

**Confirmed: 2D Final Exam:  
Thursday 18<sup>th</sup> March 11:30-2:30 PM WLH 2005**

**Course Review 14<sup>th</sup> March 10am WLH 2005 (TBC)**

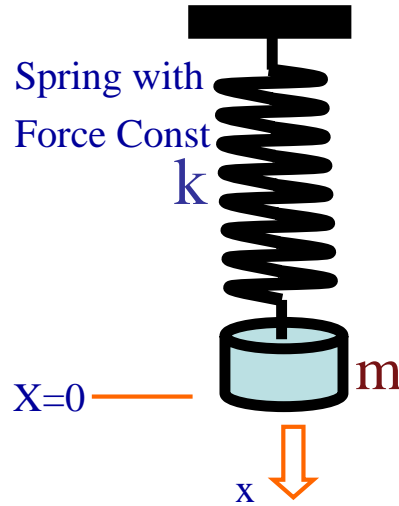
Date	Time	Read	Topic	HW problems for the week	Location
Monday	11:00 am	Ch 5	Quantum Mechanics in 1 Dimension		WLH 2005
Tuesday	8:00 pm	Ch 5	Quantum Mechanics in 1 Dimension	Ch 5 :20, 21, 25, 30, 33, 34, 35, 39, 40	WLH 2005
Wednesday	11:00 am	Ch 6	Tunneling Phenomenan	Read Section 6.1	WLH 2005
Wednesday	3:00 pm	Ch 5	Discussion	-	WLH 2005
Thursday	5:00-6:20 pm	-	Problem Session		Peterson 108
Friday	11:00am	-	Quiz	Ch 5	WLH 2005



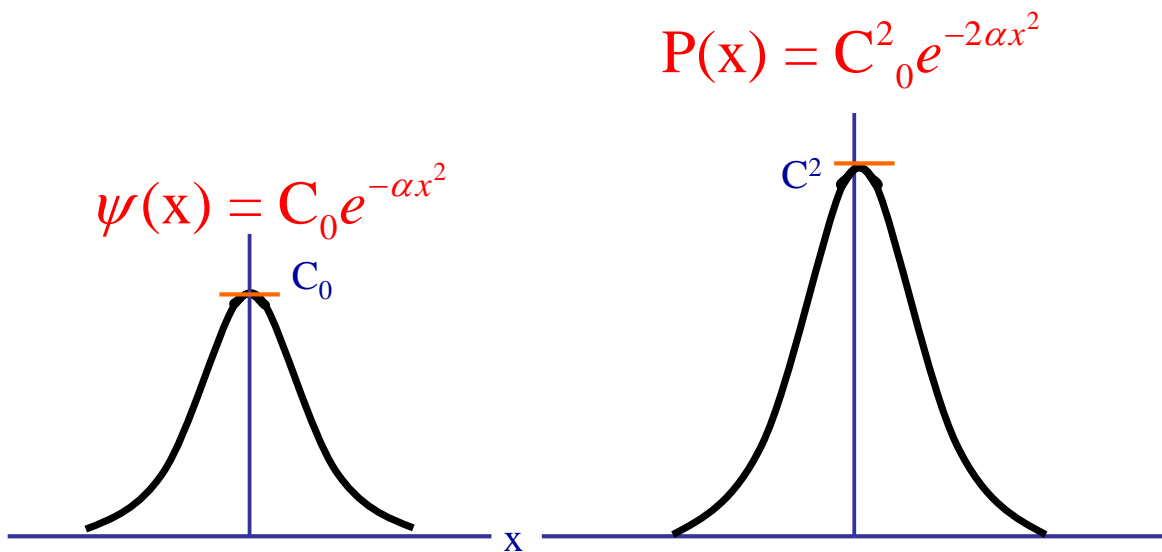
**Physics 2D Lecture Slides  
Lecture 25: Mar 2<sup>nd</sup>**

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UCSD Physics**

# Simple Harmonic Oscillator: Quantum and Classical



## Quantum Picture: Harmonic Oscillator



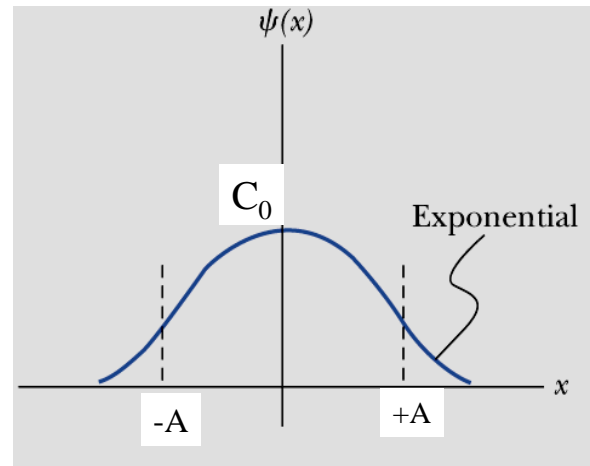
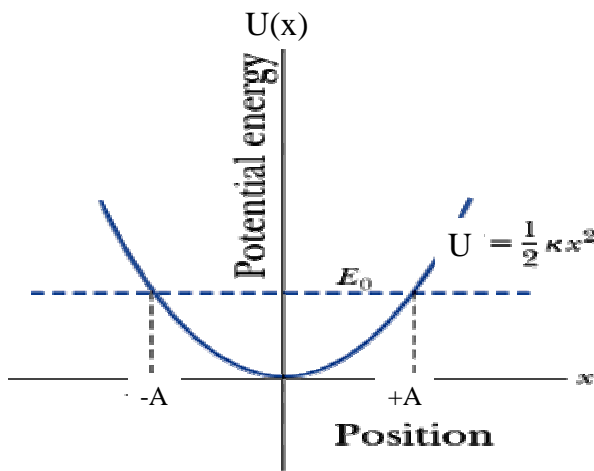
How to Get  $C_0$  &  $\alpha$  ?? ... Try plugging in the wave-function into  
the time-independent Schr. Eqn.

## Quantum Harmonic Oscillator In Pictures

$$E = KE + U(x) = \frac{1}{2} \hbar \omega > 0 \text{ for } n=0$$

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 Harmonic Oscillator compared

- Limits of classical vibration  $\Rightarrow$  Turning Points

Classical oscillator : at  $x = \pm A$ , changes all KE into potential energy of spring

$$\text{Total energy } E(x = \pm A) = \text{KE}(x = \pm A) + U(x = \pm A) = 0 + \frac{1}{2} m \omega^2 A^2$$

For Quantum Oscillator : Total Energy  $E = \frac{1}{2} \hbar \omega$ ;

$$\text{comparing classical and quantum energies} \Rightarrow \frac{1}{2} \hbar \omega = \frac{1}{2} m \omega^2 A^2$$

$$\Rightarrow A = \sqrt{\frac{\hbar}{m \omega}};$$

Classical oscillator bound within  $-A \leq x \leq A = \sqrt{\frac{\hbar}{m \omega}}$

Cannot venture outside  $x = \pm A$  because it has no KE left

- But due to **Uncertainty principle**, Quantum Probability for particle outside classical turning points  $P(|x| > A) > 0$  !!

## Quantum Oscillator In The Classically Forbidden Territory

Calculate probability of Quantum oscillator where a Classical oscillator can't dare be !

$$\Rightarrow \text{Calculate } P(|X|>A) = \sqrt{\frac{\hbar}{m\omega}}; \quad P(|X|>A) = \int_{-\infty}^{-A} |\psi_0(x)|^2 dx + \int_A^{\infty} |\psi_0(x)|^2 dx$$

Since  $\psi_0(x) = \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{4}} e^{-\left(\frac{m\omega}{2\hbar}\right)x^2}$  is symmetric about  $x=0$

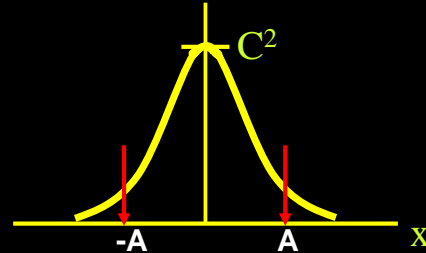
$$\Rightarrow P(|X|>A) = 2 \int_A^{\infty} |\psi_0(x)|^2 dx = 2 \left[\frac{m\omega}{\pi\hbar}\right]^{\frac{1}{2}} \int_A^{\infty} e^{-2\left(\frac{m\omega}{2\hbar}\right)x^2} dx$$

Change variable:  $z = \sqrt{\frac{m\omega}{\hbar}}x$  and write  $A = \sqrt{\frac{\hbar}{m\omega}}$

$$\Rightarrow P(|X|>A) = \frac{2}{\sqrt{\pi}} \int_1^{\infty} e^{-z^2} dz = \text{Error Fn} = \text{erfc}(1) = 0.157$$

$P(|X|>A) = 16\% \quad !!!$

Large probability to go on to the "other side" !



## 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

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

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

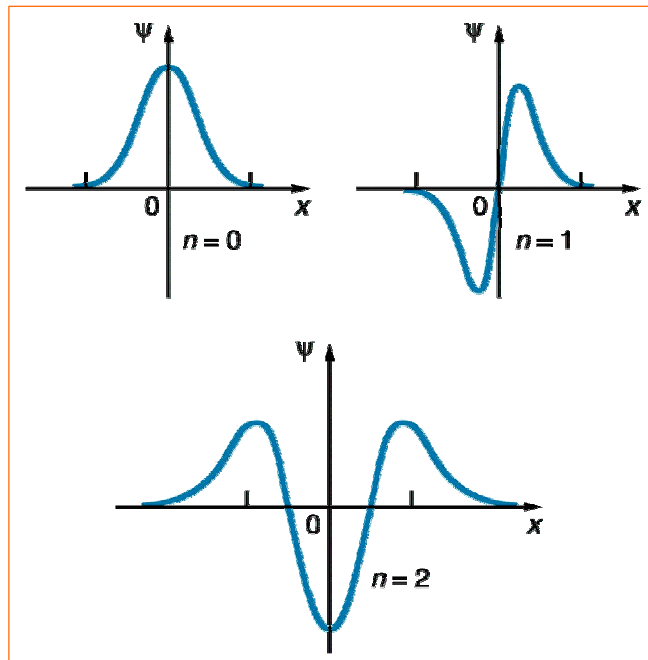
$$H_3(x) = 8x^3 - 12x$$

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

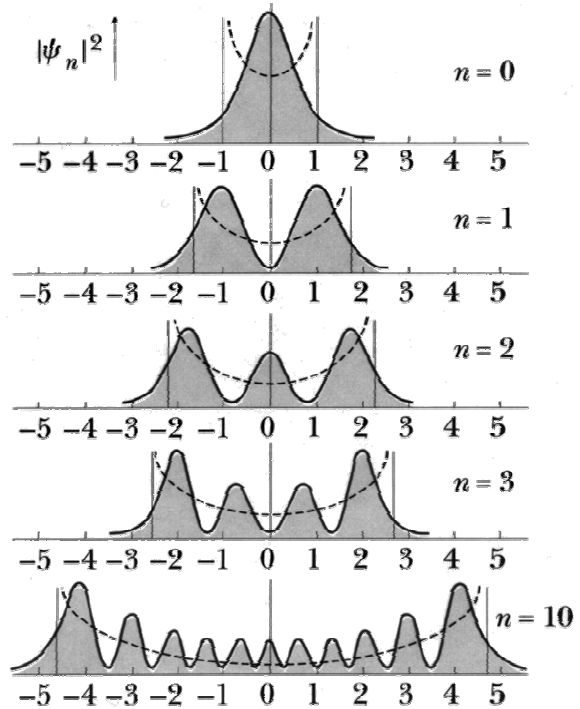
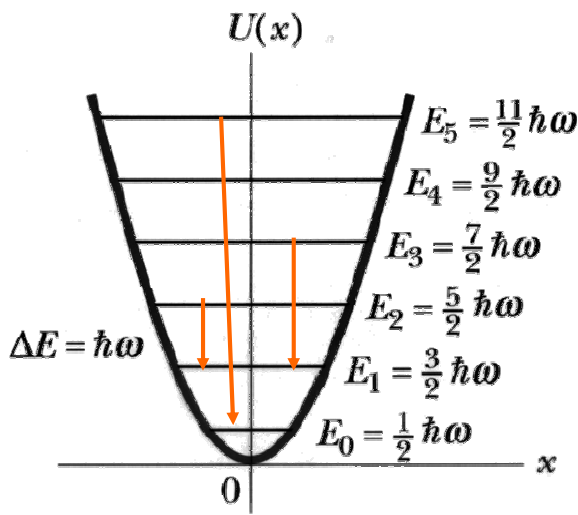
and

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

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



## Excited States of The Quantum Oscillator



Ground State Energy > 0 always

As  $n \rightarrow \infty$  classical and quantum probabilities become similar

## 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

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

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

$\sigma = \text{small} \rightarrow \text{Sharp distr.}$

Uncertainty  $\Delta X = \sigma$

## Particle in the Box, n=1, find $\langle x \rangle$ & $\Delta x$ ?

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

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

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

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

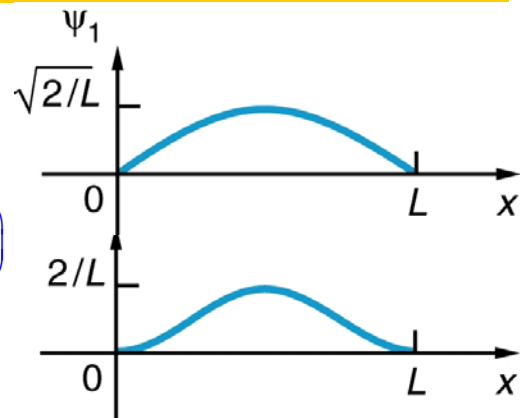
$$\Rightarrow \langle x \rangle = \frac{2L}{2\pi^2} \left[ \int_0^\pi \theta d\theta - \int_0^\pi \theta \cos 2\theta d\theta \right] \quad \text{use } \int u dv = uv - \int v du$$

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

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

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

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

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

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

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

**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 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

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.

- $[H]\Psi(x,t) = [E] \Psi(x,t)$

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

- 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

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

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

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

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!

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

## 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 : charteristic of the potential U(x,t) !

