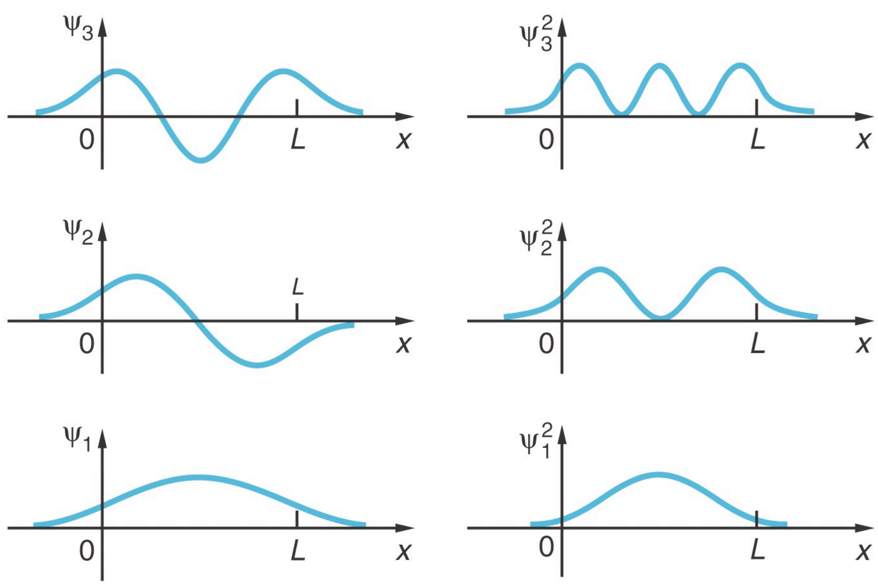
Again, coefficients A & B come from matching conditions at the edge of the walls (x =0, L)

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

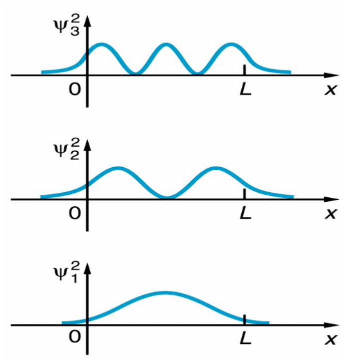
Further require Continuity of $\psi(x)$ and $\frac{d\psi(x)}{dx}$

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 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)

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

If U>>E $\Rightarrow$ Tiny penetration

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

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

If U>>E $\Rightarrow$ Tiny penetration

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

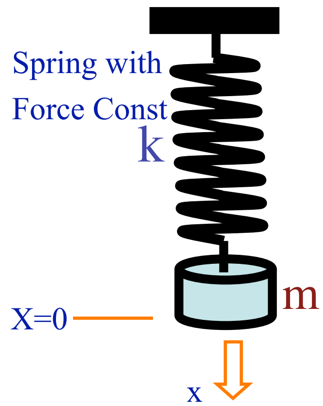
$$E_n = \frac{n^2\pi^2\hbar^2}{2m(L+2\delta)^2}, n = 1, 2, 3, 4...$$

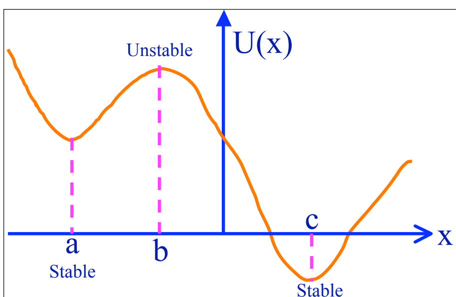
When E=U then solutions blow up

$\Rightarrow$ 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)

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

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

$\vec{F}(x=b) = 0$, $\vec{F}(x=c) = 0$ ...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 equilibrium 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: $\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x}+\frac{1}{2}m\omega^2x^2\psi(x)=E\ \psi(x)$

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

Two guesses about the simplest Wavefunction:

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

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

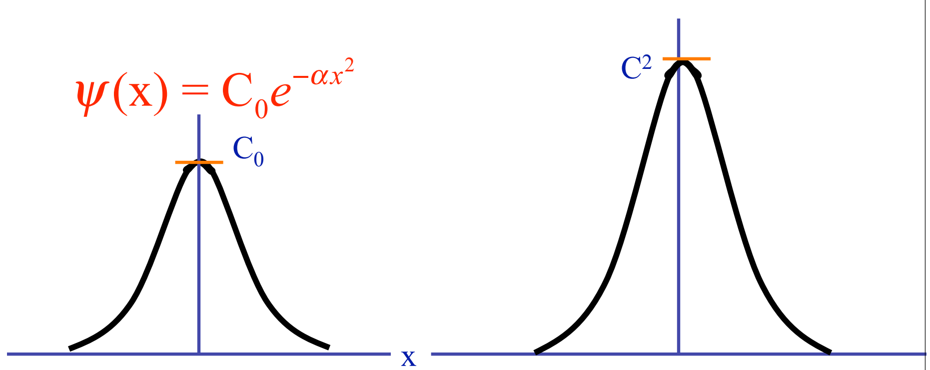
My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

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

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



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

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

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

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

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

& 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

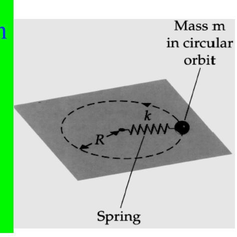
$$\Rightarrow \qquad C_0 = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}}$$

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

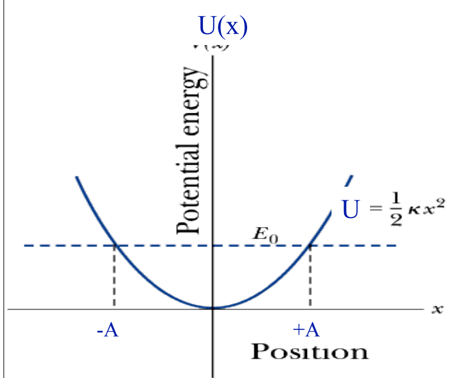
Planck's Oscillators were electrons tied by the "spring" of the mutually attractive Coulomb Force

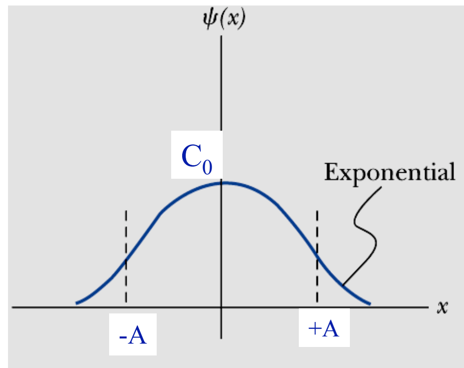


Quantum Oscillator In Pictures

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

$H_0(x)=1$

$H_1(x)=2x$

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

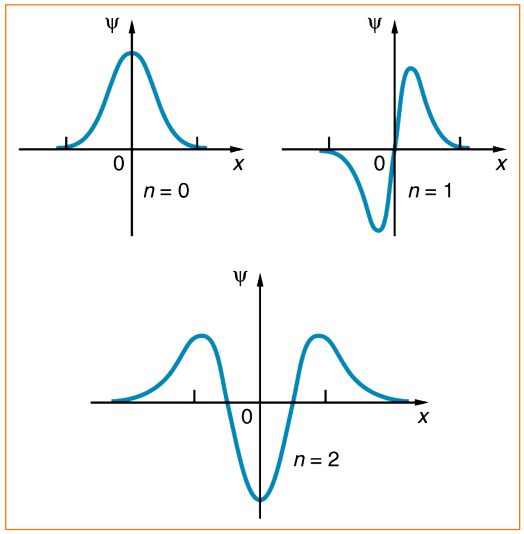
$H_3(x)=8x^3-12x$

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

and

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

Again n=0,1,2,3...∞ Quantum #



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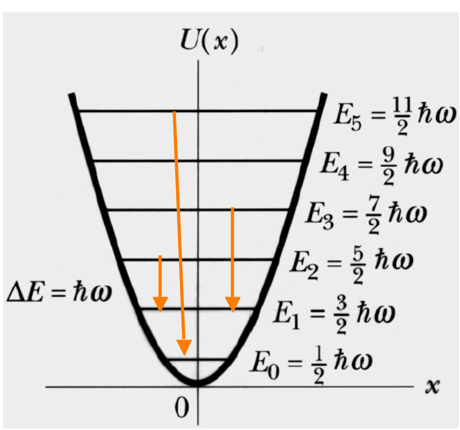

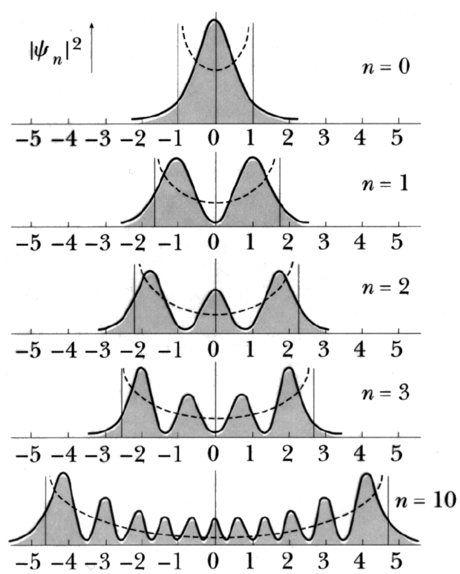

Ground State Energy >0 always