B.Sc. (Semester - 6)
Subject: Physics
Course: US06CPHY21
Quantum Mechanics

UNIT- 3 Uncertainty Principle & SHO

The Uncertainty Principle:

The uncertainty in the value of quantum mechanical observables also defined in the same way of uncertainty principle. If A is an observable and $\langle A\rangle$ its expectation or mean value in the state Ψ , then deviation is $A-\langle A\rangle$ and is the self adjoint operator. The square of this deviation gives the uncertainty of A, it is denoted by ΔA.

$$\therefore\ (\Delta A)^2 = \langle (A-\langle A\rangle)^2\rangle = \langle A^2\rangle - \langle A\rangle^2 \quad \ldots (3.1)$$

Similarly for other variable B , we can write

$$(\Delta B)^2 = \langle (B-\langle B\rangle)^2\rangle = \langle B^2\rangle - \langle B\rangle^2 \quad \ldots (3.2)$$

Here, ΔA and ΔB are not operator, but $A-\langle A\rangle$ is the square root of mean square operator. Now, this operator is represented by deviation operator D_a and D_b.

$$\therefore D_a = A - \langle A\rangle \quad \ldots (3.3)$$

$$D_b = B - \langle B\rangle \quad \ldots (3.4)$$

Now, using the positivity property of operators

$$\langle (D_a - i\lambda D_b)(D_a + i\lambda D_b)\ \rangle \geq 0 \quad \ldots (3.5)$$

λ is a real parameter.

Let we expand the product as,

$$\langle {D_a}^2 + i\lambda D_a D_b - i\lambda D_b D_a + \lambda^2 {D_b}^2\rangle$$

Now taking the differentiation with respect to λ and equating to zero, we get

$$\langle 0 + iD_aD_b - iD_bD_a + 2\lambda\, {D_b}^2\rangle = 0$$

$$\therefore\ \langle i[D_a, D_b]\rangle + 2\lambda\,\langle D_b\rangle^2 = 0$$

$$\therefore \lambda = \frac{\langle -i[D_a, D_b]\rangle}{2\,\langle D_b\rangle^2} \quad \ldots. (3.6)$$

Substituting this value of λ in equation (3.5), we get

$$\langle {D_a}^2 + i\,\frac{\langle -i[D_a, D_b]\rangle}{2\,\langle D_b\rangle^2} D_aD_b - i\,\frac{\langle -i[D_a, D_b]\rangle}{2\,\langle D_b\rangle^2} D_bD_a + \frac{\langle -i[D_a, D_b]\rangle^2}{4\langle {D_b}^2\rangle^2}{D_b}^2\rangle \geq 0$$

$$\langle {D_a}^2 + \frac{\langle [D_a, D_b]\rangle}{2\,\langle D_b\rangle^2} D_aD_b - \frac{\langle [D_a, D_b]\rangle}{2\,\langle D_b\rangle^2} D_bD_a + \frac{\langle [D_a, D_b]\rangle^2}{4\langle {D_b}^2\rangle}\rangle \geq 0$$

$$\therefore\ \langle {D_b}^2\rangle + \frac{\langle [D_a, D_b]\rangle\,\langle [D_a, D_b]\rangle}{4\langle {D_b}^2\rangle} \geq 0$$

$$\therefore 4\,\langle {D_a}^2\rangle\,\langle {D_b}^2\rangle + \langle [D_a, D_b]\rangle^2 \geq 0 \quad \ldots (3.7)$$

From equation (3.3), we have

$${D_a}^2 = A^2 - 2A\,\langle A\rangle + \langle A\rangle^2$$

$$\therefore \langle {D_a}^2\rangle = \langle A^2\rangle - 2\langle A\rangle\langle A\rangle + \langle A\rangle^2$$

$$= \langle A^2\rangle - 2\langle A\rangle^2 + \langle A\rangle^2$$

$$\therefore \langle {D_a}^2\rangle = \langle A^2\rangle - \langle A\rangle^2 \qquad \dots (3.8)$$

Similarly, $$\langle {D_b}^2\rangle = \langle B^2\rangle - \langle B\rangle^2 \qquad \dots (3.9)$$

Now,

$$[D_a, D_b] = [A - \langle A\rangle, B - \langle B\rangle]$$
$$= [A, B] - [\langle A\rangle, B] - [A, \langle B\rangle] + [\langle A\rangle, \langle B\rangle]$$
$$\therefore [D_a, D_b] = [A, B] \qquad \dots (3.10)$$

Here, other terms vanish by the property of commutators.

Now, using equations (3.8), (3.9) & (3.10) in (3.7), we get

$$4\,[\langle A^2\rangle - \langle A\rangle^2][\langle B^2\rangle - \langle B\rangle^2] + \langle [A, B]\rangle^2 \geq 0$$

Using equations (3.1) & (3.2) in above relations, we get

$$4\,(\Delta A)^2(\Delta B)^2 + \langle [A, B]\rangle^2 \geq 0$$
$$\therefore 4\,(\Delta A)^2(\Delta B)^2 \geq -\langle [A, B]\rangle^2$$
$$\therefore (\Delta A)^2(\Delta B)^2 \geq -\frac{1}{4}\langle [A, B]\rangle^2 \qquad \dots (3.11)$$
$$\therefore (\Delta A)(\Delta B) \geq -\frac{1}{2}\langle [A, B]\rangle \qquad \dots (3.12)$$

This is the product of uncertainty in A and B and is of the order of commutator $[A, B]$. Equation (3.12) gives the general statement of the uncertainty principle for any pair of observables A, B.

If A, B are a canonically conjugate pair of operators, it is characterized by

$$[A, B] = i\hbar \qquad \dots (3.13)$$

Then, equation (3.12) becomes

$$(\Delta A)(\Delta B) \geq \frac{1}{2}\hbar \qquad \dots (3.14)$$

Here, sign is not important.

Now, $$[x, p_x] = i\hbar$$

$$\left.\begin{aligned} \therefore (\Delta x)(\Delta p_x) &= \frac{\hbar}{2} \\ (\Delta y)(\Delta p_y) &= \frac{\hbar}{2} \\ (\Delta z)(\Delta p_z) &= \frac{\hbar}{2} \end{aligned}\right\} \qquad \dots . (3.15)$$

- **Example:** Prove that the same state of all the component of $\vec{L}$ is impossible.

  Now, we have

$$[L_x, L_y] = i\hbar L_z \qquad \dots . (3.16)$$

Now, consider a function ϕ which satisfies both the eigen equation of L_x and L_y.

$$\therefore L_x\,\phi = m_x\phi \qquad \dots . (3.17)$$

and $$L_y\,\phi = m_y\phi \qquad \dots . (3.18)$$

Now, multiplying equation (3.17) by L_y and (3.18) by L_x and subtracting we get,

$$L_y\,L_x\,\phi = L_y\,m_x\phi$$
$$L_x\,L_y\,\phi = L_x\,m_y\phi$$

$$\left(L_y\, L_x\ - L_x\, L_y\right)\phi = L_y\, m_x\phi - L_x\, m_y\phi$$

$$\therefore \left(L_x\, L_y\ - L_y\, L_x\right)\phi = m_y L_x\phi - m_x L_y\phi$$

$$= m_y m_x\phi - m_x m_y\phi = 0$$

$$\therefore \left[L_x, L_y\right]\phi = 0 \qquad \text{....}(3.19)$$

Now, comparing this equation (3.19) with (3.16), we get

$$\left[L_x, L_y\right]\phi = \ i\hbar L_z\phi = 0$$

$$\therefore L_z\phi = 0 \qquad \text{...}(3.20)$$

Similarly, if we repeat the calculation for L_x and L_y, we must have

$$L_z\phi = 0$$

and $$L_y\phi = 0$$

Hence, if any two components of angular momentum have same eigen state and applying this eigen state on third component then results will be zero. Thus, the eigen state of all the three components of angular momentum will not be same.

States with Minimum Value for Uncertainty Product:

We have obtained the uncertainty principle $(\Delta x)(\Delta p) \geq \frac{1}{2}\hbar$ using the positive property

$$\langle (D_a - i\lambda D_b)(D_a + i\lambda D_b)\ \rangle \geq 0 \qquad \text{...}(3.25)$$

If the L.H.S of this equation becomes zero then the product of uncertainty will be zero. For this we must have the state function $\Psi(x)$ such that

$$(D_a + i\lambda D_b)\Psi = 0 \qquad \text{...}(3.26)$$

$$\text{If } A = x, \qquad B = \ -i\hbar\frac{d}{dx} \qquad \text{...}(3.27)$$

Then,

$$D_a = x - \ \langle x\rangle \qquad \text{...}(3.28)$$

$$D_b = p_x - \ \langle p_x\rangle \qquad \text{...}(3.29)$$

$$\langle {D_b}^2\rangle = \langle p_x^2\rangle - \langle p_x\rangle^2 \qquad \text{...}(3.30)$$

$$(\Delta p_x)^2 = \langle p_x^2\rangle - \langle p_x\rangle^2 \qquad \text{...}(3.31)$$

We also know that,

$$\therefore \lambda = \frac{-i\langle [x, p_x]\rangle}{2\,(\Delta p_x)^2} \qquad \text{....}(3.32)$$

Here,

$$[D_a, D_b] = [A, B] = [x, p_x]$$

$$\therefore \lambda = \frac{(-i)(i\hbar)}{2\,(\Delta p_x)^2} \qquad \text{....}(3.33)$$

Substituting equations (3.28), (3.29) & (3.33) in equation (3.26), we get

$$\left[x - \langle x\rangle + \frac{(i)(-i)(i\hbar)}{2\,(\Delta p_x)^2}(p_x - \ \langle p_x\rangle)\right]\Psi = 0$$

Substituting $\quad p_x = -i\hbar\frac{d}{dx}\quad$ and arranging the terms, we get

$$\left[x - \langle x\rangle + \frac{(i\hbar)}{2\,(\Delta p_x)^2}\left(-i\hbar\frac{d}{dx} - \langle p_x\rangle\right)\right]\Psi = 0$$

$$\therefore\ \left[x - \langle x\rangle + \frac{\hbar^2}{2\,(\Delta p_x)^2}\frac{d}{dx} - \frac{i\hbar}{2\,(\Delta p_x)^2}\langle p_x\rangle\right]\Psi = 0$$

$$\therefore\ \left[\frac{\hbar^2}{2\,(\Delta p_x)^2}\frac{d}{dx} + x - \langle x\rangle - \frac{i\hbar}{2\,(\Delta p_x)^2}\langle p_x\rangle\right]\Psi = 0$$

$$\therefore\ \frac{d\Psi}{dx} + \left\{\frac{2\,(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle) - \frac{i\,\langle p_x\rangle}{\hbar}\right\}\Psi = 0 \qquad \dots(3.34)$$

$$\therefore\ \frac{d\Psi}{dx} = -\left\{\frac{2\,(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle) - \frac{i\,\langle p_x\rangle}{\hbar}\right\}\Psi$$

$$\therefore\ \frac{d\Psi}{\Psi} = -\left\{\frac{2\,(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle) - \frac{i\,\langle p_x\rangle}{\hbar}\right\}dx$$

Integrating on both the sides, we get

$$\ln\Psi = -\left\{\frac{2\,(\Delta p_x)^2}{\hbar^2}\left(\frac{x^2}{2} - \langle x\rangle\,x\right) - \frac{i\,\langle p_x\rangle}{\hbar}x\right\}$$

$$= -\left\{\frac{(\Delta p_x)^2}{\hbar^2}(x^2 - 2\,x\,\langle x\rangle\,) - \frac{i\,\langle p_x\rangle}{\hbar}x\right\}$$

$$= -\left\{\frac{(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle)^2 - \frac{(\Delta p_x)^2}{\hbar^2}\langle x\rangle^2 - \frac{i\,\langle p_x\rangle}{\hbar}x\right\}$$

$$\therefore\ \Psi = N\exp\left\{-\frac{(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle)^2 - \frac{i\,\langle p_x\rangle}{\hbar}x\right\} \qquad \dots(3.35)$$

Here the factor $\frac{(\Delta p_x)^2}{\hbar^2}$ is contain in constant N.

The wave function is normalized

$$i.e.\int|\Psi|^2\,dx = 1 \text{ in } N \text{ is chosen as}$$

$$N = \left[\frac{2\,(\Delta p_x)^2}{\pi\,\hbar^2}\right]^{1/4} \qquad \dots(3.36)$$

$$\therefore\ |\Psi|^2 = \left(\frac{2\,(\Delta p_x)^2}{\pi\,\hbar^2}\right)^{1/2}\ \exp\left[-\frac{2(\Delta p_x)^2}{\hbar^2}(x - \langle x\rangle)^2\right] \qquad \dots(3.37)$$

Equation (3.35) gives the normalized wave function for which $(\Delta x)(\Delta p_x)$ has the minimum value $\frac{\hbar}{2}$. Note that Ψ has the form of a Gaussian function 'modulated' by the oscillatory factor $\exp\left[\frac{i\,\langle p_x\rangle}{\hbar}x\right]$.

For minimum uncertainty

$$(\Delta x)(\Delta p_x) = \frac{\hbar}{2}$$

$$\therefore\ \Delta p_x = \frac{\hbar}{2(\Delta x)} \qquad \dots(3.38)$$

Substituting this value of Δp_x in equation (3.37), we get

$$|\Psi|^2 = \left(\frac{2\,\hbar^2}{4(\Delta x)\,\pi\,\hbar^2}\right)^{1/2} \exp\left[-\frac{2\,\hbar^2}{4(\Delta x)\ \hbar^2}(x - \langle x\rangle)^2\right]$$

$$\therefore \quad |\Psi|^2 = [2\,\pi\,(\Delta x)^2\,]^{-1/2} \exp\left[-\frac{(x - \langle x\rangle)^2}{2(\Delta x)^2}\right] \qquad \ldots (3.39)$$

Since $|\Psi|^2$ is negligibly small outside a region having dimensions of the order $\Delta x = \left(\hbar/_{2\Delta p_x}\right)$, the wave function (3.35) is said to describe a minimum uncertainty wave packet.

Commuting Observables; Removal of Degeneracy:

Consider an eigen equation

$$A\phi_a = a\phi_a \qquad \ldots . (3.40)$$

Let us consider another operator B which commute with A. Now operator B on both the sides we have

$$BA\phi_a = aB\phi_a \qquad \ldots . (3.41)$$

But, $BA = AB$

$$\therefore A\,(B\phi_a) = a(\,B\phi_a) \qquad \ldots . (3.42)$$

Thus, not only ϕ_a, but $B\phi_a$ also is an eigenstate of A belonging to the same eigenvalue a. If 'a' happens to be a non-degenerate eigen value, there is only one eigen function belonging to it and hence $B\phi_a$ must be a constant multiple of ϕ_a, say

$$B\phi_a = b\phi_a \qquad \ldots . (3.43)$$

This means that ϕ_a is also an eigen function of B, belonging to eigen values b. Thus, any eigen function belonging to a non-degenerate eigen value of a pair of commuting operator A, B is necessarily an eigen function of the other operator.

It is possible to choose a basic set of r eigen functions in such a way that each of them is an eigen function of B. In this manner one can obtain a complete set of simultaneous eigen functions ϕ_{ab} for any pair of commuting observable A, B.If the r independent eigen functions belonging to a given degenerate eigen value 'a' are characterized by r distinct value of b, then we say that the degeneracy of a is completely removed.

If it is not removed then we have to introduce another observable C.
ϕ_{abc},........and $\phi_{a'b'c'}$ are identical if and only if $a = a', b = b', c = c', \ldots\ldots$ It is obvious that if each ϕ_{abc} is individually normalized, the set of all such simultaneous eigen functions forms an orthonormal set

$$\int \phi^*_{abc\ldots}\,\phi_{a'b'c'\ldots}d\tau = \ \delta_{aa'}, \delta_{bb'}, \delta_{cc'}, \ldots . \qquad \ldots . (3.44)$$

Evolution of System with Time; Constants of The Motion:

The time dependent Schrodinger equation is

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = \ -\frac{\hbar^2}{2m}\nabla^2\Psi(\vec{r},t) + V(\vec{r})\Psi(\vec{r},t) \qquad \ldots (3.45)$$

Here,

$$-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) = \ H_{op}$$

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = H_{op}\Psi(\vec{r},t) \qquad \dots (3.46)$$

H_{op} is called Hamiltonian operator. Ψ is a function of $\vec{r}$ and t.

The solution of equation (3.45) is

$$\Psi(\vec{r},t) = u(\vec{r})\, \phi(t) \qquad \dots (3.47)$$

where, $$\phi(t) = Ne^{-iEt/\hbar} \qquad \dots (3.48)$$

The expectation value of operator does not depend on time. For example, operator A_{op}

$$\langle A \rangle = \int \Psi^*(\vec{r},t)\, H_{op}\Psi(\vec{r},t)\ d\tau$$

$$= \int u^*(\vec{r})\, \phi^*(t)\, A_{op}u(\vec{r})\, \phi(t)\ d\tau$$

$$= \int u^*(\vec{r})\, e^{iEt/\hbar}\, A_{op}u(\vec{r})\, e^{-iEt/\hbar}\ d\tau$$

Hence, if an operator is not depending on time, then

$$\langle A \rangle = \int u^*(\vec{r})\ A_{op}\, u(\vec{r})\ \ d\tau \qquad \dots (3.49)$$

- **Postulate-4:**

The state Ψ varies with time in a manner determined by the Schrodinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = H_{op}\Psi \qquad \dots (3.50)$$

where H_{op} is the Hamiltonian operator. The basic dynamical variable $\vec{r}$ and $\vec{p}$ do not change with time.

Consider operator A_{op} which are explicitly time dependent.

$$\frac{d}{dt}\langle A(\vec{r},\vec{p},t)\rangle = \frac{d}{dt}\int \Psi^*(\vec{r},t)\, A_{op}\Psi(\vec{r},t)\ d\tau$$

$$\therefore \frac{d}{dt}\langle A(\vec{r},\vec{p},t)\rangle = \int \frac{\partial \Psi^*}{\partial t} A(\vec{r},\vec{p},t)\,\Psi\, d\tau + \int \Psi^* \frac{\partial A_{op}}{\partial t}\Psi\ d\tau + \int \Psi^*\, A_{op}\ \frac{\partial \Psi}{\partial t}\, d\tau \qquad \dots (3.51)$$

But,

$$i\hbar \frac{\partial \Psi}{\partial t} = H_{op}\Psi \qquad \dots (3.52)$$

and, $$-i\hbar \frac{\partial \Psi^*}{\partial t} = \left(H_{op}\Psi\right)^* \qquad \dots (3.53)$$

Using equations (3.52) & (3.53) in equation (3.51), we have

$$\frac{d}{dt}\langle A\rangle = \int -\frac{1}{i\hbar}\left(H_{op}\Psi\right)^* A_{op}\,\Psi\, d\tau + \int \Psi^* \frac{\partial A_{op}}{\partial t}\Psi\ d\tau + \int \Psi^*\, A_{op}\left(\frac{1}{i\hbar}\ H_{op}\Psi\right) d\tau$$

But, H_{op} is Hermitian

$$\therefore \frac{d}{dt}\langle A\rangle = \int -\frac{1}{i\hbar}\ \Psi^* H_{op}\, A_{op}\,\Psi\, d\tau + \int \Psi^* \frac{\partial A_{op}}{\partial t}\Psi\ d\tau + \int \Psi^*\, A_{op}\ \frac{1}{i\hbar}\ H_{op}\Psi d\tau$$

$$\therefore \frac{d}{dt}\langle A\rangle = \int \Psi^* \left\{\frac{1}{i\hbar}\left[A_{op}, H_{op}\right] + \frac{\partial A_{op}}{\partial t}\right\}\Psi\, d\tau \qquad \dots (3.54)$$

Thus, the rate of change of the expectation value of any dynamical variable A may be obtained as the expectation value of $(i\hbar)^{-1}[A,H] + \frac{\partial A}{\partial t}$. This operator may be taken to represent the dynamical variable $\frac{dA}{dt}$.

$$\left(\frac{dA}{dt}\right)_{op} = \frac{1}{i\hbar}[A_{op}, H_{op}] + \frac{\partial A_{op}}{\partial t} \qquad \dots (3.55)$$

If A is any dynamical variable which is not explicitly time-dependent then $\frac{dA_{op}}{dt} = 0$ and it commutes with H , then $\langle A \rangle$ is independent of time. Such A is said to be a ***conserved quantity*** or ***constant of motion***.

Non-Interacting and Interacting Systems:

Suppose we have two system. The two systems may be two individual particles or a particle and an atom or two atoms. Let us use the symbol '1' to denote the dynamical variables for the first system and '2' for the other. The Hamiltonian of the combined system will depend on both the sets of variables.

$$\therefore H(1,2) = H_1(1) + H_2(2) \qquad \dots (3.56)$$

Then the systems are said to be non-interacting because they do not influence each other.

If system 1 is an eigen state $u(1)$ of $H_1(1)$ and 2 is in an eigenstate $v(2)$ of $H_2(2)$ then

$$H_1(1)\, u(1) = E_1\, u(1) \text{ and } H_2(2)\, v(2) = E_2\, v(2) \qquad \dots (3.57)$$

Then,

$$\begin{aligned} H(1,2)\, u(1)v(2) &= [H_1(1)\, u(1)]\, v(2) + u(1)[H_2(2)\, v(2)] \\ &= E_1\, u(1)\, v(2) + u(1)\, E_2\, v(2) \\ &= [E_1 + E_2]\, u(1)\, v(2) \end{aligned}$$

$$\therefore H(1,2)\, u(1)v(2) = E\, u(1)v(2) \qquad \dots (3.58)$$

Here, $E = E_1 + E_2$

Thus, the eigen functions of the combined system consisting of two non- interacting subsystems are products of the eigen functions of the individual subsystems, while the energy eigenvalue E is a sum of E_1 and E_2.

If the systems 1 and 2 interact mutually, then $H(1,2)$ can not be separated but interaction part is introduced as

$$H(1,2) = H_1(1) + H_2(2) + H'(1,2) \qquad \dots (3.59)$$

Here, $H'(1,2)$ is the interaction part of the Hamiltonian and $H_1(1) + H_2(2)$ is the free part.

Systems of Identical Particles:

If we have a system of N identical particles then total Hamiltonian is $H(1,2, \dots . N)$. If any two particles interchange or exchange the H_{op} will not be change. As a result $\Psi(1,2, \dots . N)$ will not effected.

We use new operator P_{ij} for exchange of particles. It is known as exchange operator.

$$P_{ij}\Psi(1,2, \dots . i, j, \dots . N) = \Psi(1,2, \dots . i, j, \dots . N) \qquad \dots (3.60)$$

If we operate again then,

$$P_{ij}\, P_{ij}\Psi(1,2, \dots . i, j, \dots . N) = P_{ij}\, \Psi(1,2, \dots . i, j, \dots . N)$$

$$\therefore\ P_{ij}\, P_{ij}\Psi(1,2, \dots . i, j, \dots . N) = \Psi(1,2, \dots . i, j, \dots . N)$$

Here, we use equation (3.60)

$$P_{ij}^{\,2}\Psi(1,2,\dots.i,j,\dots.N) = \Psi(1,2,\dots.i,j,\dots.N) \quad \dots(3.61)$$

$$\therefore\ P_{ij}^{\,2} = 1$$

The eigen equation of the exchange operator is given by

$$P\phi = \lambda\phi \quad \dots(3.62)$$

$$\text{and} \quad P^2\phi = \lambda^2\phi \quad \dots(3.63)$$

comparing equations (3.62) & (3.63), we get

$$\lambda^2 = \lambda$$

$$\therefore\ \lambda = \pm 1$$

There are two possible eigen values ± 1 for exchange operator of the eigen functions ϕ_+ and ϕ_-.

$$\left.\begin{aligned} P\,\phi_+ &= \phi_+ \\ and\ \ P\,\phi_- &= \phi_- \end{aligned}\right\} \quad \dots(3.64)$$

Now,

$$PH(1,2,\dots.i,j,\dots.N)\Psi(1,2,\dots.i,j,\dots.N) = H(1,2,\dots.i,j,\dots.N)\Psi(1,2,\dots.i,j,\dots.N)$$

$$= H(1,2,\dots.i,j,\dots.N)P\Psi(1,2,\dots.i,j,\dots.N)$$

$$\therefore PH = HP$$

$$\therefore PH - HP = 0$$

$$\therefore\ [P,H] = 0$$

Hence, P and H have the same eigen functions. If H has eigen function $\Psi(1,2,\dots.i,j,\dots.N)$ then

$$P\Psi(1,2,\dots.i,j,\dots.N) = \pm\Psi(1,2,\dots.i,j,\dots.N)$$

Here, ϕ_+ and ϕ_- are symmetric and antisymmetric respectively under interchange of the particles.

We conclude that the wave function ϕ must belong to one of the types:

(a) The totally symmetric (even) type which remains unchanged $(\lambda = \pm 1)$ under any interchange of particles or
(b) Totally antisymmetric (odd) type which changes sign $(\lambda = -1)$ with the interchange of any pair of particles.

The elementary particles in nature are classified in two ways

(a) Those which always have totally antisymmetric wave functions and
(b) Those which have totally symmetric wave functions.

- The particles which have symmetric wave functions are called **Bosons**, which obey the Bose-Einstein statistics. Its spin is an integer multiple of ħ. Photon, π −meson belong to this category. They are bosons.
- The particles which have antisymmetric wave functions are called **Fermions**. They obey Fermi-Dirac statistics. Its spin is half integer of ħ like $\frac{1}{2}\hbar, \frac{3}{2}\hbar, \dots \dots$. The fermions are electrons, protons, neutrons etc. The fermions obey the Pauli-exclusions principle.

The antisymmetric wave function is represented by the determinant

$$\Psi(1,2,\dots.i,j,\dots.N)=\begin{vmatrix}\Psi_a(1) & \Psi_a(2)\dots\dots\dots\dots\dots.\Psi_a(N)\\ \Psi_b(1) & \Psi_b(2)\dots\dots\dots\dots\dots.\Psi_b(N)\\ \dots\dots\dots\dots\dots\dots\dots & \dots\dots\dots\dots\dots\dots\dots\dots..\\ \dots\dots\dots\dots\dots\dots\dots & \dots\dots\dots\dots\dots\dots\dots\dots..\\ \dots\dots\dots\dots\dots\dots\dots & \dots\dots\dots\dots\dots\dots\dots\dots..\\ \Psi_z(1) & \Psi_z(2)\dots\dots\dots\dots\dots.\Psi_z(N)\end{vmatrix}$$

The Simple Harmonic Oscillator:

- **The Schrödinger equation and energy eigen values:**

The force acting on the pendulum is proportional to the displacement x. Then the motion of $\bar{e}$ is known as simple harmonic oscillator.

$$\therefore F\propto x$$
$$F=-kx$$

Where k is force constant.

$$\text{But,}\quad F=-\frac{\partial V}{\partial x}$$
$$\therefore\ -\frac{\partial V}{\partial x}=-kx$$

Integrating on both the sides with respect to x , we get

$$\therefore\ -\int\frac{dV}{dx}=-\int kx\,dx$$
$$\therefore V=\frac{1}{2}kx^2 \qquad \dots(3.65)$$

Where, force constant $k=mw^2$

Now, Hamiltonian operator is

$$H=K.E+P.E$$
$$\therefore H=\frac{1}{2}mv^2+\frac{1}{2}kx^2$$
$$\therefore H=\frac{P^2}{2m}+\frac{1}{2}kx^2$$
$$\therefore\ H=\frac{-\hbar^2\nabla^2}{2m}+\frac{1}{2}m\omega^2x^2 \qquad \dots(3.66)$$

Because $\vec{p}\rightarrow\ -i\hbar\vec{\nabla}$ and $k=\ m\omega^2$

The stationary state energies E_n and wave function $u_n(x)$ are the solution of time independent Schrodinger equation. The wave equation is given by

$$H\ u(x)=E\ u(x)$$

Using equation (3.66), we can write

$$\left[\frac{-\hbar^2}{2m}\nabla^2+\frac{1}{2}m\omega^2x^2\right]u(x)=E\ u(x)$$

For one-dimensional, we get

$$\left[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2x^2\right]u(x)=E\ u(x)$$

Multiplying both sides by $-\frac{2m}{\hbar^2}$

$$\therefore \frac{d^2u}{dx^2} - \frac{m^2\omega^2}{\hbar^2}x^2u(x) = -Eu\frac{2m}{\hbar^2}$$

$$\therefore \frac{d^2u}{dx^2} + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega^2x^2\right]u = 0 \qquad \text{...(3.67)}$$

This is the Schrodinger equation for simple harmonic oscillator.

Now take $x = \rho/\alpha$ where, $\alpha = \sqrt{\frac{m\omega}{\hbar}}$

Substituting this value in above equation, we get

$$\frac{d^2u}{d\rho^2}\alpha^2 + \frac{2m}{\hbar^2}\left[E - \frac{1}{2}m\omega^2\frac{\rho^2}{\alpha^2}\right]u = 0$$

$$\therefore \frac{d^2u}{d\rho^2}\alpha^2 + \frac{2mE}{\hbar^2}u - \frac{m^2\omega^2\rho^2}{\hbar^2\alpha^2}u = 0$$

$$\therefore \frac{d^2u}{d\rho^2} + \frac{2mE}{\alpha^2\hbar^2}u - \frac{m^2\omega^2}{\hbar^2}\frac{\rho^2}{\alpha^4}u = 0$$

Substituting the value of $\alpha = \sqrt{\frac{m\omega}{\hbar}}$ in above equation, we have

$$\therefore \frac{d^2u}{d\rho^2} + \frac{2mE}{\frac{m\omega}{\hbar}\hbar^2}u - \frac{m^2\omega^2}{\hbar^2}\frac{\rho^2}{\frac{m^2\omega^2}{\hbar^2}}u = 0$$

$$\therefore \frac{d^2u}{d\rho^2} + \frac{2Eu}{\hbar\omega} - \rho^2u = 0$$

Taking $\frac{2E}{\hbar\omega} = \lambda$, dimension less quantity.

Because $E = h\nu = \left(\frac{h}{2\pi}\right)(2\pi\nu) = \hbar\omega$

$$\therefore \frac{d^2u}{d\rho^2} + [\lambda - \rho^2]u = 0 \qquad \text{...(3.68)}$$

This is the dimension less Schrodinger equation.

- **To examine the asymptotic behaviour of wave function $u(x)[x = \pm\infty]$:**

Asymptotic behaviour means the behaviour of wave function for large value of x.

For simplicity put $\rho = x$

The solution of this equation is $u(x) = e^{-x^2/2}$

Another solution is $u(x) = e^{x^2/2} \to \infty$, when $x \to \infty$.

Therefore, we interpolate in the solution

$$\therefore u(x) = e^{-x^2/2}\,\phi(x) \qquad \text{...(3.69)}$$

Substituting this solution in equation (3.68). Here $\phi(x)$ is unknown polynomials.

$$\therefore \frac{d^2}{dx^2}\left[e^{-x^2/2}\,\phi(x)\right] + [\lambda - x^2]\left[e^{-x^2/2}\,\phi(x)\right] = 0$$

$$\therefore \frac{d}{dx}\left[e^{-x^2/2}\frac{d\phi(x)}{dx} + \phi(x)e^{-x^2/2}\left(-\frac{1}{2}2x\right)\right] + [\lambda - x^2]e^{-x^2/2}\,\phi(x) = 0$$

$$\therefore e^{-x^2/2}\,\frac{d^2\phi(x)}{dx^2} + e^{-x^2/2}(-x)\frac{d\phi}{dx} - \frac{d\phi}{dx}\,x\,e^{-x^2/2} - \phi(x)e^{-x^2/2} + x^2\phi(x)e^{-x^2/2}$$
$$+ [\lambda - x^2]e^{-x^2/2}\,\phi(x) = 0$$

$$\therefore \frac{d^2\phi}{dx^2} - 2x\,\frac{d\phi}{dx} + (\lambda - 1)\,\phi(x) = 0 \qquad \dots (3.70)$$

❖ **Series Solution:**

Let us now obtain the series solution of equation (3.70). Suppose its series solution is given by

$$\phi(x) = \sum_{n=0}^{\infty} a_n\ x^{n+s} \qquad \dots (3.71)$$

$$\therefore\ \phi'(x) = \sum_{n=0}^{\infty} a_n\,(n+s)\,x^{n+s-1}$$

and $$\phi''(x) = \sum_{n=0}^{\infty} a_n\,(n+s)\,(n+s-1)x^{n+s-2}$$

substituting these values in equation (3.70), we get

$$\sum_{n=0}^{\infty}[(n+s)\,(n+s-1)x^{n+s-2} - 2x\,(n+s)\,x^{n+s-1} + (\lambda-1)x^{n+s}\,]\,a_n = 0$$

$$\therefore \sum_{n=0}^{\infty}[(n+s)\,(n+s-1)x^{n+s-2} - 2\,(n+s)\,x^{n+s} + (\lambda-1)x^{n+s}\,]\,a_n = 0 \qquad \dots (3.72)$$

Now, equating the lowest power of x to zero by putting $n = 0$.

$$\therefore s(s-1)\,a_0 = 0$$

But , $a_0 \neq 0$

$$\therefore s(s-1) = 0$$

$$\therefore s = 0 \quad or \quad s = 1$$

Now, put $s = 0$ in equation (3.72)

$$\sum_{n=0}^{\infty}[n\,(n-1)\,x^{n-2} - 2\,n\,x^n + (\lambda-1)x^n\,]\,a_n = 0 \qquad \dots (3.73)$$

Now, equating the general coefficient of x^n to zero

$$\therefore\ (n+2)(n+1)a_{n+2} - [2n - (\lambda-1)]a_n = 0$$

$$\therefore\ (n+2)(n+1)a_{n+2} = [2n - \lambda + 1]a_n$$

$$\therefore \frac{a_{n+2}}{a_{n+1}} = \frac{2n - (\lambda-1)}{(n+2)(n+1)} \qquad \dots (3.74)$$

This formula is known as recurrence formula.

For $n \to \infty$, if the ratio of two successive coefficient tends to zero, then the series is called convergent series.

$$\phi(x) = \sum a_n\,x^n$$
$$= a_0 + a_2x^2 + a_4x^4 + \cdots \dots \dots .. + a_kx^k + a_{k+2}x^{k+2} + \cdots \dots$$

Here k is ∞

$$\therefore \frac{a_{k+2}}{a_k} = \frac{2k}{k^2} = \frac{2}{k} \to 0$$

We know that,

$$e^t = 1 + t + \frac{t^2}{2!} + \frac{t^3}{3!} + \cdots \ldots \ldots$$

Take $t = x^2$

$$\therefore e^{x^2} = 1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \cdots \ldots \ldots . + \frac{x^k}{\left(\frac{k}{2}\right)!} + \frac{x^{k+2}}{\left(\frac{k+2}{2}\right)!} + \cdots \ldots \ldots$$

The ratio of two successive coefficients is

$$\frac{x^{k+2}}{x^k} = \frac{\left(k + {}^2\!/_2\right)!}{\left({}^k\!/_2\right)!} = \frac{2}{k} \to 0 \quad as\ k \to \infty$$

The behaviour of the coefficient is series $\phi(x)$ is exactly the same as in the series for e^{x^2}.

$$\therefore u(x) = e^{-x^2/_2}\, \phi(x)$$
$$= e^{-x^2/_2}\, e^{x^2}$$
$$= e^{-x^2/_2} \to \infty \quad when\ x \to \infty$$

The above function will be unacceptable wave function. In order to avoid this situation the value of λ is chosen in such a way that the power series for $\phi(x)$ gets cut-off after certain number of terms, thereby making $\phi(x)$ a polynomials.

For example,

$$\phi(x) = a_0 + a_2x^2 + a_4x^4 + \cdots \ldots \ldots \ldots \ldots + a_kx^k + a_{k+2}x^{k+2} + \cdots \ldots ..$$

If we want to terminate the series after three terms, then the coefficients $a_6, a_8, a_{10}, \ldots$ should be zero.

This could happen only when the numerator in recursion relation is zero. Now, put $n = 4$ in recursion relation

$$\frac{a_6}{a_4} = \frac{8 - (\lambda - 1)}{6 \times 5} = \frac{8 - (\lambda - 1)}{30}$$
$$\therefore a_6 = \frac{8 - (\lambda - 1)}{30} a_4$$
$$\therefore Numerator = 8 - (\lambda - 1) = 0$$
$$\therefore \lambda - 1 = 8$$
$$\therefore \lambda = 9$$
$$\therefore \lambda = 2n + 1$$

We can say that, for $\lambda = 9$ the series will terminate after three terms.

The value of λ which make the series to cut-off at n^{th} terms is

$$\lambda = 2n + 1$$

But,

$$\lambda = \frac{2E}{\hbar\omega}$$
$$\therefore E = \frac{1}{2}\hbar\omega\lambda$$
$$\therefore E = \frac{1}{2}\hbar\omega(2n + 1)$$
$$\therefore E = \hbar\omega\left(n + \frac{1}{2}\right) \qquad \ldots .(3.75)$$

$$where, n = 0,1,2, \dots \dots$$

This gives energy eigen values of simple harmonic oscillator.

For $n = 0$,

$$E = \frac{1}{2}\hbar\omega$$

It is known as the zero-point energy.

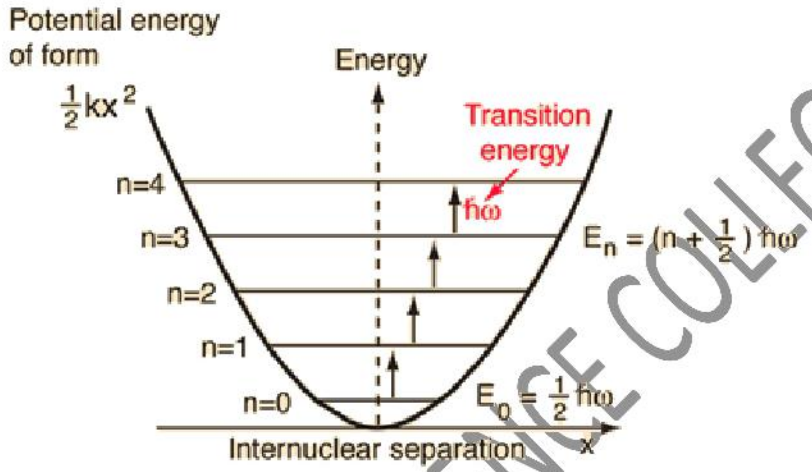

Fig:3.1

The stationary states of simple harmonic oscillator are characterized by equally spaced energy levels.

A constant spacing between successive energy levels is $\hbar\omega = \frac{h}{2\pi} 2\pi\nu = h\nu$ is exactly what had been postulated by Max Plank.

The wave mechanical treatment gives definite non-zero value for the ground state energy $E_0 = \frac{\hbar\omega}{2}$. This is called zero-point energy.

➢ Orthonormality:

The orthonormality property of the set of functions is

$$(u_m, u_n) = \int u_m^*(x)\, u_n(x)\, dx = \delta_{mn} \qquad \dots .(3.76)$$

To prove this property of the stationary state wave functions $u_n(x)$ we make use of known properties of Hermite polynomials. The generating function $G(\rho, h)$ of the Hermite polynomials defines as

$$G(\rho, h) = \sum_{n=0}^{\infty} \frac{1}{n!} H_n(\rho) h^n \qquad \dots (3.77)$$

$$= e^{(-h^2 + 2\rho h)} \qquad \dots (3.78)$$

Here, h is a parameter. $H_n(\rho)$ is the coefficient of $\frac{h^n}{n!}$ In the expansion of $e^{-h^2+2\rho h}$.

Now, consider the integral

$$\int_{-\infty}^{+\infty} G(\rho,h)G(\rho,h')e^{-\rho^2}\,d\rho \qquad \dots(3.79)$$

Now, substituting equations (3.77) & (3.78) in (3.79), we get

$$\sum_m \sum_n \frac{h^m h'^n}{m!\,n!} \int_{-\infty}^{+\infty} H_m(\rho)H_n(\rho)e^{-\rho^2}\,d\rho = \int_{-\infty}^{+\infty} e^{-\rho^2}\,e^{-h^2+2\rho h}e^{-h'^2+2\rho h'}\,d\rho$$

$$= \int_{-\infty}^{+\infty} e^{-\rho^2+2\rho(h+h')-(h^2+h'^2)}\,d\rho \qquad \dots.(3.80)$$

$$\therefore \sum_m \sum_n \frac{h^m h'^n}{m!\,n!} \int_{-\infty}^{+\infty} H_m(\rho)H_n(\rho)e^{-\rho^2}\,d\rho = \sqrt{\pi}\sum_m \sum_n \frac{2^n h^m h'^n}{n!}\delta_{mn} \qquad \dots(3.81)$$

Now, equating the coefficient of $h^m h'^n$ on both the sides, we get

$$\int_{-\infty}^{+\infty} H_m(\rho)H_n(\rho)e^{-\rho^2}\;d\rho = \sqrt{\pi}\,2^n\,m!$$

$$\therefore \int_{-\infty}^{+\infty} H_m(\rho)H_n(\rho)e^{-\rho^2}\;d\rho = \sqrt{\pi}\,2^n\,n!\,\delta_{mn} \qquad \dots.(3.82)$$

This is the orthogonal property of wave function of simple harmonic oscillator.

Question Bank

Multiple choice questions:

(1) According to general statement of uncertainty principle if ΔA and ΔB give the uncertainty in the measurement of A and B then $(\Delta A)^2(\Delta B)^2 \geq$ _______

(a) $\frac{\mathbf{1}}{\mathbf{4}}\langle[\boldsymbol{A},\boldsymbol{B}]\rangle^2$ (b) $\hbar$

(c) I$\hbar$ (d) $\frac{1}{2}\langle[A,B]\rangle^2$

(2) If A & B are a canonically conjugate pair of operator, then $[A,B] =$ _______

(a) *I$\hbar$/2* (b) ***I$\hbar$***

(c) $\hbar$ (d) *2i$\hbar$*

(3) The same state of all the components of _____ operator is impossible

(a) $\vec{P}$ (b) $\vec{\boldsymbol{L}}$

(c) $\vec{K}$ (d) $\vec{\nabla}$

(4) The value of constant of integration for Box normalized momentum eigen function is __________

(a) $^1/_{2\sqrt{L}}$ (b) $^{\mathbf{1}}/_{\sqrt{\boldsymbol{L}}}$

(c) $^1/_{\sqrt{\pi}}$ (d) $^1/_{\sqrt{2\pi}}$

(5) Time dependent Schrodinger equation in shorter form is given by Hu = _______

(a) Eu^2 (b) E

(c) EH (d) **Eu**

(6) Force acting on the pendulum is proportional to _________

(a) Velocity (b) **displacement**

(c) Time (d) acceleration

(7) Hamiltonian operator for simple harmonic oscillator is $H =$ ___________

(a) **$\frac{p^2}{2m}+\frac{1}{2}kx^2$** (b) $\frac{p^2}{2m}$

(c) $\frac{1}{2}kx^2$ (d) $\frac{p^2}{2m}+kx$

(8) Potential of harmonic oscillator is $V =$ __________

(a) mgh (b) **$\frac{1}{2}kx^2$**

(c) $\frac{p^2}{2m}$ (d) kx

(9) Energy eigen value of simple harmonic oscillator is given by E = _________

(a) $\hbar\nu$ (b) **$\left(n+\frac{1}{2}\right)\hbar\omega$**

(c) $N\hbar\nu$ (d) $\hbar\omega$

(10) The zero point energy for simple harmonic oscillator is E = _________

(a) $\hbar\omega$ (b) **$\frac{1}{2}\hbar\omega$**

(c) $\frac{3}{2}\hbar\omega$ (d) $\frac{5}{2}\hbar\omega$

(11) The ground state energy for simple harmonic oscillator is E = _________

(a) $\hbar\omega$ (b) **$\frac{1}{2}\hbar\omega$**

(c) $\frac{3}{2}\hbar\omega$ (d) $\frac{5}{2}\hbar\omega$

Short Questions:

1. Show that if the components of angular momentum Lx and Lyhave the same eigen function than they are commutative operators
2. State the uncertainty principle for operators A and B
3. Set up the Hamiltonian for simple harmonic oscillator
4. Write the dimension less Schrodinger equation for simple harmonic oscillator
5. Draw the energy level diagram of simple harmonic oscillator

Long Questions:

1. State uncertainty principle and discuss it for quantum mechanical observables.
2. Prove that the same state of all the component of $\vec{L}$ is impossible
3. Derive the dimension less Schrodinger equation for simple harmonic oscillator
4. Set up the Hamiltonian of simple harmonic oscillator and derive the expression of its energy eigen value