

Bound Problems in the real world

From the Schrödinger Equation in 3D to the angular momentum

Schrödinger Equation in 3D

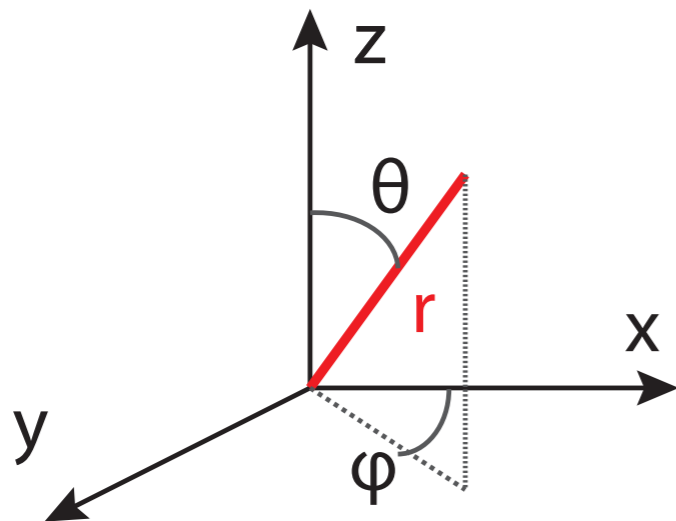
- We write the time-independent Schrödinger equation

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

- in spherical coordinates

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

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



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

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

- In spherical coordinates we have:

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

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

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

- 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:

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

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

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

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

1) Angular Equation

- The normalized angular eigenfunctions are then Spherical Harmonic functions

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

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

$$P_0^0(\cos\theta) = 1$$

$$P_0^1(\cos\theta) = \cos\theta$$

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

Spherical Harmonics

$|Y_0^0(\theta, \phi)|$



$\text{Re}(Y_0^0(\theta, \phi))$



$|Y_1^0(\theta, \phi)|$



$|Y_1^1(\theta, \phi)|$



$\text{Re}(Y_1^0(\theta, \phi))$



$\text{Re}(Y_1^1(\theta, \phi))$



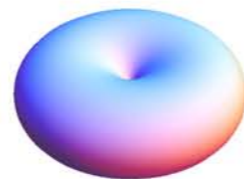
$|Y_2^0(\theta, \phi)|$



$|Y_2^1(\theta, \phi)|$



$|Y_2^2(\theta, \phi)|$



$\text{Re}(Y_2^0(\theta, \phi))$



$\text{Re}(Y_2^1(\theta, \phi))$



$\text{Re}(Y_2^2(\theta, \phi))$



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