4E : The Quantum Universe

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Measurement Expectation: Statistics Lesson

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

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

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 $\rightarrow$ Sharp distr.

Uncertainty ΔX = σ

Particle in the Box, n=1, find <x> & Δx ?

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

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

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

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

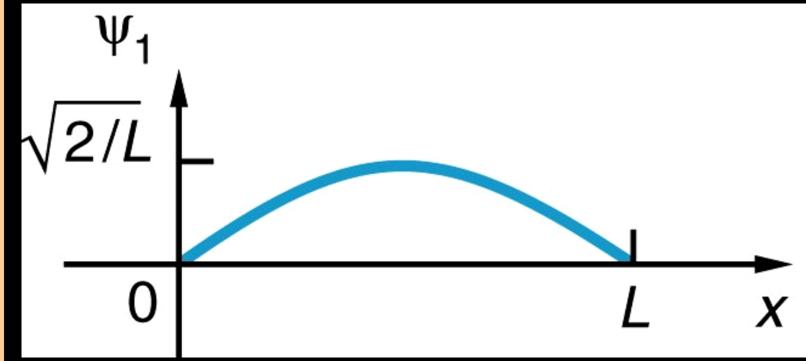
$$\Rightarrow <x>=\frac{2L}{2\pi^2}\left[\int_0^{\pi}\theta d\theta \;-\; \int_0^{\pi}\theta\cos 2\theta d\theta\right] \quad \text{use } \int udv=uv-\int vdu$$

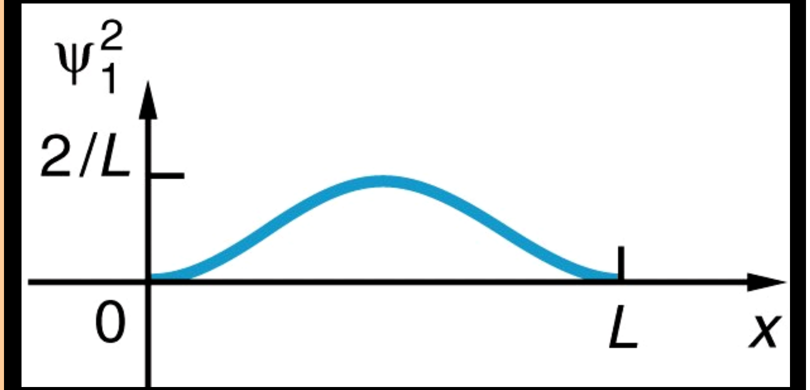
$$\Rightarrow <x>=\frac{L}{\pi^2}\left(\frac{\pi^2}{2}\right)=\frac{L}{2} \quad \text{(same result as from graphing } \psi^2(x))$$

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

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

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 about the Observable 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: $[X] = x$, $[P] = \frac{\hbar}{i}\frac{d}{dx}$

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

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	$i\hbar\frac{\partial}{\partial t}$

Operators → Information Extractors

Plug & play form

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

gives the value of average mometum in the following way:

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

Similerly :

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

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

Similerly

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

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

[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]Ψ(x,t) = [E] Ψ(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

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

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

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

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 <p> = 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!

$$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x) \qquad \& \qquad \psi^*_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$$

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

$$< p >= \frac{\hbar}{i}\frac{2}{L}\frac{n\pi}{L}\int_{-\infty}^{\infty} \sin(\frac{n\pi}{L}x)\cos(\frac{n\pi}{L}x)dx$$

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

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

We knew THAT before doing any math !

Quiz 1: What is the <p> for the Quantum Oscillator in its symmetric ground state

Quiz 2: What is the <p> for the Quantum Oscillator in its asymmetric first excited state

But what about the <KE> of the Particle in Box ?

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

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

Why ? What gives ?

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

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

$$<KE> = <\frac{p^2}{2m}> \neq 0 \; ; \quad \text{not} \quad \frac{<p^2>}{2m} \quad !$$

Be careful when being "lazy"

Quiz: what about <KE> 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.

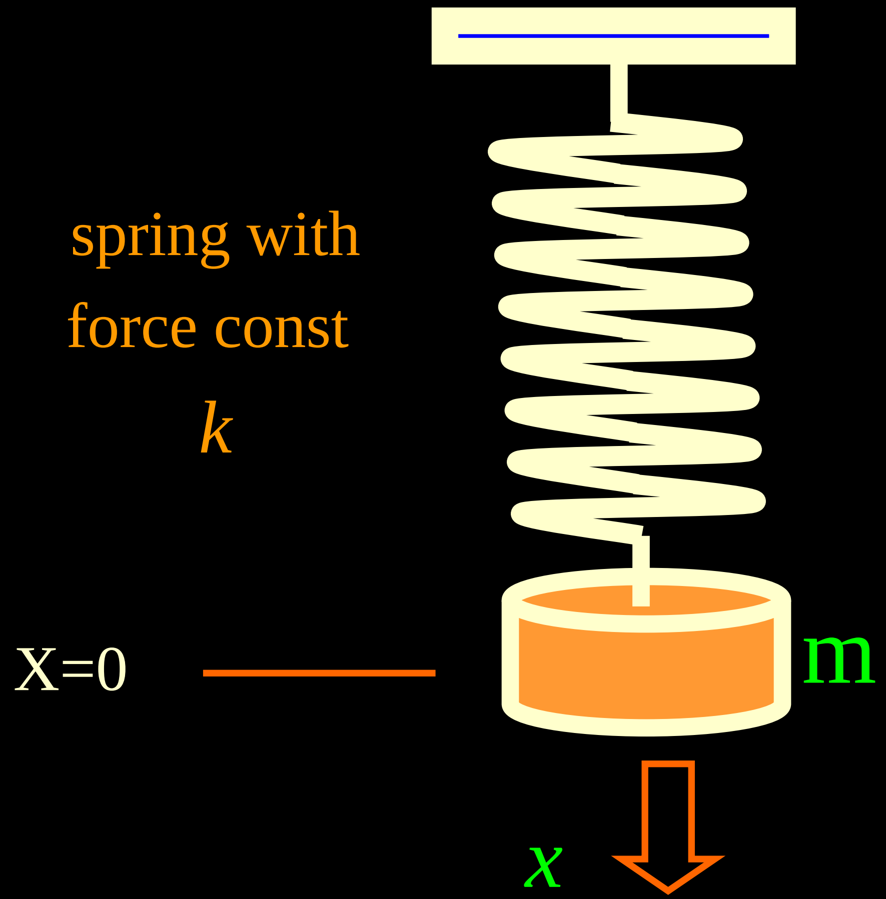
These are called "stationary" states because Prob is independent of time

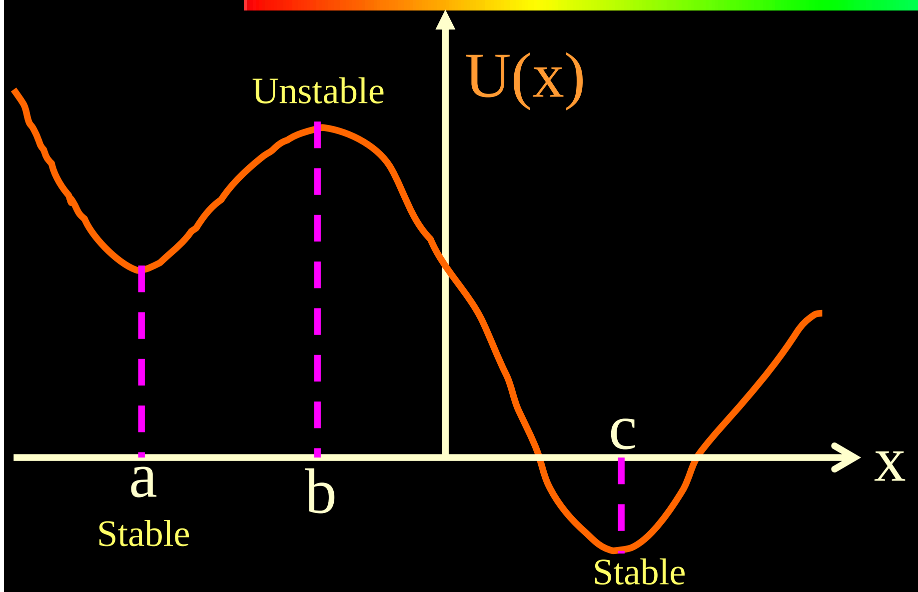
Examples : Particle in a box (why?)

: Quantum Oscillator (why?)

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

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:

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

Stable Equilibrium: General Form :

$$U(x) = U(a) + \frac{1}{2}k(x-a)^2$$

$$\text{Rescale} \Rightarrow U(x) = \frac{1}{2}k(x-a)^2$$

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

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

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

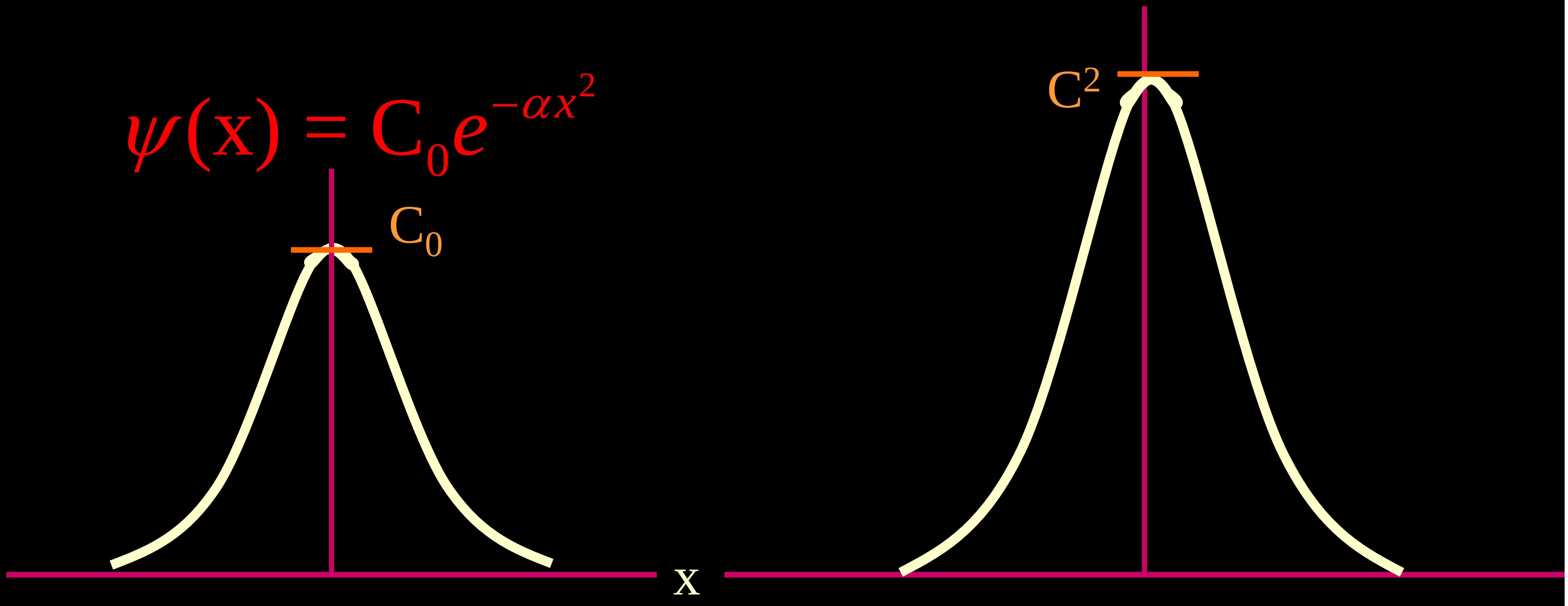
My guess: $\psi(\mathrm{x}) = \mathrm{C}_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

Quantum Picture: Harmonic Oscillator

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

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



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

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 $\alpha \Rightarrow$

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

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

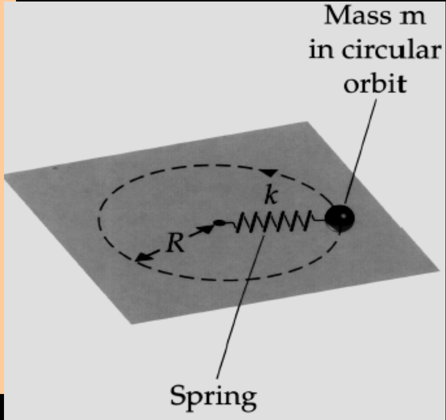
$$\Rightarrow \qquad C_0 = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}}$$

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

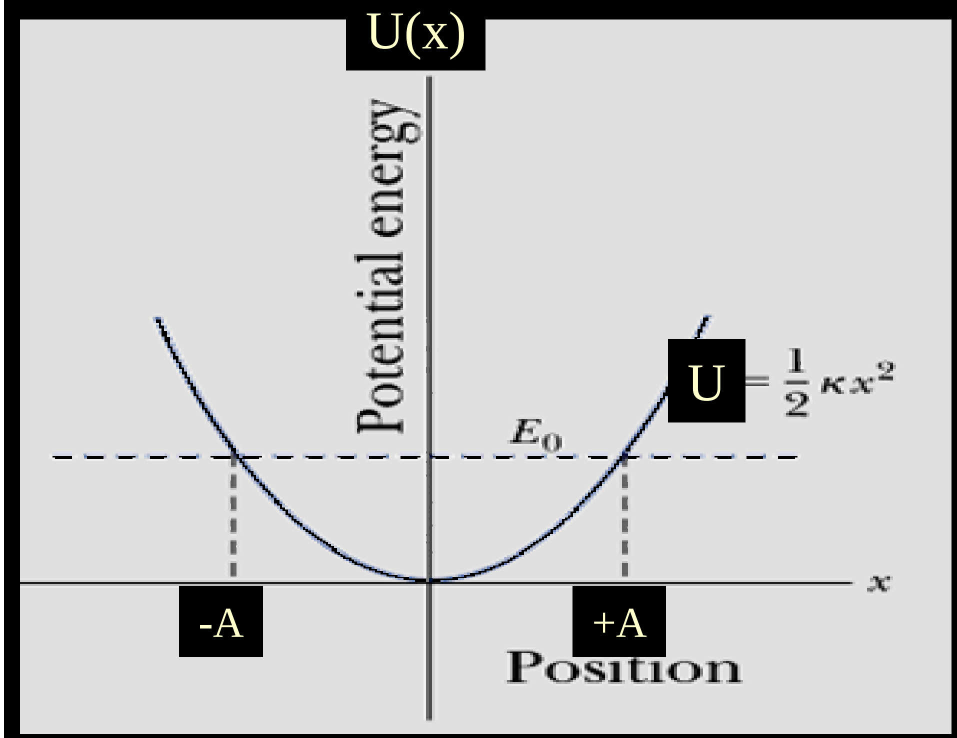
Planck's Oscillators were electrons tied by the "spring" of the mutually attractive Coulomb Force

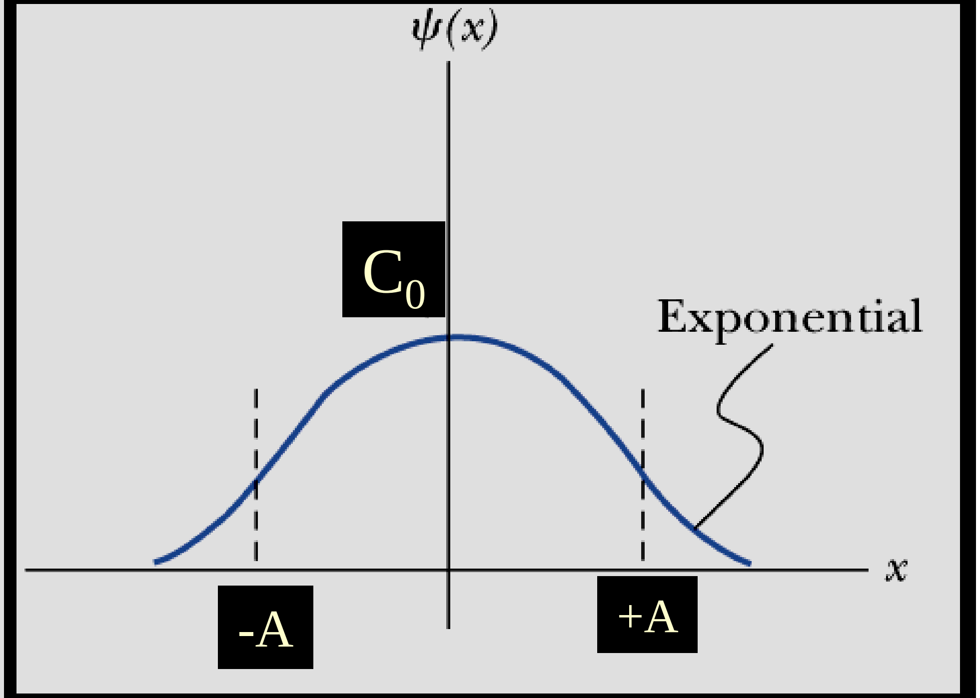


Quantum Oscillator In Pictures

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

$H_0(x)=1$

$H_1(x)=2x$

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

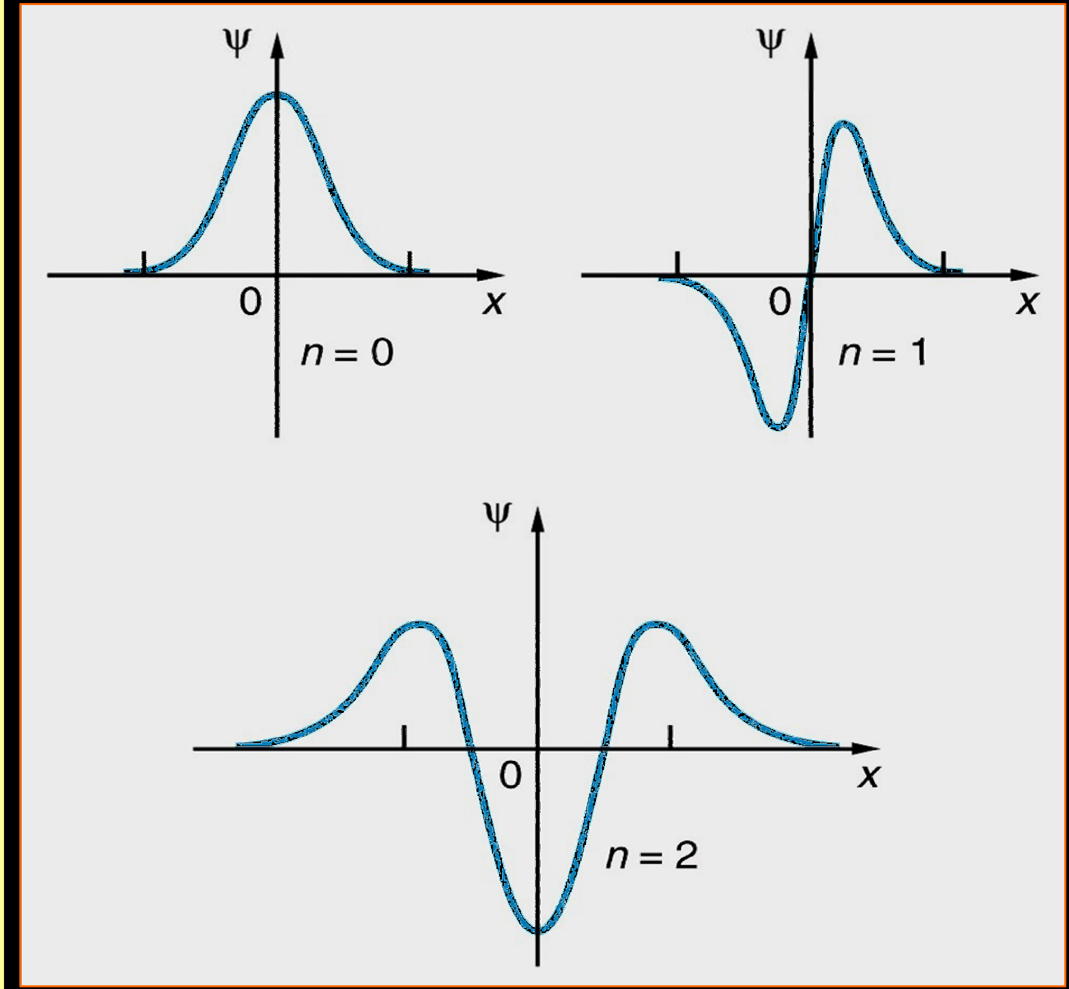
$H_3(x)=8x^3-12x$

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

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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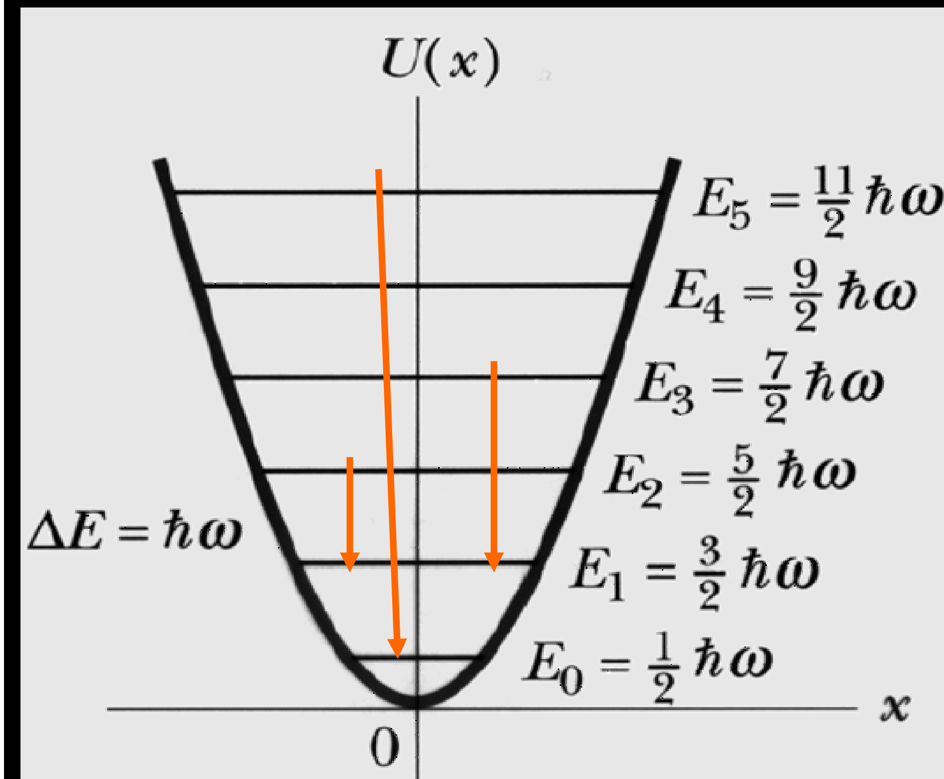

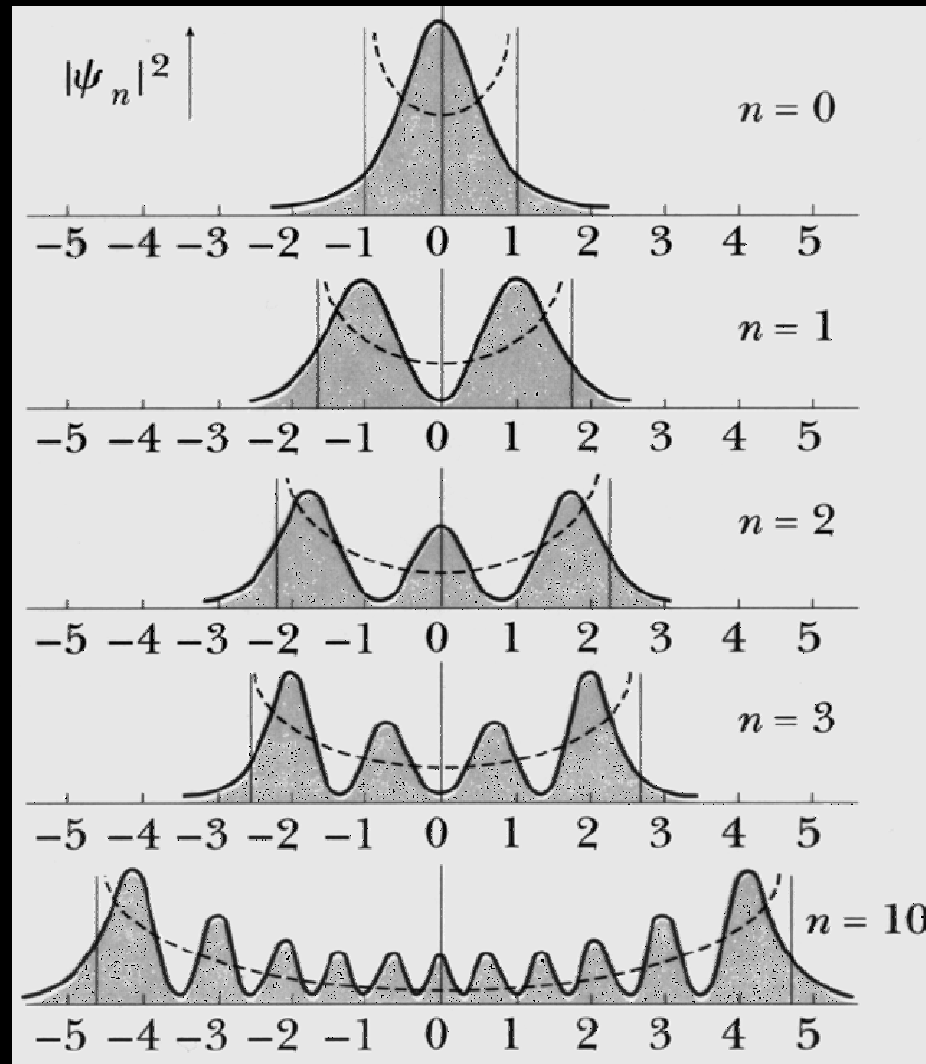

Ground State Energy >0 always

As n → ∞ classical and quantum probabilities become similar

The Case of a Rusty "Twisted Pair" of Naked Wires & How Quantum Mechanics Saved ECE Majors !

- Twisted pair of Cu Wire (metal) in virgin form
- Does not stay that way for long in the atmosphere
  - Gets oxidized in dry air quickly Cu →Cu_2O
  - In wet air Cu → $Cu(OH)_2$ (the green stuff on wires)
- Oxides or Hydride are non-conducting ..so no current can flow across the junction between two metal wires
- No current means no circuits → no EE, no ECE !!
- All ECE majors must now switch to Chemistry instead & play with benzene !!! Bad news !