Rigid Rotor (2D & 3D)

QM

CM

Quiz

TSE

↓

SE

↓

Exact problems

↓

H-atom

Linear Momentum ⟷ Angular momentum

free particle $\quad V=0 \leftarrow \quad \hat{H} = \frac{1}{2I}\hat{L}_z \cdot \hat{L}_z$

$\hat{p}_x \longleftrightarrow \hat{L}_z$

? ?

"x" $\quad$ "ϕ"

Δp_x

distance $\quad$ Angle

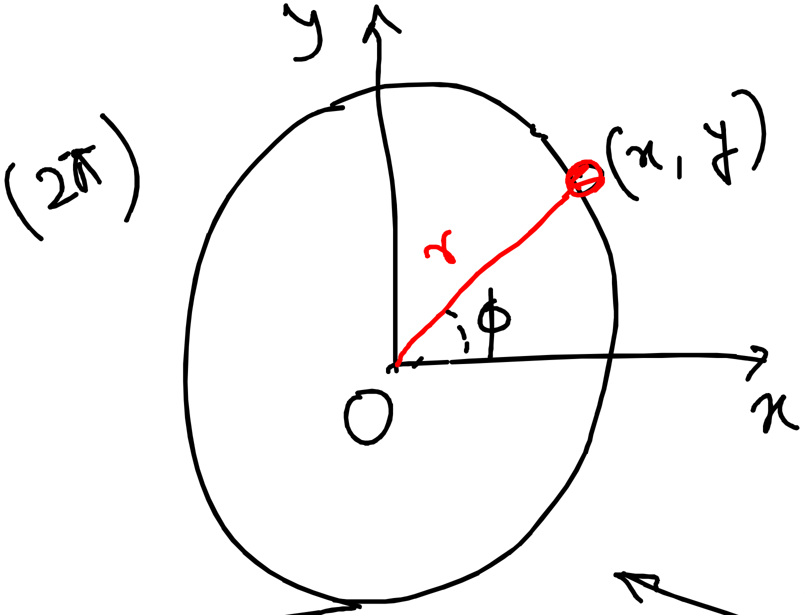
$\Delta L_z \cdot \Delta \phi$

$\hat{H}\Psi = E\Psi$

(r, ϕ)

$\Psi(\phi)$

$$\hat{H} = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2}$$



$\Psi(x, y)$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)$$

(x, y)

r is const.

$r = \sqrt{x^2 + y^2}$

$x = r\cos\phi;\ y = r\sin\phi$

xy plane

to r, ϕ plane

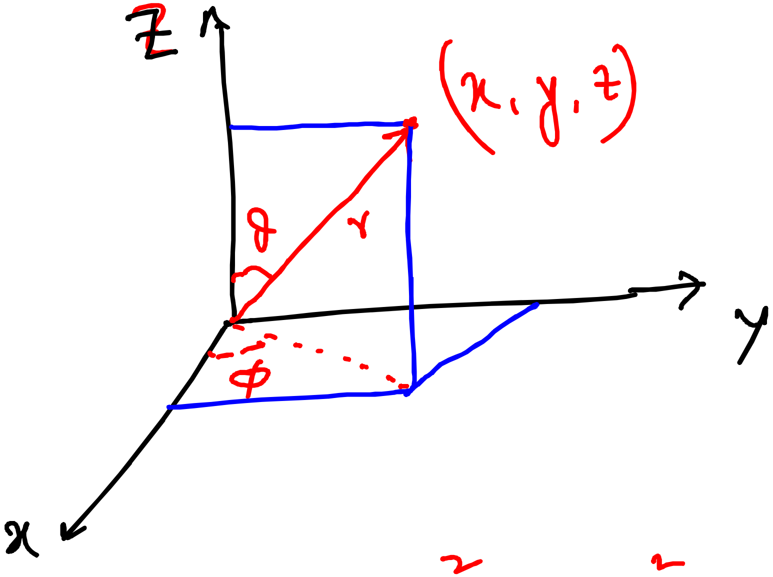
$\Psi(\phi)$

2D problem

→ 3D rotor problem

"θ" → (π)

Cartesian ⟷ Spherical



$$z = r\cos\theta$$
$$x = r\sin\theta\cdot\cos\phi$$
$$y = r\sin\theta\cdot\sin\phi$$
$$r = \sqrt{x^2+y^2+z^2}$$

Laplacian. $\nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2} = \left(\dfrac{\partial^2}{\partial r^2} + \dfrac{2}{r}\dfrac{\partial}{\partial r} + \dfrac{1}{r^2}\Lambda^2\right)$

Legendrian. $\Lambda^2 = \left(\dfrac{\partial^2}{\partial\theta^2} + \cot\theta\dfrac{\partial}{\partial\theta} + \dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\phi^2}\right)$

Volume element $\rightarrow$ $\underline{r^2\,dr\,d\theta\,\sin\theta\cdot d\phi}$

2D.

$$\hat{H} = \frac{1}{2I}\hat{L}_z^2 \qquad V = 0 \qquad \hat{H}\psi(\phi) = E\psi(\phi)$$

$$\frac{d^2\psi}{d\phi^2} = -\frac{2IE}{\hbar^2}\psi(\phi)$$

Like 1D particle (free) soln.

x

$$\psi(\phi) = A.\exp(ik\phi) + B\exp(-ik\phi)$$

where $k = \left(\frac{2IE}{\hbar^2}\right)^{1/2}$

rotating in opposite direction

Take one of them

$$\psi(\phi) = A.\exp(ik\phi)$$

$$\psi(0) = \psi(2\pi)$$

$$\int_0^{2\pi} \psi^* \cdot \psi \, d\phi = 1 \quad \& \quad \psi(0) = \psi(2\pi)$$

$$A \cdot \exp(0) = A \cdot \exp(2\pi i k)$$

$$\exp\left(2\pi i \,(\text{integer})\right) = 1$$

$$I = mr^2$$

$$\Rightarrow \frac{1}{\hbar}\sqrt{2IE} = \underline{\text{integer}} = m_l$$

$$\frac{L_z^2}{2I} \leftarrow E_{m_l} = \frac{\hbar^2 m_l^2}{2I} \qquad m = 0, \pm 1, \pm 2, \ldots$$

$$\boxed{L_z = m_l \hbar}$$

$$\psi_{m_l} = A \cdot \exp(i m_l \phi).$$

$$m_l = 0, \pm 1, \ldots, \pm m_l, \ldots$$

Degeneracy $\rightarrow \pm |m_l|$

$\Delta L_z = 0$ $\because$ $E_0 = 0$ definite & continuous values of E & L_z

$\Delta\phi \rightarrow \infty$

$\int_0^{2\pi} d\phi \, |\psi_{m_\ell}(\phi)|^2 = 1 \rightarrow A = \frac{1}{\sqrt{2\pi}}$

$\boxed{|\psi_{m_\ell}(\phi)|^2 = \frac{1}{2\pi}} \rightarrow$ no ϕ dependence

$\boxed{\hat{H}\psi_{m_\ell}(\phi) = E_{m_\ell}\psi_{m_\ell}(\phi)} \longleftrightarrow \hat{L}_z \psi_{m_\ell}(\phi) = \hbar m_\ell \psi_{m_\ell}(\phi)$

$\psi(\theta, \phi)$ $\leftarrow L_z$

3D rotor

2 quantum numbers

$$\psi(\theta, \phi) = \psi(\theta, \phi + 2\pi) = \psi(\theta + \pi, \phi)$$

$$\hat{H} = -\frac{\hbar^2}{2I} \Lambda^2$$

$$-\frac{\hbar^2}{2I} \Lambda^2 \psi(\theta, \phi) = E \psi(\theta, \phi)$$

$$\Lambda^2 \psi(\theta, \phi) = -\frac{2IE}{\hbar^2} \psi(\theta, \phi)$$

Separation of variables:

$$\psi(\theta, \phi) \equiv Y_{l m_l}(\theta, \phi) = S(\theta) . T(\phi)$$

$$S(\theta) = S(\theta + \pi) \quad \& \quad \underline{T(\phi) = T(\phi + 2\pi)}$$

$$T_{m_\ell}(\phi) = \frac{1}{\sqrt{2\pi}} \exp(i m_\ell \phi) \; ; \; m_\ell = 0, \pm 1, \pm 2, \ldots \pm \ell, \ldots$$

$$\ell = 0, 1, 2 \ldots$$

$2\ell + 1$

$$E_{m_\ell} = \frac{m_\ell^2 \hbar^2}{2I} \qquad I = mr^2$$

$$L_z = m_\ell \hbar$$

$$\Delta L_z \cdot \Delta\phi \geq \hbar/2$$

$S_{\ell m_\ell}(\theta)$ = Associated Legendre polynomials.

$$\hat{L}^2 \leftarrow \hat{L}_z^2 + \hat{L}_x^2 + \hat{L}_y^2$$

Uniform probability density independent of ϕ for $T_{m_\ell}(\phi) \rightarrow |T_{m_\ell}(\phi)|^2 = \frac{1}{2\pi}$