# Bound Problems in the real world

From the Schrödinger Equation in 3D to the angular momentum

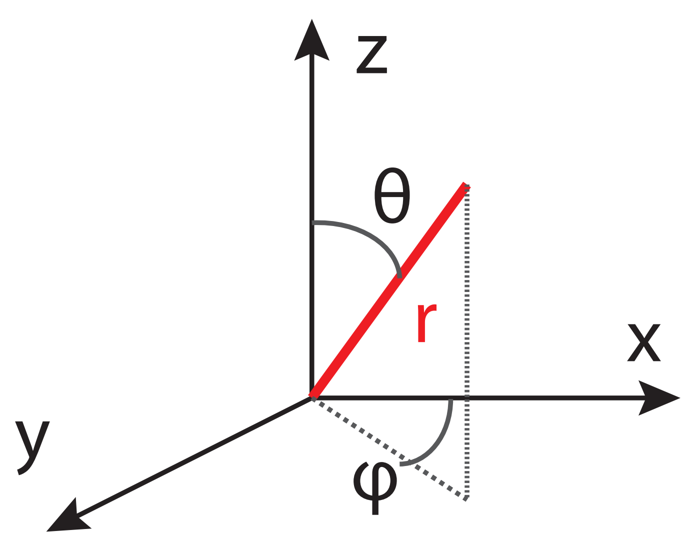
# Schrödinger Equation in 3D

- We write the time-independent Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(x,y,z)\right)\psi(x) = E\psi(x)$$

- in spherical coordinates

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\phi^2}\right]\psi(r,\theta,\phi)$$




$$= [E - V(r)]\psi(r,\theta,\phi)$$

# Schrodinger Equation in 3D

- Assumption: $$V(r, \vartheta, \varphi) = V(r)$$

- By using separation of variables, we find

1) an angular equation

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2} = -l(l+1)Y(\theta, \phi)$$

2) a radial equation

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2m\,r^2}{\hbar^2}(V - E) = l(l+1)$$

# 1) Angular Equation: Angular Momentum Operator

- Consider the classical angular momentum and the related quantum operator

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} = -i\hbar \hat{\vec{r}} \times \hat{\vec{\nabla}}$$

- In spherical coordinates we have:

$$L_x = i\hbar \left( \sin\varphi \frac{\partial}{\partial\vartheta} + \cot\vartheta \cos\varphi \frac{\partial}{\partial\varphi} \right),$$

$$\hat{L}_y = -i\hbar \left( \cos\varphi \frac{\partial}{\partial\vartheta} - \cot\vartheta \sin\varphi \frac{\partial}{\partial\varphi} \right)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial\varphi}$$

- And the magnitude of the angular momentum $|\hat{\vec{L}}|^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ is

$$\hat{L}^2 = -\hbar^2 \left[ \frac{1}{\sin\vartheta} \frac{\partial}{\partial\vartheta} \left( \sin\vartheta \frac{\partial}{\partial\vartheta} \right) + \frac{1}{\sin^2\vartheta} \frac{\partial^2}{\partial\varphi^2} \right]$$

# 1) Angular Equation

- We identify the angular equation as the eigenvalue equation for the orbital angular momentum:

$$-\hbar^2 \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial Y}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2 Y}{\partial\phi^2} \right] = \hbar^2 l(l+1) Y(\theta,\phi)$$

$$\rightarrow \quad L^2 Y = \hbar^2 l(l+1) Y(\theta,\phi)$$

- We solve the differential equation by separation of variables, $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$

$$\frac{d^2\Phi}{d\phi^2} = -m^2\Phi(\phi) \qquad \sin\theta \frac{d}{d\theta}\left( \sin\theta \frac{d\Theta}{d\theta} \right) = \left[ m^2 - l(l+1)\sin^2\theta \right] \Theta(\theta)$$

# 1) Angular Equation

- The normalized angular eigenfunctions are then Spherical Harmonic functions

$$Y_l^m(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\,P_l^m(\cos\theta)\,e^{im\phi}$$

- where $P_l^m(\cos\theta)$ are Legendre Polynomials. For example:

$$P_0^0(\cos\theta) = 1 \qquad P_0^1(\cos\theta) = \cos\theta \qquad P_0^{\pm 1}(\cos\theta) = \sin\theta$$

# Spherical Harmonics