QUANTUM DYNAMICS

Describe the variable or parameter that specify the state of a physical system
Describe the evolution of Quantum system with time

In classical mechanics the dynamical state of a physical system is defined by the set of dynamical variables such as position, momentum, velocities etc

The equation of motion which describes evolution of physical system with time is a differential equation of these variables (position, momentum, velocities). The state of a system at any time can be determined by this differential equations by the state of the system at any initial time t_0
This is known as dynamical postulate:

In Quantum Mechanics the state of physical system is represented by a vector known as state vector ($|\psi\rangle$ or $\langle\psi|$), it is defined in abstract hilbert space. Therefore equation of motion for a quantum mechanical system could be a differential equation of a state vector. But these are not observable quantities, are not state vectors. But these are expectation values of a set of hermitian operator corresponding to dynamical variables.

Equation of motion in quantum mechanics should be concerned with evolution of these expectation values with time.

Consider an operator $\hat{A}$ corresponding to a dynamical variable. Expectation value of this operator in the state ψ is $\langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle$. Here the variation of $\langle \hat{A} \rangle$ can takes place in any time in any of the following ways.

1) The state vector ψ changes with time, but $\hat{A}$ remains unchanged

2) Operator $\hat{A}$ changes with time and ψ remains constant

3) Both ψ and $\hat{A}$ can change with time.

THE SCHRODINGER PICTURE :-

Let ψ is a function of t, $\hat{A}$ is not a function of t. The equation of motion is then equation for ψ, the value of $\psi(t)$ at any time 't' is determined by $\psi(t_0)$ at a given initial time 't_0'. 'ψ' is a vector in linear vector space, the relation b/w $\psi(t)$ and $\psi(t_0)$ is prescribed by <u>Evolution Operator</u> (we also call it as time dependent operator) 'U'

Properties of Evolution Operator:-

1) The operator $\hat{U}$ is a linear operator

2) The operator $\hat{U}$ preserves principle of superposition.
ie, if a state vector at initial time 't_0' can be written as

$$|\psi(t_0)\rangle = \sum_i a_i |\phi_i(t_0)\rangle$$

Since the operator $\hat{U}$ gives a new state at time 't'. When it acts on the state $|\psi(t_0)\rangle$ ie. the new state $|\psi(t)\rangle$ =

$$|\psi(t)\rangle = \hat{U}|\psi(t_0)\rangle$$
$$= \hat{U}\sum_i a_i |\phi_i(t_0)\rangle$$
$$= \sum_i a_i \hat{U}|\phi_i(t_0)\rangle$$
$$|\psi(t)\rangle = \sum_i a_i |\phi_i(t)\rangle$$

which proves the preservation of principle of superposition

3) $\hat{U}$ is found to be Unitary operator

4) $\hat{U}$ preserves the norm ie at time 't_0', we have the norm of the state, $\langle\psi(t_0)|\psi(t_0)\rangle$ and at time 't' $\langle\psi(t)|\psi(t)\rangle$.

fundamental dynamic postulate the state

$$|\psi(t)\rangle = \hat{U}(t,t_0)|\psi(t_0)\rangle$$

$$\langle\psi(t)| = \langle\psi(t_0)|\hat{U}^{+}(t,t_0)$$

Consider the norm.

$$\langle\psi(t)|\psi(t)\rangle = \langle\psi(t_0)|UU^{+}(t,t_0)|\psi(t_0)\rangle$$

$$= \langle\psi(t_0)|\psi(t_0)\rangle$$

Which shows U^{+} also preserves the norm.

Applying Hamiltonean operator $\hat{H}$ to the state vector $\psi(t)$

$$\hat{H}\psi = \hat{E}\psi$$

$$\hat{H}\psi = i\hbar\frac{\partial\psi(t)}{\partial t}$$

time dependent schrodinger equation

$$\hat{H}\psi = i\hbar\frac{\partial\psi(t)}{\partial t}$$

Rearranging

$$\frac{d\psi}{dt} = \frac{1}{i\hbar}\hat{H}\psi$$

$$\frac{d\psi}{\psi} = \frac{1}{i\hbar}\hat{H}dt$$

Integrating the above equation with respect to 't' between the limits t and to on both sides

$$\int_{\psi(t_0)}^{\psi(t)}\frac{d\psi(t)}{\psi} = \frac{1}{i\hbar}\int_{t}^{t_0}\hat{H}\,dt$$

$$\ln\psi\Big|_{\psi(t_0)}^{\psi(t)} = \frac{\hat{H}t}{i\hbar}\Big|_{t_0}^{t}$$

$$\ln\psi(t) - \ln\psi(t_0) = \frac{\hat{H}}{i\hbar}(t-t_0)$$

$$\ln\left(\frac{\psi(t)}{\psi(t_0)}\right) = \frac{\hat{H}(t-t_0)}{i\hbar}$$

$$\frac{\psi(t)}{\psi(t_0)} = e^{\hat{H}(t-t_0)/i\hbar}$$

$$\psi(t) = \psi(t_0)\, e^{-i\hat{H}(t-t_0)/\hbar}$$

we know that $\psi(t) = \hat{U}\,\psi(t_0)$

Then $\hat{U}(t_0) = \underline{\underline{\psi(t_0)\, e^{-i\hat{H}(t-t_0)/\hbar}}}$ is the value of evolution operator.

we know that

$$\hat{H}\,|\psi(t_0)\rangle = i\hbar\,\frac{\partial|\psi(t_0)\rangle}{\partial t}$$

Applying the $\hat{U}$ operator to the state vector $\psi(t_0)$

$$\hat{U}\hat{H}\,|\psi(t_0)\rangle = \hat{U}\left(i\hbar\,\frac{\partial|\psi(t_0)\rangle}{\partial t}\right)$$

$$\hat{H}\hat{U}\,|\psi(t_0)\rangle = i\hbar\,\hat{U}\left|\frac{\partial\psi(t_0)}{\partial t}\right\rangle$$

$$\hat{H}\hat{U}\,|\psi(t_0)\rangle = i\hbar\,\frac{\partial\hat{U}}{\partial t}|\psi(t_0)\rangle$$

then $\boxed{\hat{H}\hat{U} = i\hbar\,\frac{\partial U}{\partial t}}$.

EQUATION OF MOTION IN SCHRODINGER'S PICTURE:-

The expectation value of an operator $\hat{A}$ can be written as $\langle\hat{A}\rangle = \langle\psi(t)|\hat{A}|\psi(t)\rangle$

$$\frac{d}{dt}\langle\hat{A}\rangle = \frac{d}{dt}\left(\langle\psi(t)|\hat{A}|\psi(t)\rangle\right) \quad \text{—— ①}$$

From the schrodinger time independent equation

$$\hat{H}|\psi(t)\rangle = i\hbar\,\frac{\partial|\psi(t)\rangle}{\partial t} = i\hbar\,\frac{d|\psi(t)\rangle}{dt}$$

$$\frac{d}{dt}|\psi(t)\rangle = \left|\frac{d\psi(t)}{dt}\right\rangle$$

$$H|\psi(t)\rangle = i\hbar\left|\frac{d\psi(t)}{dt}\right\rangle$$

$$\left|\frac{d}{dt}\psi(t)\right\rangle = \frac{1}{i\hbar} H|\psi(t)\rangle \quad \text{in the ket space}$$

$$\left\langle \frac{d\psi(t)}{dt}\right| = \langle \psi(t)| \frac{\hat{H}^{+}}{-i\hbar} \quad \text{in Bra space}$$

$$= \langle \psi(t)| \frac{\hat{H}}{-i\hbar} \quad \text{since } \hat{H}^{+} = \hat{H}$$

— (2)

(1) $\Rightarrow$ $$\frac{d}{dt}\langle A\rangle = \left\langle \frac{d\psi(t)}{dt}\right|\hat{A}|\psi(t)\rangle + \langle\psi(t)|\hat{A}\left|\frac{d\psi(t)}{dt}\right\rangle$$

From (2)

$$\frac{d}{dt}\langle A\rangle = \langle\psi(t)|\left(\frac{H}{-i\hbar}\right)|\hat{A}|\psi(t)\rangle + \langle\psi(t)|\hat{A}\left|\frac{H}{i\hbar}\psi(t)\right\rangle$$

$$= \langle\psi(t)|\left(\frac{\hat{H}\hat{A}}{-i\hbar} + \frac{\hat{A}\hat{H}}{i\hbar}\right)|\psi(t)\rangle$$

$$= \frac{1}{i\hbar}\langle\psi(t)|(\hat{H}\hat{A} - \hat{A}\hat{H})|\psi(t)\rangle$$

$$= \frac{1}{i\hbar}\langle\psi(t)|[\hat{A},\hat{H}]|\psi(t)\rangle$$

$\therefore$ $\boxed{\frac{d\langle\hat{A}\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle}$ is the equation of motion

in Schrodinger picture.

Comparing the above equation with the equation of motion for the dynamical variables A in classical mechanics, we can see that the expectation value of the operator obey the same equation of motion in Quantum mechanics as the dynamical variables in classical mechanics, we identify → $\left[\frac{\text{commutator bracket}}{i\hbar}\right]$ = Poisson bracket in Quantum mechanics

For the time dependent forces the equation of motion

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle[\hat{A},\hat{H}]\rangle + \left\langle\frac{d\hat{A}}{dt}\right\rangle$$

If A commutes with $\hat{H}$ of the system, then $\hat{A}$ is called as constant of motion ie

$$\frac{d\langle A\rangle}{dt} = 0 \implies \langle\hat{A}\rangle = \text{constant}$$

THE HEISENBIRG PICTURE:-

In order to distinguish the state vector and operators in Heisenburg picture from those of Schrodinger picture we use subscript H.

If ψ is the state vector and A_H is the operator then from Schrodinger formulation,

$$\langle\hat{A}\rangle = \langle\psi(t)|\hat{A}|\psi(t)\rangle \quad \text{--- (1)}$$

$$|\psi(t)\rangle = \hat{U}|\psi(t_0)\rangle \quad \text{--- (2)}$$

$$\langle\psi(t)| = \langle\psi(t_0)|U^{+} \quad \text{--- (3)}$$

substitute equation (2) and (3) in equation (1)

$$\langle\hat{A}\rangle = \langle\psi(t_0)|U^{+}AU|\psi(t_0)\rangle$$

consider $\hat{U}^{+}\hat{A}\hat{U} = \hat{A}_H$

$$\langle\hat{A}\rangle = \langle\psi(t_0)|\hat{A}_H|\psi(t_0)\rangle \quad \text{--- (4)}$$

differentiating equation (4) with respect to t

$$\frac{d\langle\hat{A}\rangle}{dt} = \frac{d}{dt}\left(\langle\psi(t_0)|\hat{A}_H|\psi(t_0)\rangle\right)$$

$$= \frac{d}{dt}\left(\langle\psi(t_0)|\hat{U}^{+}\hat{A}\hat{U}|\psi(t_0)\rangle\right)$$

$$\frac{d\langle\hat{A}\rangle}{dt} = \langle\psi(t_0)|\frac{d}{dt}(\hat{U}^{+}\hat{A}\hat{U})|\psi(t_0)\rangle$$

$$\frac{d\langle A\rangle}{dt} = \langle\psi(t_0)| U^{+} A \frac{dU}{dt} |\psi(t_0)\rangle + \langle\psi(t_0)| \frac{dU^{+}}{dt} A U |\psi(t_0)\rangle \quad \text{--- (5)}$$

From the differentiation of evolution operator

$$\hat{U} = e^{-\frac{i\hat{H}(t-t_0)}{\hbar}} \qquad U^{+} = e^{\frac{i\hat{H}(t-t_0)}{\hbar}}$$

$$\frac{dU}{dt} = -\frac{i\hat{H}}{\hbar} e^{-\frac{i\hat{H}(t-t_0)}{\hbar}} \qquad \frac{dU^{+}}{dt} = \frac{i\hat{H}}{\hbar} e^{\frac{i\hat{H}(t-t_0)}{\hbar}}$$

$$= -\frac{i\hat{H}\hat{U}}{\hbar} \qquad = \frac{i\hat{H}}{\hbar}\hat{U}^{+}$$

$$\frac{dU}{dt} = \frac{\hat{H}\hat{U}}{i\hbar} \qquad \frac{dU^{+}}{dt} = -\frac{\hat{H}U^{+}}{i\hbar}$$

(5) $\Rightarrow$ $\langle\psi(t_0)| -\frac{\hat{H}U^{+}}{i\hbar} AU |\psi(t_0)\rangle + \langle\psi(t_0)| \hat{U}^{+} A \frac{\hat{H}\hat{U}}{i\hbar} |\psi(t_0)\rangle$

$$\frac{d\langle A\rangle}{dt} = \frac{d}{dt}\langle\psi(t_0)| U^{+}AHU - HU^{+}AU |\psi(t_0)\rangle$$

$$= \frac{d}{dt}\langle\psi(t_0)| \hat{A}_H\hat{H} - H\hat{A}_H |\psi(t_0)\rangle$$

$$= \frac{d}{dt}\langle\psi(t_0)| [\hat{A}_H, H] |\psi(t_0)\rangle$$

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle [A_H, H]\rangle \quad \text{--- (6)}$$

If $\hat{A}_H$ depends explicitly on time then,

$$\frac{d\hat{A}_H}{dt} = \frac{\partial\hat{A}_H}{\partial t} + \frac{1}{i\hbar}\langle [A_H, H]\rangle \quad \text{--- (7)}$$

Equation (6) and (7) are called Heisenberg equations of motion for the operator $\hat{A}_H$

(6) and (7) are identical in form. The only difference is In the place of poisson bracket in (7) is taken by the commutator bracket in (6)

From the definition of poisson's bracket

$$\{F, H\} = \frac{\partial F}{\partial q}\frac{\partial H}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial H}{\partial q} = \frac{\partial F}{\partial t}$$

where p and q are basic canonical transformations.

Or we can write $\{q_i, p_j\} = \delta_{ij}$

$$[q_i, p_j] = i\hbar\, \delta_{ij}$$

The relation between poisson's bracket and commutator bracket is $\{A, H\} = \frac{[A, H]}{i\hbar}$

Find the equation of motion considering

(i) $\hat{A} = \hat{P}_x$ (ii) $\hat{A} = x$

(i) From the schrodinger picture

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle [A, H]\rangle$$

$$= \frac{1}{i\hbar}\left\langle \left[\hat{P_x}, \left(\frac{\hat{P}_x^2}{2m} + V(x)\right)\right]\right\rangle$$

$$= \frac{1}{i\hbar}\left\langle \left[\hat{P_x}, \frac{P_x^2}{2m}\right] + \left[\hat{P_x}, V(x)\right]\right\rangle$$

$$[A, BC] = [A, B]C + B[A, C]$$

consider

$$\left[\hat{P_x}, \frac{P_x P_x}{2m}\right] = \frac{1}{2m}\left[[\hat{P_x}\hat{P_x}]\hat{P_x} + \hat{P_x}[\hat{P_x}, \hat{P_x}]\right]$$

$$= \underline{\underline{0}} \qquad \because [\hat{P_x}, \hat{P_x}] = 0$$

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle [\hat{P_x}, V(x)]\rangle$$

$$= \frac{1}{i\hbar}(P_x V(x) - V(x) P_x)$$

$$= \frac{1}{i\hbar}(\hat{P_x} V(x)\psi(x) - V(x) P_x \psi(x))$$

$$= \frac{1}{i\hbar}\left(-i\hbar\frac{\partial}{\partial x}(V(x)\psi(x)) - V(x)\left(-i\hbar\frac{\partial\psi(x)}{\partial x}\right)\right)$$

$$\psi(x)\frac{d\langle A\rangle}{dt} = -\psi(x)\frac{\partial V(x)}{\partial x}$$

$$\frac{d\langle A\rangle}{dt} = -\frac{\partial V(x)}{\partial x}$$

$$\boxed{\frac{d\langle A\rangle}{dt} = -\frac{\partial V}{\partial x}}$$

(ii) $\hat{A} = x$

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\langle[A, H]\rangle$$

$$= \frac{1}{i\hbar}\left\langle\left[\hat{x}, \left(\frac{P_x^2}{2m} + V(x)\right)\right]\right\rangle$$

$$= \frac{1}{i\hbar}\left\langle\left[\hat{x}, \frac{P_x^2}{2m}\right] + [\hat{x}, V(x)]\right\rangle$$

consider

$$\left[\hat{x}, \frac{P_x^2}{2m}\right] = \frac{1}{2m}\left[[\hat{x}, \hat{P}_x]\hat{P}_x + \hat{P}_x[\hat{x}, \hat{P}_x]\right]$$

$$= \frac{1}{2m}\left[i\hbar\hat{P}_x + \hat{P}_x i\hbar\right]$$

$$= \frac{2i\hbar\hat{P}_x}{2m}$$

$$= \frac{i\hbar\hat{P}_x}{m}$$

$$[\hat{x}, V(x)] = 0$$

$$\frac{d\langle A\rangle}{dt} = \frac{1}{i\hbar}\left[\frac{i\hbar P_x}{m}\right]$$

$$\boxed{\frac{d\langle A\rangle}{dt} = \frac{\langle P_x\rangle}{m}}$$

ONE DIMENSIONAL SIMPLE HARMONIC OSCILLATOR

The difference between schrodinger and Heisenburg picture can be illustrated by applying these two methods to the solution of problem of Linear Harmonic oscillator, for which the Hamiltonian is given by,

$$\hat{H} = \frac{P_x^2}{2m} + \frac{1}{2} k x^2$$

$$= \frac{P_x^2}{2m} + \frac{1}{2} m\omega^2 x^2 \quad \text{—— (1)}$$

Our aim is to solve this problem ie find the eigen values and eigen vectors of the operator H. Dirac introduced a new method where he used new operators to solve this problem. These operators can generate all the eigen vectors of Hamiltonian operator from any given eigen ~~value~~ vector. These eigenvectors will define the matrix representation. Hamiltonian is found to be the diagonal of this matrix representation. This method is also known as second quantization.

These operators are,

$$\hat{a} = \frac{1}{\sqrt{2m\omega\hbar}} \left[m\omega x + i\hat{p} \right] \quad \text{—— (2)}$$

$$\hat{a}^+ = \frac{1}{\sqrt{2m\omega\hbar}} \left[m\omega x - i\hat{p} \right] \quad \text{—— (3)}$$

add equation (2) and (3)

$$\hat{a} + \hat{a}^+ = \frac{1}{\sqrt{2m\omega\hbar}} (2m\omega x) \quad \text{—— (4)}$$

Subtract equation (3) from (2)

$$\hat{a} - \hat{a}^+ = \frac{1}{\sqrt{2m\omega\hbar}} (2i\hat{p}) \quad \text{—— (5)}$$

④ $\Rightarrow \dfrac{\sqrt{2}\sqrt{m}\sqrt{\omega}}{\sqrt{\hbar}}\hat{x} = \hat{a}+\hat{a}^{+}$

Therefore $\hat{x} = \dfrac{(\hat{a}+\hat{a}^{+})\sqrt{\hbar}}{\sqrt{2m\omega}} = \sqrt{\dfrac{\hbar}{2m\omega}}(\hat{a}+\hat{a}^{+})$

⑤ $\Rightarrow (\hat{a}-\hat{a}^{+}) = \dfrac{\sqrt{2}\, i\hat{p}}{\sqrt{m\omega\hbar}}$

$$\hat{p} = \sqrt{\frac{m\omega\hbar}{2}}\,\frac{1}{i}(\hat{a}-\hat{a}^{+})$$

Consider $[a, a^{+}] = \left[\dfrac{1}{\sqrt{2\omega m\hbar}}(m\omega\hat{x}+i\hat{p}), \dfrac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat{x}-i\hat{p})\right]$

$$= \left(\frac{1}{\sqrt{2m\omega\hbar}}\right)^2\left[(m\omega\hat{x}+i\hat{p}), (m\omega\hat{x}-i\hat{p})\right]$$

$$= \frac{1}{2m\omega\hbar}\left[[m\omega\hat{x}, m\omega\hat{x}] - [m\omega\hat{x}, i\hat{p}] + [i\hat{p}, m\omega\hat{x}] - [i\hat{p}, i\hat{p}]\right]$$

$$= \frac{1}{2m\omega\hbar}\left[0 - m\omega i(i\hbar) - m\omega i(i\hbar) - 0\right]$$

$$= \frac{1}{2m\omega\hbar}\left[2m\omega\hbar\right] = 1$$

$\therefore [a, a^{+}] = 1$

Consider $[a^{+}, a] = \left[\dfrac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat{x}-i\hat{p}), \dfrac{1}{\sqrt{2m\omega\hbar}}(m\omega\hat{x}+i\hat{p})\right]$

$$= \frac{1}{2m\omega\hbar}\left[(m\omega\hat{x}-i\hat{p}), (m\omega\hat{x}+i\hat{p})\right]$$

$$= \frac{1}{2m\omega\hbar}\left[[m\omega\hat{x}, m\omega\hat{x}] + [m\omega\hat{x}, -i\hat{p}] - [i\hat{p}, m\omega\hat{x}] - [i\hat{p}, i\hat{p}]\right]$$

$$= \frac{1}{2m\omega\hbar}\left[0 - (m\omega\hbar) - (m\omega\hbar) - 0\right]$$

$$= \frac{1}{2m\omega\hbar}\left[-2m\omega\hbar\right]$$

$$\therefore \left[a^{+}, a\right] = -1$$

To find the Hamiltonean in terms of a and a^{+} :-

First we will find the value of aa^{+}.

Consider $$aa^{+} = \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + m\omega\hat{x}i\hat{p} - ipm\omega\hat{x} + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + im\omega(\hat{p}\hat{x} - \hat{x}\hat{p}) + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + im\omega[\hat{p}, \hat{x}] + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + im\omega(-i\hbar) + p^2\right\}$$

$$aa^{+} = \frac{m^2\omega^2\hat{x}^2}{2m\omega\hbar} + \frac{m\omega\hbar}{2m\omega\hbar} + \frac{p^2}{2m\omega\hbar}$$

$$= \frac{m\omega^2\hat{x}^2}{2\omega\hbar} + \frac{1}{2} + \frac{p^2}{2m\omega\hbar}$$

$$= \frac{1}{\omega\hbar}\left\{\frac{p^2}{2m} + \frac{m\omega^2\hat{x}^2}{2}\right\} + \frac{1}{2}$$

Therefore $$aa^{+} = \frac{1}{\hbar\omega}\left[\hat{H}\right] + 1/2 \quad \text{———} \quad (2)$$

where $\hat{H} = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}$ in the Hamiltonean operator for One Dimensional Simple Harmonic oscillator

Now consider $\hat{a}^+\hat{a} = \frac{1}{2m\omega\hbar}\left\{(m\omega\hat{x} - i\hat{p})(m\omega\hat{x} + i\hat{p})\right\}$

$$\hat{a}^+\hat{a} = \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + m\omega\hat{x}\,i\hat{p} - i\hat{p}\,m\omega\hat{x} + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 - im\omega(\hat{p}\hat{x} - \hat{x}\hat{p}) + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + im\omega(\hat{x}\hat{p} - \hat{p}\hat{x}) + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + im\omega[\hat{x},\hat{p}] + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 + im\omega(i\hbar) + p^2\right\}$$

$$= \frac{1}{2m\omega\hbar}\left\{m^2\omega^2\hat{x}^2 - m\omega\hbar + p^2\right\}$$

$$\hat{a}^+\hat{a} = \frac{1}{\omega\hbar}\left\{\frac{m\omega^2x^2}{2} + \frac{p^2}{2m}\right\} - \frac{1}{2}$$

$$\hat{a}^+\hat{a} = \frac{1}{\omega\hbar}[\hat{H}] - 1/2$$

Now,

$$aa^+ + a^+a = \frac{2\hat{H}}{\hbar\omega} + \left(\frac{1}{2} - \frac{1}{2}\right)$$

$$= \frac{2\hat{H}}{\hbar\omega}.$$

$$aa^+ - a^+a = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} + \frac{1}{2} - \frac{\hat{H}}{\hbar\omega}$$

$$= \frac{1}{4}$$

Therefore $\hat{H} = \frac{\hbar\omega(aa^+ + a^+a)}{2}$ —— (x)

To find $[\hat{a}, \hat{H}]$

$$[\hat{a}, \hat{H}] = \left[a, \hbar\omega \frac{(aa^+ + a^+a)}{2} \right] \quad \text{(from (11))}$$

we have $[A, (BC)] = [A,B]C + B[A,C]$

$$[\hat{a}, \hat{H}] = \frac{\hbar\omega}{2} \left\{ [\hat{a}, \hat{a}\hat{a}^+] + [\hat{a}, \hat{a}^+\hat{a}] \right\}$$

consider $[\hat{a}, \hat{a}\hat{a}^+] = [\hat{a}\,\hat{a}]\,a^+ + \hat{a}\,[\hat{a}, \hat{a}^+]$

$$= 0 + \hat{a} = \underline{\underline{\hat{a}}}$$

$$[\hat{a}, \hat{a}^+\hat{a}] = [a, a^+]a + a^+[a, a]$$

$$= \hat{a} + 0 = \underline{\underline{\hat{a}}}$$

Then $[\hat{a}, \hat{H}] = \frac{\hbar\omega}{2} \left\{ \hat{a} + \hat{a} \right\}$

$$= \underline{\underline{\hbar\omega\hat{a}}}$$

Similarly find $[\hat{a}^+, \hat{H}] = \left[\hat{a}^+, \frac{\hbar\omega}{2} (aa^+ + a^+a) \right]$

$$= \frac{\hbar\omega}{2} \left\{ [\hat{a}^+, \hat{a}\hat{a}^+] + [\hat{a}^+, \hat{a}\hat{a}^+] \right\}$$

consider $[\hat{a}^+, \hat{a}\hat{a}^+] = [\hat{a}^+, \hat{a}]\,\hat{a}^+ + \hat{a}\,[\hat{a}^+, \hat{a}^+]$

$$= (-1)\,a^+ + 0$$

$$= \underline{\underline{-\hat{a}^+}}$$

$$[\hat{a}^+, \hat{a}^+, \hat{a}] = [\hat{a}^+\hat{a}^+]\,\hat{a} + \hat{a}^+[\hat{a}^+, \hat{a}]$$

$$= 0 + \hat{a}^+(-1) = \underline{\underline{-\hat{a}^+}}$$

$$\therefore [\hat{a}^+, \hat{H}] = \frac{\hbar\omega}{2}(-2\hat{a}^+) = \underline{\underline{-\hbar\omega\hat{a}^+}}$$

Meaning of $[a, \hat{H}]$:-

let $\hat{H}$ acting on $|\psi_{En}\rangle$ ie

$$\hat{H}|\psi_{En}\rangle = E_n|\psi_{En}\rangle \quad \text{—— (5)}$$

where $\hat{H}$ is Hamiltonean of Harmonic oscillator with eigen value E_n which is nothing but energy.

we know that $[a, \hat{H}] = \hbar\omega\hat{a}$

$$[a, \hat{H}]|\psi_{En}\rangle = \hbar\omega\hat{a}|\psi_{En}\rangle$$

$$(\hat{a}\hat{H} - \hat{H}\hat{a})|\psi_{En}\rangle = \hbar\omega\hat{a}|\psi_{En}\rangle$$

$$\hat{a}\hat{H}|\psi_{En}\rangle - \hat{H}\hat{a}|\psi_{En}\rangle = \hbar\omega\hat{a}|\psi_{En}\rangle$$

From (5)

$$\hat{a}E_n|\psi_{En}\rangle - \hat{H}\hat{a}|\psi_{En}\rangle = \hbar\omega\hat{a}|\psi_{En}\rangle$$

$$\hat{H}\hat{a}|\psi_{En}\rangle = \hat{a}E_n|\psi_{En}\rangle - \hbar\omega\hat{a}|\psi_{En}\rangle \quad \text{—— (6)}$$

$$\hat{H}\hat{a}|\psi_{En}\rangle = (E_n - \hbar\omega)\hat{a}|\psi_{En}\rangle$$

From equation (6) we can analyse that $\hat{a}|\psi_{En}\rangle$ is also an eigen state of $\hat{H}$ but belongs to the eigen value $(E_n - \hbar\omega)$. It means that if the operator $\hat{a}$ acts on any state it is converted into a new state which is nothing but lower energy state.

* Suppose $\hat{a}$ acts once again on $\hat{a}|\psi_{En}\rangle$ ie $\hat{a}\hat{a}|\psi_{En}\rangle$ we will get a new state $|\psi_{En-2\hbar\omega}\rangle$ ie $\hat{a}\hat{a}|\psi_{En}\rangle = |\psi_{En-2\hbar\omega}\rangle$ which implies that $\hat{a}$ acts on any state its energy value reduces by a factor $\hbar\omega$. ie It destroys one quanta or one particle. Therefore $\hat{a}$ is called destruction operator or anhilation operator

* If a acts on any state $|\psi_{En}\rangle$ 'n' times ie

$$a^n|\psi_{En}\rangle \longrightarrow |\psi_{En-n\hbar\omega}\rangle$$ then it may reach the ground state $|\psi_{E0}\rangle$

Since $|\psi_{E0}\rangle$ is the ground state or minimum energy state then a acting on $|\psi_{E_0}\rangle$ does not have any meaning in quantum mechanics because there is no energy state below the ground state. Therefore $\hat{a}|\psi_{E_0}\rangle = 0$.

Meaning of $[a^+, \hat{H}]$:-

Consider $\hat{H}|\psi_{E_n}\rangle = E_n|\psi_{E_n}\rangle$.

we know that $[a^+, \hat{H}] = -\hbar\omega\hat{a}^+$

$$[a^+, \hat{H}]|\psi_{E_n}\rangle = -\hbar\omega\hat{a}^+|\psi_{E_n}\rangle$$

$$(a^+\hat{H} - \hat{H}a^+)|\psi_{E_n}\rangle = -\hbar\omega\hat{a}^+|\psi_{E_n}\rangle$$

$$a^+\hat{H}|\psi_{E_n}\rangle - \hat{H}a^+|\psi_{E_n}\rangle = -\hbar\omega\hat{a}^+|\psi_{E_n}\rangle$$

$$a^+E_n|\psi_{E_n}\rangle - \hat{H}\hat{a}^+|\psi_{E_n}\rangle = -\hbar\omega\hat{a}^+|\psi_{E_n}\rangle$$

$$\hat{H}\hat{a}^+|\psi_{E_n}\rangle = \hbar\omega a^+|\psi_{E_n}\rangle + a^+E_n|\psi_{E_n}\rangle$$

$$\hat{H}a^+|\psi_{E_n}\rangle = (E_n + \hbar\omega)a^+|\psi_{E_n}\rangle \quad \text{——— (7)}$$

From (7) we can observe that when a^+ acts on any state its energy value is increased by the factor $\hbar\omega$, which is nothing but a higher energy state.

$$\hat{a}^+|\psi_{E_n}\rangle \longrightarrow |\psi_{E_n + \hbar\omega}\rangle$$

Therefore a^+ is called creation operator

* If $\hat{a}^+$ acts on $|\psi_{E_n}\rangle$ n times ie

$$(a^+)^n|\psi_{E_n}\rangle \longrightarrow |\psi_{E_n + n\hbar\omega}\rangle$$

<u>To find the zero point energy</u> :-

we know that $a^+|\psi_{E_0}\rangle = 0$

If a^+ acts on $\hat{a}|\psi_{E_0}\rangle$ state then

$$\hat{a}^+\hat{a}|\psi_{E_0}\rangle = 0$$

$$\left(\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}\right)|\psi_{E_0}\rangle = 0$$

$$\frac{\hat{H}}{\hbar\omega}|\psi_{E_0}\rangle - \frac{1}{2}|\psi_{E_0}\rangle = 0$$

$$\frac{\hat{H}}{\hbar\omega}|\psi_{E0}\rangle = \frac{1}{2}|\psi_{E0}\rangle$$

$$\hat{H}|\psi_{E0}\rangle = \frac{\hbar\omega}{2}|\psi_{E0}\rangle$$

we know that $\hat{H}\psi = E_0\psi$

$$E_0|\psi_{E0}\rangle = \frac{\hbar\omega}{2}|\psi_{E0}\rangle$$

On comparing, we get

$$E_0 = \frac{\hbar\omega}{2} \quad \text{—— (8)}$$

which represents the zero point energy or ground state of harmonic Oscillator

Let us take $\hat{a}$ acting on ψ_{En} ie

$$\hat{a}|E_n\rangle = |n\rangle \quad \text{and} \quad |\psi_{En-\hbar\omega}\rangle = |n-1\rangle$$

when $\hat{a}$ acts on $|\psi_{En}\rangle$ it reduces the energy state by a factor $\hbar\omega$ ie

$$\hat{a}|n\rangle \longrightarrow |n-1\rangle$$

$$\hat{a}|\psi_n\rangle \longrightarrow |\psi_{En-\hbar\omega}\rangle$$

when $\hat{a}$ acts on n^{th} energy state, the state is converted into $(n-1)$ energy state

$$\hat{a}|n\rangle = \alpha_n|n-1\rangle$$

where α_n is eigen value of operator $\hat{a}$.

To find the value of α_n (Eigen value of $\hat{a}$) :-

consider $\hat{a}|n\rangle = \alpha_n|n-1\rangle$ —— (9)

$\langle n|\hat{a}^{+} = \langle n-1|\alpha_n^{*}$ —— (10)

consider (10) x (9)

$$\langle n|\hat{a}^{+}\hat{a}|n\rangle = \langle n-1|\alpha_n^{*}\alpha_n|n-1\rangle$$

$$\langle n|\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}|n\rangle = |\alpha_n|^2\langle n-1|n-1\rangle$$

Since $(n-1)^{th}$ state is normalised state.

$\langle n-1|n-1\rangle = 1$ then

$$\langle n|\frac{\hat{H}}{\hbar\omega} - \frac{1}{2}|n\rangle = |\alpha_n|^2$$

$$\langle n|\frac{\hat{H}}{\hbar\omega}|n\rangle - \frac{1}{2}\langle n|n\rangle = |\alpha_n|^2$$

$$\frac{1}{\hbar\omega}\langle n|\hat{H}|n\rangle - \frac{1}{2} = |\alpha_n|^2$$

$$\frac{1}{\hbar\omega}\langle n|E_n|n\rangle - \frac{1}{2} = |\alpha_n|^2$$

$$\frac{E_n}{\hbar\omega}\langle n|n\rangle - \frac{1}{2} = |\alpha_n|^2$$

$$\frac{E_n}{\hbar\omega} - \frac{1}{2} = |\alpha_n|^2$$

In case of Harmonic oscillator

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$\frac{\left(n+\frac{1}{2}\right)\hbar\omega}{\hbar\omega} - \frac{1}{2} = |\alpha_n|^2$$

$$n = |\alpha_n|^2$$

$$\alpha_n = \sqrt{n}$$

where n is the quantum number

substituting in $\hat{a}|n\rangle = \alpha_n|n-1\rangle$ from (9)

$$\hat{a}|n\rangle = \sqrt{n}\,|n-1\rangle \quad \text{—— (12)}$$

Equation (12) is the eigen equation for anhilation operator $\hat{a}$ with eigen value $\sqrt{n}$

To find eigen value of a^+:-

we know that $|\psi_{E_n}\rangle = |n\rangle$

and $|\psi_{E_n+\hbar\omega}\rangle = |n+1\rangle$

Since we know $a^+|\psi_{E_n}\rangle \longrightarrow |\psi_{E_n+\hbar\omega}\rangle$

$$a^+|n\rangle \longrightarrow |n+1\rangle$$

Take β_n be the eigen value of a^+ so that

$$a^+|n\rangle = \beta_n|n+1\rangle \quad \text{——— (13)}$$

$$\langle n|\hat{a} = \langle n+1|\beta_n^* \quad \text{——— (14)}$$

consider (13) (14)

$$\langle n|\hat{a}a^+|n\rangle = \langle n+1|\beta_n^*\beta_n|n+1\rangle$$

$$\langle n|\frac{\hat{H}}{\hbar\omega}+\frac{1}{2}|n\rangle = |\beta_n|^2$$

$$\frac{1}{\hbar\omega}\langle n|\hat{H}|n\rangle + \langle n|\tfrac{1}{2}|n\rangle = |\beta_n|^2$$

$$(\because \hat{H} = (n+\tfrac{1}{2})\hbar\omega)$$

$$\left(\frac{n+1/2}{\hbar\omega}\right)\hbar\omega + \frac{1}{2} = |\beta_n|^2$$

$$n+1 = |\beta_n|^2$$

$$\beta_n = \sqrt{n+1}$$

where n is the quantum number

Substituting in $a^+|n\rangle = \beta_n|n+1\rangle$

$$a^+|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

For example: $a^+|0\rangle = \sqrt{0+1}\,|0+1\rangle$

$$= \sqrt{1}\,|1\rangle = |1\rangle = \frac{1}{\sqrt{1}}a^+|0\rangle$$

$$a^+|1\rangle = \sqrt{2}\,|2\rangle = |2\rangle = \frac{1}{\sqrt{2}}a^+|1\rangle$$

$$a^+|2\rangle = \sqrt{3}\,|3\rangle = |3\rangle = \frac{1}{\sqrt{3}}a^+|2\rangle$$

$$a^+|3\rangle = \sqrt{4}\,|4\rangle = |4\rangle = \frac{1}{\sqrt{4}}a^+|3\rangle$$

$$= \frac{1}{\sqrt{4}}a^+\left(\frac{1}{\sqrt{3}}a^+|2\rangle\right)$$

$$= \frac{1}{\sqrt{4}}\frac{1}{\sqrt{3}}a^+a^+|2\rangle$$

$$= \frac{1}{\sqrt{4}}\frac{1}{\sqrt{3}}\frac{1}{\sqrt{2}}a^+a^+a^+|1\rangle$$

$$= \frac{1}{\sqrt{4}}\frac{1}{\sqrt{3}}\frac{1}{\sqrt{2}}a^+a^+a^+\left(\frac{1}{\sqrt{1}}a^+|0\rangle\right)$$

$$\text{or } |4\rangle = \frac{1}{\sqrt{4!}}(a^+)^4|0\rangle$$

In general $|n\rangle = \frac{1}{\sqrt{n!}} (a^+)^n |0\rangle$.

which is called occupation representation

Matrix Representation of Hamiltonian $\hat{H}$ of Harmonic Oscillator:-

To represent Hamiltonian $\hat{H}$ in terms of matrix form first we need to find matrix representation of annihilation and creation operator

$$\hat{H} = \frac{\hbar\omega}{2} (a a^+ + a^+ a)$$

$\hat{a}$	0	1	2	3	4 ...
0	$\langle 0\|a\|0\rangle$	$\langle 0\|a\|1\rangle$	$\langle 0\|a\|2\rangle$	$\langle 0\|a\|3\rangle$	$\langle 0\|a\|4\rangle$ ...
1	$\langle 1\|a\|0\rangle$	$\langle 1\|a\|1\rangle$	$\langle 1\|a\|2\rangle$	$\langle 1\|a\|3\rangle$	$\langle 1\|a\|4\rangle$ ...
2	$\langle 2\|a\|0\rangle$	$\langle 2\|a\|1\rangle$	$\langle 2\|a\|2\rangle$	$\langle 2\|a\|3\rangle$	$\langle 2\|a\|4\rangle$ ...
3	$\langle 3\|a\|0\rangle$	$\langle 3\|a\|1\rangle$	$\langle 3\|a\|2\rangle$	$\langle 3\|a\|3\rangle$	$\langle 3\|a\|4\rangle$ ...
4	$\langle 4\|a\|0\rangle$	$\langle 4\|a\|1\rangle$	$\langle 4\|a\|2\rangle$	$\langle 4\|a\|3\rangle$	$\langle 4\|a\|4\rangle$ ...
⋮		⋮	⋮	⋮	⋮

1st row $\langle 0|a|0\rangle = \langle 0| \times 0 = 0$

$\langle 0|a|1\rangle = \langle 0|\sqrt{1}|0\rangle = \sqrt{1}\langle 0|0\rangle = \sqrt{1}$

$\langle 0|a|2\rangle = \langle 0|\sqrt{2}|1\rangle = \sqrt{2}\langle 0|1\rangle = 0$

$\langle 0|a|3\rangle = \langle 0|\sqrt{3}|2\rangle = \sqrt{3}\langle 0|2\rangle = 0$

$\langle 0|a|4\rangle = \langle 0|\sqrt{4}|3\rangle = \sqrt{4}\langle 0|3\rangle = 0$

Similarly we can find for other rows.

$\hat{a}$	0	1	2	3	4 ...
0	0	$\sqrt{1}$	0	0	0 ...
1	0	0	$\sqrt{2}$	0	0 ...
2	0	0	0	$\sqrt{3}$	0 ...
3.	0	0	0	0	$\sqrt{4}$ ...

Representation of a^+ matrix form

a^+	0	1	2	3	4	...
0	$\langle 0\|a^+\|0\rangle$	$\langle 0\|a^+\|1\rangle$	$\langle 0\|a^+\|2\rangle$	$\langle 0\|a^+\|3\rangle$	$\langle 0\|a^+\|4\rangle$	...
1	$\langle 1\|a^+\|0\rangle$	$\langle 1\|a^+\|1\rangle$	$\langle 1\|a^+\|2\rangle$	$\langle 1\|a^+\|3\rangle$	$\langle 1\|a^+\|4\rangle$	...
2	$\langle 2\|a^+\|0\rangle$	$\langle 2\|a^+\|1\rangle$	$\langle 2\|a^+\|2\rangle$	$\langle 2\|a^+\|3\rangle$	$\langle 2\|a^+\|4\rangle$	...
3	$\langle 3\|a^+\|0\rangle$	$\langle 3\|a^+\|1\rangle$	$\langle 3\|a^+\|2\rangle$	$\langle 3\|a^+\|3\rangle$	$\langle 3\|a^+\|4\rangle$	...
4	$\langle 4\|a^+\|0\rangle$	$\langle 4\|a^+\|1\rangle$	$\langle 4\|a^+\|2\rangle$	$\langle 4\|a^+\|3\rangle$	$\langle 4\|a^+\|4\rangle$	...
⋮	⋮	⋮	⋮	⋮	⋮	

1st row $\quad \langle 0|a^+|0\rangle = \langle 0|\sqrt{1}|1\rangle = \sqrt{1}\langle 0|1\rangle = 0$

$\langle 0|a^+|1\rangle = \langle 0|\sqrt{2}|2\rangle = \sqrt{2}\langle 0|2\rangle = 0$

⋮

IInd row :- $\langle 1|a^+|0\rangle = \langle 1\sqrt{1}|1\rangle = \sqrt{1}\cdot 1 = \sqrt{1} = 1$

$\langle 1|a^+|1\rangle = \langle 1|\sqrt{2}|2\rangle = 0.$

$\langle 1|a^+|2\rangle = \langle 1\sqrt{3}|3\rangle = 0$

⋮

Similarly we can find all other elements

a^+	0	1	2	3	4	...
0	0	0	0	0	0	...
1	$\sqrt{1}$	0	0	0	0	...
2	0	$\sqrt{2}$	0	0	0	...
3	0	0	$\sqrt{3}$	0	0	...
4	0	0	0	$\sqrt{4}$	0	...
⋮	⋮	⋮	⋮	⋮	⋮	

$$\hat{a}\hat{a}^{+} = \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & & & & & \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

$$\hat{a}\hat{a}^{+} = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 3 & 0 & \cdots \\ 0 & 0 & 0 & 4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

$$a^{+}a = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} 0 & \sqrt{1} & 0 & 0 & 0 & \cdots \\ 0 & 0 & \sqrt{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & \sqrt{3} & 0 & \cdots \\ 0 & 0 & 0 & 0 & \sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

$$a^{+}a = \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

Therefore matrix representation of Hamiltonian $\hat{H}$ is given by

$$\hat{H} = \frac{\hbar\omega}{2}(aa^{+} + a^{+}a)$$

$$= \frac{\hbar\omega}{2} \begin{bmatrix} 0 & 0 & 0 & 0 & \cdots \\ 0 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 2 & 0 & \cdots \\ 0 & 0 & 0 & 3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 2 & 0 & 0 & \cdots \\ 0 & 0 & 3 & 0 & \cdots \\ 0 & 0 & 0 & 4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

$$= \frac{\hbar\omega}{2} \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots \\ 0 & 3 & 0 & 0 & \cdots \\ 0 & 0 & 5 & 0 & \cdots \\ 0 & 0 & 0 & 7 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

Therefore $$\hat{H} = \begin{bmatrix} \frac{\hbar\omega}{2} & 0 & 0 & 0 & \cdots \\ 0 & \frac{3\hbar\omega}{2} & 0 & 0 & \cdots \\ 0 & 0 & \frac{5\hbar\omega}{2} & 0 & \cdots \\ 0 & 0 & 0 & \frac{7\hbar\omega}{2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix}$$

ANGULAR MOMENTUM :-

In classical mechanics the angular momentum of particle is given by $\vec{L} = \vec{r} \times \vec{p}$

where $\vec{r}$ = position vector and

$\vec{p}$ = momentum of the particle

$L_x = yP_z - zP_y$, $L_y = zP_z - xP_z$, $L_z = xP_y - yP_x$.

Then we have commutation relation

$[L_x, x] = 0$ $\quad [L_x, y] = i\hbar z$ $\quad [L_x, z] = +i\hbar y$

$[L_y, x] = -i\hbar z$ $\quad [L_y, y] = 0$ $\quad [L_y, y] = i\hbar x$

$[L_z, x] = i\hbar y$ $\quad [L_z, y] = -i\hbar x$ $\quad [L_z, z] = 0$

The commutation relation between angular momentum and linear momentum

$[L_x, P_x] = 0$ $\quad [L_x, P_y] = i\hbar P_z$ $\quad [L_x, P_z] = -i\hbar P_y$

$[L_y, P_x] = -i\hbar P_z$ $\quad [L_y, P_y] = 0$ $\quad [L_y, P_z] = i\hbar P_x$

$[L_z, P_x] = i\hbar P_y$ $\quad [L_z, P_y] = -i\hbar P_x$ $\quad [L_z, P_z] = 0$

The commutation relation between two angular momentum

$[L_x, L_x] = 0$ $\quad [L_x, L_y] = i\hbar L_z$ $\quad [L_x, L_z] = -i\hbar L_y$

$[L_y, L_x] = -i\hbar L_z$ $\quad [L_y, L_y] = 0$ $\quad [L_y, L_z] = +i\hbar L_x$

$[L_z, L_x] = i\hbar L_y$ $\quad [L_z, L_y] = -i\hbar L_x$ $\quad [L_z, L_z] = 0$

$[L^2 L_x] = [L.L, L_x] = 0 \rightarrow [L_x^2 + L_y^2 + L_z^2, \ldots] = 0$

Similarly,

$[L^2, L_x] = 0$, $[L^2, L_y] = 0$ $[L^2, L_z] = 0$

$[L^2, \hat{H}] = 0$ $[L_z, \hat{H}] = 0.$

Thus the components of angular momentum operator don't commute among themselves, though they commutes with the square of angular momentum operator

The commutation relation determine the quantum properties of angular momentum ie Eigen value and Eigen vectors are completely determined by the commutation relation and the general properties of Hilbert space

Therefore commutation relation are only taken for the different defination of the angular momentum operator

EIGEN VALUES AND EIGEN FUNCTIONS OF L^2 ~~AND~~ L_z:-

We know that L^2 commute with L_x L_y L_z.

$[L^2, L_x] = 0$ $[L^2, L_y] = 0$, $[L^2, L_z] = 0$

In general $[L^2, L] = 0$

So L^2 is compatible with each component of 'L' and we can write eigen equation

$L^2 f = \lambda f$ ——— ①

Similarly, $L_z f = \mu f$ ——— ②

Using Ladder operator technique.

Let $L_{\pm} = L_x \pm iL_y$ ——— (3)

ie $L_+ = L_x + iL_y$ and $L_- = L_x - iL_y$

Its commutator with L_z is

$$[L_z, L_{\pm}] = [L_z, L_x \pm iL_y]$$

$$= [L_z, L_x] \pm [L_z, iL_y]$$

consider $[L_z, L_+] = [L_z, L_x] + [L_z, iL_y]$

$$= i\hbar L_y + i^2 \hbar L_x$$

$$= i\hbar (L_y - iL_x)$$

$$[L_z, L_-] = [L_z, L_x] - [L_z, iL_y]$$

$$= i\hbar (L_y + L_x)$$

Therefore $[L_z, L_{\pm}] = i\hbar (L_y \mp iL_x)$ ——— (4)

Therefore $L_{\pm} f$ is an eigen function of L_z with the new eigen value $(\mu \pm \hbar)$

$L_+ \rightarrow$ is called raising operator, because it increases the eigen value of L_z by $\hbar$

$L_- \longrightarrow$ is called 'lowering operator because it lowers the eigen value by $\hbar$

Similarly $[L^2, L_{\pm}] = [L^2, L_x \pm iL_y]$

$$= [L^2, L_x] \pm [L^2, iL_y]$$

consider $[L^2, L_+] = [L^2, L_x] + [L^2, iL_y]$

$$= 0 + 0 = \underline{\underline{0}}$$

$[L^2, L_-] = [L^2, L_x] - [L^2, iL_y] = 0 - 0 = \underline{\underline{0}}$

(5)

Therefore $[L^2, L_\pm] = 0$. ——

$L^2(L_\pm f) = L_\pm(L^2 f) = L_\pm(\lambda f) = \lambda(L_\pm f)$

If f is an eigen function of L^2 and L_z, then f also a eigen function of $L_\pm f$.

From (4) we can write $L_z(L_\pm f) = L_\pm(L_z f)$

$= L_\pm(\mu f)$

$= (L_x \pm i L_y)(\mu f)$

$$L_z(L_\pm f) = (L_z L_\pm - L_\pm L_z) f + L_\pm L_z f$$

$$= \pm \hbar L_\pm f + L_\pm (L_z f)$$

$$= \pm \hbar (L_\pm f) + \mu (L_\pm f)$$

$$L_z(L_\pm f) = (\pm\hbar + \mu)(L_\pm f) \quad \text{—— (7)}$$

For a given value of λ we can obtain a ladder of states with each rung separated from its neighbours by 1 unit of $\hbar$ in the eigen value of L_z

There exist a top rung f_t such that,

$$L_+ f_t = 0 \quad \text{—— (8)}$$

Let $\hbar l$ be the eigen value of L_z at the top rung

ie where $f = f_t \Rightarrow \mu = \hbar l$ &

$$L_z f_t = \mu f_t$$

$$= (\hbar l) f_t$$

Then $L^2 f_t = \lambda f_t$

Consider $L_\pm L_\mp = (L_x \pm i L_y)(L_x \mp i L_y)$

$$= L_x^2 + L_y^2 \pm (L_x L_y - L_y L_x)$$

First let us consider $L_+L_- = (L_x + iL_y)(L_x - iL_y)$

$$= L_x^2 - iL_xL_y + iL_yL_x + L_y^2$$

$$= L_x^2 - i(L_xL_y - L_yL_x) + L_y^2$$

$$= L_x^2 - i[L_x, L_y] + L_y^2$$

$$= L_x^2 - i(i\hbar L_z) + L_y^2$$

$$= L_x^2 + \hbar L_z + L_y^2$$

Now consider $L_-L_+ = (L_x - iL_y)(L_x + iL_y)$

$$= L_x^2 + iL_xL_y - iL_yL_x + L_y^2$$

$$= L_x^2 + i(L_xL_y - L_yL_x) + L_y^2$$

$$= L_x^2 - i(L_yL_x - L_xL_y) + L_y^2$$

$$= L_x^2 - i[L_y, L_x] + L_y^2$$

$$= L_x^2 - i(-i\hbar L_z) + L_y^2$$

$$= L_x^2 - \hbar L_z + L_y^2$$

$$[L_+, L_-] = (L_x + iL_y)(L_x - iL_y) - (L_x - iL_y)(L_x + iL_y)$$

$$= L_x^2 + \hbar L_z + L_y^2 - (L_x^2 - \hbar L_z + L_y^2)$$

$$= 2\hbar L_z$$

$$[L_+, L_z] = [L_x, L_z] + i[L_y, L_z]$$

$$= -i\hbar L_y + i(i\hbar L_x)$$

$$= -\hbar(L_x + iL_y)$$

$$= -\hbar L_+$$

Therefore $L_\pm L_\mp = L_x^2 + L_y^2 \mp \hbar L_z$ —— (9)

Now we have

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$L_x^2 + L_y^2 = L^2 - L_z^2$$

From (9) $\Rightarrow$ $L_\pm L_\mp = L^2 - L_z^2 \mp \hbar L_z$ —— (10)

Therefore $L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$

From the eigen equation for top rung f_t (from (1))

$$L^2 f_t = \lambda f_t$$

Substitute L^2 (from (10))

$$(L_\pm L_\mp + L_z^2 \mp \hbar L_z) f_t = L_\pm L_\mp f_t + L_z^2 f_t - \hbar L_z f_t$$

$$= (L_z f_t)^2 + \hbar(\hbar l)$$

$$= ((\hbar l)^2 + \hbar^2 l) f_t$$

$$= (\hbar^2 l^2 + \hbar^2 l) f_t$$

$$L^2 f_t = \hbar^2 l(l+1) f_t = \lambda f_t \quad \text{—— (11)}$$

Therefore $\lambda = l(l+1)\hbar^2$ is the eigen value of L^2 for top rung f_t

Equation (11) gives the eigen value of L^2 in terms of maximum eigen value of L_z i.e. $L^2 f_t = l(l+1)\hbar^2 f_t$ —— (11)(b)

Similarly, For bottom rung f_b

$$L_- f_b = 0 \quad \text{—— (12)}$$

Let $L_z f_b = (\hbar l') f_b$

$$L^2 f_b = \lambda f_b \quad \text{—— (13)}$$

Substitute the value of L^2 in equation (13)

$$L^2 = L_{\pm} L_{\mp} + L_z^2 \mp \hbar L_z$$

(13) $\Rightarrow$ $(L_{\pm} L_{\mp} + L_z^2 \mp \hbar L_z) f_b = (L_{\pm} L_{\mp}) f_b + L_z^2 f_b \mp \hbar L_z f_b$

$$= L_z^2 f_b - \hbar(\hbar l') f_b$$

$$= \left[(\hbar l')^2 - \hbar^2 l'\right] f_b$$

$$= (\hbar^2 l'^2 - \hbar^2 l') f_b$$

$$L^2 f_b = \hbar^2 l'(l'-1) f_b = \lambda f_b \quad \text{—— (14)}$$

Therefore $\lambda = \hbar^2 l'(l'-1)$

Compare the equation (14) and (11)(b)

$$l'(l'-1)\hbar^2 = l(l+1)\hbar^2$$

The possible value of l' are $l' = (l+1)$ or $l' = -l$

when $l' = l+1$,

$$(l+1)(l+1-1) = \underline{l(l+1)}$$

when $l' = -l$

$$(-l)(-l-1) = l(l+1)$$

$$l(l+1) = \underline{l(l+1)}$$

For top rung (step) f_t,

Eigen value of $L^2 = l(l+1)\hbar^2$

Eigen value of $L_z = l\hbar$

For bottom rung (step) f_b, If $l' = (l+1)$

Eigen value of $L^2 = l'(l'-1)\hbar^2$

$$= (l+1)(l+1-1)\hbar^2 = \underline{l(l+1)\hbar^2}$$

Similarly, $L_z = (l+1)\hbar$.

Since eigen value of L_z are $m\hbar$, where ... in N integer steps

In particular, It follows that $l = -l + N \Rightarrow N = 2l$

$$l = \frac{N}{2}$$

$\Rightarrow$

therefore l must be an integer or half integer

For General angular momentum operator J.

$J^2 = j(j+1)\hbar^2$, where j takes the values $0, 1/2, 1, 3/2, \ldots$

According to bohr's atomic model

For an orbiting electron we have to take the value

$l = 0, 1, 2, 3 \ldots$ and $j = 1/2, 3/2$. spin angular momentum.

For orbital momentum, we have to take integer values only.

Example For $l = 2$

$$m_l = -l \text{ to } +l$$

$$= -2, -1, 0, 1, 2$$

$$L_z = -2\hbar, -\hbar, 0, \hbar, 2\hbar$$

$$L^2 = l(l+1)\hbar^2 = 2(2+1)\hbar^2 = 6\hbar^2$$

$|L| = \sqrt{6}\hbar$ is the length of the $\vec{L}$ vector

When a system with magnetic dipole moment is placed in a magnetic field, the interaction energy is quantized. The magnetic dipole moment vector and angular momentum vector will orient only in certain prefered angles, such that L_z value is quantised (integral multiple of $\hbar$)

Potential Energy $V = (\vec{\mu} \cdot \vec{B})$

$$V = |\vec{\mu}||\vec{B}| \cos\theta$$

If $\vec{L}$ is the angular momentum of the particle

$$|\vec{\mu}| = \frac{e|\vec{L}|}{2m}$$

Potential energy $V = B \cdot \frac{e|\vec{L}|}{2m} \cos\theta$

$$V = \frac{eB}{2m} (\vec{L} \cdot \cos\theta)$$

$$= \frac{e\vec{B}\,\vec{L_z}}{2m}$$

$$V = \frac{e\vec{B}\,(\hbar m_l)}{2m}$$

Totally 2 quantum numbers are required to define L^2 and L_z ie l and m_l

ACTION OF L_+ ON $|l, m_l\rangle$:-

Denoting simultaneous eigen state of 2 operator L^2 and L_z by $|l, m_l\rangle$

we know that $L^2 f = l(l+1)\hbar^2 f$

$L_z f = m_l \hbar f$ where $m_l = -l$ to $+l$

$$L^2 Y_l^{m_l} = l(l+1)\hbar^2 Y_l^{m_l}$$

$$L^2 |l, m_l\rangle = l(l+1)\hbar^2 |l, m_l\rangle \quad \text{——— (1)}$$

Also $L_z Y_l^{m_l} = m_l \hbar Y_l^{m_l}$

$$L_z |l, m_l\rangle = m_l \hbar |l, m_l\rangle \quad \text{——— (2)}$$

For orbital angular momentum j

$$J^2 |j, m_j\rangle = j(j+1)\hbar^2 |j, m_j\rangle$$

$$J_z |j, m_j\rangle = m_j \hbar |j, m_j\rangle$$

when L_+ acts on the state $|l, m_l\rangle$

* L^2 remains same
* But L_z is increased by an amount $\hbar$

$\longrightarrow |l, m_l+1\rangle$ —— (3)

Therefore $L_+ |l, m_l\rangle$ —— (4)

Similarly $L_- |l, m_l\rangle \longrightarrow |l, m_l - 1\rangle$ —— (5)

Let us consider $L_+ |l, m_l\rangle = C_+ |l, m_l+1\rangle$ —— (6)

In Bra space $\langle l, m_l | L_+^{+} = \langle l, m_l+1 | C_+^{*}$

(6)×(5) $\Rightarrow \langle l, m_l | L_+^{+} L_+ | l, m_l\rangle = \langle l, m_l+1 | C_+^{*} C_+ | l, m_l+1\rangle$

$$\langle l, m_l | L_+^{+} L_+ | l, m_l\rangle = |C_+|^2 \langle l, m_l+1 | l, m_l+1\rangle$$

$$= |C_+|^2 \cdot 1$$

$$|C_+|^2 = \langle l, m_l | L_- L_+ | l, m_l\rangle$$

$$= \langle l, m_l | (L_x - iL_y)(L_x + iL_y) | l, m_l\rangle$$

$$= \langle l, m_l | (L_x^2 + iL_xL_y - iL_yL_x + L_y^2) | l, m_l\rangle$$

$$= \langle l, m_l | (L_x^2 + i(L_xL_y - L_yL_x) + L_y^2) | l, m_l\rangle$$

$$= \langle l, m_l | (L_x^2 + i[L_x, L_y] + L_y^2) | l, m_l\rangle$$

$$= \langle l, m_l | (L_x^2 + L_y^2 + i(i\hbar L_z)) | l, m_l\rangle$$

$$= \langle l, m_l | (L_x^2 + L_y^2 - \hbar L_z) | l, m_l\rangle$$

we have $L^2 = L_x^2 + L_y^2 + L_z^2$

$$L_x^2 + L_y^2 = L^2 - L_z^2$$

$$|C_+|^2 = \langle l, m_l | (L^2 - L_z^2 - \hbar L_z) | l, m_l\rangle$$

$$|C_+|^2 = \langle l, m_l | L^2 | l, m_l\rangle - \langle l, m_l | L_z^2 | l, m_l\rangle - \hbar\langle l, m_l | L_z | l, m_l\rangle$$

$$= l(l+1)\hbar^2 \langle l, m_l | l, m_l\rangle - (m_l\hbar)^2 \langle l, m_l | l, m_l\rangle$$

$$- \hbar (m_l\hbar) \langle l, m_l | l, m_l\rangle$$

$$= l(l+1)\hbar^2 - m_l^2\hbar^2 - m_l\hbar^2$$

$$|C_+|^2 = \left[l(l+1) - m_l(m_l+1) \right] \hbar^2$$

$$= \left[l^2 + l - m_l^2 - m_l \right]\hbar^2$$

$$= \left[l^2 - m_l^2 + (l - m_l) \right]\hbar^2$$

$$= \left[(l+m_l)(l-m_l) + (l-m_l) \right]\hbar^2$$

$$|C_+| = \sqrt{(l-m_l)(l+m_l+1)}\ \hbar$$

$$L_+|l,m_l\rangle = \sqrt{(l-m_l)(l+m_l+1)}\ \hbar\ |l,m_l+1\rangle$$

ACTION OF L_- ON $|l,m_l\rangle$:-

Let $L_-|l,m_l\rangle = C_-|l,m_l-1\rangle$ — ①

In Bra space $\langle l,m_l|L_-^+ = \langle l,m_l-1|C_-^*$ — ②

② × ① => $\langle l,m_l|L_-^+ L_-|l,m_l\rangle = \langle l,m_l-1|C_-^* C_-|l,m_l-1\rangle$

$$\langle l,m_l|(L_x+iL_y)(L_x-iL_y)|l,m_l\rangle = (C_-^* C_-)\langle l,m_l-1|l,m_l-1\rangle$$

$$|C_-|^2 = \langle l,m_l|(L_x^2 - iL_xL_y + iL_yL_x + L_y^2)|l,m_l\rangle$$

$$= \langle l,m_l|(L_x^2 + L_y^2 + (-i)(i\hbar L_z)|l,m_l\rangle$$

we have $L^2 = L_x^2 + L_y^2 + L_z^2$

$$L_x^2 + L_y^2 = L^2 - L_z^2$$

$$|C_-|^2 = \langle l,m_l|(L^2 - L_z^2 + \hbar L_z)|l,m_l\rangle$$

$$= \langle l,m_l|L^2|l,m_l\rangle - \langle l,m_l|L_z^2|l,m_l\rangle + \hbar\langle l,m_l|L_z|l,m_l\rangle$$

$$= l(l+1)\hbar^2 - m_l^2\hbar^2 + \hbar m_l \hbar$$

$$|C|^2 = \left[l(l+1) - m_l(m_l-1)\right]\hbar^2$$

$$|C_-|^2 = \sqrt{l(l+1) - m_l(m_l-1)}\ \hbar$$

$$L_-|l, m_l\rangle = \sqrt{l(l+1) - m_l(m_l-1)}\ \hbar\,|l, m_l-1\rangle$$

Consider $l(l+1) - m_l(m_l-1) = l^2 + l - m_l^2 + m_l$

$$= (l^2 - m_l^2) + (l + m_l)$$

$$= (l+m_l)(l-m_l) + (l+m_l)$$

$$= (l+m_l)(l-m_l+1)$$

Therefore $L_-|l, m_l\rangle = \sqrt{(l+m_l)(l-m_l+1)}\ \hbar\,|l, m_l-1\rangle$

In general,

$$L_\pm|l, m_l\rangle = \sqrt{(l\pm m_l)(l\mp m_l+1)}\ \hbar\,|l, m_l\rangle$$

SPIN ANGULAR MOMENTUM :-

The electron is a structureless point particle, and its spin angular momentum can not be decomposed into orbital angular momenta of constituent parts. The elementary particles carry intrinsic angular momentum (S) in addition to their extrinsic angular momentum (L). The electron in a atom possesses an intrinsic angular momentum in a addition to orbital angular momentum

In classical mechanics, a rigid object admits two kinds of angular momentum

1) orbital angular momentum associated with motion of centre of mass

2) Spin angular momentum associated with motion about the centre of mass

Projection of these spin moments on z axis can have the value $S_z = m_s \hbar$ where $m_s = \pm 1/2$

The minimum measurable components of spin angular momentum in units of $\hbar$ is called the spin of the particle, denoted by S.

From fundamental commutation relation

$$[S_x, S_y] = i\hbar S_z$$

$$[S_y, S_z] = i\hbar S_x$$

$$[S_z, S_x] = i\hbar S_y$$

It follows that eigen vectors of S^2 and S_z satisfy

$$S^2 | s, m \rangle = \hbar^2 s(s+1) | s, m \rangle$$

$$S_z | s, m_s \rangle = \hbar m | s, m_s \rangle$$

$$S_\pm | s\, m_s \rangle = \hbar \sqrt{s(s+1) - m_s(m_s \pm 1)} \, | s\, m_s \pm 1 \rangle$$

where $S_\pm = S_x \pm i S_y$

But eigen vectors are not spherical harmonics and there is no reason to exclude the half integer value of S and m_s

$$S = 0\ \tfrac{1}{2}, 1, \tfrac{3}{2}, \ldots$$

$$m_s = -s, -s+1, \ldots s-1, s$$

Electron has spin angular momentum $(1/2)\hbar$

Electron has a magnetic moment which is given by spin magnetic moment

$$\mu = \frac{-ges}{2m}$$

where $m \rightarrow$ mass of the electron

$g \longrightarrow$ Landés g-factor

$s \longrightarrow$ Spin angular momentum operator

Spin 1/2

Examples for spin half particles:-

* Protons
* Nuetrons
* Electrons
* quarts
* leptons.

The spin angular momentum give rise to an intrinsic magnetic momentum μ_s it is given by $\mu_s = \frac{-e}{m}\vec{s}$

There are two eigen state which we calls

$|1/2, 1/2\rangle \longrightarrow$ spin up

$|1/2, -1/2\rangle \longrightarrow$ spin down

Using these basis vectors, the general state of a spin-1/2 particle can be expressed as two element column matrix

$$\chi = \begin{pmatrix} a \\ b \end{pmatrix} = a\chi_+ + b\chi_-$$

where $\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \longrightarrow$ Spin up

$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \longrightarrow$ Spin down

Matrix representation of S^2:

Spin operators become 2x2 matrix which is nothing but their effect on χ_+ and χ_-

$$S^2|\chi_+| = s(s+1)\hbar^2|\chi_+>$$
$$= \frac{1}{2}(1/2+1)\hbar^2|\chi_+>$$
$$S^2|\chi_+> = 3/4\,\hbar^2|\chi_+>$$

$$S^2|\chi_-> = s(s+1)\hbar^2|\chi_->$$
$$= \frac{1}{2}(1/2+1)\hbar^2|\chi_->$$
$$S^2|\chi_-> = 3/4\,\hbar^2|\chi_->$$

If we write S^2 as matrix

$$S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix}$$

$$S^2|\chi_+> = 3/4\,\hbar^2|\chi_+> = \begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} c \\ e \end{pmatrix} = \begin{pmatrix} 3/4\,\hbar^2 \\ 0 \end{pmatrix}$$

$$\therefore \quad c = 3/4\,\hbar^2 \quad \text{and} \quad e = 0$$

Similarly, $S^2|\chi_-> = \frac{3}{4}\hbar^2|\chi_->$

$$\Rightarrow \begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3}{4}\hbar^2\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} d \\ f \end{pmatrix} = \begin{pmatrix} 0 \\ 3/4\,\hbar^2 \end{pmatrix}$$

$$d = 0 \quad \text{and} \quad f = (3/4)\hbar^2$$

Therefore $S^2 = (3/4)\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

Matrix representation of S_z:-

Similarly we can evaluate $S_z|\chi_+> = m_s\hbar|\chi_+>$
$$= \frac{1}{2}\hbar|\chi_+>$$
$$S_z|\chi_-> = m_s\hbar|\chi_->$$
$$= -\frac{1}{2}\hbar|\chi_->$$

Let us consider $S_z = \begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}$

we have $S_z |\chi_+\rangle = \frac{1}{2}\hbar |\chi_+\rangle$

$$\begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{2}\hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} c' \\ e' \end{pmatrix} = \begin{pmatrix} \hbar/2 \\ 0 \end{pmatrix}$$

Similarly, $S_z \chi_- = -\frac{1}{2}\hbar |\chi_-\rangle$

$$\begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{1}{2}\hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} d' \\ f' \end{pmatrix} = \begin{pmatrix} 0 \\ -\hbar^2/2 \end{pmatrix}$$

Therefore $S_z = \begin{pmatrix} c' & d' \\ e' & f' \end{pmatrix}$

$$S_z = \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix}$$

$$\Rightarrow S_z = \hbar/2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{—— (I)}$$

we have $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$

$$S_x = \frac{S_+ + S_-}{2} \qquad S_y = \frac{S_+ - S_-}{2i}$$

$$S_\pm |s, m_s\rangle = \hbar \sqrt{s(s+1) - m_s(m_s \pm 1)}\, |s, m_s \pm 1\rangle$$

where $S_\pm = S_x \pm iS_y$

For spin up state,

$$S_+ |1/2, 1/2\rangle = \hbar \sqrt{1/2(1/2+1) - 1/2(1/2+1)}\, |1/2, 3/2\rangle$$

$$S_+ |1/2, 1/2\rangle = \hbar \begin{pmatrix} 0 \\ 0 \end{pmatrix} = 0 \quad \text{——— (a)}$$

For spin down state :-

S_+ acts on spin down results in spin up. ie

$$S_+ |1/2, -1/2\rangle = \hbar \sqrt{1/2(1/2+1) - (-1/2)(-1/2+1)}\ |1/2, 1/2\rangle$$

$$= \hbar \sqrt{3/4 + 1/4}\ |1/2, 1/2\rangle$$

$$S_+ |1/2, -1/2\rangle = \hbar\ |1/2, 1/2\rangle$$

$$S_+ \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

let us take $S_+ = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$

therefore $\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$\begin{pmatrix} b \\ d \end{pmatrix} = \begin{pmatrix} \hbar \\ 0 \end{pmatrix} \Rightarrow \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \text{——— (b)}$$

From (a) and (b) we have

$$S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

consider $S_- |s, m_s\rangle = \hbar \sqrt{s(s+1) - m_s(m_s - 1)}\ |s, m_s - 1\rangle$

For spin up state.

$$S_- |1/2, 1/2\rangle = \hbar \sqrt{1/2(1/2+1) - (1/2)(1/2 - 1)}\ |1/2, m_s - 1/2\rangle$$

$$= \hbar \sqrt{3/4 + 1/4}$$

$$S_- |1/2, 1/2\rangle = \hbar\ |1/2, -1/2\rangle$$

$$\begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} a' \\ c' \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \text{—— (c)}$$

For spin down state

$$S_-|1/2, -1/2\rangle = \hbar\sqrt{\tfrac{1}{2}(\tfrac{1}{2}+1) - (-\tfrac{1}{2})(-\tfrac{1}{2}-1)}\;|1/2, 1/2\rangle$$

$$S_-|1/2, -1/2\rangle = 0 = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

Therefore $\begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$

$$\begin{matrix} b' \\ d' \end{matrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} \quad \text{—— (d)}$$

From the equations (c) and (d) we get

$$S_- = \begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix}$$

$$S_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

Substitute the value of S_+ and S_- in equations of S_x and S_y

ie $\quad S_x = \dfrac{S_+ + S_-}{2}$ and $S_y = \dfrac{S_+ - S_-}{2i}$

$$= \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \frac{\hbar}{2}\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad = \frac{-i}{2}\hbar\left[\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\right]$$

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{—— (II)} \qquad = \frac{-i}{2}\hbar\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{—— (III)}$$

From equations (I) (II) and (III) we have

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x$$

$$S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y$$

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$$

where $\frac{\hbar}{2}\sigma_x$, $\frac{\hbar}{2}\sigma_y$, $\frac{\hbar}{2}\sigma_z$ are called as pauli's spin matrices.

Any arbitrary state ie spin up or spin down can be written as

$$\chi = a\chi_+ + b\chi_-$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = a\begin{pmatrix} 1 \\ 0 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} a \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ b \end{pmatrix}$$

$$\Rightarrow |a^2| + |b^2| = 1$$

we have $\vec{S} = S_x\hat{i} + S_y\hat{j} + S_z\hat{k}$

$$= \frac{\hbar}{2}\sigma_x\hat{i} + \frac{\hbar}{2}\sigma_y\hat{j} + \frac{\hbar}{2}\sigma_z\hat{k}$$

$$= \frac{\hbar}{2}(\sigma_x\hat{i} + \sigma_y\hat{j} + \sigma_z\hat{k})$$

$$\vec{S} = \frac{\hbar}{2}(\vec{\sigma})$$

PROPERTIES OF PAULI SPIN MATRICES :-

Consider $\frac{\hbar}{2}\sigma_x$, $\frac{\hbar}{2}\sigma_y$, $\frac{\hbar}{2}\sigma_z$, pauli's spin matrices

here $\sigma_x, \sigma_y, \sigma_z$ are called generator of spin

The properties of paulis spin matrices are given below :-

1) These $\sigma_x, \sigma_y, \sigma_z$ donot commute with each other.

we know that $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$

$S_x = \frac{\hbar}{2}\sigma_x$ $\quad S_y = \frac{\hbar}{2}\sigma_y$, $\quad S_z = \frac{\hbar}{2}\sigma_z$

Let us consider $[S_x, S_y] = i\hbar S_z$ —— (*)

In matrix form $[\sigma_x, \sigma_y] = \sigma_x \sigma_y - \sigma_y \sigma_x$

$$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} - \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} i & 0 \\ 0 & i \end{pmatrix} - \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$$

$$= \begin{pmatrix} 2i & 0 \\ 0 & -2i \end{pmatrix} = 2i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= 2i\,\sigma_z \quad \text{—— (1)}$$

From equation (*) we have

$$[S_x, S_y] = i\hbar S_z$$

$$S_x S_y - S_y S_x = i\hbar S_z$$

$$\left(\frac{\hbar}{2}\sigma_x\right)\left(\frac{\hbar}{2}\sigma_y\right) - \left(\frac{\hbar}{2}\sigma_y\right)\left(\frac{\hbar}{2}\sigma_x\right) = i\hbar S_z$$

$$\frac{\hbar^2}{4}(\sigma_x \sigma_y - \sigma_y \sigma_x) = i\hbar S_z$$

$$[\sigma_x, \sigma_y] = i\hbar S_z \frac{4}{\hbar^2}$$

$$= \frac{4 i S_z}{\hbar}$$

$$= \frac{\overset{2}{\cancel{4}}\, i}{\hbar}\left(\frac{\hbar}{\cancel{2}}\sigma_z\right)$$

$$[\sigma_x, \sigma_y] = 2i\sigma_z \quad \text{—— (2)}$$

From (1) and (2) we have

$$[S_x, S_y] = i\hbar S_z$$

2) The value of $\sigma^2 = 3I$

$\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$

$= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$\sigma^2 = 3\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = 3I$

Therefore $\underline{\sigma^2 = 3I}$

3) σ_i is Hermitian ie σ_x σ_y and σ_z are Hermitian

Let us consider σ_x, σ_y, and σ_z are hermitian ie

$\sigma_x = \sigma_x^+$, $\sigma_y = \sigma_y^+$, $\sigma_z = \sigma_z^+$

we have $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

σ_x^+ is conjugate transpose of $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

ie $\sigma_x^+ = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

Here $\underline{\sigma_x^+ = \sigma_x}$

σ_y^+ = conjugate transpose of $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

ie conjugate of $\begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} \Rightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

Therefore $\underline{\sigma_y^+ = \sigma_y}$

$\sigma_z^+ \rightarrow$ conjugate transpose of $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$=$ conjugate $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$\sigma_z^+ = \sigma_z$

Therefore σ_i is Hermitian

iv) Pauli's spin matrices are normalized.

Consider $\sigma_x \sigma_x^* = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I$

Similarly $\sigma_y \sigma_y^* = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix} =$

$$= \begin{pmatrix} 0-1 & 0 \\ 0 & -1 \end{pmatrix} = -I$$

$$\sigma_z \sigma_z^* = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \underline{\underline{I}}$$

Therefore Pauli's spin matrices are normalized

5) σ^2 commutes with σ_i

w.k.T $\sigma^2 = \sigma_x^2 + \sigma_y^2 + \sigma_z^2$

$$[\sigma_x^2 + \sigma_y^2 + \sigma_z^2, \sigma_x] = [\sigma_x^2, \sigma_x] + [\sigma_y^2, \sigma_x] + [\sigma_z^2, \sigma_x]$$

$$= [\sigma_x \sigma_x, \sigma_x] + [\sigma_y \sigma_y, \sigma_x] + [\sigma_z \sigma_z, \sigma_x]$$

we have the formula

$$[AB, C] = A[B, C] + [A, C]B.$$

$$[\sigma_x^2 + \sigma_y^2 + \sigma_z^2, \sigma_x] = \sigma_x [\sigma_x, \sigma_x] + [\sigma_x, \sigma_x]\sigma_x$$

$$+ \sigma_y [\sigma_y, \sigma_x] + [\sigma_y, \sigma_x]\sigma_y$$

$$+ \sigma_z [\sigma_z, \sigma_x] + [\sigma_z, \sigma_x]\sigma_z$$

$$= 0 + 0 + \sigma_y(-2i\sigma_z) + -2i\sigma_z\sigma_y$$

$$+ \sigma_z(2i\sigma_y) + 2i\sigma_y\sigma_z$$

$$= 0$$

Therefore σ^2 commutes with σ_x

Similarly we can show σ^2 commutes with σ_y and σ_z

Therefore In general σ^2 commutes with σ_i

6) Pauli's Spin matrices are linearly Indipendent

$a\sigma_x + b\sigma_y + c\sigma_z = 0$ also a, b, c should be equal to zero. ie

$$a\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + b\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} + c\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\begin{pmatrix} 0+0+c & a-ib+0 \\ a+ib+0 & 0+0+c(-c) \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$$\Rightarrow \begin{pmatrix} c & a-ib \\ a+ib & -c \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

$c = 0$

$$a + ib = 0$$
$$a - ib = 0$$
$$\overline{a = 0.}$$

Therefore $a + ib = 0$

$0 + ib = 0$

$\therefore \underline{\underline{b = 0}}$ $(\because i \neq 0)$

Therefore Pauli's matrices are linearly independent

Problem:-

1) Prove that $(\sigma \cdot \vec{A})(\sigma \cdot \vec{B}) = \vec{A}\cdot\vec{B} + i\sigma(\vec{A}\times\vec{B})$

Given $\vec{\sigma}$ commutes with both $\vec{A}$ and $\vec{B}$

where $\vec{A}$ and $\vec{B}$ are vectors

From Levi Cevita relation

$$[\sigma_i, \sigma_j] = 2i\,\epsilon_{ijk}\,\sigma_x \quad \text{——— (1)}$$

Eqn (1) is called commutation relation between spin matrices

$$\sigma_i \sigma_j = \sigma_j \sigma_i = 2i \epsilon_{ijk} \sigma_k \quad \text{——— (2)}$$

By Anti commutation relation,

$$\{\sigma_i, \sigma_j\} = \sigma_i \sigma_j + \sigma_j \sigma_i = 2\delta_{ij} \quad \text{——— (3)}$$

such that

consider (2) + (3)

$$2\sigma_i \sigma_j = 2\delta_{ij} + 2i \epsilon_{ijk} \sigma_k$$

$$\sigma_i \sigma_j = \delta_{ij} + i \epsilon_{ijk} \sigma_k \quad \text{——— (4)}$$

Given σ_i commutes with $\vec{A}$ and $\vec{B}$

let

$$\sigma_i \vec{A_i} - A_i \sigma_i = 0.$$

$$\sigma_j \vec{B_j} - B_j \sigma_j = 0$$

consider $(\sigma . \vec{A})(\sigma \vec{B}) = \left(\sum_i \sigma_i A_i\right)\left(\sum_j \sigma_j B_j\right)$

$$= \sum_i \sum_j (\sigma_i A_i)(\sigma_j B_j)$$

$$= \sum_i \sum_j A_i B_j \sigma_i \sigma_j$$

$$= \sum_i \sum_j A_i B_j \left(\delta_{ij} + i \epsilon_{ijk} \sigma_k\right)$$

$$= \sum_i \sum_j A_i B_j \delta_{ij} + i \sum_i \sum_j A_i B_j \epsilon_{ijk} \sigma_k$$

$$= A_1 B_1 + A_2 B_2 + A_3 B_3 + i \{ \epsilon_{123} A_1 B_1 \sigma_3 \} + \epsilon_{132} A_1 B_3 \sigma_2$$

$$+ \epsilon_{312} A_3 B_2 \sigma_2 + \epsilon_{213} A_2 B_1 \sigma_3 + \epsilon_{231} A_2 B_3 \sigma_1 + \epsilon_{321} A_3 B_2 \sigma_1 \}$$

$$(\sigma . \vec{A})(\sigma \vec{B}) = A_1 B_1 + A_2 B_2 + A_3 B_3 + i \{ A_1 B_1 \sigma_3 + (-1) A_1 B_1 \sigma_2$$

$$+ A_3 B_1 \sigma_2 + (-) A_3 B_2 \sigma_1 + (-1) A_2 B_1 \sigma_3 + A_2 B_3 \sigma_1 \}.$$

$$= A_1 B_1 + A_2 B_2 + A_3 B_3 + i \{ \sigma_1 (A_2 B_3 - A_3 B_2) - \sigma_2 (A_1 B_3 - B_1 A_3) + \sigma_3 (A_1 B_2 - B_1 A_2) \}$$

$= A_1B_1 + A_2B_2 + A_3B_3 + i\{\sigma \cdot (\vec{A} \times \vec{B})\}$

Therefore $(\sigma \cdot \vec{A})(\sigma \cdot \vec{B}) = (\vec{A} \cdot \vec{B}) + i\{\sigma \cdot (\vec{A} \times \vec{B})\}$

---

2) Show that If $|j, m\rangle$ is an eigen state of J^2 and J_z

Then a) $\langle J_x \rangle = \langle J_y \rangle = 0$

b) $\langle J_x^2 \rangle = \langle J_y^2 \rangle = \frac{\hbar}{2}[j(j+1) - m^2]$

Solution :-

$J_+ = J_x + iJ_y$ —— ①

$J_- = J_x + iJ_y$ —— ②

Equation ① and + ②

$2J_x = J_+ + J_-$

$J_x = \frac{J_+ + J_-}{2}$

Equation ① - ②

$2J_y = \frac{J_+ - J_-}{i}$

$J_y = \frac{J_+ - J_-}{2i}$

To find the expectation of value of J_x

$\langle J_x \rangle = \langle j, m | J_x | j, m \rangle$

$\langle J_x \rangle = \langle j, m | \frac{J_+ + J_-}{2} | j, m \rangle$

$= \frac{1}{2} \langle j, m | J_+ + J_- | j, m \rangle$

$= \frac{1}{2} \{ \langle jm | J_+ | j, m \rangle + \langle jm | J_- | j, m \rangle \}$

$= \frac{1}{2} \{ \langle jm | \sqrt{j(j+1) - m(m+1)}\, \hbar | j, m+1 \rangle$

$+ \langle jm | \sqrt{j(j+1) - m(m-1)}\, \hbar | j, m \rangle \}$

$\langle J_x \rangle = \frac{1}{2}\{0 + 0\} = 0$

Similarly $\langle J_y \rangle = 0$ and $\langle J_x^2 \rangle$,

3) For two electron system (Like ...)

Show that $(\vec{S_1} \cdot \vec{S_2}) = \begin{cases} -3/4\,\hbar^2 & \text{for } {}^1S_0 \text{ singlet state} \\ 1/4\,\hbar^2 & \text{for } {}^3S_1 \text{ Triplet state} \end{cases}$

The net spin vector is $\vec{S} = \vec{S_1} + \vec{S_2}$

In singlet state (antiparallel) $\uparrow\downarrow$,

$S = 1/2 - 1/2 = 0$

Then multiplicity of orientation $= (2S+1)$

$= 2(0)+1 = \underline{\underline{1}}$

$\Rightarrow {}^1S_0$

In triplet state (parallel spin) $\uparrow\uparrow, \downarrow\downarrow$,

$S = 1/2 + 1/2 = 1$

Then multiplicity orientation $= (2S+1) = (2(1)+1) = \underline{\underline{3}}$

$\Rightarrow {}^3S_1$

$\vec{S} \cdot \vec{S} = (\vec{S_1} + \vec{S_2}) \cdot (\vec{S_1} + \vec{S_2})$

$|\vec{S}|^2 = |\vec{S_1}|^2 + |\vec{S_2}|^2 + 2(\vec{S_1} \cdot \vec{S_2})$

The eigen value of spin angular momentum

$S(S+1)\hbar^2 = S_1(S_1+1)\hbar^2 + S_2(S_2+1)\hbar^2 + 2(\vec{S_1} \cdot \vec{S_2})$ —— ①

Take $S_1 = S_2 = 1/2$

Then equation ① becomes

$S(S+1)\hbar^2 = \frac{1}{2}(3/2)\hbar^2 + 1/2(3/2)\hbar^2 + 2(\vec{S_1} \cdot \vec{S_2})$

$S(S+1)\hbar^2 = \frac{3}{2}\hbar^2 + 2(\vec{S_1} \cdot \vec{S_2})$ —— ②

For singlet state, $S = 0$, then

② $\Rightarrow$ $0 = 3/2\,\hbar^2 + 2(\vec{S_1} \cdot \vec{S_2})$

$2(\vec{S_1} \cdot \vec{S_2}) = -3/2\,\hbar^2$

$(\vec{S_1} \cdot \vec{S_2}) = -3/4\,\hbar^2$

ADDITION OF ANGULAR MOMENTUM :- (CLEBSCH GORDAN COEFFICIENT)

Let J_1 and J_2 be two independent angular momentum of a system containing two electrons. Then J_1 & J_2

* may be both are orbital angular momentum } of 2 electrons
* may be both are spin angular momentum }
* orbital & spin of single electron

Since J_1 and J_2 are independent. We have the commutation relation

$$[J_1, J_2] = 0$$

$$[J_1^2, J_2^2] = 0$$

$$[J_1^2, J_2] = 0$$

$$[J_2^2, J_2] = 0$$

Thus for this system there are four commuting operators J_1, J_2, J_{1z}, J_{2z} ie in a particular state of system these four quantities can be measured simultaneously without any uncertainity. The simultaneous eigen state for these four operators can be represented as.

(i) $|j_1, j_2, m_1, m_2\rangle$

(ii) $|j_1, m_1, j_2, m_2\rangle$

(iii) $|j_1, m_1\rangle |j_2, m_2\rangle$

where $m_1 = -j_1$ to $+j_1$

$m_2 = -j_2$ to $+j_2$

$J_1^2 |j_1 m_1, j_2, m_2\rangle = \hbar^2 j_1(j_1+1)|j_1, m_1 j_2 m_2\rangle$

$J_2^2 |j_1 m_1 j_2 m_2\rangle = \hbar^2 j_2(j_2+1)|j_1 m_1 j_2 m_2\rangle$

For triplet state, $S=1$

$$2\hbar^2 = \frac{3}{2}\hbar^2 + 2(\vec{S_1}\cdot\vec{S_2})$$

$$\frac{1}{2}\hbar^2 = 2(\vec{S_1}\cdot\vec{S_2})$$

$$(\vec{S_1}\cdot\vec{S_2}) = \frac{1}{4}\hbar^2$$

4) Prove that $[S_+, S_-] =$

we know that $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$

$$[S_+, S_-] = S_+S_- - S_-S_+$$

$$= (S_x + iS_y)(S_x - iS_y) - (S_x - iS_y)(S_x + iS_y)$$

$$= \cancel{S_x^2} - iS_xS_y + iS_yS_x + \cancel{S_y^2} - \cancel{S_x^2} - iS_xS_y + iS_yS_x - \cancel{S_y^2}$$

$$= -2i(S_xS_y) + 2i(S_yS_x)$$

$$= -2i(S_xS_y - S_yS_x)$$

$$= -2i[S_x, S_y] = -2i(i\hbar S_z)$$

$$= 2\hbar S_z$$

5) Prove that $[S_z, S_\pm] =$

Consider LHS $[S_z, S_\pm] = [S_z, S_x \pm iS_y]$

$$= [S_z, S_x] \pm i[S_z, S_y]$$

$$= i\hbar S_y \mp i(i\hbar S_x)$$

$$= \pm i\hbar(S_x \cdot -iS_y)$$

$$= \pm i\hbar S_\pm$$

$J_{1z}|j_1 m_1 j_2 m_2\rangle = m_1\hbar |j_1 m_1 j_2 m_2\rangle$

$J_{2z}|j_1 m_1 j_2 m_2\rangle = m_2\hbar |j_1 m_1 j_2 m_2\rangle$

This basis is more appropriate when the two system J_1 & J_2 are non interacting each other. Under such circumstances m_1, m_2 are (good) quantum number. But if there exist an internal interaction in the composite system the total angular momentum is given by

$\vec{J} = \vec{J_1} + \vec{J_2}$ then

$[J^2, J_z] = 0$

$[J^2, J_1^2] = 0$

$[J^2, J_2^2] = 0$

The orthonormal eigen kets of J^2 and J_z can be written as $|j, m\rangle$. Since J^2 commutes with J_z, J_1^2, J_2^2, they formed another complete set. Represented by $|j_1, j_2, j, m\rangle$

For a given value of j_1 and j_2 one can write after interaction $|j_1, j_2, j, m\rangle = |j, m\rangle$

Here j may vary from $j_1 + j_2 \rightarrow j_1 - j_2$

Final state of the system due to the interaction between angular momentum vectors can be expressed as linear combination of initial state before interaction.

ie, $|j_1 j_2, m_1 m_2\rangle = \sum_{m m_2} C_{m_1 m_2} |j_1 j_2, j, m\rangle$

where $C_{m_1 m_2} = \langle j_1 j_2, m_1 m_2 | j_1 j_2, j, m\rangle$

are called Clebsch Gordan coefficient

$|j_1, j_2, j, m\rangle = \sum_{m m_2} \langle j_1 j_2, m_1 m_2 | j_1 j_2 j, m\rangle | j_1 j_2 m_1 m_2\rangle$

$$= \sum_{m_1 m_2} |j_1 j_2 m_1 m_2\rangle\langle j_1 j_2 m_1 m_2 | j_1 j_2, j, m\rangle$$

where $\sum_{m_1 m_2} |j_1\, j_2\, m_1 m_2\rangle\langle j_1\, j_2\, m_1 m_2| = I$

Therefore $|j_1 j_2\, m_1 m_2\rangle$ forms a complete set or it form a basis. Therefore we can solve the problem of adding two angular momentum by determining Clebsh Gordan coefficients.

These coefficients are also called wigner coefficient or vector coupling coefficient

Therefore Final state $= \sum_{m_1 m_2}$ C-G coefficient X Initial state

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PROBLEMS

1) Add $j_1 = 1/2$ and $j_2 = 1/2$ for hydrogen molecule

solution :-

Given - $j_1 = 1/2$ and $j_2 = 1/2$

The value of $m_1 = 1/2$ and $m_1 = -1/2$

$m_2 = 1/2$ and $-1/2$

For the first electron, the initial state.

$|j_1, m_1\rangle = |1/2, 1/2\rangle_{①}$ and $|1/2, -1/2\rangle_{②}$

For the second electron initial states are

$|j_2, m_2\rangle = |1/2, 1/2\rangle_{②}$ and $|1/2, -1/2\rangle_{②}$

After interaction the possible values are

$j = j_1 + j_2 \xrightarrow{to} j = j_1 - j_2$

ie $\frac{1}{2} + \frac{1}{2} \xrightarrow{to} \frac{1}{2} - \frac{1}{2}$

1 to 0

ie 1 and 0.

If $j = 1$ then $m = +1, 0, -1$

and if $j = 0$ then $m = 0$.

Therefore final states are

$$\left.\begin{aligned} |j, m\rangle &= |1, +1\rangle \\ &= |1, 0\rangle \\ &= |1, -1\rangle \end{aligned}\right\} \text{for } (j_1 + j_2)$$

$$= |0, 0\rangle \longrightarrow \text{for } (j_1 - j_2)$$

Final state $= \sum_{m_1 m_2}$ C-G coefficient × intial state

$$|1, 1\rangle = c_1 |1/2, 1/2\rangle_{①} + |1/2, 1/2\rangle_{②} \quad \text{——— ①}$$

$$|1, 0\rangle = c_2 |1/2, 1/2\rangle_{①} + |1/2, -1/2\rangle_{②} + c_3 |1/2, -1/2\rangle_{①} |1/2, +1/2\rangle_{②} \quad \text{——— ②}$$

$$|1, -1\rangle = c_4 |1/2, -1/2\rangle_{①} |1/2, -1/2\rangle_{②} \quad \text{——— ③}$$

$$|0, 0\rangle = c_5 |1/2, 1/2\rangle_{①} |1/2, -1/2\rangle_{②} + c_6 |1/2, -1/2\rangle_{①} |1/2, 1/2\rangle_{②} \quad \text{——— ④}$$

$$\begin{bmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \\ |0,0\rangle \end{bmatrix} = \begin{bmatrix} c_1 & 0 & 0 & 0 \\ 0 & c_2 & c_3 & 0 \\ 0 & 0 & 0 & c_4 \\ 0 & c_5 & c_6 & 0 \end{bmatrix} \begin{bmatrix} |1/2, 1/2\rangle_{①} \, |1/2, 1/2\rangle_{②} \\ |1/2, 1/2\rangle_{①} \, |1/2, -1/2\rangle_{②} \\ |1/2, -1/2\rangle_{①} \, |1/2, +1/2\rangle_{②} \\ |1/2, -1/2\rangle_{①} \, |1/2, -1/2\rangle_{②} \end{bmatrix}$$

To find C_1:-

$① \Rightarrow |1,1\rangle = C_1 |1/2, 1/2\rangle_{①} |1/2, 1/2\rangle_{②}$ ——— ⑤

In Bra space

$\langle 1,1| = C_1^* \langle 1/2\, 1/2|_{①} \langle 1/2, 1/2|_{②}$ ——— ⑥

$⑥ \times ⑤ \Rightarrow \langle 1,1|1,1\rangle = C_1^* C_1 \{\langle 1/2, 1/2|1/2, 1/2|1/2\, 1/2|1/2, 1/2\rangle$

$1 = |C_1|^2$

$\underline{C_1 = 1}$

To find C_2:-

we have $|1,1\rangle, C_1 |1/2, 1/2\rangle_{①} |1/2\, 1/2\rangle_{②}$

consider $J_- |1,1\rangle = C_1 (J_{1-} + J_{2-}) |1/2\, 1/2\rangle_{①} |1/2, 1/2\rangle_{②}$

$J_- |j, m\rangle = \sqrt{(j+m)(j-m+1)}\, \hbar\, |j, m-1\rangle$

Therefore $J_1 |1,1\rangle = \sqrt{(1+1)(1-1+1)}\, \hbar\, |1, 1-1\rangle = \sqrt{2}\, \hbar |1,0\rangle$

ie $\sqrt{2}\, \hbar |1,0\rangle = C_1 \{J_{1-} |1/2, 1/2\rangle_{①} |1/2, 1/2\rangle_{②} + J_{2-} |1/2, 1/2\rangle_{①} |1/2, 1/2\rangle_{②}\}$

J_{1-} is not applicable to $|1/2, 1/2\rangle_{②}$ ie 2nd electron,

$\therefore \sqrt{2}\, \hbar |1,0\rangle = C_1 \{|1/2, 1/2\rangle_{②} J_{1-} |1/2, 1/2\rangle_{①} + |1/2, 1/2\rangle_{①} J_{2-} |1/2, 1/2\rangle_{②}\}$

$= C_1 \{|1/2, 1/2\rangle_{②} \sqrt{(1/2+1/2)(1/2-1/2+1)}\, \hbar\, |1/2, 1/2-1\rangle_{②} +$

$|1/2, 1/2\rangle_{①} \sqrt{(1/2+1/2)(1/2-1/2+1)}\, \hbar\, |1/2, 1/2-1\rangle_{②}\}$

$\sqrt{2}\, \hbar |1,0\rangle = C_1 \{\hbar |1/2, -1/2\rangle_{①} |1/2, +1/2\rangle_{②} + \hbar |1/2, -1/2\rangle_{②} |1/2, 1/2\rangle_{①}\}$

$$\Rightarrow \langle 1,0|0,0\rangle = c_2^* c_5 \langle 1/2,1/2|1/2,1/2\rangle\langle 1/2,-1/2|1/2,-1/2\rangle + c_2^* c_6 \langle 1/2,1/2|1/2,-1/2\rangle\langle 1/2,-1/2|1/2,1/2\rangle + c_3^* c_5 \langle 1/2,-1/2|1/2,1/2\rangle\langle 1/2,1/2|1/2,-1/2\rangle + c_3^* c_6 \langle 1/2,-1/2|1/2,-1/2\rangle\langle 1/2,1/2|1/2,1/2\rangle$$

$$0 = c_2^* c_5 + c_3^* c_6$$

$$0 = \frac{1}{\sqrt{2}} c_5 + \frac{1}{\sqrt{2}} c_6$$

$$\underline{\underline{c_5 = -c_6}}$$

consider equation (4) braspace

$$\langle 0,0| = c_5^* \langle 1/2,1/2|_{①} \langle 1/2,-1/2|_{②} + c_6^* \langle 1/2,-1/2|_{①} \langle 1/2,1/2|_{②} \quad \text{——} (12)$$

(12) x (4) $\langle 00|00\rangle = c_5^* c_5 + c_6^* c_6$

$$1 = |c_5|^2 + |c_6|^2$$

Substituting $c_5 = -c_6$

$$1 = 2|c_6| = \frac{1}{\sqrt{2}}$$

Therefore $c_5 = \frac{-1}{\sqrt{2}}$

$$\begin{bmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \\ |0,0\rangle \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \end{bmatrix} \begin{bmatrix} |1/2,1/2\rangle_{①} |1/2,1/2\rangle_{②} \\ |1/2,1/2\rangle_{①} |1/2,-1/2\rangle_{②} \\ |1/2,-1/2\rangle_{①} |1/2,1/2\rangle_{②} \\ |1/2,-1/2\rangle_{①} |1/2,-1/2\rangle_{②} \end{bmatrix}$$

Dividing the whole equation by $\sqrt{2}$ and put c_1 =

$$|1,0\rangle = \frac{1}{\sqrt{2}}|1/2,1/2\rangle|1/2,1/2\rangle + \frac{1}{\sqrt{2}}|1/2,-1/2\rangle|1/2,1/2\rangle \quad \text{——} (7)$$

On comparing (2) and (7)

$$c_2 = \frac{1}{\sqrt{2}} \quad \text{and} \quad c_3 = \frac{1}{\sqrt{2}}$$

To find c_4:-

Consider $|1,-1\rangle = c_4|1/2,-1/2\rangle_{(1)}|1/2,-1/2\rangle_{(2)}$ —— (8)

In Bra space

$$\langle 1,-1| = c_4^* \langle 1/2,-1/2|_{(1)} \langle 1/2,-1/2| \quad \text{——} (9)$$

$(9)\times(8) \Rightarrow \langle 1,-1|1,-1\rangle = c_4^* c_4 \{\langle 1/2,-1/2|\langle 1/2,-1/2|1/2,-1/2\rangle|1/2,-1/2\rangle\}$

$$1 = c_4^* c_4 \{1\}$$

$$1 = |c_4|^2$$

Therefore $\underline{\underline{c_4 = 1}}$

To find c_5 and c_6

consider $|0,0\rangle = c_5|1/2,1/2\rangle_{(1)}|1/2,-1/2\rangle_{(2)} + c_6|1/2,-1/2\rangle_{(1)}|1/2,1/2\rangle_{(2)}$

Also one more final state which is having same eigen state as that of $|0,0\rangle$ is $|1,0\rangle$: ie

(2) $\Rightarrow |1,0\rangle = c_2|1/2,1/2\rangle_{(1)}|1/2,-1/2\rangle_{(2)} + c_3|1/2,-1/2\rangle_{(1)}|1/2,1/2\rangle_{(2)}$ —— (10)

In Bra space

$$\langle 1,0| = c_2^* \langle 1/2,1/2|_{(1)} \langle 1/2,-1/2|_{(2)} + c_3^* \langle 1/2,-1/2|_{(1)} \langle 1/2,+1/2|_{(2)} \quad \text{——} (11)$$

(11) x (4) ~~⇒~~

2) $j_1 = 1$ and $j_2 = 1/2$, Add j_1 and j_2

Solution :-

Given $j_1 = 1$ and $j_2 = 1/2$

For $j_1 = 1$, $m_1 = +1, 0, -1$

$j_2 = 1/2$ $m_2 = 1/2, -1/2$

The initial states of first election are

$|1,1\rangle_{①}$ $|1,0\rangle_{①}$ and $|1,-1\rangle_{①}$

Initial states of second electron :

$|1/2, 1/2\rangle_{②}$ and $|1/2, -1/2\rangle_{②}$

After interaction the final states are

$j \longrightarrow j_1 + j_2 \longrightarrow j_1 - j_2$

$1 + 1/2 \longrightarrow 1 - 1/2$

$3/2 \longrightarrow 1/2$

If $j = 3/2$ $m = 3/2$ to $-3/2$

i.e $m = 3/2, 1/2, -1/2, -3/2$

If $j = 1/2$ $m = 1/2, -1/2$

The final states are,

$|3/2, 3/2\rangle$ $|3/2, 1/2\rangle$ $|3/2, -1/2\rangle$ $|3/2, -3/2\rangle$ $|1/2, 1/2\rangle$ $|1/2, -1/2\rangle$

$|3/2, 3/2\rangle = C_1 |1,1\rangle_{①} |1/2, 1/2\rangle_{②}$ —— ①

$|3/2, 1/2\rangle = C_3 |1,0\rangle_{①} |1/2, 1/2\rangle_{②} + C_2 |1,1\rangle_{①} |1/2, -1/2\rangle_{②}$ —— ②

$|3/2, -1/2\rangle = C_4 |1,0\rangle_{①} |1/2, -1/2\rangle_{②} + C_5 |1,-1\rangle_{①} |1/2, 1/2\rangle_{②}$ —— ③

$|3/2, -3/2\rangle = C_6 |1,-1\rangle_{①} |1/2, -1/2\rangle_{②}$ —— ④

$$|{}^1\!/_2, {}^1\!/_2\rangle = c_7 |1,1\rangle_{①} |{}^1\!/_2, -{}^1\!/_2\rangle_{②} + c_8 |1,0\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②} \quad ⑤$$

$$|{}^1\!/_2, -{}^1\!/_2\rangle = c_9 |1,0\rangle_{①} |{}^1\!/_2, -{}^1\!/_2\rangle_{②} + c_{10} |1,-1\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②} \quad ⑥$$

$$\begin{bmatrix} |{}^3\!/_2, {}^3\!/_2\rangle \\ |{}^3\!/_2, {}^1\!/_2\rangle \\ |{}^3\!/_2, -{}^1\!/_2\rangle \\ |{}^3\!/_2, -{}^3\!/_2\rangle \\ |{}^1\!/_2, {}^1\!/_2\rangle \\ |{}^1\!/_2, -{}^1\!/_2\rangle \end{bmatrix} = \begin{bmatrix} c_1 & 0 & 0 & 0 & 0 & 0 \\ 0 & c_2 & c_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_4 & c_5 & 0 \\ 0 & 0 & 0 & 0 & 0 & c_6 \\ 0 & c_7 & c_8 & 0 & 0 & 0 \\ 0 & 0 & 0 & c_9 & c_{10} & 0 \end{bmatrix} \begin{bmatrix} |1,1\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②} \\ |1,1\rangle_{①} |{}^1\!/_2, -{}^1\!/_2\rangle_{②} \\ |1,0\rangle_{①} |{}^1\!/_2, +{}^1\!/_2\rangle_{②} \\ |1,0\rangle_{①} |{}^1\!/_2, -{}^1\!/_2\rangle_{②} \\ |1,-1\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②} \\ |1,-1\rangle_{①} |{}^1\!/_2, -{}^1\!/_2\rangle_{②} \end{bmatrix}$$

To find c_1:-

consider eqn ① $|{}^3\!/_2, {}^3\!/_2\rangle = c_1 |1,1\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②}$ —— ①

In Bra space

$$\langle {}^3\!/_2, {}^3\!/_2| = c_1^* \underset{①}{\langle 1,1|} \underset{②}{\langle {}^1\!/_2, {}^1\!/_2|} \quad ⑦$$

$$⑦ \times ① \Rightarrow \langle {}^3\!/_2, {}^3\!/_2 | {}^3\!/_2, {}^3\!/_2\rangle = c_1^* c_1 \langle 1,1|1,1\rangle \langle {}^1\!/_2, {}^1\!/_2 | {}^1\!/_2, {}^1\!/_2\rangle$$

$$1 = |c_1|^2$$

$$\underline{\underline{c_1 = 1}}$$

To find c_2 and c_3:-

consider equation ① $J_- |{}^3\!/_2, {}^3\!/_2\rangle = c_1 (J_{1-} + J_{2-}) |1,1\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②}$

we know that

$$J_- |j,m\rangle = \sqrt{(j+m)(j-m+1)}\, \hbar\, |j, m-1\rangle$$

$$\sqrt{({}^6\!/_2)(1)}\, \hbar\, |{}^3\!/_2, {}^1\!/_2\rangle = c_1 \left\{ J_{1-} |1,1\rangle_{①} |{}^1\!/_2, {}^1\!/_2\rangle_{②} + |1,1\rangle_{①} J_{2-} |{}^1\!/_2, {}^1\!/_2\rangle_{②} \right\}$$

$$\sqrt{3}\hbar\,|3/2,1/2\rangle = \{\sqrt{(2)(1)}\,\hbar\,|1,0\rangle_{①}|1/2,1/2\rangle_{②} + |1,1\rangle_{①}\hbar\,|1/2,-1/2\rangle\}$$

$$|3/2,1/2\rangle = \frac{\sqrt{2}}{\sqrt{3}}|1,0\rangle_{①}|1/2,1/2\rangle_{②} + \sqrt{1/3}\,|1,1\rangle_{①}|1/2,-1/2\rangle_{②}$$

comparing it with equation

$$c_3 = \sqrt{2/3} \quad \text{and} \quad c_2 = \frac{1}{\sqrt{3}}.$$

To find C_4 and C_5:-

consider equation ②, operate J_{2-} on eqn ②

$$J_-|3/2,1/2\rangle = (J_{1-}+J_{2-})\frac{1}{\sqrt{3}}|1,1\rangle_{①}|1/2,-1/2\rangle_{②} +$$

$$(J_{1-}+J_{2-})\sqrt{2/3}\,|1,0\rangle_{①}|1/2,1/2\rangle_{②}$$

$$\sqrt{(3/2+1/2)(3/2-1/2+1)}\,\hbar\,|3/2,-1/2\rangle = \frac{1}{\sqrt{3}}\Big[\sqrt{2(1)}\,\hbar\,|1,0\rangle_{①}|1/2,-1/2\rangle_{②} + 0\Big] + \sqrt{2/3}\Big[\sqrt{(1)(2)}\,\hbar\,|1,-1\rangle_{①}|1/2,1/2\rangle_{②} + \sqrt{(1)(1)}\,\hbar\,|1/2,-1/2\rangle_{①}|1,0\rangle_{②}\Big]$$

$$\sqrt{(2)(2)}\,|3/2,-1/2\rangle = \frac{1}{\sqrt{3}}\sqrt{2}\,|1,0\rangle_{①}|1/2,-1/2\rangle_{②} + \sqrt{2/3}\Big[\sqrt{2}\,|1,-1\rangle_{①}|1/2,1/2\rangle_{②} + |1/2,-1/2\rangle_{①}|1,0\rangle_{②}\Big]$$

$$|3/2,-1/2\rangle = \frac{1}{\sqrt{6}}|1,0\rangle_{①}|1/2,-1/2\rangle_{②} + \frac{1}{\sqrt{3}}|1,-1\rangle_{①}|1/2,+1/2\rangle_{②} + \frac{1}{\sqrt{6}}|1/2,-1/2\rangle_{①}|1,0\rangle_{②}$$

$$|3/2,-1/2\rangle = \frac{2}{\sqrt{6}}|1,0\rangle_{①}|1/2,-1/2\rangle_{②} + \frac{1}{\sqrt{3}}|1,-1\rangle_{①}|1/2,1/2\rangle_{②}$$

Therefore $C_4 = \sqrt{2/3}$ and $C_5 = \frac{1}{\sqrt{3}}$

To find ~~C_7 and C_8~~ C_6 :-

consider eqn (4)

$|3/2, -3/2\rangle = C_6 \, |1,-1\rangle_{①} \, |1/2, -1/2\rangle_{②}$ ——— (8)

In Bra space

$\langle 3/2, -3/2| = C_6^* \, \langle 1,-1|_{①} \, \langle 1/2, -1/2|_{②}$

(8) × (4) => $\langle 3/2, -3/2 | 3/2, -3/2\rangle = C_6^* C_6 \langle 1,-1|1,-1\rangle \langle 1/2,-1/2|1/2,-1/2\rangle$

$1 = |C_6|^2$

$C_6 = \underline{\underline{1}}$

To find C_7 and C_8:- consider (5) in Bra space

$\langle 1/2, 1/2| = \langle 1,1|_{①} \langle 1/2, +1/2| C_7^* + C_8^* \langle 1,0|_{①} \langle 1/2, 1/2|_{②}$ ——— (9)

(5) × (9) => $1 = |C_7|^2 + |C_8|^2$

Take eqn (2) in Braspace

$\langle 3/2, 1/2| = \langle 1,1|_{①} \langle 1/2, -1/2| C_2^* + \langle 1,0| \langle 1/2, 1/2| C_3^*$ ——— (10)

(10) × (5) => $0 = C_7 C_2^* + C_8 C_3^*$

$0 = C_7 \left(\frac{1}{\sqrt{3}}\right) + C_8 \left(\sqrt{2/3}\right)$

$\frac{C_7}{\sqrt{3}} = -\sqrt{\frac{2}{3}} \, C_8$

$C_8 = \frac{C_7}{\sqrt{2}}$

$1 = |C_7|^2 + \left|\frac{C_7}{\sqrt{2}}\right|^2 => 2 = 3|C_7|^2$

$|C_7|^2 = \frac{2}{3}$

$C_7 = \sqrt{2/3}$

$$c_8 = -\sqrt{2/3} \times \frac{1}{\sqrt{2}} = -\frac{1}{\sqrt{3}}$$

$$c_7 = \sqrt{2/3} \quad \text{and} \quad c_8 = -\frac{1}{\sqrt{3}}$$

To find c_9 and c_{10}

consider the equation ⑥ in Bra space

$$\langle 1/2, -1/2| = \langle 1,0| \langle 1/2, -1/2| c_9^* + \langle 1,-1| \langle 1/2, 1/2| c_{10}^* \quad \text{— (11)}$$

⑥ × ⑪ $\Rightarrow$ $1 = |c_9|^2 + |c_{10}|^2$

Take equation ③ in Braspace

$$\langle 3/2; 1/2| = \langle 1,0| \langle 1/2, -1/2| c_4^* + \langle 1,-1| \langle 1/2, 1/2| c_5^* \quad \text{— (12)}$$

⑥ × ⑫ $\Rightarrow$ $0 = c_4^* c_9 + c_5 c_{10}$

$$0 = \sqrt{2/3}\, c_9^* + \frac{1}{\sqrt{3}} c_{10}$$

$$-\sqrt{2}\, c_9 = c_{10}$$

we have $1 = |c_9|^2 + |c_{10}|^2$

$$1 = |c_9|^2 + |\sqrt{2}\, c_9|^2$$

$$1 = 3|c_9|^2$$

$$c_9 = \frac{1}{\sqrt{3}} \quad \text{and}$$

$$c_{10} = -\sqrt{2/3}$$

Therefore

$$\begin{bmatrix} |3/2, 3/2\rangle \\ |3/2, 1/2\rangle \\ |3/2, -1/2\rangle \\ |3/2, -3/2\rangle \\ |1/2, 1/2\rangle \\ |1/2, -1/2\rangle \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1/\sqrt{3} & \sqrt{2/3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2/3} & \sqrt{1/3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \sqrt{2/3} & -\sqrt{1/3} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{3}} & \sqrt{2/3} & 0 \end{bmatrix} \begin{bmatrix} |1,1\rangle_{①} |1/2, 1/2\rangle_{②} \\ |1,1\rangle_{①} |1/2, -1/2\rangle_{②} \\ |1,0\rangle_{①} |1/2, 1/2\rangle_{②} \\ |1,0\rangle_{①} |1/2, -1/2\rangle_{②} \\ |1,-1\rangle_{①} |1/2, +1/2\rangle_{②} \\ |1,-1\rangle_{①} |1/2, -1/2\rangle_{②} \end{bmatrix}$$