Quantum Rules

Instead of Newton's laws relating Force and acceleration, we have

The Schroodinger equation

$$H\Psi(\vec{r},t) = E\Psi(\vec{r},t)$$

H = Hamiltonian operator

E = Energy Eigenvalue

$\Psi(\vec{r},t)$ = probability "Amplitude"

(1) Such that $|\Psi(\vec{r},t)|^2 \Delta x \Delta y \Delta z \Delta t$

represents the probability that particle will be within "region" x to $x+\Delta x$, y to $y+\Delta y$, z to $z+\Delta z$ and t to $t+\Delta t$

H and $\psi(\vec{r},t)$ change with

E such that

$$H\psi = E\psi \quad \text{for any } E$$

H is an <u>operator</u>, E is a #

in general $\psi(\vec{r},t)$ can be written

$$\psi(\vec{r},t) = \psi(\vec{r})\,\Phi(t)$$

where $\Phi(t)$ is usually:

$$\Phi(t) = e^{-iE_n/\hbar}$$

and $\psi(\vec{r})$ depends on the type of "potential" $U(\vec{r})$

Note that H can be written

2 ways:

1) a time dependent form
2) a position dependent form.

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ex: let $E = K + U = K$ (Free particle)

Then $H\psi(x)\Phi(t) = \frac{p^2}{2m}\psi(x)\Phi(t)$

if $\psi = A\sin(kx+\phi)e^{-\frac{ip^2}{2m\hbar}t}$ $\quad k = \frac{2\pi}{\lambda} = \frac{p}{\hbar}$

Then if $\boxed{H = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2}}$

$$H\psi = \frac{-\hbar^2}{2m}(-k^2)\psi(x)\Phi(t) = \frac{p^2}{2m}\psi(x)\Phi(t)$$

$$\Rightarrow \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} \quad \Rightarrow p = \hbar k$$

if $\boxed{H = -\frac{\hbar}{i}\frac{d}{dt}}$

Then $H\psi = -\psi(x)\frac{\hbar}{i}\frac{d}{dt}\Phi(t)$

$$= \psi(x)\frac{-\hbar}{i}\frac{-ip^2}{2m\hbar}\Phi(t)$$

$$= \psi(x)\Phi(t)\frac{p^2}{2m} = E\psi(x)\Phi(t)$$

usual approach: solve the "Time independent" part of the SEQ $\psi(\vec{r})$ and put in the Time dependent part later.

$$\psi_n(\vec{r},t) = \psi_n(\vec{r}) e^{\frac{-iE_n}{\hbar}t}$$

for "infinite square well"

Use $\psi_n(\vec{r}) = A_n \sin(k_n x + \phi)$

But $\psi_n(0) = \psi_n(L) = 0$

$\Rightarrow \phi = 0$

$\Rightarrow k_n L = n\pi$

$\Rightarrow k_n = \frac{n\pi}{L}$ $\quad \left(P_n = \frac{n\hbar\pi}{L} \right)$

$E_n = \frac{P_n^2}{2m} = \frac{n^2\hbar^2\pi^2}{2mL^2}$

Also

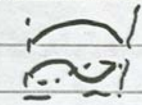
$$\sum_{i=1}^{N} |\psi(x)|^2 \Delta x_i = 1$$

$N \to \infty$ $\quad \int A_n^2 \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$

$$A_n = \sqrt{\frac{2}{L}}$$

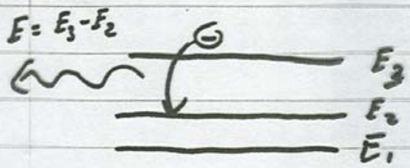
So for the infinite square well

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



etc

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} = n^2 E_1$$



$$\psi(x,t) = \sqrt{\frac{2}{L}}\sin\frac{n\pi x}{L}\, e^{-\frac{i n^2 E_1}{\hbar}t}$$

What about a different potential?

ex: Harmonic oscillator

$$E = K + U = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

$$H\psi = \left(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{K\text{ operator}} + \frac{1}{2}kx^2\right)\psi_n(x) = \underbrace{E_n}_{\#}\,\psi_n(x)$$

Solution? Try $A_n e^{-B_n x^2}$ & plug in.

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1.e. $\frac{\partial \psi}{\partial x} = Ae^{-Bx^2}(2Bx)$

$$\frac{\partial^2 \psi}{\partial x^2} = -2BAe^{-Bx^2} + (2Bx)^2 Ae^{-Bx^2}$$

$$= 2B(2Bx^2-1)\psi$$

$$H\psi = \frac{-\hbar^2}{2m}(2Bx^2-1)\cancel{\psi} + \left(\frac{kx^2}{2}\right)\cancel{\psi} = E_n \cancel{\psi}$$

$$-\frac{\hbar^2}{2m}4B^2x^2 + \frac{\hbar^2}{2m}(2B) = E_n - \frac{kx^2}{2}$$

Works only if

A) $\frac{\hbar^2}{2m}(2B) = E_n$

B) $\frac{\hbar^2}{2m}4B^2 = \frac{k}{2}$ equate coef.

A) $\Rightarrow B = \frac{mE_n}{\hbar^2}$

B) $\Rightarrow B^2 = \frac{mk}{4\hbar^2}$ let $k = m\omega_0^2$

$$B^2 = \frac{m^2\omega_0^2}{4\hbar^2} \Rightarrow B = \frac{m\omega_0}{2\hbar}$$

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So $E_n = \frac{\hbar^2 \beta}{m} = \frac{\hbar^2}{m}\left(\frac{m\omega_0}{2\hbar}\right) = \frac{\hbar\omega_0}{2}$

So $\psi_n(x) = A_n e^{-\frac{m\omega_0}{2\hbar}x^2} e^{-\frac{i}{\hbar}\left(\frac{\hbar\omega_0}{2}\right)t}$

to find A_n set $t=0$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = A_n^2 \int_{-\infty}^{\infty} e^{-\frac{m\omega_0}{\hbar}x^2} dx = \underline{1}$$

N.K $\int_{-\infty}^{\infty} e^{-u^2} du = \sqrt{\pi}$

let $\frac{m\omega_0 x^2}{\hbar} = u^2$, $u = \sqrt{\frac{m\omega_0}{\hbar}}\, x$

$du = \sqrt{\frac{m\omega_0}{\hbar}}\, dx$, $dx = \sqrt{\frac{\hbar}{m\omega_0}}\, du$

$$\Rightarrow A_n^2 \int_{-\infty}^{\infty} e^{-u^2} du \sqrt{\frac{\hbar}{m\omega_0}} = A_n^2 \sqrt{\frac{\hbar}{m\omega_0}} \sqrt{\pi} = 1$$

$$A_n = \left(\frac{m\omega_0}{\pi\hbar}\right)^{\frac{1}{4}}$$

So we have

1) $$\psi_n(x) = \left(\frac{\hbar}{m\omega_0\pi}\right)^{\frac{1}{4}} e^{-\frac{m\omega_0}{2\hbar}x^2}$$

$$E = \frac{\hbar\omega_0}{2}$$

is reality an entire "class" of

functions solve the S.E.Q.

$$\psi_n(x) = A_n \mathcal{H}_n(\xi)\, e^{-\xi^2/2}$$

where H_n is the n^{th} order "Hermite Polynomial"

$$\xi_n = \bar{a}\,d_n = \sqrt{\frac{m\omega_0}{\hbar}}\, x$$

and the "Energy Eigenfunctions" are

$$E_n = (n + \tfrac{1}{2})\hbar\omega_0$$

for $n = 1$ we get Solution (1) at top

this is the ground state.

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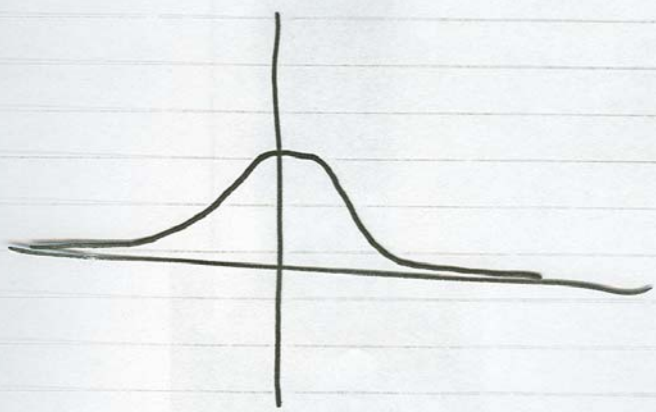
Harmonic oscillator results)

1) $E_n = \hbar\omega_0(n+\frac{1}{2})$ $\quad \hbar\omega_0 = hf$

$\Delta E = E_{n+1} - E_n = \hbar\omega_0$ (Planck!)

2) is ground state

$$\psi_n = A_n e^{-\frac{\rho^2}{2}} = A_n e^{-\frac{m\omega_0}{2\hbar}x^2}$$



This is a "gaussian" wave packet

standard gaussian: $\psi_n = A e^{-\left(\frac{x}{2\sigma}\right)^2}$

so that $\sigma = \sqrt{\frac{\hbar}{2m\omega_0}}$