Elementary Quantum Machanics.

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De Broglie Hypothesis

In 1924 ~~which~~ ~~Lewis~~ Louis de Broglies give the energy relation between classical and his shows that sub-atomic like electrons are shows both the properties of wave and matter. That's why the relation is called wave particle dual nature.

According to planks theory

$$E = h\nu \quad \text{......} \quad (1)$$

According to clasical mechanics.

$$E = mc^2 \quad \text{......} \quad (2)$$

Where m = mass of electron
c = velocity of light $(3.8 \times 10^{-8}\ m/sec$

From eqn (1) and (2)

$$h\nu = mc^2$$

But we have,

$$\nu = \frac{c}{\lambda} \quad \text{......} \quad (3)$$

Then eqn (3) becomes.

$$\frac{hc}{\lambda} = mc^2$$

$$\frac{h}{\lambda} = mc$$

$$\lambda = \frac{h}{mc} \quad \text{------------} \quad (4)$$

$$\lambda = \frac{h}{p} \quad \text{------------} \quad (5)$$

so, we can write

$$\lambda = \frac{h}{mv} = \frac{h}{mc} = \frac{h}{p} \quad \text{------------} \quad (6)$$

Addition and Substitution operator

1) Addition

$$(\hat{A} + \hat{B}) f(x) = \hat{A} f(x) + \hat{B} f(x)$$

A

$$(\hat{A} - \hat{B}) f(x) = \hat{A} f(x) - \hat{B} f(x)$$

Multiplication operator

$$\hat{A} \cdot \hat{B} f(x) = \hat{A} (f(x)) . \hat{B} f(x) = f' . f' = f''$$

$$\hat{A} \cdot \hat{B} f(x) \neq \hat{B} \cdot \hat{A} f(x)$$

Linear operator

$$\hat{A} \left[f(x) + g(x) \right] = \hat{A} f(x) + \hat{A} g(x)$$

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c is constant.

$$\hat{A}[c.f(x)] = c\hat{A}f(x)$$

* IMP Energy operator or Hamiltonian operator $(\hat{H})$

According to a classical mechanics a total energy is represented by 'H' and it is nothing but sum of kinetic energy and potential energy.

$$H = K.E, P.E$$

$$H = \frac{1}{2}mv^2$$

$$H = T + V \quad \text{------} \quad (1)$$

Corresponding operator eqⁿ (1) is

$$\hat{H} = \hat{T} + \hat{V} \quad \text{------} \quad (2)$$

But we have,

$$K.E = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m}$$

$$(\because p = mv)$$

$$\text{------} \quad (3)$$

also the v have,

$V = (x, y, z)$ three coordinate

Thefor the partical mass m moving in three dimentional space the classical momment

Function H can be given terms of momentum (P) along x, y and z axis.

$$H = \frac{1}{2m}\left(P_x^2 + P_y^2 + P_z^2\right) + V(x,y,z) \quad \text{------} (4)$$

corresponding eqⁿ

$$\hat{H} = \frac{1}{2m}\left(\hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2\right) + \hat{V}(x,y,z) \quad \text{---------} (5)$$

Then the momentum operator is,

$$\hat{P}_x = \frac{h}{2\pi i}\frac{\partial}{\partial x}$$

$$\hat{P}_y = \frac{h}{2\pi i}\frac{\partial}{\partial y}$$

$$\hat{P}_z = \frac{h}{2\pi i}\frac{\partial}{\partial z}$$

$$\hat{P}_x^2 = \left(\frac{h}{2\pi i}\frac{\partial}{\partial x}\right)\cdot\left(\frac{h}{2\pi i}\frac{\partial}{\partial x}\right)$$

$$= \frac{-h^2}{4\pi^2}\frac{\partial^2}{\partial x^2} \quad \left(\because i^2 = -1\right)$$

similarly

$$\hat{P}_y^2 = \left(\frac{-h^2}{4\pi^2}\frac{\partial^2}{\partial y^2}\right)$$

$$\hat{p}_z^2 = \frac{-h^2}{4\pi^2} \frac{\partial^2}{\partial z^2}$$

Only feel the value in eqn ⑤

$$\hat{H} = \frac{-h^2}{8\pi^2 m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x,y,z) \quad \text{--- ⑦}$$

eq ⑦ is form of Hamiltonian operator.

$$\hat{H} = \frac{-h^2}{8\pi^2 m} \nabla^2 + V(x,y,z) \quad \text{--- ⑧}$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

∇^2 Lapaleason operator

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* Schrodinger wave equation :—

Schrodinger is argued scientis. if microscopic particale like electrone could behave as like wave and hence eqn of a wave on motion could be succesfully applied them.

He used classical independet eqn. The eqn is ~~best~~ basd on the electron moving around nucleus as a ~~strong~~ standing wave with λ along x axis.

We have eqⁿ of standing wave.

$$\psi = A \sin \frac{2\pi x}{\lambda} \quad \text{-------- (1)}$$

Where ψ = amplitude of wave
A = constant
x = displacement along x axis
λ = wavelength.

Differtiat eqⁿ (1) with respect to x.

$$\frac{\partial \psi}{\partial x} = A \frac{2\pi}{\lambda} \cos \frac{2\pi x}{\lambda} \quad \text{-------- (2)}$$

Taking (2) eqⁿ with respect to x.

$$\frac{\partial^2 \psi}{\partial x^2} = - A \frac{4\pi}{\lambda^2} \sin \frac{2\pi x}{\lambda} \quad \text{-------- (3)}$$

From eqⁿ (1) and (3)

$$\frac{\partial^2 \psi}{\partial x^2} = - \frac{4\pi^2}{\lambda^2} \psi \quad \text{-------- (4)}$$

electron is moving with speed v and mass m hence.

$$K.E. = \frac{1}{2} mv^2 = \frac{1}{2} \frac{m^2v^2}{m} \quad \text{-------} (5)$$

According to Debroglie Hypothesis

$$\lambda = \frac{h}{mv}$$

$$\lambda^2 = \frac{h^2}{m^2v^2}$$

$$m^2v^2 = \frac{h^2}{\lambda^2} \quad \text{-------} (6)$$

Feels this value in eq^n

$$K.E = \frac{h^2}{2\lambda^2 . m} \quad \text{-------} (7)$$

From eq^n (4) $\frac{\partial^2 x}{\partial x^2} = \frac{-4\pi^2}{\lambda^2} \psi$

$$\lambda^2 = \frac{-4\pi \psi}{\partial^2 \psi / \partial x^2} \quad \text{-------} (8)$$

Feel the value of eq^n (8) in and (7)

$$K.E = -\frac{h^2}{2m \frac{4\pi^2 \psi}{\partial^2 x / \partial x^2}}$$

$$K.E = \frac{-h^2}{8m\pi^2\psi} \frac{\partial^2\psi}{\partial x^2} \quad \text{--------- (9)}$$

Now total energy of electron,

$$E = K.E + P.E$$

$$E = K.E + V$$

$$K.E = E - V \quad \text{--------- (10)}$$

From eq^n (9) and (10)

$$E - V = \frac{-h^2}{8m\pi^2\psi} \frac{\partial^2\psi}{\partial x^2}$$

Now we have changing sign througout.

$$-(E-V) = \frac{h^2}{8\pi^2 m\psi} \frac{\partial^2\psi}{\partial x^2}$$

$$\frac{\partial^2\psi}{\partial x^2} = -(E-V) \frac{8\pi^2 m\psi}{h^2}$$

$$\frac{\partial^2\psi}{\partial x^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \quad \text{--------- (11)}$$

eq^n (11) is independent schodingear eq^n along x axis for electron moving along x, y and z axis the schodinger eq^n becomes.

Give the characterstic or propertie of wave function.

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$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \quad \text{---------- (12)}$$

$$\nabla^2\psi + \frac{8\pi^2 m}{h^2}(E-V)\psi = 0 \quad \text{---------- (13)}$$

Properties of characterstic

i) The physical interpretation $\psi \cdot \psi^*$ or ψ^2 imposes the restriction of accepte the vale. of ψ.

1) The wave function ψ must be single value at any point.

2) The wave function must always remains ∞ if infanite value is assingned to ψ then ψ^2 will be infinite and that means there is infinite probabitity of a ~~finite~~ finding of a particle.

3) The total probability of finding a electron some is must be unity.

* $\int \psi^2 \, dv = 1$

* $\int \psi \cdot \psi^* \, dv = 1$

4) The wave function ψ must be contineous because the probabitity of value of finding a any point is single value, and therefore it should not be change suddenly. that means function must be contineous.

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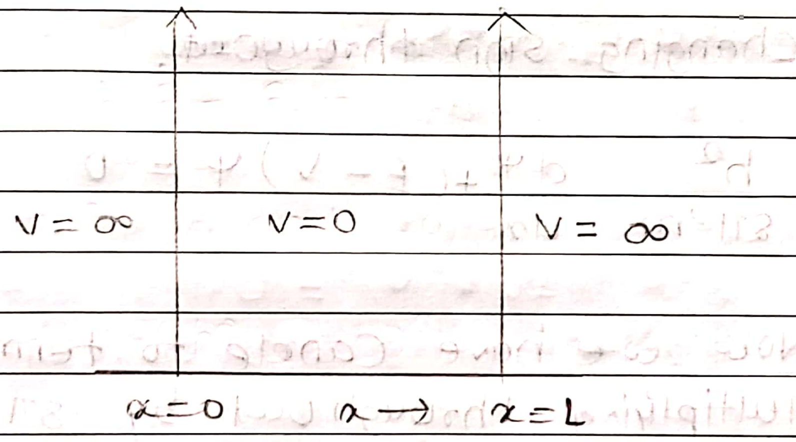
If wave function satisfied all these condition then it is called wave function.

3 marks

* Partical in 1 D box

consider a particle which is allowed to move in limitting space such a model is called particle in 1 D box.



Consider a particle is moving in 1 Dimention box of length L with infinite hight of wall is ∞. The potettial energy inside the box is 0 and outside the box is ∞, Here the particle moves in the Length L,

The energy operater is given by.

$$\hat{H}\psi = E\psi \quad ------ (1)$$

Where $\hat{H}$ is Haimantonial operator, having

$$\hat{H} = -\frac{h^2}{8\pi^2 m}\frac{d}{dx} + v \quad ------ (2)$$

from eqn ① and ②

$$-\frac{h^2}{8\pi^2 m}\frac{d\psi}{dx} + V\psi = E\psi$$

$$-\frac{h^2}{8\pi^2 m}\frac{d\psi}{dx} + V\psi - E\psi = 0$$

Changing sign througout,

$$\frac{h^2}{8\pi^2 m}\frac{d\psi}{dx} + (E - V)\psi = 0$$

Now we have cancle to term.
Multipliying through out by $\frac{8\pi^2 m}{h^2}$

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0 \quad \text{------ (3)}$$

eqn ③ is a ~~soo~~dinger eqn as particle moving axis in a 1D box.

since, particle is discontinus is conveniant to consider the ~~sodinger~~ eqn schrodinger eqn where sodinger eqn outside the box when potential energy is given as $V = \infty$. Then eqn ③ becomes.

$$\frac{d^2\psi}{d^2x} + \frac{8\pi^2 m}{h^2}(E - \infty)\psi = 0$$

------ (4)

$$\frac{d^2\psi}{dx^2} + \frac{h^2}{8\pi^2 m}$$

$$\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + (E - \infty)\psi = 0$$

$$\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + E\psi \; \infty\psi = 0$$

Rearranging above eqⁿ.

$$\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} - \infty\psi = -E\psi$$

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} + \infty\psi = E\psi \quad \text{--------} \quad (5)$$

The sodienges eqⁿ inside the box where $V = 0$,

from eqⁿ (5)

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} = E\psi \quad \text{--------} \quad (6)$$

$$-\frac{h^2}{8\pi^2 m} \frac{d^2\psi}{dx^2} - E\psi = 0 \quad \text{--------} \quad (7)$$

Due to infinity large potential energy beyond the boundry of the box partical has no change in the region. $x<0$ and $x>0$, i.e ψ^2 and hence ψ is must be zero

Since ψ must be contineous hence eqn (7) becomes.

$$\frac{d^2\psi}{dx^2} + \frac{8\pi^2 m}{h^2} E\psi = 0 \quad \text{------ (8)}$$

Now these eqn

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{------ (9)}$$

$$k^2 = \frac{8\pi^2 m}{h^2} E$$

$$E = \frac{k^2 h^2}{8\pi^2 m} \quad \text{------ (10)}$$

The eqn (8) (9) is satisfied by function like $\sin kx$ and $\cos kx$ all of ~~ead~~ which are finite and single value.

They are fullfill in the well behavoed function they we have,

$$\psi = A\sin kx + B\cos kx \quad \text{------ (11)}$$

where A and B is arbitrary constant.

The value of A, B and k can be determing by applying boundry for above eqn.

$x=0$ and $\psi=0$

$$0 = A\sin 0.k + B\cos 0.k$$

$$0 = 0 + B$$

$$B = 0 \quad \text{-------------} \quad (12)$$

from eqn (11) and eqn (12)

$$\psi = A\sin kx$$

Now put the value $x=L$

$$\psi = A\sin kL \quad \text{---------} \quad (13)$$

$$0 = A\sin kL$$

~~so we can fill~~

Both A and B are zero that mean zero, which is not fact solution of eqn (13)

$$kL = n\pi \quad \text{---------} \quad (14) \quad (n \neq 0)$$

$$k = \frac{n\pi}{L}$$ fill this value in eqn (13)

$$\cancel{0 = A\sin n\pi}$$

$$\psi = A\sin \frac{n\pi}{L} x \quad \text{---------} \quad (14)$$

Now we have eqn

$$E = \frac{k^2 h^2}{8\pi^2 m}$$

$$E = \frac{n^2 \pi^2}{L^2} \cdot \frac{h^2}{8\pi^2 m}$$

$$E = \frac{n^2 h^2}{8mL^2} \quad \text{------------ (15)}$$

where $n = 1, 2, 3 \ldots\ldots n$ etc.
If in above eqn h, m L are constant
∴ The energy is depends on only the value of n and the lowest energy of particle

$$E = \frac{h^2}{8mL^2} \quad \text{------------ (16)}$$

(zero point energy)

Give