E.F. Deveney/BSC Physics PH402 Quantum

3-D particle in a Box

Note Title 4/15/2006

Q.M. story .... $\hat{H}\Psi = i\hbar \frac{\partial \Psi}{\partial t}$

is energy eigenstates

$\hat{H}\psi = E\psi \qquad \Psi = e^{-i\frac{E_n t}{\hbar}}\psi(x) =$ Stationary states

& $\Psi =$ great complete basis for even time dep part

& $[\hat{H}, \hat{A}] = 0$ means observables of $\hat{A}$, a, also eigenvalue of energy eigenstates

all 1-D so far.....

recall $\Psi(x,t)$ Born prob condition

$$\int_{-\infty}^{+\infty} \Psi^*(x,t)\,\Psi(x,t)\,dx = 1$$

must consider Ψ over all of 1-D space

now in 3-D $\Psi(x,y,z,t)$

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \Psi^*(x,y,z,t)\,\Psi(x,y,z,t)\,dx\,dy\,dz = 1$$

$$= \int_{-\infty}^{\infty} \Psi^*\Psi\,d^3\vec{r} = 1$$

The entire Formalism, including expectations follows ...

$$\langle\hat{O}\rangle = \int_{-\infty}^{+\infty} \Psi^*\hat{O}\,\Psi\,d^3\vec{r}$$

and $\Rightarrow$

$$\hat{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}$$

$$\vdots$$

$$\hat{H}\psi(x,y,z) = E\,\psi(x,y,z)$$

w/ $$\Psi_{tot}(x,y,z,t) = e^{-i\frac{E_n t}{\hbar}}\,\psi(x,y,z)$$

So thats the plan

$\hat{H}\psi(x,y,z) = E\,\psi(x,y,z)$ is Cartesian Symmetry

or whatever coordinates are most convenient

$\hat{H}\psi(r,\theta,\phi) = E\,\psi(r,\theta,\phi)$ = Spherical Symmetry

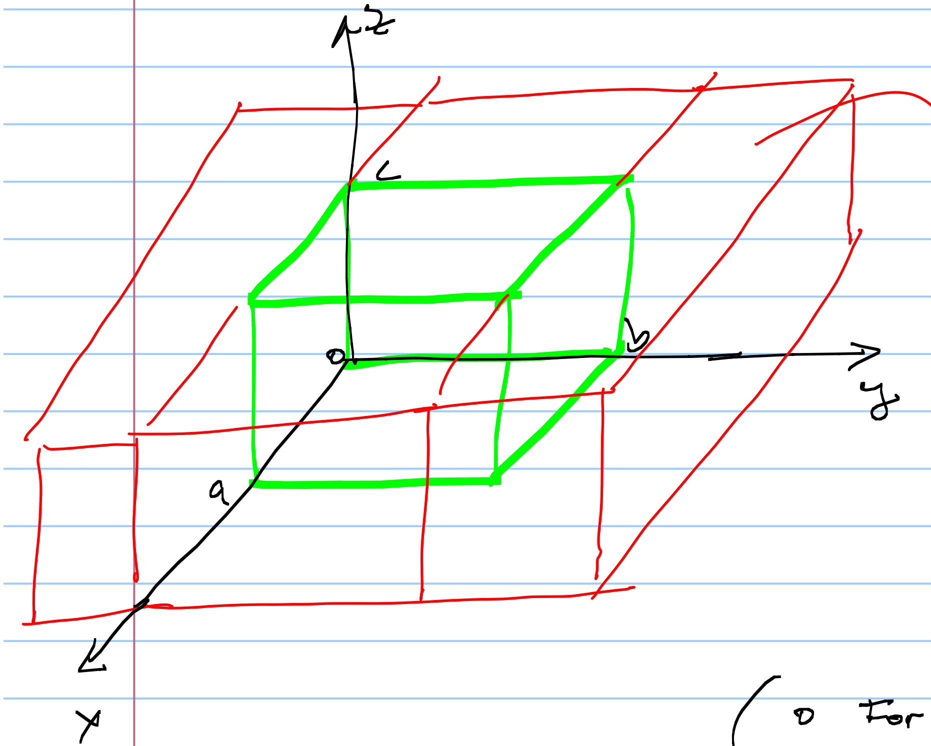
$\hat{H}\psi(r,\phi,z) = E\,\psi(r,\phi,z)$ = Cylindrical Symmetry

Of course, $\hat{H} = E_T = \frac{p^2}{2m} + V$ + anything else

must also be expressed in those coordinates

1st

3-D Schrö time-Indep Problem = Particle in ∞ — 3-D Box!



These are all electrical potential "walls" w/ $V_0 \to \infty$

So $V(\vec{r}) = V(x,y,z) = \begin{cases} 0 & \text{for } 0<x<a \\ & \phantom{\text{for }} 0<y<b \\ & \phantom{\text{for }} 0<z<c \\ \infty & \text{for } x \geq a \\ & \phantom{\text{for }} y \geq b \\ & \phantom{\text{for }} z \geq c \end{cases}$

and

Clearly... the cartesian symmetry is most convenient coordinate system to use.

OK you've got 3-D $V(\vec{r})$

Recall our 3-D $\frac{\hat{p}^2}{2m}$

$$* \quad -i\hbar \frac{\partial}{\partial x} = \text{1-D } \hat{p}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = \text{1-D } \frac{\hat{p}^2}{2m}$$

so $\quad$ 3-D $\vec{p} = -i\hbar\left(\frac{\partial}{\partial x}\hat{i} + \frac{\partial}{\partial y}\hat{j} + \frac{\partial}{\partial z}\hat{k}\right)$

or $\quad -i\hbar\vec{\nabla}$ $\quad$ "Del" operator

now $\quad E_k = \frac{p^2}{2m}$ $\quad$ so 3-D $= \frac{\vec{p}\cdot\vec{p}}{2m}$

$$\frac{(-i\hbar)^2\,\vec{\nabla}\cdot\vec{\nabla}}{2m} =$$

$$= \frac{-i\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

$$= \frac{-\hbar^2}{2m}\nabla^2$$

Ok: $\quad \hat{H}\,\psi_n(x,y,z) = E_n\,\psi_n(x,y,z)$

already anticipating Quantized eigen energies!

$$= \left(-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right)\psi_n(x,y,z) = E_n\,\psi_n$$

$$= \frac{-\hbar^2}{2m}\left(\frac{\partial^2\psi_n}{\partial x^2} + \frac{\partial^2\psi_n}{\partial y^2} + \frac{\partial^2\psi_n}{\partial z^2}\right) + V\,\psi_n = E_n\,\psi_n$$

ok

$\Downarrow$

$$\frac{\partial^2 \psi_n}{\partial x^2} + \frac{\partial^2 \psi_n}{\partial y^2} + \frac{\partial^2 \psi_n}{\partial z^2} = \frac{-2mE_n}{\hbar^2}\psi_n$$

OK.... what next? solve for $\psi_n(x,y,z)$

How?

Separation of variables $\Rightarrow$ good place to start & build a general bases set

OK $\boxed{\psi_n(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)}$

Same old thing sub into orig prob

$$\psi_y(y)\psi_z(z)\frac{\partial^2 \psi_x}{\partial x^2} + \psi_x(x)\psi_z(z)\frac{\partial^2 \psi_y}{\partial y^2} + \psi_x(x)\psi_y(y)\frac{\partial^2 \psi_z}{\partial z^2} = \frac{-2mE_n\psi_n}{\hbar^2}$$

Next again, same old trick divide everything by $\frac{1}{\psi_x\psi_y\psi_z}$

$$\frac{1}{\psi_x}\frac{\partial^2 \psi_x}{\partial x^2} + \frac{1}{\psi_y}\frac{\partial^2 \psi_y}{\partial y^2} + \frac{1}{\psi_z}\frac{\partial^2 \psi_z}{\partial z^2} = \frac{-2mE_n}{\hbar^2}$$

Now watch

$$f(x) + f(y) + f(z) = \frac{-2mE_n}{\hbar^2}$$

a) $$f(x) = \frac{-2mE_n}{\hbar^2} - f(y) - f(z)$$

or

b) $$f(y) = \frac{-2mE_n}{\hbar^2} - f(x) - f(z)$$

or

c) $$f(z) = \frac{-2mE_n}{\hbar^2} - f(y) - f(z)$$

Now as before, if x, y & z are independent variables

say

$$f(x=2) = \frac{-2mE_n}{\hbar^2} - f(y = \text{anything}) - f(z = \text{anything})$$

only way that this can happen is

if each, $f(x)$, $f(y)$ & $f(z)$ are = to constants!

OR:

$$\left.\begin{aligned} \frac{1}{\psi_x}\frac{d^2\psi_x}{dx^2} &= C_x \\ \frac{1}{\psi_y}\frac{d^2\psi_y}{dy^2} &= C_y \\ \frac{1}{\psi_z} = \frac{d^2\psi_z}{dz^2} &= C_z \end{aligned}\right\}$$

This is only way a, b & c could be TRUE!

So.... recombining

$$\frac{1}{\psi_x}\frac{\partial^2\psi_x}{\partial x^2} + \frac{1}{\psi_y}\frac{\partial^2\psi_y}{\partial y^2} + \frac{1}{\psi_z}\frac{\partial^2\psi_z}{\partial z^2} = \frac{-2mE_n}{\hbar^2}$$

$$C_x + C_y + C_z = \frac{-2mE_n}{\hbar^2}$$

Now so maybe

$$\frac{-\hbar^2}{2m}\left[C_x + C_y + C_z\right] = E_n$$

$$E_x = \frac{-\hbar^2}{2m}C_x$$

$$E_y = \frac{-\hbar^2}{2m}C_y$$

$$E_z = \frac{-\hbar^2}{2m}C_z$$

So.....

$$\frac{1}{\psi_x}\frac{d^2\psi_x}{dx^2} = C_x = \frac{2m}{\hbar^2}E_x$$

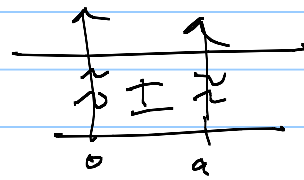
$$\frac{1}{\psi_y}\frac{d^2\psi_y}{dy^2} = C_y = \frac{-2m}{\hbar^2}E_y$$

$$\frac{1}{\psi_z}\frac{d^2\psi_z}{dz^2} = C_z = \frac{-2m}{\hbar^2}E_z$$

For x: $\psi_x'' = \frac{-2m}{\hbar}E_x\psi_x$

$\psi_x'' + \frac{2m}{\hbar^2}E_x\psi_x \Rightarrow$ Look Familiar?

of course... 1-D schrö, 1-D ∞ well



$$\hat{H}\psi_n = E_n\psi_n$$

Region I only

$$\psi'' + A\psi = 0$$

$$A = \frac{2m}{\hbar^2}(E_n - \cancel{V}), \quad V \to 0$$

& we got $\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$ $\quad 0 \le x \le a$

otherwise 0

$$E_n = \frac{\hbar^2\pi^2}{2ma^2}n^2 \; ; \; n = 1, 2, 3 \ldots$$

So!

$$\psi_x(x) \propto \sin\left(\frac{n_x\pi x}{a}\right) \quad \text{w/} \quad E_{n_x} = \frac{\hbar^2\pi^2}{2ma^2}n_x^2$$

* note
  n = # of 1/2 λ's now in 3-D!
  So 3-D particle has to fit 1/2 λ's in all 3-directions

$$\psi_y(y) \propto \sin\left(\frac{n_y\pi y}{b}\right) \quad \text{w/} \quad E_{n_y} = \frac{\hbar^2\pi^2}{2mb^2}n_y^2$$

$$\psi_z(z) \propto \sin\left(\frac{n_z\pi z}{c}\right) \quad \text{w/} \quad E_{n_z} = \frac{\hbar^2\pi^2}{2mc^2}n_z^2$$

Therefore... particle in 3-D ∞ potential Box

$$\hat{H}\psi_n = E_n \psi_n$$

$$\psi_{n\,(n_x,n_y,n_z)}(x,y,z) = \psi_x(x)\,\psi_y(y)\,\psi_z(z)$$

$$= A \sin\left(\frac{n_x \pi x}{a}\right) \sin\left(\frac{n_y \pi y}{b}\right) \sin\left(\frac{n_z \pi z}{c}\right)$$

toss all the contsants together into 1 Big constant That will have to be our normalization constant anyway

$$= \sqrt{\frac{8}{\text{Volume}}} = \sqrt{\frac{8}{abc}}$$

= H.W. prob 6.1

w/ $E_{n(n_x,n_y,n_z)} = E_x + E_y + E_z = \left(\frac{h^2\pi^2}{2m}\right)\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$

$$\left.\begin{array}{l} n_x = 1, 2, 3 \ldots \\ n_y = 1, 2, 3 \ldots \\ n_z = 1, 2, 3 \ldots \end{array}\right\} \text{all independently!}$$

That's it! Looks like 3 linearly indep 1-D solns multiplied together! & it is!

* n_x, n_y, n_z = # ½ wavelengths That fit in that direction.

* Last pt ⇓

Check out if Box = cube, $a=b=c$

Then

$$E_{n\,(n_x,n_y,n_z)} = \frac{\hbar^2\pi^2}{2ma^2}\left(n_x^2+n_y^2+n_z^2\right)$$

$$\psi_{n\,(n_x,n_y,n_z)} = \sqrt{\frac{8}{a^3}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)$$

note if $\left.\begin{matrix} n_x=1 \\ n_y=1 \\ n_z=2 \end{matrix}\right\} \psi_{1,1,2}$ & $E_{1,1,2}$

then $\left.\begin{matrix} n_x=1 \\ n_y=2 \\ n_z=1 \end{matrix}\right\} \psi_{1,2,1}$ & $E_{1,2,1}$

Note $\psi_{1,1,2} \neq \psi_{1,2,1}$

But $E_{1,1,2} = E_{1,2,1}$

This Happens often! That for 2 different wave functions

$\psi_a \neq \psi_b$ = Degenerate energy states:

But $E_a = E_b$

Same energy, different wavefunctions!

Note: ⇘

Degeneracies appear when there are symmetries!

Cube = very symmetric

Symmetric system

$$\left.\begin{matrix}\psi_1\\ \psi_2\\ \psi_3\end{matrix}\right\}\text{all not equal but } E_1 = E_2 = E_3$$

Now if you break the symmetry somehow.

$$\underbrace{E_1 \neq E_2 \neq E_3}_{\text{all}}$$

Look different!

WOW!

Now BIGGER PICTURE

VERY SYMMETRIC

$(\psi_1, \psi_2 \ldots \psi_n)$

all same E

$\Downarrow$ Break Symmetry

$$\left.\begin{matrix}\psi_1 & \psi_2 & \ldots & \psi_n\\ E_1 & E_2 & \ldots & E_n\end{matrix}\right\}\text{Everything Look different}$$

Supersymmetry

Fermions Bosons

example TOE

everything

= E&M weak nuc strong nuc gravity

ex:

Supersymmetry

Broken Symmetry

Fermions

Bosons

TOE (Theory of everything)

electroweak Broken symmetry

Grand unification Broken Symmetry

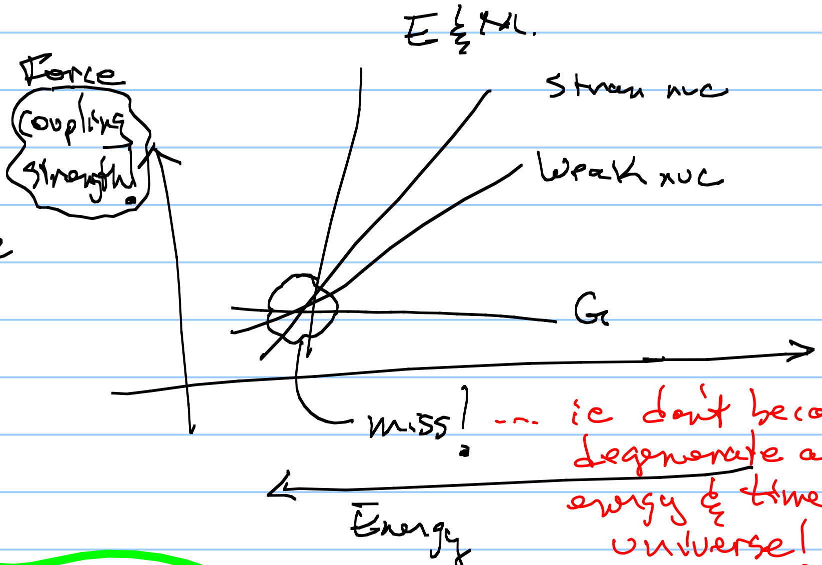
E & M Force

WEAK nuc Force

Strong nuc Force

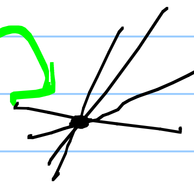
Gravity

Note



... ie don't become degenerate at HUGE energy & time of early universe!

Bob is make super symmetric they meet EXACTLY!



HUGE!