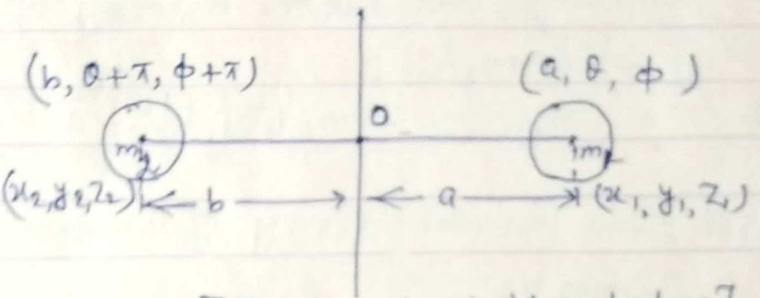
# Rigid rotator with free axis

The system consisting of two spherical particles attached together and separated by a finite fixed distance and capable of rotating about an axis passing through the centre of mass and normal to the plane containing the two particles constitute a rigid rotator. If these two particles are constrained to remain in the plane, then the direction of the axis of rotation is fixed and the system is called the rigid rotator with fixed axis. If the plane of these two particles can move, then the axis of rotation is free to take any position in the space and so the system is called the rigid rotator with free axis.

Considering two spherical masses $m_1$ and $m_2$ at a fixed distance apart and rotating about an axis passing through a fixed point O as shown in fig.




[Free axis rigid rotator]

Let the co-ordinates of two masses with respect to origin O be $(x_1, y_1, z_1)$ and $(x_2, y_2, z_2)$. a be the distance of mass $m_1$ from O and b be the distance of mass $m_2$ from O then the polar co-ordinates can be expressed as $(a, \theta, \phi)$ and $[b, (\theta+\pi), (\phi+\pi)]$.

The Cartesian co-ordinates are related to the respective polar co-ordinates by the relations:

$$x_1 = a\sin\theta\cos\phi \qquad x_2 = b\sin(\pi+\theta)\cos(\pi+\phi) = b\sin\theta\cos\phi$$

$$y_1 = a\sin\theta\sin\phi \qquad y_2 = b\sin(\pi+\theta)\cdot\sin(\pi+\phi) = b\sin\theta\cdot\sin\phi$$

$$z_1 = a\cos\theta \qquad z_2 = b\cos(\pi+\theta) = -b\cos\theta$$

The Kinetic energy of the particle of mass $m_1$ is given by

$$T_1 = \frac{1}{2} m_1 \left[ \left(\frac{dx_1}{dt}\right)^2 + \left(\frac{dy_1}{dt}\right)^2 + \left(\frac{dz_1}{dt}\right)^2 \right] \quad \text{(1)}$$

$$\frac{dx_1}{dt} = a\left[\cos\theta \cos\phi \left(\frac{d\theta}{dt}\right) - \sin\theta \sin\phi \left(\frac{d\phi}{dt}\right)\right]$$

$$\frac{dy_1}{dt} = a\left[\cos\theta \sin\phi \left(\frac{d\theta}{dt}\right) + \sin\theta \cos\phi \left(\frac{d\phi}{dt}\right)\right]$$

$$\frac{dz_1}{dt} = -a \sin\theta \left(\frac{d\theta}{dt}\right)$$

Hence $\left(\frac{dx_1}{dt}\right)^2 + \left(\frac{dy_1}{dt}\right)^2 + \left(\frac{dz_1}{dt}\right)^2$

$$= a^2\left[\cos^2\theta \left(\frac{d\theta}{dt}\right)^2 + \sin^2\theta \left(\frac{d\phi}{dt}\right)^2 + \sin^2\theta \left(\frac{d\theta}{dt}\right)^2\right]$$

$$= a^2\left[\left(\frac{d\theta}{dt}\right)^2 + \sin^2\theta \left(\frac{d\phi}{dt}\right)^2\right]$$

$$\therefore T_1 = \frac{1}{2} m_1 a^2 \left[\left(\frac{d\theta}{dt}\right)^2 + \sin^2\theta \left(\frac{d\phi}{dt}\right)^2\right] \quad \text{(2)}$$

Similarly, the Kinetic energy of the particle of mass $m_2$ is

$$T_2 = \frac{1}{2} m_2 b^2 \left[\left(\frac{d\theta}{dt}\right)^2 + \sin^2\theta \left(\frac{d\phi}{dt}\right)^2\right] \quad \text{(3)}$$

The total Kinetic energy of the two masses is given by

$$T = T_1 + T_2$$

$$= \left[\left(\frac{d\theta}{dt}\right)^2 + \sin^2\theta \left(\frac{d\phi}{dt}\right)^2\right] \left(\frac{1}{2} m_1 a^2 + \frac{1}{2} m_2 b^2\right) \quad \text{(4)}$$

If we put $I = m_1 a^2 + m_2 b^2$;
= moment of inertia about free axis, then equation (4) reduces to

$$T = \frac{1}{2} I \left\{\left(\frac{d\theta}{dt}\right)^2 + \sin^2\theta \left(\frac{d\phi}{dt}\right)^2\right\} \quad \text{(5)}$$

The Kinetic energy is same as that of a single particle of mass I moving on the surface of a sphere of unit radius.

The general Schrodinger wave equation in spherical co-ordinates is given by

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\cdot\frac{\partial^2\psi}{\partial\phi^2}+\frac{2m}{\hbar^2}(E-V)\psi=0 \quad (6)$$

As $r$ is constant, hence first factor $\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)=0$ i.e. $(r=1)$

and since there is no force acting on the rotator, $V=0$.

Therefore, the Schrodinger wave equation for a rigid rotator becomes

$$\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2I}{\hbar^2}E\psi=0$$

where $[m=I]$ — (7)

Solution of wave equation

The solution of equation (7) can be obtained by the method of separation of variables

Assume, $\psi(\theta,\phi)=\Theta(\theta)\Phi(\phi)=\Theta\Phi$ — (8)

where $\Theta$ is a function of $\theta$ alone and $\Phi$ is a function of $\phi$ alone.

Putting equation (8) in (7) and dividing both sides by $\Theta\Phi/\sin^2\theta$, we have,

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\frac{2IE}{\hbar^2}\sin^2\theta=-\frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\phi^2} \quad (9)$$

L.H.S is a function of $\theta$ alone while R.H.S is a function of $\phi$ alone. Therefore, if this equation is to be satisfied, both sides must be equal to the same constant $m^2$ (say)

(4)

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\frac{2IE}{\hbar^2}\sin^2\theta=m^2 \quad \text{--- (10)}$$

and $-\frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\phi^2}=m^2$

or $m^2+\frac{1}{\Phi}\cdot\frac{\partial^2\Phi}{\partial\phi^2}=0$

or $$\frac{\partial^2\Phi}{\partial\phi^2}+m^2\Phi=0 \quad \text{--- (11)}$$

The solution of equation (11) may be represented as —

$$\Phi=Ae^{im\phi} \quad \text{--- (12)}$$

where $m=0,\pm1,\pm2,\pm3,\ldots$

The A is any arbitrary constant which may be chosen in such a way that the function $\Phi$ is normalized i.e

$$\int_0^{2\pi}\Phi\Phi^*\,d\phi=1$$

or $$\int_0^{2\pi}Ae^{im\phi}\cdot Ae^{-im\phi}\,d\phi=1$$

$$A^2\int_0^{2\pi}d\phi=1$$

$$A^2\cdot2\pi=1$$

$$A=\frac{1}{\sqrt{2\pi}} \quad \text{--- (13)}$$

Hence equation (12) is written as —

$$\Phi=\frac{1}{\sqrt{2\pi}}e^{im\phi}; \quad \text{--- (14)}$$

Multiplying equation (10) by $\frac{\Theta}{\sin^2\theta}$, we get —

$$\frac{1}{\sin\theta}\cdot\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right)+\left(\frac{2IE}{\hbar^2}-\frac{m^2}{\sin^2\theta}\right)\Theta=0 \quad \text{--- (15)}$$

This equation can be solved by the following substitution

$\cos\theta = x$, $\sin\theta = \sqrt{1-x^2}$ or $\sin^2\theta = 1-x^2$

$$\frac{\partial x}{\partial \theta} = -\sin\theta$$

$$dx = -\sin\theta \, \partial\theta$$

$$\frac{\partial x}{\partial \theta} = -\sin\theta$$

$$\frac{\partial \Theta}{\partial \theta} = \frac{\partial \Theta}{\partial x} \cdot \frac{\partial x}{\partial \theta} = -\sin\theta \cdot \frac{\partial \Theta}{\partial x}$$

$$\sin\theta \frac{\partial \Theta}{\partial \theta} = -\sin^2\theta \cdot \frac{\partial \Theta}{\partial x} = -(1-x^2)\frac{\partial \Theta}{\partial x}$$

$-\frac{1}{\sin\theta}$ and $\frac{\partial}{\partial \theta} = -\sin\theta \frac{\partial}{\partial x}$

or $-\frac{1}{\sin\theta} \cdot \frac{\partial}{\partial \theta} = \frac{\partial}{\partial x}$

$$+\frac{\partial}{\partial x}\left\{(1-x^2)\frac{\partial \Theta}{\partial x}\right\} + \left\{\lambda - \frac{m^2}{(1-x^2)}\right\}\Theta = 0 \quad (16)$$

where $\lambda = \frac{2IE}{\hbar^2} = l(l+1)$

Equation (16) is known as Legendre's equation ~~whose solution is~~ The solution of above equation contains a factor called associated Legendre function $P_l^m(x)$ which may be defined as

$$P_l^m(x) = (1-x^2)^{m/2} \frac{d^m}{dx^m} P_l(x)$$

where $P_l(x)$ is Legendre polynomial of degree $l$. Hence the solution of equation (16) is written as

$$\Theta = B P_l^m(x) = B P_l^m(\cos\theta) \quad (17)$$

where B is constant which may be a normalising factor.

According to orthogonal properties of associated Legendre's polynomials, we have

$$\int_{-1}^{+1} P_k^m(x) P_l^m(x)\, dx = \frac{2}{2l+1} \cdot \frac{(l+m)!}{(l-m)!} \text{ for } K = l \quad (18)$$

(6)

According to normalising condition

$$\int_{-1}^{+1} \Theta_{ml} \Theta_{ml}^{*} \, d\theta = 1$$

i.e. $B^2 \int_{-1}^{+1} P_l^m(x) \cdot P_l^m(x) \, dx = 1$

i.e. $B^2 \cdot \frac{2}{2l+1} \cdot \frac{(l+m)!}{(l-m)!} = 1$

i.e. $B = \sqrt{\frac{(2l+1)}{2} \cdot \frac{(l-m)!}{(l+m)!}}$ ; ——— (19)

Substituting (19) in (17)

$$\Theta_l^m(\theta) = \sqrt{\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m)!}} \cdot P_l^m(\cos\theta) \quad \text{——— (20)}$$

The complete wavefunction or eigenfunction for the rigid rotator is given by

$$\psi_{lm}(\theta, \phi) = \Theta(\theta) \, \Phi(\phi)$$

$$\therefore \boxed{\psi_{lm}(\theta, \phi) = \sqrt{\frac{2l+1}{2} \cdot \frac{(l-m)!}{(l+m)!}} \cdot \frac{1}{\sqrt{2\pi}} P_l^m(\cos\theta) \, e^{im\phi}}$$

**Eigen values or energy levels of the rigid rotator**

Eigenvalue of $\psi_{lm}$ is

$$\frac{2IE_l}{\hbar^2} = l(l+1)$$

$$E_l = \frac{\hbar^2}{2I} l(l+1) \quad \text{where } l = 0, 1, 2, \ldots$$

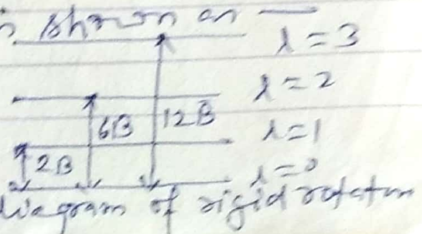
When $l = 0$, $E_0 = 0$

$l = 1$, $E_1 = \frac{\hbar^2}{2I} \cdot 2 = 2B$

$l = 2$, $E_2 = \frac{\hbar^2}{2I} \cdot 6 = 6B$

$l = 3$, $E_3 = \frac{\hbar^2}{2I} \cdot 12 = 12B$

The energy level diagram is shown as




Energy level diagram of rigid rotator