

1. Quantization of Rotational Energy of Diatomic Molecules

Classical Treatment : While treating the rotational motion of a diatomic molecule, it can be adopted a model of rigid rotator where the two masses m_1 and m_2 representing the masses of the two atoms are connected through a rigid rod of length r equal to the distance between the two atoms of the molecule. Let this rigid rotator be rotated around an axis perpendicular to its own axis and passing through the centre of gravity as shown in Fig 1

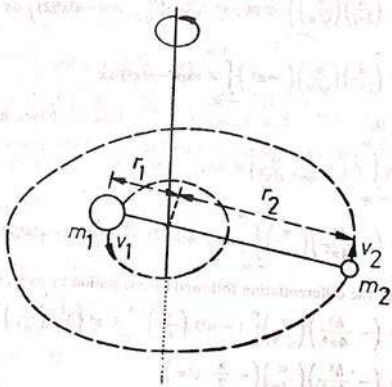


Figure1: The model of a rigid rotator

Let v_1 and v_2 be the respective velocities of the two particles with which they are rotating around the axis. The kinetic energy of the rotator is

$$T = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2 \quad \dots\dots\dots (1)$$

For the two particles of rigid rotator,

$$v_1 = r_1 \omega \quad \dots\dots\dots (2)$$

$$v_2 = r_2 \omega \quad \dots\dots\dots (3)$$

Where ω is the angular velocity of the particles, and r_1 and r_2 are the respective distances of the two masses from the centre of gravity of the molecule. Substitution of Eqs. (2) & (3) in Eq.(1) gives

$$\begin{aligned} T &= \frac{1}{2} m_1 (r_1 \omega)^2 + \frac{1}{2} m_2 (r_2 \omega)^2 \\ &= \frac{1}{2} (m_1 r_1^2 + m_2 r_2^2) \omega^2 \\ &= \frac{1}{2} I \omega^2 \quad \dots\dots\dots (4) \end{aligned}$$

Where I is the moment of inertia of the system, by definition,

$$I = \sum_1 m_i r_i^2$$

The moment of inertia I can be written in terms of the distance r between the two atoms. From the location of centre of gravity, it can be written-

$$m_1 r_1 = m_2 r_2 \quad \dots\dots\dots(5)$$

$$\text{Since } r_1 + r_2 = r, \quad \dots\dots\dots(6)$$

we have,

$$r_1 = \frac{m_2}{m_1 + m_2} r \quad \dots\dots\dots(7)$$

$$r_2 = \frac{m_1}{m_1 + m_2} r \quad \dots\dots\dots(8)$$

Substituting Eq. (7) and Eq. (8) in the expression

$$I = m_1 r_1^2 + m_2 r_2^2$$

We get ,

$$\begin{aligned} I &= m_1 \left(\frac{m_2}{m_1 + m_2} r \right)^2 + m_2 \left(\frac{m_1}{m_1 + m_2} r \right)^2 \\ &= \left(\frac{m_1 m_2}{m_1 + m_2} \right) r^2 \\ &= \mu r^2 \quad \dots\dots\dots(9) \end{aligned}$$

Where μ is the reduced mass of the system and is equal to $m_1 m_2 / (m_1 + m_2)$.

Alternatively, it may be written as

$$\frac{1}{\mu} = \left(\frac{1}{m_1} + \frac{1}{m_2} \right) \quad \dots\dots\dots(10)$$

The kinetic energy expression $T = 1/2 I \omega^2$ is the rotational counter part of the kinetic energy expression $T = 1/2 m v^2$ with I taking the place of m and ω taking the place of v . Similar analog between the linear momentum and the angular momentum gives

Angular momentum, $L=I\omega$ (11)

The kinetic energy of the system (Eq. 4) can be written in terms of angular momentum of the system as follows

$$T = \frac{1}{2} I\omega^2 = \frac{(I\omega)^2}{2I} = \frac{L^2}{2I} \dots\dots\dots (12)$$

Classically speaking, the kinetic energy of the rotator can have any value since ω can possess any value. This is, however, not true in the framework of quantum mechanics. In the later, it can be shown that the energies are quantized.

Quantum Mechanical Treatment

The classical kinetic energy of the rigid rotator can be written as

$$T = \frac{1}{2} m_1 v_1^2 + \frac{1}{2} m_2 v_2^2$$

$$= \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2}$$

Where p_1 and p_2 are the linear momenta of the two particles of rigid rotator. For a rotator rotating freely, the potential energy is zero and hence its total energy is equal to its kinetic energy, i.e.,

$$E = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2}$$

Or
$$E = \frac{p_{x_1}^2 + p_{y_1}^2 + p_{z_1}^2}{2m_1} + \frac{p_{x_2}^2 + p_{y_2}^2 + p_{z_2}^2}{2m_2} \dots\dots\dots (14)$$

Where p_x , p_y and p_z are the three components of linear momentum always x-,y-, z- and z- axes perpendicular to each other. Replacing ps with the corresponding quantum mechanical operators, we get

$$H_{op} = - \frac{h^2}{8\pi^2 m_1} \left[\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} \right] - \frac{h^2}{8\pi^2 m_2} \left[\frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2} \right] \dots\dots\dots (15)$$

It is convenient to express the rotation of a diatomic molecule in terms of the internal coordinates which are defined as

$$x = x_2 - x_1$$

$$y = y_2 - y_1$$

$$z = z_2 - z_1$$

$$\frac{\partial^2}{\partial x_1^2} = \left(\frac{\partial}{\partial x_1}\right)^2 = \left\{\frac{\partial x}{\partial x_1} \frac{\partial}{\partial x}\right\}^2 = \left\{(-1) \frac{\partial}{\partial x}\right\}^2 = \frac{\partial^2}{\partial x^2}$$

Similar expressions can be written for other differentials. Substituting these in Eq. (15), we get

$$\begin{aligned} H_{op} &= -\frac{h^2}{8\pi^2 m_1} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) - \frac{h^2}{8\pi^2 m_2} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \\ &= -\frac{h^2}{8\pi^2} \left(\frac{1}{m_1} + \frac{1}{m_2}\right) \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \\ &= -\frac{h^2}{8\pi^2 \mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \end{aligned} \dots\dots\dots(16)$$

The Schrodinger equation for the rigid rotator is given by

$$-\frac{h^2}{8\pi^2 \mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \psi = E \psi \dots\dots\dots(17)$$

It is convenient to transform the above equation into spherical coordinates with m_1 at the centre and m_2 at the position r, θ and ϕ (fig.2). The transformation equation are

$$\begin{aligned} x &= r \sin \theta \cos \phi \\ y &= r \sin \theta \sin \phi \\ z &= r \cos \theta \end{aligned}$$

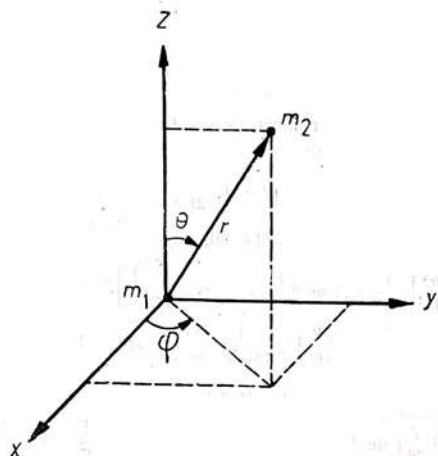


Fig. Cartesian and Spherical coordinates

This transformation is lengthy; only the transformed expression is given below.

$$-\frac{\hbar^2}{8\pi^2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\psi=E\psi \quad \dots\dots\dots (18)$$

Since the distance r between the two masses of the rotator remains constant, the derivative with respect to r will not appear in (Eq.18). Thus, Eq. 18 reduces to

$$-\frac{\hbar^2}{8\pi^2\mu r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]Y(\theta,\varphi)=EY(\theta,\varphi) \quad \dots\dots\dots (19)$$

Where the function ψ has been replaced a function by $Y(\theta,\varphi)$, known as spherical harmonics which depends only on the coordinates θ and φ . Eq.19 can be written as

$$\left[-\frac{\hbar^2}{4\pi^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}\right]Y=(2EI)Y \quad \dots\dots\dots (20)$$

Now according to (Eq. 12) ,we have

$$2EI=L^2 \quad \dots\dots\dots (21)$$

and moreover, the operation on the left hand side of Eq. (20) represents the operator of square of angular momentum. Hence, Eq.(20) may be written as

$$L_{op}^2 Y = L^2 Y \quad \dots\dots\dots(22)$$

The solution of Eq.22 provides the following expression for the quantized values of L^2 .

$$L^2 = J(J + 1) \left(\frac{\hbar}{2\pi}\right)^2 \quad \dots\dots\dots(23)$$

Where J is the quantum number, The corresponding expression for the energy will be

$$E = \frac{L^2}{2I} = J(J + 1) \frac{1}{2I} \left(\frac{\hbar}{2\pi}\right)^2 \quad \dots\dots\dots(24)$$

Substituting Eq. (23) in Eq. (20), we get

$$\left[-\frac{\hbar^2}{4\pi^2}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}\right]Y = J(J + 1) \left(\frac{\hbar}{2\pi}\right)^2 Y$$

or $\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\varphi^2} + J(J + 1) Y = 0 \quad \dots\dots\dots(25)$

Multiplying throughout by $\sin^2\theta$, we get

$$\sin \theta \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial Y}{\partial \theta} \right) + J(J + 1) \sin^2 \theta Y + \frac{\partial^2 Y}{\partial \phi^2} = 0 \quad \dots\dots\dots(26)$$

If we defined the function $Y(\theta, \phi)$ as a product of two functions $\Theta(\theta)$ and $\Phi(\phi)$, then we have

$$\Phi \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + J(J + 1) \Phi \sin^2 \theta \Theta + \Theta \frac{d^2 \Phi}{d\phi^2} = 0 \quad \dots\dots\dots(27)$$

Note: $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$
 $\partial Y / \partial \theta = \Phi (d \Theta / d \theta)$

Dividing throughout by $\Theta\Phi$ and rearranging, we have

$$\frac{1}{\Theta} \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + J(J + 1) \sin^2 \theta = - \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} \quad \dots\dots\dots(28)$$

Now the left hand side of Eq. 28 involves only θ whereas the right hand side involves only ϕ . These two terms will be equal when both are equal to the same constant, say m^2 . Thus, we have

$$\frac{1}{\Theta} \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + J(J + 1) \sin^2 \theta = m^2 \quad \dots\dots\dots(29)$$

and

$$- \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m^2 \quad \dots\dots\dots(30)$$

Qualitative Solution of Eq. 29 and Eq. 30

Equation (30) can be written as

$$\frac{d^2\phi}{d\varphi^2} = -m^2\phi \quad \dots\dots\dots(31)$$

The solution of this equation is

$$\Phi_m = A \exp\{im\varphi\} \quad \dots\dots\dots(32)$$

Boundary condition for the function ϕ : When the angle φ is replaced by $(\varphi+2\pi)$, the same set of points in space is obtained. So the boundary condition is

$$\phi(\varphi+2\pi)=\phi(\varphi) \quad \dots\dots\dots(33)$$

Hence $A\exp\{im(\varphi+2\pi)\}=A\exp\{im\varphi\}$

Or $\exp\{im2\pi\}=1 \quad \dots\dots\dots(34)$

Since $\exp\{im2\pi\} = \cos(2\pi m) + i(\sin 2\pi m)$, Eq (34) will be true only when the constant m has a value of zero or a positive or negative integer, i.e,

$$m = 0, \pm 1, \pm 2. \quad \dots\dots\dots(35)$$

The value of A in Eq.(32) can be determined by normalizing the function ϕ , such that

$$\int_0^{2\pi} \Phi_m^* \Phi_m d\varphi = 1$$

or $A^* A \int_0^{2\pi} \exp(-im\varphi) \exp(im\varphi) d\varphi = 1$

or $|A|^2 (2\pi) = 1$

or $A = \frac{1}{\sqrt{2\pi}}$

Thus, the solution of Eq. (31) is

$$\Phi_m = \frac{1}{\sqrt{2\pi}} \exp\{im\varphi\}$$

$$m = 0, \pm 1, \pm 2, \dots \quad \dots\dots\dots(36)$$

A few normalized ϕ_m functions are given in table 1.

Table 1: A few normalized ϕ_m Functions

m	Φ_m
0	$1/\sqrt{2\pi}$
+ 1	$(1/\sqrt{2\pi}) \exp(i\varphi)$
- 1	$(1/\sqrt{2\pi}) \exp(-i\varphi)$
+ 2	$(1/\sqrt{2\pi}) \exp(i2\varphi)$
- 2	$(1/\sqrt{2\pi}) \exp(-i2\varphi)$

(2) Solution of Equation (29):

Equation (29) can be written in a more familiar form by defining a variable

$$\xi = \cos \theta$$

Thus

$$\frac{d}{d\theta} = \frac{d\xi}{d\theta} \cdot \frac{d}{d\xi} = (-\sin \theta) \frac{d}{d\xi}$$

$$\sin^2 \theta = 1 - \cos^2 \theta = 1 - \xi^2$$

and the function $\Theta(\theta) \equiv P(\xi)$

With the above relations, Eq(29) modify to

$$\frac{1}{P} \left[- (1 - \xi^2) \right] \frac{d}{d\xi} \left[- (1 - \xi^2) \frac{dP}{d\xi} \right] + J(J + 1)(1 - \xi^2) = m^2$$

Dividing by $(1-\xi^2)/P$ and rearranging, we get

$$\frac{d}{d\xi} \left[(1 - \xi^2) \frac{dP}{d\xi} \right] + \left[J(J + 1) - \frac{m^2}{(1 - \xi^2)} \right] P = 0 \quad \dots\dots\dots(37)$$

or

$$(1 - \xi^2) \frac{d^2P}{d\xi^2} - 2\xi \frac{dP}{d\xi} + \left[J(J + 1) - \frac{m^2}{1 - \xi^2} \right] P = 0 \quad \dots\dots\dots(37)$$

Equation (37) is a differential equation called the associated Legendre equation. The various solution $P(\xi)$ of this equation are in the form of polynomial series, each of which must be restricted to a finite number of terms if the solution is to remain finite everywhere. This

condition ultimately leads to the requirement that J be restricted to non-negative integer values, i.e

$$J=0,1,2,3,\dots\dots\dots(38)$$

The solution P are the associated Legendre Polynomials $P_J^{|m|}$ of degree J and order m and are given by the relation

$$P = P_J^{|m|} = (1 - \xi^2)^{|m|/2} \frac{d^{|m|}}{d\xi^{|m|}} P_J \dots\dots\dots(39)$$

Where P_J is the Legendre Polynomial whose form depends only on integer J and is given by

$$P_J = \frac{1}{2^J J!} \frac{d^J}{d\xi^J} (\xi^2 - 1)^J \dots\dots\dots(40)$$

Besides J being a positive integer, the present solution P of the function Θ also requires that the $|m| \leq J$ if the functions are not vanish. This follows immediately from the fact that the differential $(d^{|m|} P_J/d\xi^{|m|})$ will become zero if m is greater than J (Eq. 40). Thus, the two quantum conditions are

$$J = 0, 1, 2, 3, \dots \dots\dots(38)$$

$$m = 0, \pm 1, \pm 2, \pm 3, \dots, \pm J \dots\dots\dots(41)$$

Hence m can have (2J+1) values for a given value of J.

Now the function $\Theta(\theta)$ are identical to the solutions of the associated Legendre Polynomials i.e the Eq. (39). However, the functions as given by Eq.(39) are not normalized. On normalizing Eq. (39) through the expression

$$\int_0^\pi \Theta^* \Theta \sin\theta d\theta = m \dots\dots\dots(42)$$

$$\Theta_{J,|m|} = \left[\frac{(2J+1)(J-|m|)!}{2(J+|m|)!} \right]^{1/2} P_J^{|m|} \dots\dots\dots(43)$$

The function Θ depends on the values of two quantum numbers J and m . The exact form of the function $\Theta_{J,m}$ for from Eq. the given values of J and m can be determined from Eq. (42), Eq.(39) and Eq. (40).

Problem1: Determine the form of the function Θ for $J=2$ and $m=0$.

The function is given by Eq.42 is

$$\Theta_{2,0} = \left[\frac{(2 \times 2 + 1)}{2} \cdot \frac{2!}{2!} \right]^{1/2} P_2^{(0)}$$

Where $P_2^{(0)}$ from Eq. 39 is given by

$$P_2^{(0)} = (1 - \xi^2)^0 \frac{d^0}{d\xi^0} P_2 = P_2$$

and P_2 from Eq. 40 is given by

$$\begin{aligned} P_2 &= \frac{1}{2^2(2!)} \frac{d^2}{d\xi^2} (\xi^2 - 1)^2 \\ &= \frac{1}{2^2(2!)} \frac{d}{d\xi} \{ 2(\xi^2 - 1) 2\xi \} \\ &= \frac{1}{2^2(2!)} [2(2\xi)(2\xi) + 2(\xi^2 - 1) 2] \\ &= \frac{1}{8} [12\xi^2 - 4] = \frac{3}{2} \xi^2 - \frac{1}{2} \end{aligned}$$

Hence

$$\begin{aligned} \Theta_{2,0} &= \left(\frac{5}{2} \right)^{1/2} \left(\frac{3}{2} \xi^2 - \frac{1}{2} \right) \\ &= \left(\sqrt{\frac{2 \times 5}{2 \times 2}} \right) \left(\frac{1}{2} (3\xi^2 - 1) \right) \\ &= \frac{\sqrt{10}}{4} (3\xi^2 - 1) \end{aligned}$$

Since $\xi = \cos\theta$, we have

$$\Theta_{2,0} = \frac{\sqrt{10}}{4} (3 \cos^2 \theta - 1)$$

Following the method given in Problem 1, the other functions with different values of J and m can be determined. Table 2 includes some of these functions.

Table 2: A few normalized $\theta_{J,m}$ functions

J	m	$\theta_{J,m}$
0	0	$\sqrt{2}/2$
1	0	$(\sqrt{6}/2) \cos \theta$
1	± 1	$(\sqrt{3}/2) \sin \theta$
2	0	$(\sqrt{10}/4) (3 \cos^2 \theta - 1)$
2	± 1	$(\sqrt{15}/2) \sin \theta \cos \theta$
2	± 2	$(\sqrt{15}/4) \sin^2 \theta$

Physical Significance of the constant J: From Eq.23,

$$L^2 = J(J + 1) \left(\frac{h}{2\pi} \right)^2$$

$$L = \sqrt{J(J + 1)} (h/2\pi)$$

Thus, the constant J is the quantum number which stands for the quantization of total angular momentum of the system. This constant also represents the quantization of energy since

$$E = \frac{L^2}{2I} = J(J + 1) \frac{h^2}{8\pi^2 I} \dots\dots\dots(24)$$

The minimum allowed value of J is zero, for which L as well as E has zero value. Thus, in the present case angular momentum L can have a precise value. Thus, however, does not violate the uncertainty principle since the angles of orientation, θ and ϕ are completely unspecified.

Physical Significance of the constant m: In order to understand the physical significance of the constant m, let the function $(1/\sqrt{2\pi}) \exp(im\phi)$ be operated by an operator of the z-component of angular momentum. The operator in spherical coordinate system has the form.

$$(L_z)_{op} = \frac{h}{2\pi i} \frac{\partial}{\partial \varphi} \dots\dots\dots(43)$$

Thus,

$$\begin{aligned} (L_z)_{op} \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} &= \frac{h}{2\pi i} \frac{\partial}{\partial \varphi} \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} \\ &= m \frac{h}{2\pi} \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} \dots\dots\dots(44) \end{aligned}$$

Equation (44) represents an eigenvalue problem, where the z-component of angular momentum has precise values and is given by the relation

$$L_z = m \left(\frac{h}{2\pi} \right) \dots\dots\dots(45)$$

Hence the constant m represents the quantization of the z-component of the angular momentum. Accordingly to Eq. (44), the permitted values of m are 0, ±1, ±2, Again, precise values of the z-component of angular momentum (i.e., the orientation angle θ of the angular momentum with the z-axis) are allowed. This also does not violate the uncertainty principle as the angle φ is completely unspecified.

Relation between the Constants J and m: The relation between J and m can also be determined following the procedure given below:

Now

$$(L_z)_{op} \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} = m \frac{h}{2\pi} \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\}$$

Therefore

$$\begin{aligned} (L_z)_{op}^2 \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} &= (L_z)_{op} \left\{ m \frac{h}{2\pi} \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} \\ &= m^2 \left(\frac{h}{2\pi} \right)^2 \left\{ \frac{1}{\sqrt{2\pi}} \exp(im\varphi) \right\} \dots\dots\dots(46) \end{aligned}$$

That is , the square of the z-component of angular momentum is $(mh/2\pi)^2$.

Since the angular momentum is a vector, it can be written as

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

or

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

or

$$\left[J(J+1) - m^2 \right] \left(\frac{h}{2\pi} \right)^2 = L_x^2 + L_y^2 \quad \dots\dots\dots (47)$$

The right hand side of Eq.(47) is a positive quantity as it consists of a sum of squares. It, therefore, follows that the left hand side of this equation should also be a positive quantity, for which it must be

$$J(J+1) - m^2 \geq 0 \quad \dots\dots\dots(48)$$

This condition will be fulfilled provided $|m| \leq J$

Thus the values of m are restricted to $m = 0, \pm 1, \pm 2, \dots, \pm J$, i.e., m can have (2J+1) values. All states with different values of m but the same value of J are degenerate (i.e., they have same energy) as the energy of the system depends only on the quantum number J

Pictorial Representations : Since m_z is confined to the (2J+1) discrete values J, (J-1),.....-(J-1),-J for a given value of J, it implies that the orientations of the angular momentum vector of magnitude $\sqrt{J(J+1)} (h/2\pi)$ in space is such that its component along the z-axis can have a value of $m_z(h/2\pi)$, where m_z can take any value out of J, J-1,.....-(J-1),-J. The angular momentum being a vector quantity can be shown by an arrow whose length is proportional to the magnitude of the angular momentum and which points in a direction perpendicular to the plane of rotation. Thus, the orientations of the angular momentum vector and also the corresponding orientation of the plane of rotation may take only a discrete range of values, as shown in Figure 3 for J=1. This leads to what is known as the *space quantization* . The angle θ between the angular momentum vector and the z-axis is given by the relation

$$\sqrt{J(J+1)} \cos \theta = m_z \quad \dots\dots\dots(49)$$

In fig3, the orientations of angular momentum vectors labeled as (i) and (ii) are in the plane of paper. For m_z not equal to zero the angular momentum vector can also point out of the plane of paper making the same angle θ with the z-axis. These orientations are shown under the labeling (iii). Thus , any vector on the conical surfaces will have a value of $\sqrt{2} (h/2\pi)$ for the total angular momentum and $\pm (h/2\pi)$ for the z-component of angular momentum. The fact that the angular momentum may lie anywhere on the cone is in agreement with the uncertainty principle (angle θ has a precise value but not the angle ϕ).

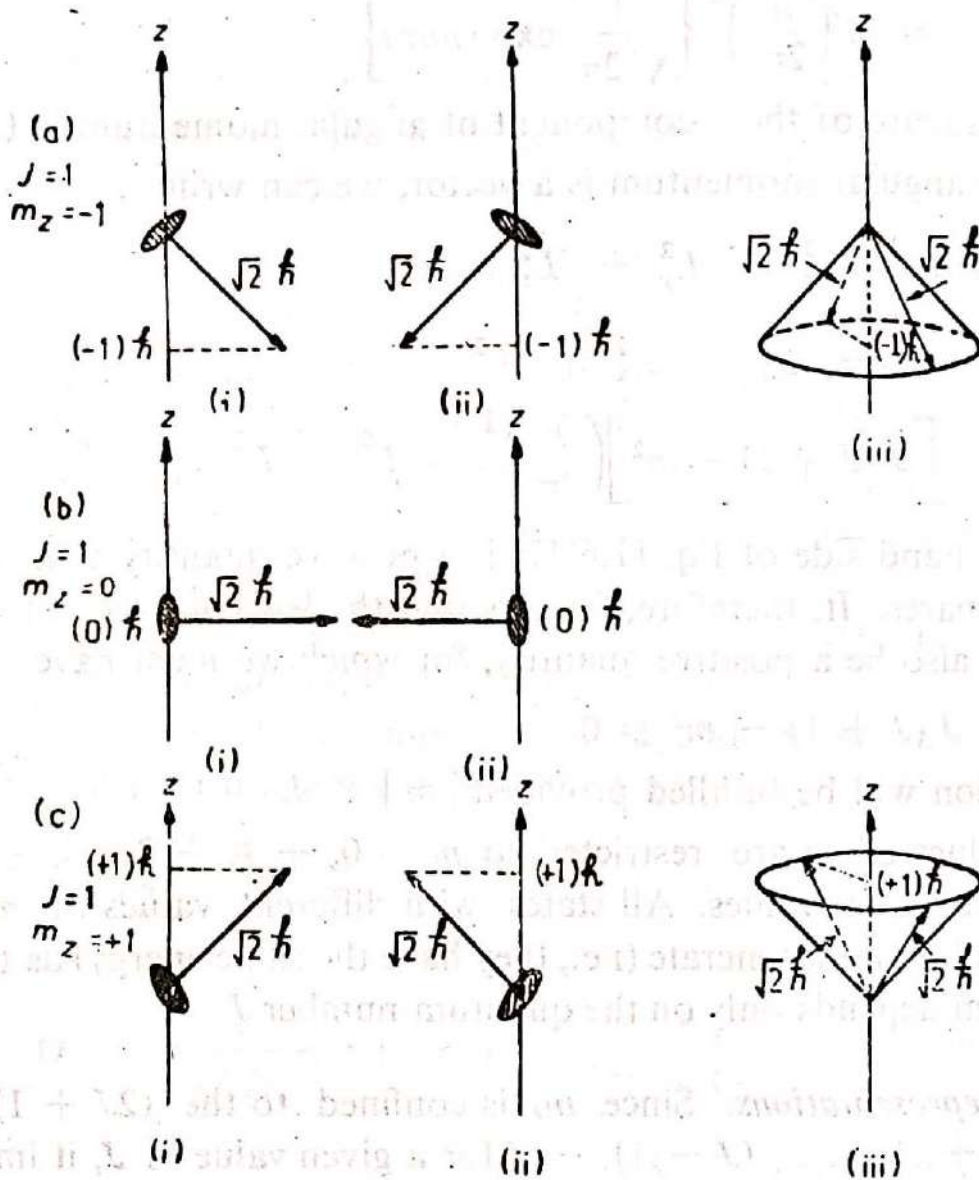


Figure 3: Possible orientations of angular momentum vectors for $J=1$

.....End.....