Rigid Rotator

I. Planar

The Laplacian in plane polar coordinators is

$$x = \rho cos\theta; \quad y = \rho sin\theta$$

$$\rho = \left(x^2 + y^2\right)^{\frac{1}{2}}; \quad tan\theta = y/x$$

$$^2 = \frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial 2}{\partial\theta^2}$$

For a rigid rotator

$$\rho = \rho_e$$

$$\boxed{H_{r.r.} = \frac{-\hbar^2}{2\mu r_e^2}\frac{\partial^2}{\partial\theta^2}} \qquad - \quad \text{angular kinetic energy}$$

$$H_{r.r.}\,\Phi(\theta) = \lambda\Phi(\theta)$$

By inspection $\quad \Phi(\theta) = Ne^{\,ia\theta}$

Then $\quad$ Hrr $\Phi = +\frac{\hbar^2}{2\mu r_e^2}a^2\Phi; \;\; \lambda = \frac{\hbar^2}{2\mu r_e^2}a^2$

Boundary condition. $\Phi(\theta + 2\pi) = \Phi(\theta)$.

Thus

$$e^{i\theta a} = e^{i(\theta + 2\pi)a} \qquad e^{i\,2\pi a} = 1$$

$$a = 0, \pm 1, \pm 2, \ldots \text{etc} \qquad a \quad m \text{ (integer)}$$

$$\Phi_m(\theta) = N e^{im\theta}.$$

Normalization: $\int_0^{2\pi} d\theta \, |\Phi_m|^2 = 1$

$$N^2 \int_0^{2\pi} d\theta = 2\pi N^2 = 1 \text{\_\_\_\_\_\_\_} N = \frac{1}{\sqrt{2\pi}}$$

<u>Summary</u> $\Phi_m(\theta) = \frac{1}{\sqrt{2\pi}} e^{im\theta}; \qquad m = 0, \pm 1, \pm 2, \ldots$

$$E_m = \frac{\hbar^2 m^2}{2\mu r_e^2}$$

II. Three dimensional

Need ∇^2 in spherical polar coordinates. Before that recall team class. ____?

$\boldsymbol{L} = \boldsymbol{r} \times \boldsymbol{p}$

$$\begin{vmatrix} i & j & k \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} :$$

$$\begin{aligned} L_x &= yP_z - zP_y \\ L_y &= zP_x - xP_z \\ L_z &= xP_y - yP_x \end{aligned}$$

:

Qm: replace with operators $\qquad P_\alpha = -i\hbar \frac{\partial}{\partial \alpha}$

<u>Commutation relations:</u>

$$\begin{aligned} [L_x, L_y] &= i\hbar\, L_z \\ [L_z, L_x] &= i\hbar\, L_y \\ [L_y, L_z] &= i\hbar\, L_x \end{aligned}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 \qquad [L_\alpha, L^2] = 0 \qquad \alpha = x, y,$$