Physics 2D Lecture Slides
Lecture 24: Feb 28th 2005

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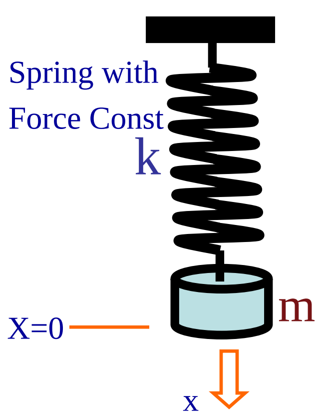
Simple Harmonic Oscillator: Quantum and Classical Pictures Compared



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 amplitude A changes E

E can take any value & if A $\rightarrow$ 0, E $\rightarrow$ 0
Max. KE at x = 0, KE= 0 at x= $\pm$ 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: $\boxed{\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x}+\frac{1}{2}m\omega^2x^2\psi(x)=E\ \ \psi(x)}$

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

Two guesses about the simplest Wavefunction:

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

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

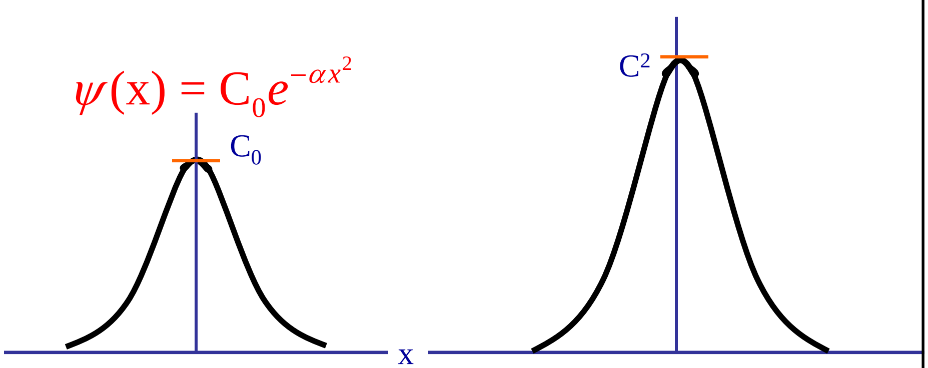
My guess: $\psi(x) = C_0 e^{-\alpha x^2}$; Need to find C_0 & α :

What does this wavefunction & PDF look like?

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

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

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

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

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

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

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

$\boxed{E = \frac{1}{2}\hbar\omega = hf}$!!!!......(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 $\displaystyle\int_{-\infty}^{+\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}$ (dont memorize this)

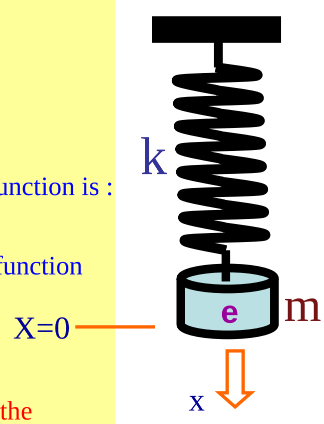
Identifying $a = \dfrac{m\omega}{\hbar}$ and using the identity above

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

Hence the Complete NORMALIZED *groundstate* 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

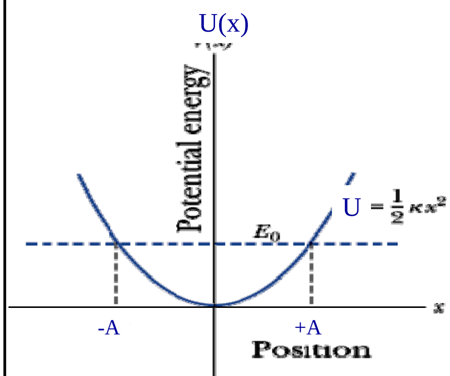


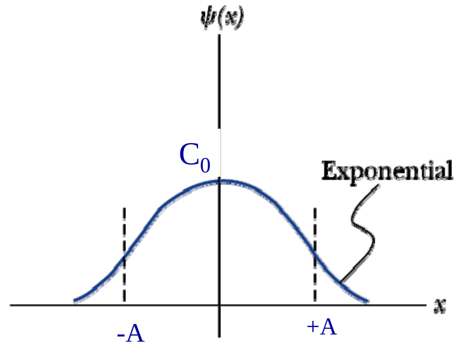
Planck's Oscillators were electrons tied by the "spring" of the mutually attractive Coulomb Force

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 Harmonic Oscillator compared

- Limits of classical vibration $\Rightarrow$ Turning Points

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

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

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

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

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

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

Cannot venture outside x = ±A because it has no KE left

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

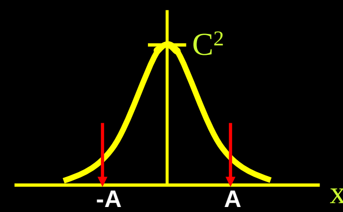
Quantum Oscillator In The Classically Forbidden Territory

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

$\Rightarrow$ Calculate P(|X|>A = $\sqrt{\frac{\hbar}{m\omega}}$) ; 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)= $\frac{2}{\sqrt{\pi}}\int_{1}^{\infty} e^{-z^2} dz$ = Error Fn=erfc(1)=0.157

P(|X|>A) =16% !!!

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

$H_0(x)=1$

$H_1(x)=2x$

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

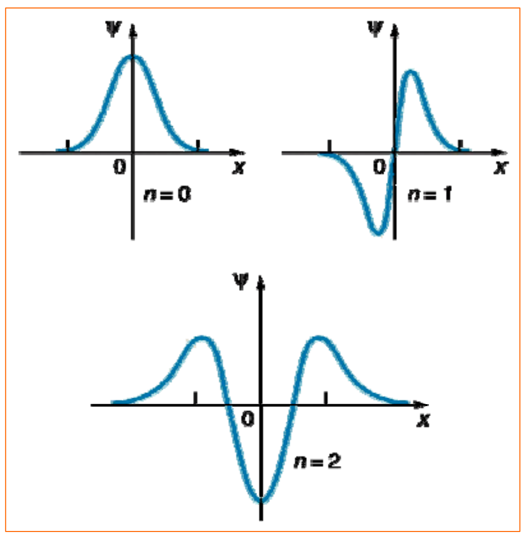
$H_3(x)=8x^3-12x$

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

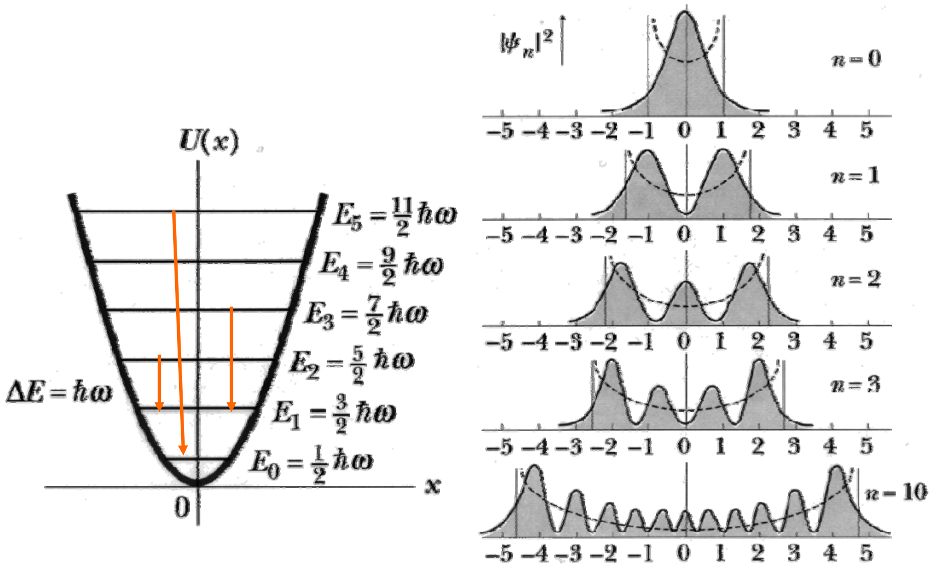
and

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

Again n=0,1,2,3...∞ Quantum #



Excited States of The Quantum Oscillator



Ground State Energy >0 always

As n → ∞ 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

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

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 distribution:
= scatter around the average

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

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

σ = small → Sharp distr.

Uncertainty $\Delta X = \sigma$

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

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

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

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

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

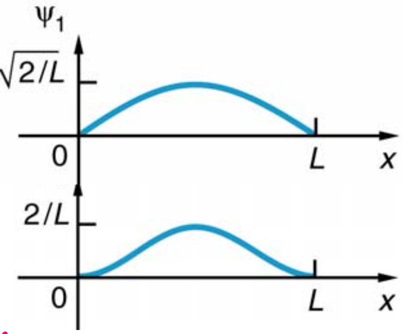
$\Rightarrow <x>=\frac{2L}{2\pi^2}\left[\int_0^\pi \theta d\theta\ -\ \int_0^\pi \theta\cos 2\theta d\theta\right]$ use $\int udv=uv-\int vdu$

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

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

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

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

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

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

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 Rigid 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!

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

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

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

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

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

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

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

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

Be careful when being "lazy"

Quiz: what about <KE> 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

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

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

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

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

Stationary State: Putting Humpty Dumpty Back Togather

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

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

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

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

$\Rightarrow \phi(t) = \phi(0)e^{-\frac{iE}{\hbar}t}$; $\phi(0)$ = constant= 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 = 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) !