RIGID ROTATOR

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Rigid Rotator

Let us examine the three-dimensional rigid rotator. Consider two particles of masses m_1 and m_2 joined about an axis passing through a point O. The particle of mass m_1 is at a distance r_1 from O and the other particle is at a distance r_2 from O and $r_1 + r_2 = R$ (Fig. 1). Such a system is called a *rigid rotator* because the distances r_1 and r_2 are fixed. The magnitude of the vibration of a diatomic molecule is generally small compared with the equilibrium bond length so the rigid rotator is a good first approximation.

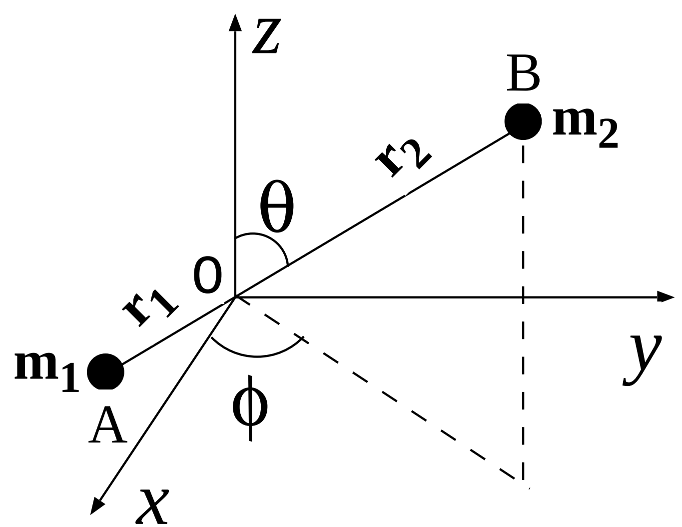

Figure 1: Parameters of the rigid rotator AB.

Hamiltonian and Schrödinger Equation

Let us denote the coordinates of the two particles with respect to the origin O as (x_1, y_1, z_1) and (x_2, y_2, z_2), respectively. The classical equation of motion for the rigid rotator is

$$\text{Kinetic Energy (K.E)} = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 = \frac{1}{2}\left(m_1 r_1^2 + m_2 r_2^2\right)\omega^2 \ , \tag{1}$$

where $v_1 = r_1\omega$, $v_2 = r_2\omega$ and ω is the angular frequency of rotation. Thus, $\mathrm{K.E.} = I\omega^2/2$ where $I = m_1 r^2 + m_2 r_2^2$ is the moment of inertia. The potential of the system is zero because there is no external force on the system and hence $H = I\omega^2/2$.

The system is spherically symmetric; therefore, it is convenient to deal it in spherical polar coordinates. In this coordinates system the coordinates of the particles are (a, θ, ϕ) and $(b, \pi - \theta, \pi + \phi)$, respectively. We have

$$x_1 = a\sin\theta\cos\phi, \quad x_2 = b\sin\theta\cos\phi, \tag{2a}$$

$$y_1 = a\sin\theta\sin\phi, \quad y_2 = b\sin\theta\sin\phi, \tag{2b}$$

$$z_1 = a\cos\theta, \quad z_2 = -b\cos\theta. \tag{2c}$$

Hamiltonian and Schrödinger Equation

The component of velocity of the particles are

$$
\begin{aligned}
v_{1x} &= \frac{\mathrm{d}x_1}{\mathrm{d}t} = a\left(\cos\theta\,\cos\phi\,\frac{\mathrm{d}\theta}{\mathrm{d}t} - \sin\theta\,\sin\phi\,\frac{\mathrm{d}\phi}{\mathrm{d}t}\right)\;, && \text{(3a)}\\
v_{1y} &= \frac{\mathrm{d}y_1}{\mathrm{d}t} = a\left(\cos\theta\,\sin\phi\,\frac{\mathrm{d}\theta}{\mathrm{d}t} + \sin\theta\,\cos\phi\,\frac{\mathrm{d}\phi}{\mathrm{d}t}\right)\;, && \text{(3b)}\\
v_{1z} &= \frac{\mathrm{d}z_1}{\mathrm{d}t} = -a\sin\theta\,\frac{\mathrm{d}\theta}{\mathrm{d}t}\;. && \text{(3c)}
\end{aligned}
$$

Then

$$
v_1^2 = v_{1x}^2 + v_{1y}^2 + v_{1z}^2 = r_1^2\left(\dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2\right)\;. \tag{4}
$$

Similarly, $v_2^2 = r_2^2\left(\dot{\theta}^2 + \sin^2\theta\,\dot{\phi}^2\right)$. Then the total kinetic energy of the two particles is written as

$$
\begin{aligned}
\text{K.E.} &= T_1 + T_2 = \frac{1}{2}\left(m_1 r_1^2 + m_2 r_2^2\right)\left(\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2\right)\\
&= \frac{1}{2} I\left(\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2\right)\;. && \text{(5)}
\end{aligned}
$$

Hamiltonian and Schrödinger Equation

For a particle of mass I moving on the surface of a sphere of radius r the kinetic energy is given by

$$\mathrm{K.E.} \quad = \quad \frac{1}{2} I\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right)=\frac{1}{2} I r^2\left(\dot{\theta}^2+\sin^2\theta\, \dot{\phi}^2\right) . \tag{6}$$

The Laplacian ∇^2 in spherical polar coordinates is

$$\nabla^2=\frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)+\frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial}{\partial \theta}\right)+\frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} . \tag{7}$$

For the rigid rotator r is constant so

$$\nabla^2=\frac{1}{\sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial}{\partial \theta}\right)+\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} . \tag{8}$$

The Hamiltonian is

$$H=-\frac{\hbar^2}{2 I}\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta}\left(\sin \theta \frac{\partial}{\partial \theta}\right)+\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}\right] . \tag{9}$$

The orientation of the rigid rotator depends only on θ and ϕ; therefore, its ψ depends only on θ and ϕ and is independent of r.

Hamiltonian and Schrödinger Equation

The Schrödinger equation $H\psi = E\psi$ takes the form

$$-\frac{\hbar^2}{2I}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\theta,\phi) = E\psi(\theta,\phi) \tag{10}$$

or

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}+\frac{2I}{\hbar^2}E\psi = 0\ . \tag{11}$$

The operator in the left-side of Eq. (10) is identified as $\vec{L}^2/2I$ where $\vec{L}^2$ is the square of the orbital angular momentum. Equation (10) implies that the eigenvalues E of the rigid rotator are $(1/2I)$ times the eigenvalues of the operator $\vec{L}^2$.

Eigenfunctions and Eigenvalues

We show that the solution of Eq. (11) is simply the spherical harmonics. We obtain the solution by variable separable method. Assume the solution of the form

$$\psi(\theta,\phi) = \Theta(\theta)\Phi(\phi)\ . \tag{12}$$

Substituting Eq. (12) in Eq. (11) and multiplying by $\sin^2\theta/(\Theta\Phi)$ we get

$$\frac{\Phi}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\,\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \frac{\Theta}{\sin^2\theta}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} + \frac{2I}{\hbar^2}E\Theta\Phi = 0\,. \tag{13}$$

That is

$$\frac{\sin\theta}{\Theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\,\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \frac{2IE}{\hbar^2}\sin^2\theta = -\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2}\ . \tag{14}$$

Since θ and ϕ are two independent variables the above equation is true only if both sides are equal to the same constant. We choose the constant as m^2. Then

$$-\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi^2}{\mathrm{d}\phi^2} = m^2\ . \tag{15}$$

The solution of it is

$$\Phi_m = A\mathrm{e}^{\pm\mathrm{i}m\phi}\ . \tag{16}$$

Eigenfunctions and Eigenvalues

A is determined from the normalization condition

$$\int_0^{2\pi} \Phi^* \Phi \, \mathrm{d}\phi = 1. \tag{17}$$

A is obtained as $1/\sqrt{2\pi}$. Equation (14) is now written as

$$\frac{\sin\theta}{\Theta} \frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta \frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) + \frac{2IE\sin^2\theta}{\hbar^2} = m^2 \tag{18}$$

or

$$-\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\frac{\sin^2\Theta}{\sin\theta}\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right) - \left(\frac{2IE}{\hbar^2} - \frac{m^2}{\sin^2\theta}\right)\Theta = 0 \, . \tag{19}$$

Substituting

$$\cos\theta = x, \quad 2IE/\hbar^2 = l(l+1) \tag{20}$$

in Eq. (19) we have

$$\left(1-x^2\right)\Theta'' - 2x\Theta' + \left[l(l+1) - \frac{m^2}{1-x^2}\right]\Theta = 0 \tag{21}$$

which is the associated Legendre differential equation.

Eigenfunctions and Eigenvalues

Let us find a solution of Eq. (21) of the form

$$\Theta(x) = \left(1 - x^2\right)^{m/2} X(x) \ . \tag{22}$$

Now Eq. (21) becomes

$$\left(1 - x^2\right) \frac{\mathrm{d}^2 X}{\mathrm{d}x^2} - 2(m+1)x \frac{\mathrm{d}X}{\mathrm{d}x} + \left[l(l+1) - m(m+1)\right] X = 0 \ . \tag{23}$$

Differentiating the Legendre differential equation

$$\left(1 - x^2\right) \frac{\mathrm{d}^2 P_l}{\mathrm{d}x^2} - 2x \frac{\mathrm{d}P_l}{\mathrm{d}x} + l(l+1)P_l = 0 \tag{24}$$

m times we get

$$\left(1 - x^2\right) \frac{\mathrm{d}^2}{\mathrm{d}x^2} \left(\frac{\mathrm{d}^m P_l}{\mathrm{d}x^m}\right) - 2(m+1)x \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{\mathrm{d}^m P_l}{\mathrm{d}x^m}\right)$$
$$+ \left[l(l+1) - m(m+1)\right] \frac{\mathrm{d}^m P_l}{\mathrm{d}x^m} = 0 \ . \tag{25}$$

Eigenfunctions and Eigenvalues

Comparing the Eq. (25) with Eq. (23) we write

$$X(x) = \frac{\mathrm{d}^m}{\mathrm{d}x^m} P_l(x) \tag{26}$$

provided m assumes only positive integers. Then the solution $\Theta_l^{(m)}$ is

$$\Theta_l^{(m)}(x) = \left(1 - x^2\right)^{|m|/2} \frac{\mathrm{d}^{|m|}}{\mathrm{d}x^{|m|}} P_l(x) = P_l^{|m|} \; . \tag{27}$$

$P_l^{|m|}$ are called *associated Legendre polynomials*. We note that since Eq. (21) does not depend on sign of m, because $P_l(x)$ are polynomials of degree l, we have $\mathrm{d}^{|m|} P_l / \mathrm{d}x^{|m|} = 0$ if $|m| > l$. Therefore, $|m| \leq l$. The orthogonality relation for the associated Legendre polynomials $\Theta_l^{|m|}$ is

$$\int_{-1}^{1} \Theta_l^{|m|} \Theta_{l'}^{|m|} \, \mathrm{d}x = \frac{(l - |m|)!}{(l + |m|)!} \frac{2}{2l + 1} \delta_{ll'} \tag{28}$$

which gives the normalization factor for $\Theta_l^{|m|}$. Now

$$\Theta_l^{|m|} \Phi_m = \left[\frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{1/2} P_l^{|m|}(\cos\theta) \, \mathrm{e}^{\mathrm{i}m\phi} \; . \tag{29}$$

Eigenfunctions and Eigenvalues

The right-side of Eq. (29) are the so-called *spherical harmonics* and are the eigenfunctions of the rigid rotator.

What are the allowed energy eigenvalues of the system? From Eq. (20)

$$E_l = \frac{\hbar^2}{2I} l(l+1) \; , \quad l = 0, 1, \cdots \; . \tag{30}$$

The energy levels are thus discrete. The separation between two successive energy levels are given by

$$\triangle E_l = E_{l+1} - E_l = \frac{\hbar^2}{2I}[l(l+1) - l(l-1)] = \frac{\hbar^2}{I}(l+1) \; . \tag{31}$$

The distance between successive energy levels increases with an increase in l. For each l the allowed values of m are $(2l+1)$. For $l = 0$ only one value of m is possible: $m = 0$. For other values of l there are $(2l+1)$ allowed values of m: $-l, -l+1, \cdots,$ $0, \cdots, l-1, l$. Therefore, each energy level is $(2l+1)$-fold degenerate.

Solved Problem

A rigid body freely rotates in the $x-y$ plane. At $t=0$ the wave function is assumed as $\psi(0)=C\sin^2\phi$ where ϕ is the angle between the x-axis and the rotator axis. Express $\psi(0)$ in terms of the eigenfunctions $\Phi_m=\frac{1}{\sqrt{2\pi}}\mathrm{e}^{\mathrm{i}m\phi}$, $m=0,\pm1,\pm2,\cdots$.

In terms of Φ_m we can write an arbitrary wave function as

$$\psi(0)=\sum_m C_m\Phi_m=C_0\Phi_0+C_1\Phi_1+C_{-1}\Phi_{-1}+C_2\Phi_2+C_{-2}\Phi_{-2}+\cdots\ . \tag{32}$$

We can rewrite the given $\psi(0)$ as

$$\begin{aligned}\psi(0) &= C\sin^2\phi=\frac{C}{2}(1-\cos 2\phi)=\frac{C}{2}-\frac{C}{4}\left(\mathrm{e}^{-\mathrm{i}2\phi}+\mathrm{e}^{-\mathrm{i}2\phi}\right)\\ &= \sqrt{2\pi}\left(\frac{C}{2}\Phi_0-\frac{C}{4}\Phi_2-\frac{C}{4}\Phi_{-2}\right)\ .\end{aligned} \tag{33}$$

Comparison of the above two equations for $\psi(0)$ gives

$$C_0=C\sqrt{\pi/2},\quad C_1=0,\quad C_{-1}=0,\quad C_2=-\frac{C\sqrt{\pi}}{2\sqrt{2}},\quad C_{-2}=-\frac{C\sqrt{\pi}}{2\sqrt{2}} \tag{34}$$

and other C_i's are zero.