

ROLL NO. - 210100166 CLASS – D3/T4

Rigid rotor is a system of 2 particles revolving around the centre of mass. So we can also take that the reduced mass is revolving around the centre of mass. Spherical coordinates is a method in which the coordinates are represented in a format of distance from the origin, angle from the z axis, and the angle between the projector from the point to XY plane and the X axis. From the Hamiltonian equation we get the Angular momentum operator.

$$\hat{H} = \frac{\hat{L}^2}{2I} = \frac{\hat{L}^2}{2\mu r_o^2}$$

We can show the Hamiltonian operator as function of theta and phi and then equate them to M and solve them individually. $L = r \times p$ this formula gives us an equation and when operated for the x and p operators gives us the angular momentum operator. When we operate the L operator on the phi function it gives an eigenvalue which is proportional to the m value, which shows it is quantized. As L is quantized the energy is also quantized

$$\epsilon_J = \frac{h}{8\pi^2 I_c} J(J+1) \text{ cm}^{-1}, \text{ where } J = 0, 1, 2, \dots$$

$$\epsilon_J = BJ(J+1) \text{ cm}^{-1}, \text{ where } B = \frac{h}{8\pi^2 I_c} = \text{Rotational Constant}$$

Hydrogen Atom:

The Schrodinger's equation in hydrogen atom is represented as

$$\left(-\frac{\hbar^2}{2M} \nabla_R^2 - \frac{\hbar^2}{2\mu} \nabla_r^2 - \frac{QZe^2}{r} \right) \Psi_{Total} = E_{Total} \cdot \Psi_{Total}$$

We can convert the following in to the relativistic equation and then we get the equation mentioned above. But in this equation, we have r which is in the x, y, z so it will be difficult to evaluate. Therefore, we again convert the equation in to the polar coordinates and finally we get the

$$\frac{1}{R} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{2\mu r QZe^2}{\hbar^2} + \frac{2\mu r^2}{\hbar^2} E_e = - \left[\frac{1}{\Theta} \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi} \frac{1}{\sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} \right]$$

and I learn how to solve radial, theta and phi part differently.