

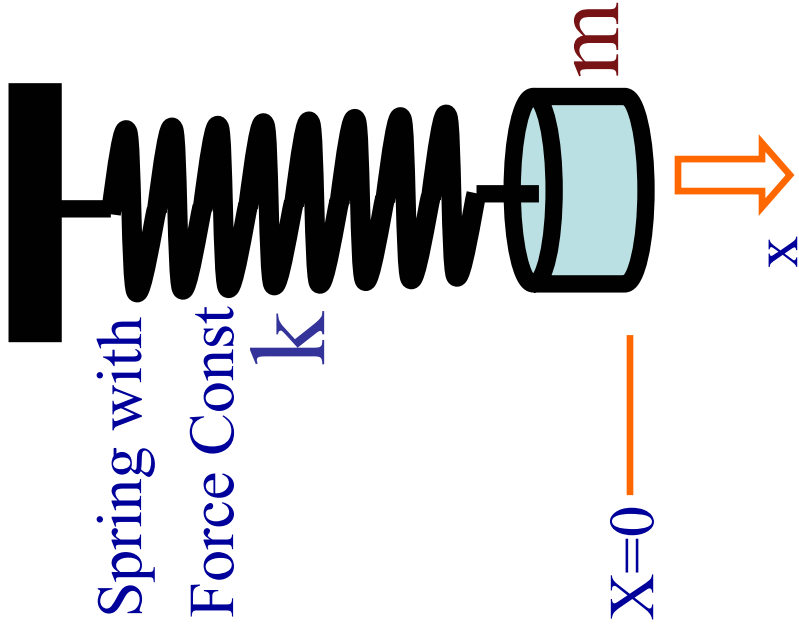


Physics 2D Lecture Slides

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Simple Harmonic Oscillator: Quantum and Classical



Quantum Picture: Harmonic Oscillator

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

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

Time Dependent Schrodinger Eqn:

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

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

What $\psi(x)$ solves this?

Two guesses about the simplest Wavefunction:

1. $\psi(x)$ should be symmetric about $x = 0$ 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?

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

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

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

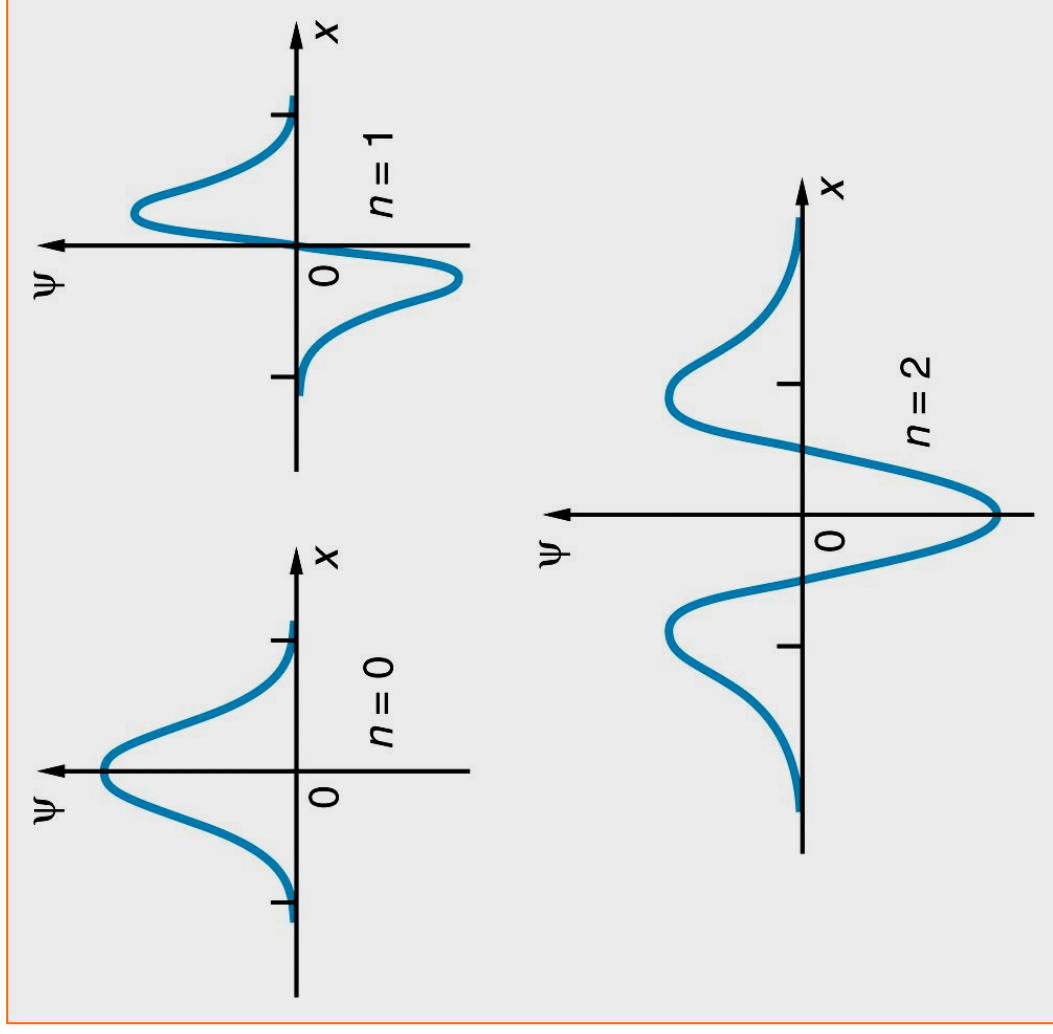
$$H_3(x) = 8x^3 - 12x$$

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

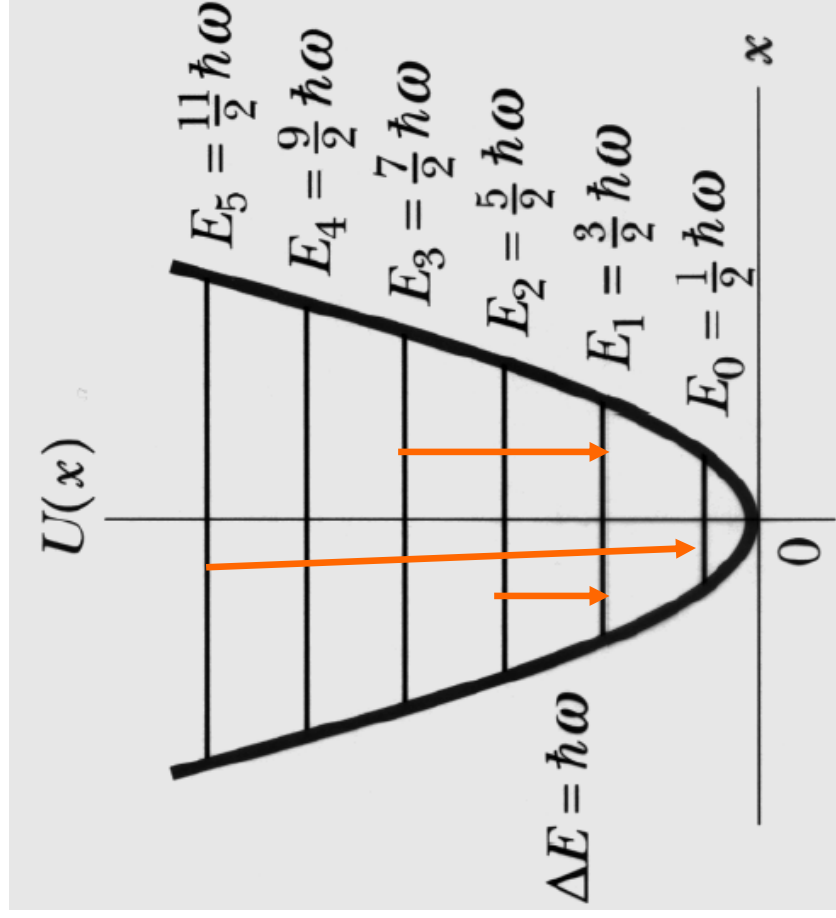
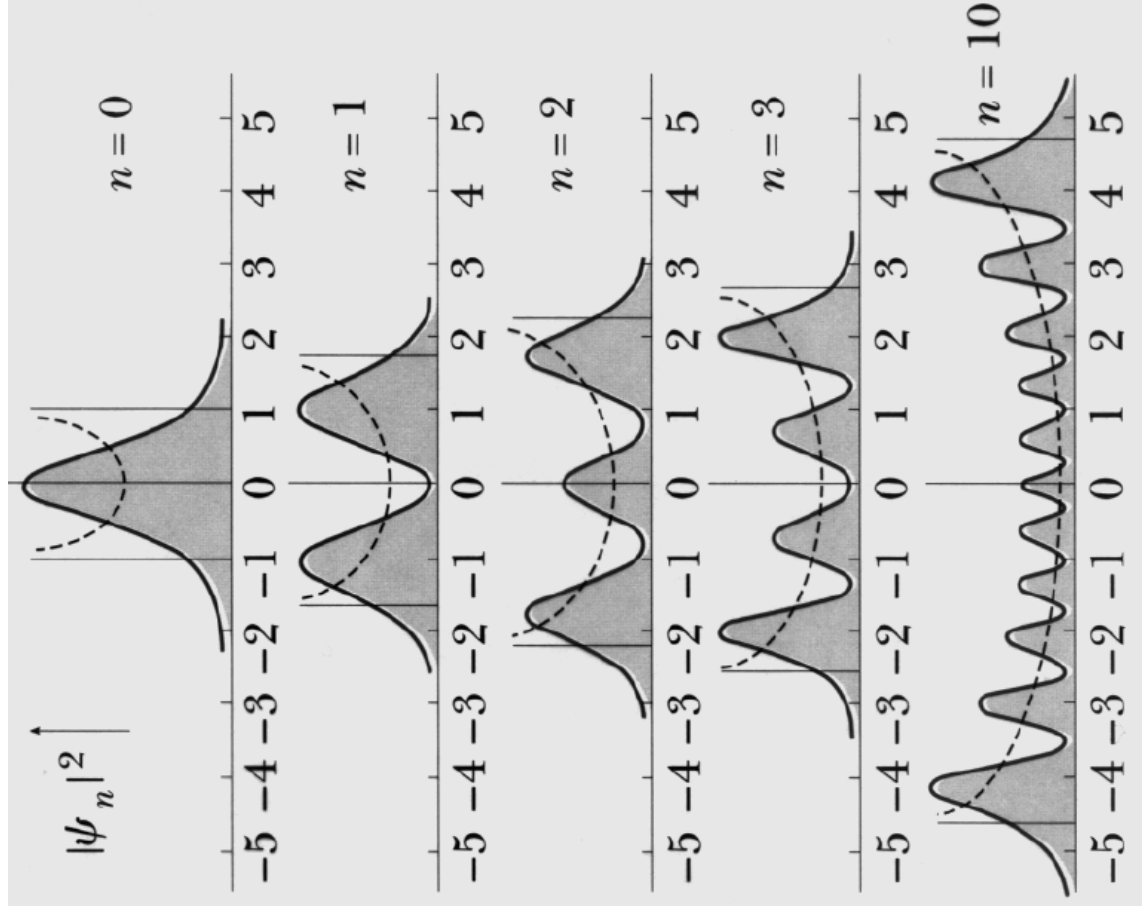
and

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

Again $n=0, 1, 2, 3, \dots, \infty$ Quantum #



Excited States of The Quantum Oscillator

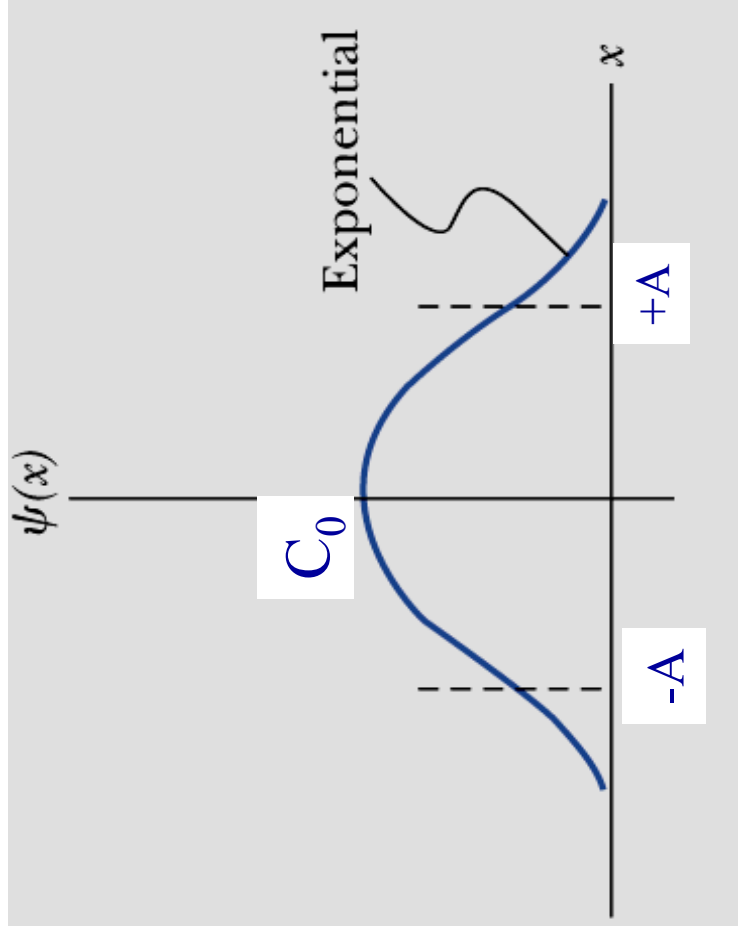
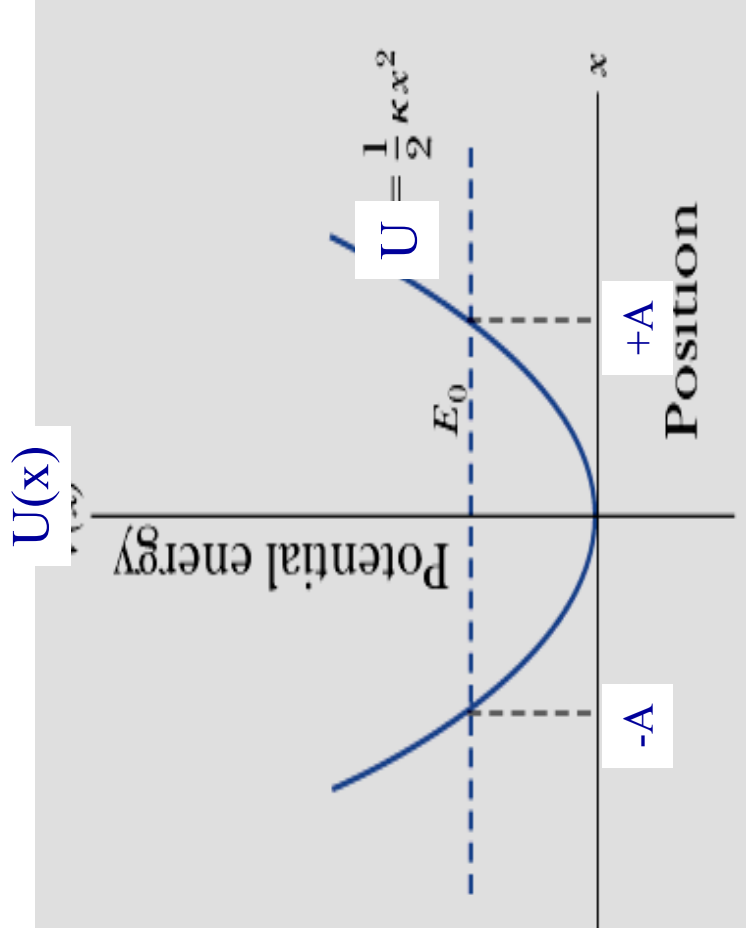


Ground State Energy > 0 always

Quantum Oscillator In Pictures

$$E = KE + U(x) > 0 \text{ for } n=0$$

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)

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

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

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

$\sigma =$ small \rightarrow Sharp distr.

Uncertainty $\Delta X = \sigma$

Particle in the Box, $n=1$, $\langle x \rangle$ & Δx ?

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

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

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

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

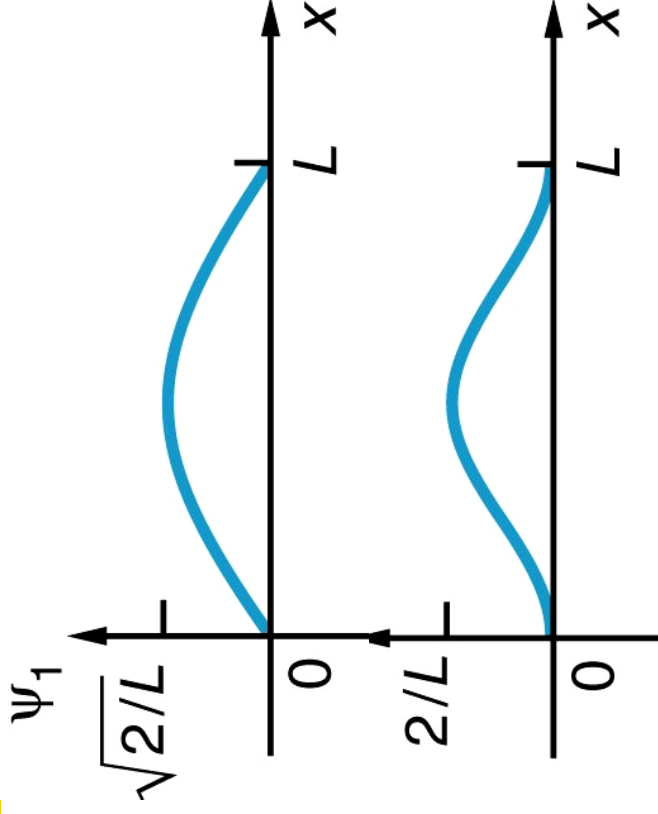
$$\Rightarrow \langle x \rangle = \frac{2L}{2\pi^2} \left[\int_0^{\pi} \theta d\theta - \int_0^{\pi} \theta \cos 2\theta d\theta \right] \text{ use } \int u dv = uv - \int v du$$

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

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

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

$\Delta X = 20\%$ 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: $[X] = x$,

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

$$[P] = \frac{\hbar}{i} \frac{d}{dx}$$

$$[E] = i\hbar \frac{\partial}{\partial t}$$

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

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

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 :

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

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

Similarly

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

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

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!

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

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

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

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

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

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

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

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

Be careful when being "lazy"

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

Does similar logic apply??

Schrodinger Eqn: Stationary State Form

- 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

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

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

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

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

Schrodinger Eqn: Stationary State Form

$$\text{Since } \frac{d}{dt}[\ln f(t)] = \frac{1}{f(t)} \frac{df(t)}{dt}$$

$$\text{In } i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t), \text{ rewrite as } \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} = \frac{E}{i\hbar} = -\frac{iE}{\hbar}$$

and integrate both sides w.r.t. time

$$\int_{t=0}^{t=t} \frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t} dt = \int_0^t -\frac{iE}{\hbar} dt \Rightarrow \int_0^t \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} dt = -\frac{iE}{\hbar}$$

$\therefore \ln \phi(t) - \ln \phi(0) = -\frac{iE}{\hbar} t$, now exponentiate both sides

$\Rightarrow \phi(t) = \phi(0)e^{-\frac{iE}{\hbar}t}$; $\phi(0) = \text{constant} = \text{initial condition} = 1$ (e.g)

$\Rightarrow \phi(t) = e^{-\frac{iE}{\hbar}t}$ & Thus $\Psi(x,t) = \psi(x)e^{-\frac{iE}{\hbar}t}$ where $E = \text{energy of system}$

Schrodinger Eqn: Stationary State Form

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

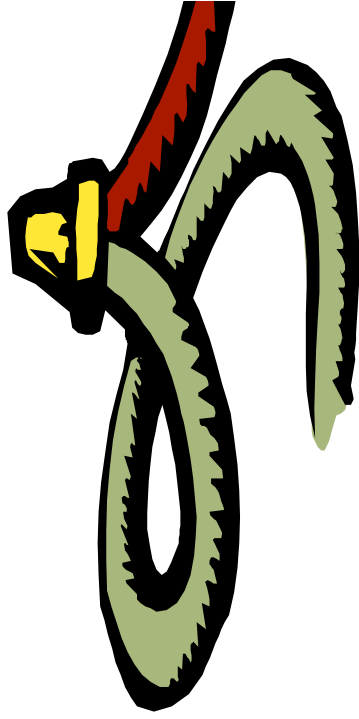
In such cases, $P(x,t)$ is INDEPENDENT of time.

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

Examples : Particle in a box (why?)
: Quantum Oscillator (why?)

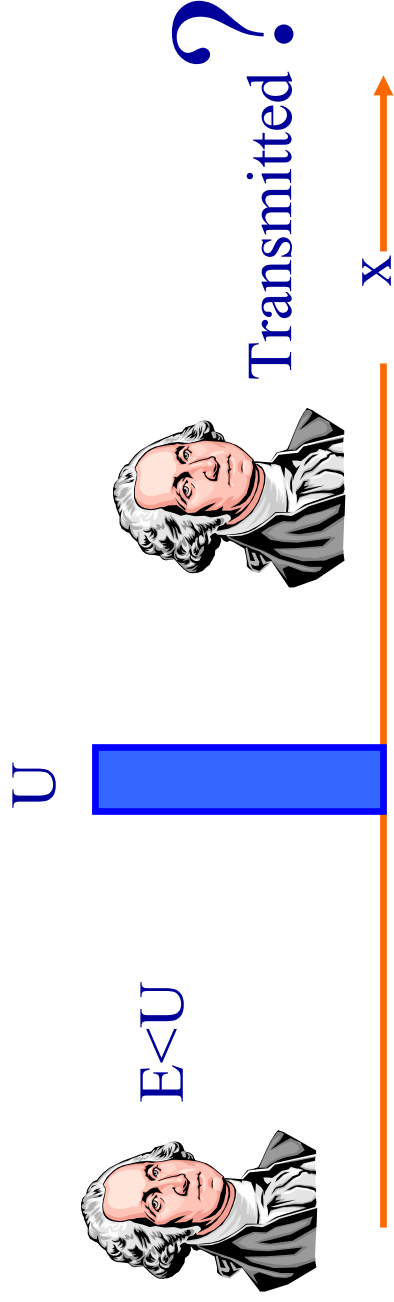
Total energy of the system depends on the spatial orientation of the system : characteristic of the potential situation !

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 $\text{Cu} \rightarrow \text{Cu}_2\text{O}$
 - In wet air $\text{Cu} \rightarrow \text{Cu}(\text{OH})_2$ (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 \rightarrow no EE, no ECE !!
- All ECE majors must now switch to Chemistry instead & play with benzene !!! Bad news !

Potential Barrier



Description of Potential

$$U = 0 \quad x < 0 \quad (\text{Region I})$$

$$U = U \quad 0 < x < L \quad (\text{Region II})$$

$$U = 0 \quad x > L \quad (\text{Region III})$$

Consider George as a “free Particle/Wave” with Energy E incident from Left
Free particle are under no Force; have wavefunctions like

$$\Psi = A e^{i(kx-wt)} \text{ or } B e^{i(-kx-wt)}$$

Wave Function Across The Potential Barrier

In Region II of Potential U

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

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

$$\text{with } \alpha^2 = \frac{\sqrt{2m(U-E)}}{\hbar}; \quad U > E \Rightarrow \alpha^2 > 0$$

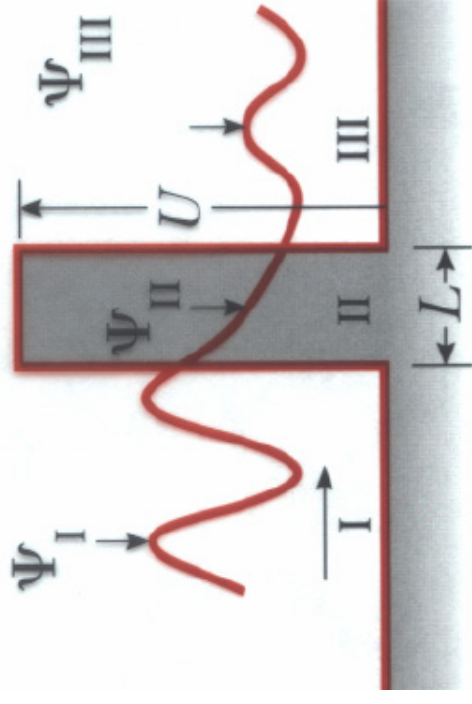
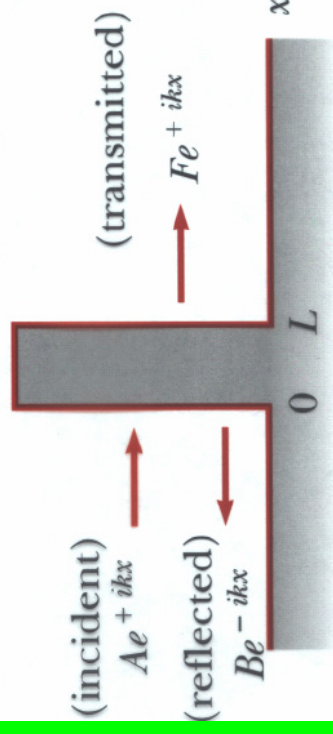
Solutions are of form $\psi(x) \propto e^{+\alpha x}$

$$\boxed{\Psi_{II}(x,t) = Ce^{+\alpha x - i\omega t} + De^{-\alpha x - i\omega t}} \quad 0 < x < L$$

To determine C & D \Rightarrow apply matching cond.

$\Psi_{II}(x,t)$ = continuous across barrier ($x=0,L$)

$$\frac{d\Psi_{II}(x,t)}{dx} = \text{continuous across barrier } (x=0,L)$$



Continuity Conditions Across Barrier

At $x = 0$, continuity of $\psi(x) \Rightarrow$

$$A+B=C+D \quad (1)$$

At $x = 0$, continuity of $\frac{d\psi(x)}{dx} \Rightarrow$

$$ikA - ikB = \alpha C - \alpha D \quad (2)$$

Similarly at $x=L$ continuity of $\psi(x) \Rightarrow$

$$Ce^{-\alpha L} + De^{+\alpha L} = Fe^{ikL} \quad (3)$$

at $x=L$, continuity of $\frac{d\psi(x)}{dx} \Rightarrow$

$$-(\alpha C)e^{-\alpha L} + (\alpha D)e^{+\alpha L} = ikFe^{ikL} \quad (4)$$

Four equations & four unknowns

Divide thruout by A in all 4 equations

\Rightarrow ratio of amplitudes \rightarrow relations for R & T

