25/11/24 Unit-5

QUANTUM MECHANICS [QM]

Classical mechanics	Quantum mechanics
1) It is approximate.	1) It is exact
2) It is macroscopic	(2) It is microscopic
3) It is deterministic	(3) It is probabilistic.
4) Momentum & energy are continuous	4) Momentum & energy are not continuous (discrete).
5) It is purely non-relativistic	6) It is relativistic

Dual Nature :-
1) Particle nature of waves
2) Wave nature of particles

Particle behaves as wave and waves behaves as particle. This is called dual nature.

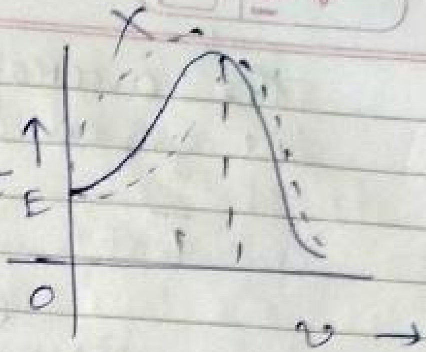
Particle nature of waves :-
Waves are behaving like particles.
Ex :- (1) black body radiation
(2) photoelectric effect (photoemission)
(3) compton scattering.

Black body radiation :-
Black body is absorber and emitter

(a) Wein's Law :- (CM)
energy density $\boxed{E(\nu)\,d\nu = A\, e^{-\frac{B\nu}{T}}\, d\nu}$

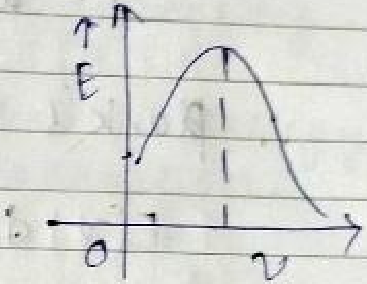
Here, ν = frequency

Conclusion :-
Wein's law is valid for high frequency & cannot explain for low frequency.
Hence, It is failed.



(b) Rayleigh-Jean's Law :- (CM)

$$\boxed{E(\nu)\,d\nu = \frac{8\pi\nu^2}{c^3}(KT)\,d\nu}$$



Conclusion:
Rayleigh-Jean's law is valid for low frequency and cannot explain for high frequency
Hence, It is failed.

Plank's Radiation Law (QM)
$h = 6.62 \times 10^{-34}$ J.S
According plank's concept, black body radiation occur due to exchange of energy between the electromagnetic wave and atomic oscillators.
- The energy of the atomic oscillator are the integral multiple of $h\nu$ where $h\nu$ is called as Quantum of energy.
h is called plank's constant
ν is frequency.

$$\boxed{E_n = nh\nu}$$

the average energy of the particles is given by

$$\overline{E} = \frac{h\nu}{e^{\frac{h\nu}{KT}} - 1}$$

K = Boltzmann constant
T = Absolute temperature

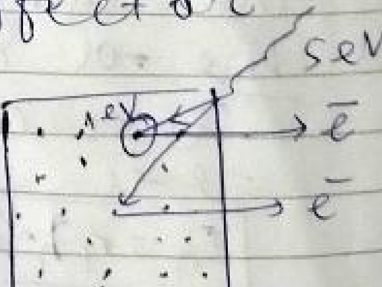
∴ Plank's radiation law is given by

$$E(\nu)\,d\nu = \frac{8\pi h\nu^3}{c^3} \cdot \frac{1}{e^{\frac{h\nu}{KT}} - 1}\,d\nu$$

∴ Plank's Law explains for both high & low frequency.

2) Photoelectric Effect (CM)

When light of suitable frequency is incident on a metallic plate or photo plate then electrons are ejected from the metallic surface and when they are subjected to electric potential, they produce electric current. This phenomenon is called photoelectric effect or photoemission.



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Characteristic

(i) It is an instantaneous process.

(ii) Maximum kinetic energy of the photo electrons depends on the frequency of the incident light.
If KE of a photoelectron varies from 0 to maximum.

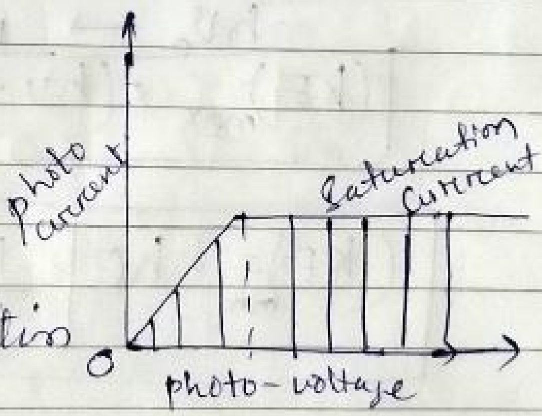
(iii) photo current depends on the intensity of the light.

(iv) Threshold frequency :- The minimum energy frequency required for photoemission.
It is denoted by (ν_0).

(v) Work function (W_0) :- The minimum energy required for photo emission.
It denoted as W_0.

$$\boxed{E_0 = W_0 = h\nu_0}$$

(vi) Saturation Current :-
photocurrent increases with photovoltage and becomes constant.
Which is known as Saturation Current.



(vii) Stopping potential (V_s)
It is the reverse potential for which the photocurrent becomes 0.

Failure of classical mechanics :-
According to the CM
(i) photoemission is not an instantaneous process
(ii) No threshold frequency is required.
(iii) KE depends on intensity not on frequency.

The above points are not valid from the experiment hence CM fails.

Einstein's photo electric effect (QM).
According to Einstein's concept, an electromagnetic wave consists of a series of particles known as photon and each photon carries a energy ($h\nu$).
let $h\nu \rightarrow$ incident energy
$h\nu_0 \rightarrow$ work function

$$\boxed{(KE)_{max} = (h\nu - h\nu_0)}$$

$$\boxed{\because \nu = \frac{c}{\lambda}}$$

$$\boxed{(KE)_{max} = hc\left[\frac{1}{\lambda} - \frac{1}{\lambda_0}\right]}$$

[C - velocity of light
. $3 \times 10^8 m/s$]

This formula is known Einstein's photo electric effect.

$\lambda_0 = 4000 Å$, $\lambda = 3000 Å$
Find $(KE)_{max} = ?$

$$(KE)_{max} = 6.62\times10^{-34}\times 3\times10^{8}\times\left[\frac{1}{3000}-\frac{1}{4000}\right]$$

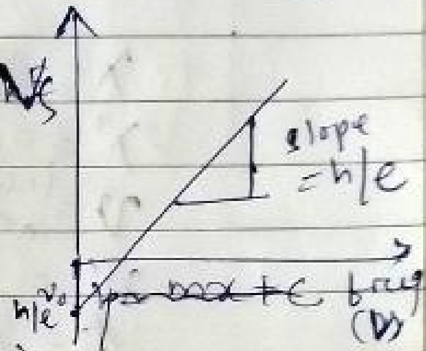
Stopping potential :-

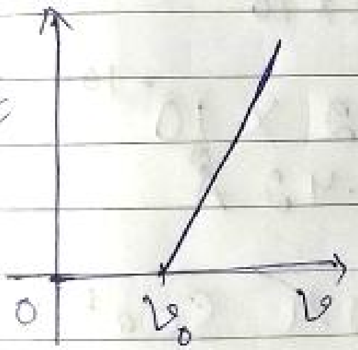
Imp

$$eV_s = (KE)_{max} = h\nu - h\nu_0$$

$$V_s = \frac{h\nu - h\nu_0}{e}$$

$$\boxed{V_s = \frac{h}{e}\nu - \frac{h}{e}\nu_0}$$





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

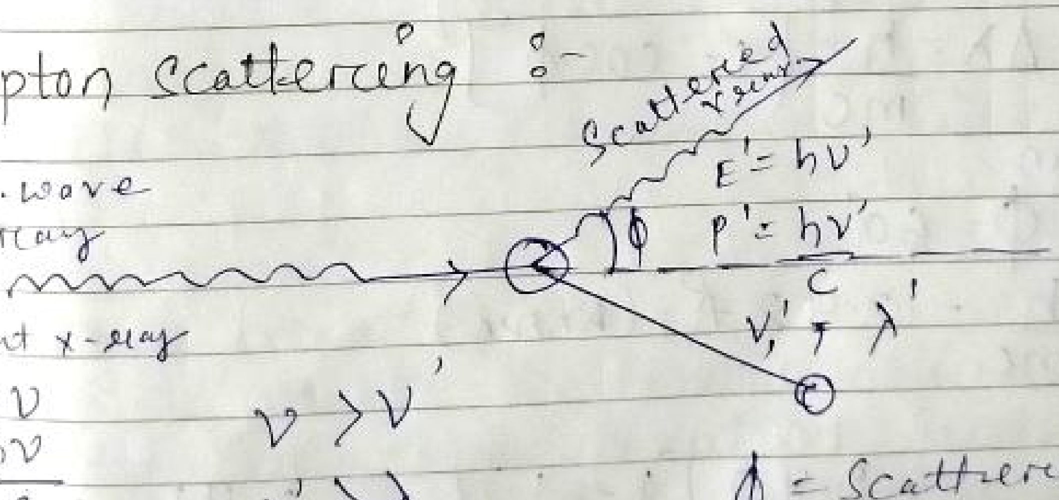
$$v^2 = \frac{2KE}{m}$$

$$\boxed{v = \sqrt{\frac{2KE}{m}}}$$

Compton scattering :-

em. wave
x-ray

incident x-ray
$E = h\nu$
$p = \frac{h\nu}{c}$
λ, ν



$\nu > \nu'$

$\lambda' > \lambda$

ϕ = Scattering angle

Change in wavelength = $\Delta\lambda = \lambda' - \lambda' = \frac{h}{m\nu}[1-\cos\phi]$
or
(Compton Shift $\Delta\lambda$)

$$\Delta\lambda = \lambda' - \lambda = \frac{h}{mc}\left[1-\cos\phi\right]$$

λ = incident wavelength
λ' = scattered wavelength
ν = incident frequency
ν' = scatted frequency
ϕ = Scatting angle

$\frac{h}{mc} = \lambda_c$ = Compton's wavelength

$\lambda_c = 6.62\times10^{-34} / 9.1\times10^{-31}\times3\times10^{8}$

$$= \frac{6.62\times10^{-32}}{2.73\times10^{-22}} = 2.42\times10^{-10} = 2.42\,\mathring{A}$$

Q. Find compton shift for Scatting angle 60°.

$$\Delta\lambda = \frac{h}{mc}\left[1-\cos\phi\right]$$

Given
$\phi = 60^\circ$
$\frac{h}{mc} = 2.42\,\mathring{A}$ (known)

$$2.42\left[1-\frac{1}{2}\right] = \frac{2.42}{2} = 1.21\,\mathring{A}\,(\mathring{A}$$

Q Incident wavelength 2.5 Å , $\phi = 30°$, find λ' & compton shift

$\lambda = 2.5$ Å

$\lambda' = ?$

$\phi = 30°$

$\Delta\lambda = 0.133 \times 2.42 = 0.324$ Å

$\Delta\lambda = \lambda' - \lambda$

$\lambda' = 0.321 + 2.5 = 2.824$ Å.

Find max & min compton shift.

$\Delta\lambda]_{max} = 4.84$ Å $\longrightarrow$ when $\phi = 180°$ (π)

$\Delta\lambda]_{min} = 0$ $\longrightarrow$ when $\phi = 0$

Wave nature of particle :-
particles are behaving like wave.

Matter wave :-
De Broglie's matter wave :-
When a particle moves with definite velocity then a matter wave is associated with the particle motion whose wavelength is given by

$$\boxed{\lambda_d = \frac{h}{p}} = \frac{h}{mv}$$ p = momentum

A bullet of mass 10gm moves with 80 m/s find the de broglie's wavelength matter the matter wave?

$m = 10gm = 10 \times 10^{-3} kg = 0.01 kg$
$v = 80 m/s$

$$\frac{6.62 \times 10^{-34}}{0.01 \times 80} = 8.275 \times 10^{-34} m$$

Different De-Broglie's wavelength :-

1. $\lambda = \frac{h}{p} = \frac{h}{mv}$

2. For electrostatic System :-

$$\lambda_d = \frac{h}{\sqrt{2mE}} = \frac{h}{\sqrt{2mVq}}$$ V = Potential diff

$q = e$

Heisenberg's Uncertainty principle :- It states that it is not possible to measure momentum and position or energy and time to a best accuracy and their relations are given by the uncertainty principle as (1) $\Delta P \cdot \Delta X \geq \frac{\hbar}{2}$

$\hbar$ = cross $= h/2\pi$

(2) $\Delta E \cdot \Delta t \geq \frac{\hbar}{2}$

Applications of uncertainty principle :-

1) Determination of ground state energy of one dimensional hormony oscillating (SHM)

2) Non-existence of electron in a nucleus.

Det^m of Ground state Energy of 1D Harmonic Oscillator :-

The total energy of harmonic oscillator

$$E = KE + PE = \frac{P^2}{2m} + \frac{1}{2}kx^2 \quad (1)$$

According to uncertainty principle

$$P \cdot x = \frac{\hbar}{2}$$

$$\Rightarrow \frac{\hbar}{2x} \quad (2)$$

∴ Using eq (2) in eq^n (1) we get

$$\boxed{E = \frac{\hbar^2}{8mx^2} + \frac{1}{2}m\omega_0^2x^2} \quad (3) \left[\because k = m\omega_0\right]$$

Ground State Energy :- It is the minimum energy of the system

From calculus the minimum energy can be obtained from the condition

$$\left.\frac{dE}{dx}\right|_{x=x_0} = 0$$

$$\Rightarrow \left[\frac{\hbar^2}{8m}\left(\frac{-2}{x^3}\right) + \frac{1}{2} m\omega_0^2 (2x)\right]_{x=x_0} = 0$$

$$\Rightarrow \frac{-\hbar^2}{4m x_0^3} + m\omega_0^2 x_0 = 0$$

$$\cancel{-}\frac{\hbar^2}{4m x_0^3} = \cancel{-} m\omega_0^2 x_0$$

$$\hbar^2 = 4m^2\omega_0^2 x_0^4$$

$$x_0^4 = \frac{\hbar^2}{4m^2\omega_0^2}$$

$$\Rightarrow \boxed{x_0^2 = \frac{\hbar}{2m\omega_0}}$$

$$\Rightarrow \boxed{x_0 = \sqrt{\frac{h}{2m\omega_0}}}$$

$\therefore$ The energy is minimum at x not equal to this value.

$$E_{gs} = E_0 = \frac{\hbar^2}{8m\left(\frac{\hbar}{2m\omega_0}\right)} + \frac{1}{2} m\omega_0^2 \left(\frac{\hbar}{2m\omega_0}\right)$$

$$\Rightarrow E_{gs} = E_0 = \frac{\hbar^2 \omega_0}{4\hbar} + \frac{1}{4}\hbar\omega_0$$

$$\Rightarrow E_{gs} = E_0 = \frac{\hbar\omega_0}{4} + \frac{\hbar\omega_0}{4}$$

$$\Rightarrow E_{gs} = E_0 = 2\left(\frac{\hbar\omega_0}{4}\right) = \frac{\hbar\omega_0}{2}$$

$$\boxed{E_0 = \frac{1}{2}\hbar\omega_0} \qquad \text{———} \quad (5)$$

From Quantum mechanics :

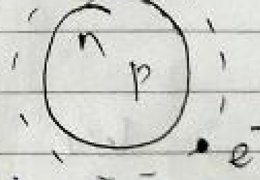
$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0 \quad , \quad n = 0, 1, 2, 3 \ldots$$

For GS, $n = 0$

$$E_0 = \frac{1}{2}\hbar\omega_0$$

2) Non- Existence of e^- in a nucleus :-

$$X = R \simeq 10^{-15}\ m$$



Generally e^- are not staying in the nucleus (only neutrons & protons are the parts of the nucleus).
In order to proove this let us presume that electrons are a part of nucleus
We know the radius of the nucleus is 10^{-15} m

Using Uncertainity principle

$$p \cdot x = \frac{\hbar}{2} \qquad (2)$$

$$\Rightarrow \quad p = \frac{\hbar}{2x} \qquad (3)$$

$$= \frac{h}{4\pi x} = \frac{h}{4\pi 10^{-15} m}$$

$$= \frac{6.62 \times 10^{-34}}{4 \times 3.14 \times 10^{-15}}$$

$$\boxed{p = 5.27 \times 10^{-20} kg \cdot m/s} \quad (4)$$

Now the energy associated with the electron is given by the relativistic formula i.e.

$$\boxed{E = \sqrt{P^2 c^2 + M_0^2 C^4}} \quad -(5)$$

p = momentum
c = velocity of light
m_0 = mass

we have, $c = 3 \times 10^8 \, m/s$
$m_0 = 9.1 \times 10^{-31}$
$p = 5.27 \times 10^{-20} \, kgm/s$

$$E = \sqrt{(5.27 \times 10^{-20})^2 (3 \times 10^8)^2 + (9.1 \times 10^{-31})^2 (3 \times 10^8)^4}$$

$$\boxed{E \simeq 10 MeV} \qquad (6)$$

From β-decay it has been observed that electrons required very small energy for emission as compared to the above value i.e. 10MeV

Hence this shows that electrons are not existing in the nucleus.

Quantum Wave function :-

Every system in QM is represented by a Quantum wave function (ψ) Sai

Characteristics of quantum wave function :-

(i) It is single valued and complex function

(ii) Its derivatives are also single value and continuous

(iii) The probability density is given by

$$\boxed{P = |\psi|^2 = \psi^* \psi}$$

ψ - Sai

ψ^* - complex conjugate of Sai

$$\boxed{\text{Total } P.D = \int_{-\infty}^{\infty} \psi^* \psi \, dx}$$

(iv) It satisfies schrodinger Equation

(v) It vanishes near the boundary (becomes 0)

Mathematically

$x \to \infty, \ \psi \to 0$

Quantum Operations :-

1. Eigen State
2. Eigen function
3. Eigen Value

4. Probability Density $\longleftrightarrow$ Normalization
5. Expectation value
Extra { 6. Operators
7. Observables

Eigen State : ψ is known as allowed or proper State

Eigen Function : every State is identified by a proper / allowed wave function known as eigen function.

Eigen Value : Every system have no. of physical quantity with allowed or proper values known as Eigen values.

$$\text{Ex:- } \underbrace{H}_{\text{operators}} \psi = \overbrace{E}^{\text{Energy Eigen value}} \underbrace{\psi}_{\text{eigen function}} \quad (\text{1D - Schrodinger } Eq^n)$$

Probability Density :

$$p = \int_{-\infty}^{\infty} \psi^* \psi \, dx$$

Ex: $\psi = ax, \quad 0 < x < 1$

Find $p = ?$ $\quad \psi^* = \psi = ax$

$$p = \int_0^1 ax \cdot ax \, dx$$

$$a^2 \int_0^1 x^2 dx = a^2 \frac{x^3}{3} \Big]_0^1 = \frac{a^2}{3}$$

$p = \frac{a^2}{3}$ (Am)

2. $\psi = 2e^{ix}$

$\psi^* = 2e^{-ix}$. $0 < x < L$

$p = \int_0^1 2e^{-ix} \cdot 2e^{ix} \, dx$

$p = 4\int_0^1 e^{-ix} \cdot e^{ix} \, dx = 4\int_0^1 dx$

$= 4[x]_0^1$

$= 4(1-0)$

$= 4$ (Am)

3. $\psi = 2\sin x$, $-\pi/2 < x < \pi/2$

$\psi^* = \psi = 2\sin x$

$p = \int 4 \sin^2 x \, dx$

$4\int_{-\pi/2}^{\pi/2} \sin^2 x \, dx$

$4\int_{-\pi/2}^{\pi/2} \frac{1-\cos 2x}{2} \, dx$

$\frac{4}{2}\int 1 - \cos 2x \, dx$

$$= 2\int_{-\pi/2}^{\pi/2} dx - 2\int_{-\pi/2}^{\pi/2} \cos 2x \, dx$$

$$= 2[x]_{-\pi/2}^{\pi/2} - \frac{2}{2}[\sin 2x]_{\pi/2}^{\pi/2}$$

$$= 2\left[\frac{\pi}{2} + \frac{\pi}{2}\right] - \left(\sin 2\left(\frac{\pi}{2}\right) + \sin 2\left(\frac{\pi}{2}\right)\right)$$

$$= \cancel{2} \times 2\frac{\pi}{\cancel{2}} - 0$$

$$= 2\pi \quad (\text{Ans})$$

3) $\psi = e^{ikx}$; $\psi^* = e^{-ikx}$ $0 < x < 1$

$p = ?$

$$p = \int_0^1 e^{-ikx} \cdot e^{ikx} \, dx$$

$$p = \int_0^1 dx$$

$$p = [x]_0^1 \Rightarrow p = 1 \quad (\text{Ans})$$

~~Expectation~~

Normalization :-

Let $= p = \int_{-\infty}^{\infty} \psi^* \psi \, dx$ $= 1 \Rightarrow$ Normalized

$= 0 \Rightarrow$ orthogonal

$= N \Rightarrow$ not normalized

Method of Normalized :-

step 1 :- 1^{st} find the probability and check for normalization.

step 2 :- let $P = \int_{-\infty}^{\infty} \psi^* \psi \, dx = N$

$$\Rightarrow \frac{1}{N} \int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

$$\Rightarrow \int_{-\infty}^{\infty} \left(\frac{\psi}{\sqrt{N}}\right)^* \left(\frac{\psi}{\sqrt{N}}\right) dx = 1$$

$\Rightarrow \frac{\psi}{\sqrt{N}}$ is normalized wavefunction.

1) $\psi = ax \quad 0 < x < 1$

$P = \frac{a^2}{3} = N \Rightarrow \frac{1}{N} = \frac{3}{a^2}$

$\frac{\psi}{\sqrt{N}} = \cancel{a}x \cdot \frac{\sqrt{3}}{\cancel{a}} = \sqrt{3}\, x$

2) $\psi = 2e^{ix}$

$P = 4 = N \Rightarrow \frac{1}{N} = \frac{1}{4} \Rightarrow \frac{1}{\sqrt{N}} = \frac{1}{2}$

$\frac{\psi}{\sqrt{N}} = \cancel{2} e^{ix} \cdot \frac{1}{\cancel{2}} = e^{ix}$ (Ans)

3) $\psi = 2\sin x \qquad -\pi/2 < x < \frac{\pi}{2}$

$p = 2\pi = N \Rightarrow \frac{1}{N} = \frac{1}{2\pi} \Rightarrow \frac{1}{\sqrt{N}} = \frac{1}{\sqrt{2\pi}}$

$\therefore \psi \cdot \frac{1}{\sqrt{N}} = 2\sin x \cdot \frac{1}{\sqrt{2\pi}}$

$= \sqrt{\frac{2}{\pi}} \sin x .$

Expectation Value :-

The expectation value of physical quantity is equal the weighted average of physical quantity with their probabilities.

let $b_1, b_2, b_3 \cdots b_n$ be the eigen values of physical quantity.

and $P_1, P_2, P_3 \cdots P_n$ are the probabilities

$\sum P_i = 1$

$$\boxed{\langle b \rangle = \frac{b_1 \times P_1 + b_2 + P_2 + b_3 * P_3 + \cdots}{\sum P = 1}}$$

Q. The energy eigen values of a system are 2eV, 5eV, 6eV respectively with corresponding probabilities 0.5, 0.2, 0.3 respectively. find expectation value of energy.

$\langle E \rangle = 0.5 \times 2 + 0.2 \times 5 + 0.3 \times 6$

$\langle E \rangle = 1 + 1 + 1.8 = 3.8\ eV$ (Ans)

The momentum eigen values are 1, 2, 3, 4 unit respectively with probabilities 0.2, 0.2, 0.3, 0.3 respectively.

$\langle P \rangle = 1 \times 0.2 + 2 \times 0.2 + 3 \times 0.3 + 0.3 \times 4$
$= 2.7$ unit

A quantum wave function is given by $\psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{3}}\psi_2 + \frac{1}{\sqrt{5}}\psi_3 + \frac{1}{\sqrt{7}}\psi_7$ if the energy eigen values are 2 eV, 3 eV, 5 eV, 7 eV respectively. Find the expectation value of energy.

square it & that is probability

$$\psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{3}}\psi_2 + \frac{1}{\sqrt{5}}\psi_3 + \frac{1}{\sqrt{7}}\psi_4 \qquad \rightarrow \tfrac{1}{2} \quad \rightarrow \tfrac{1}{3} \quad \rightarrow \tfrac{1}{5} \quad \Rightarrow \tfrac{1}{7}$$

$$\langle E \rangle = \frac{1}{2} \times 2 + \frac{1}{3} \times 3 + \frac{1}{5} \times 5 + \frac{1}{7} \times 7$$
$$= 4\ eV$$

$$\phi = \frac{1}{\sqrt{11}}\phi_1 + \frac{1}{\sqrt{22}}\phi_2 + \frac{1}{\sqrt{33}}\phi_3$$

$p = 22, 44, 66$

$$\langle p \rangle = \frac{1}{\cancel{11}} \times \cancel{22}^{\,2} + \frac{1}{\cancel{22}} \times \cancel{44}^{\,2} + \frac{1}{\cancel{33}} \times \cancel{66}^{\,2}$$
$$= 2 + 2 + 2 = 6 \text{ (Ans)}$$

Operator :-

Every physical quantity is represented by a mathematical entity which are called as the operator of that physical quantity.

physical quantity	Operators
1) Energy (E)	$i\hbar \frac{\partial}{\partial t}$
2) Momentum (P)	$-i\hbar \frac{\partial}{\partial x}$
3) PE (Potential Energy)	V
4) Position	x
5.) KE (Kinetic Energy)	$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$

~~[illegible]~~ :-

Schrodinger Equation :- (SE)

- Time dependent SE
  - 1D
  - 2D
  - 3D
- Time independent SE
  - 1D
  - 2D
  - 3D