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Quantum Mechanics in Three Dimensions

The Schrodinger Equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi = \underbrace{\left[\frac{p^2}{2m} + V(x)\right]}_{\frac{1}{2m}(P_x^2+P_y^2+P_z^2)+V(\vec{r})}\Psi$$

$$i\hbar \frac{\partial \Psi(\vec{r},t)}{\partial t} = H\Psi(\vec{r},t) \qquad \Psi(\vec{r},t)=\psi(\vec{r})\phi(t), \quad \phi(t)=e^{-\frac{Et}{\hbar}i}$$

$$\Rightarrow H\psi(\vec{r})=E\psi(\vec{r})$$

$$\Psi(\vec{r},t)=\sum_n c_n \psi_n(\vec{r})e^{-i\frac{E_n t}{\hbar}}$$

Example: infinite potential box

$$V(x,y,z)\begin{cases}0 & 0<x,y,z<a\\ \infty & \text{otherwise}\end{cases}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right)=E\psi \qquad \text{B.C.S} \quad \psi(x,y,0)=\psi(x,y,a)=\psi(x,0,z)=\psi(x,a,z)=\psi(0,y,z)=0$$

let $\psi(x,y,z)=X(x)Y(y)Z(z)$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2X}{dx^2}=E_xX$$

$$-\frac{\hbar^2}{2m}\frac{d^2Y}{dy^2}=E_yY$$

$$-\frac{\hbar^2}{2m}\frac{d^2Z}{dz^2}=E_zZ$$

$$E_x+E_y+E_z=E$$

$$E_x=\frac{\hbar^2k_x^2}{2m} \qquad E_y=\frac{\hbar^2k_y^2}{2m} \qquad E_z=\frac{\hbar^2k_z^2}{2m}$$

$$\Rightarrow X(x)=A\cos(k_x x)+B\sin(k_x x)$$

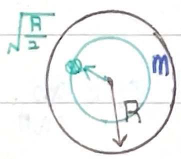
$X(0)=0 \qquad A=0$

$X(a) \qquad \rightarrow k_x a=n_x\pi$

$$\Rightarrow \psi(x,y,z)=\left(\frac{2}{a}\right)^{\frac{3}{2}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{a}\right)\sin\left(\frac{n_z\pi z}{a}\right)$$

$$E=\frac{\pi^2\hbar^2}{2ma}(n_x^2+n_y^2+n_z^2)$$

Particle on a ring



$$I=mr^2$$

$$H=-\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)}_{=\frac{\partial^2}{\partial r^2}\xrightarrow{}0+\frac{1}{r}\frac{\partial}{\partial r}\xrightarrow{}0+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}} \qquad \text{where} \quad x=r\cos\varphi,\ y=r\sin\varphi$$

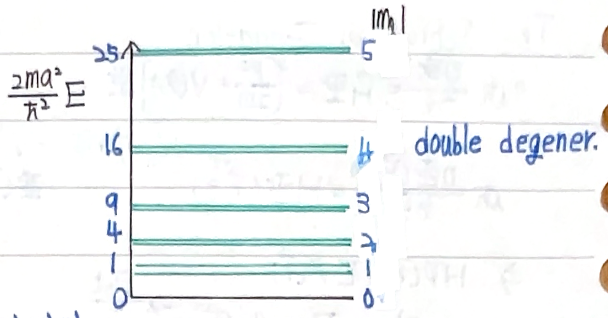
$$=-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{d^2}{d\varphi^2}=-\frac{\hbar^2}{2I}\frac{d^2}{d\varphi^2}$$

$$\Rightarrow \frac{d^2\Phi(\varphi)}{d\varphi^2}=-\frac{2EI}{\hbar^2}\Phi(\varphi)$$

$$\Rightarrow \Phi=Ae^{im_l\varphi}+Be^{im_l\phi}, \quad m_l=\sqrt{\frac{2EI}{\hbar^2}}$$

B.C.S. $\Phi(\varphi+2\pi)=\Phi(\varphi) \Rightarrow Ae^{im_l\phi}e^{2\pi im_l}+Be^{-im_l\varphi}e^{-2\pi im_l}=Ae^{im_l\varphi}+Be^{im_l\varphi}$

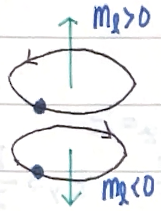
$$\Rightarrow E_{m_l} = \frac{m_l^2 \hbar^2}{2I} \quad , \quad m_l = 0, \pm 1, \pm 2, \cdots$$



classical angular momentum $I = \vec{r} \times \vec{p} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix}$

$$l_z = xP_y - yP_x = x\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) - y\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = \frac{\hbar}{i}\frac{\partial}{\partial \varphi}$$

$$l_z \Phi(m_l) = \frac{\hbar}{i}\frac{\partial}{\partial \varphi} A e^{im_l\varphi} = m_l \hbar A e^{im_l\varphi} = m_l \hbar \Phi(m_l) \qquad \text{if } B = 0$$



if $m_l > 0$, $I > 0$
if $m_l < 0$, $I < 0$

$$\int_0^{2\pi} \Phi^* \Phi \, d\varphi = |A|^2 \int_0^{2\pi} e^{-im_l\varphi} e^{im_l\varphi} d\varphi = |A|^2 \int_0^{2\pi} d\varphi = 2\pi |A|^2 \quad , \quad |A|^2 = \frac{1}{\sqrt{2\pi}}$$

$$\Rightarrow \Phi(m_l) = \frac{1}{\sqrt{2\pi}} e^{im_l\varphi} = \frac{1}{\sqrt{2\pi}} \cos(m_l\varphi + i \sin m_l\varphi)$$

$$|\Phi(m_l)|^2 = \frac{1}{2\pi}$$

1. in a state of definite angular momentum, the particle is distributed uniformly round the ring
2. E and $I \uparrow$, the number of nodes in the real and imaginary componenets $\uparrow$
3. $\Phi_{m_l}(\varphi + \pi) = (-1)^{m_l} \Phi_{m_l}(\varphi)$

at point across the diameter of the ring the w.f. differs in sign if m_l is odd
same even

$$\Phi(\varphi, t) = \frac{1}{\sqrt{2\pi}} e^{im_l\varphi} e^{-i\frac{m_l^2\hbar^2}{2I}t}$$