

$$\hat{H} = -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{e^2}{4\pi\epsilon_0 r} \quad \xrightarrow{\text{Hamiltonian for H-atom}}$$

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

$[\hat{H}, \hat{p}_x] \neq 0$ (uncertainty in energy and momentum cannot be simultaneously zero)
 Do not commute
 (momentum has no precise value)

$$\hat{H} = -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \right\} - \frac{e^2}{4\pi\epsilon_0 r}$$

$$\hat{H} = \dots + \frac{\hat{A}}{r^2} - \frac{e^2}{4\pi\epsilon_0 r}$$

$$[\hat{H}, \hat{A}] = (\hat{H}\hat{A} - \hat{A}\hat{H})$$

$$\xrightarrow{(\dots) + \frac{\hat{A}}{r^2} - \frac{1}{r^2}(\dots)}$$

$$[\text{r part of } \hat{A}, \hat{A}] + [\hat{A}/r, \hat{A}] + \left[-\frac{e^2}{4\pi\epsilon_0 r}, \hat{A} \right]$$

$\hat{A} \xrightarrow{\circ} \text{represents some physical observable}$

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

$$\frac{d\bar{L}}{dt} = \frac{d\bar{r}}{dt} \times \bar{p} + \bar{r} \times \frac{dp}{dt}$$

$$\bar{L} = \hat{i} L_x + \hat{j} L_y + \hat{k} L_z$$

$$\frac{1}{m} \bar{r} \times \bar{F} = 0$$

$$\frac{d\bar{r}}{dt} = \bar{v} = \frac{\bar{p}}{m}$$

Central
field problem

Classical Mechanics

\bar{p} along the radial direction

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

Angular momentum

(perpendicular to the plane)

Circular path $\bar{L} = \bar{p} r$
 $|L| = mvr$

$$\bar{L} = \hat{i}(y p_z - z p_y) + \hat{j}(z p_x - x p_z) + \hat{k}(x p_y - y p_x)$$

$$L_x \quad L_y \quad L_z$$

$x \leftarrow \hat{x}$
 $z \leftarrow \hat{y}$

$$\bar{r} = \hat{i} x + \hat{j} y + \hat{k} z$$

$$\bar{p} = \hat{i} p_x + \hat{j} p_y + \hat{k} p_z$$

$$\bar{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

\bar{L} is conserved $\rightarrow \bar{L}$ is constant
of motion

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x}$$

$$\hat{p}_y = -i\hbar \frac{\partial}{\partial y}$$

$$\hat{p}_z = -i\hbar \frac{\partial}{\partial z}$$

Quantum Mechanics

Operator

$$\hat{L}_x = (\hat{y} \hat{p}_z - \hat{z} \hat{p}_y) = (-i\hbar) \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) = \hat{L}_x$$

$$\hat{L}_y = (-i\hbar) \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \quad \hat{L}_z = (-i\hbar) \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

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

$$[\hat{L}_x, \hat{L}_y] = ?$$

$\neq 0$

$$\hat{L}_x = (-i\hbar) \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$\hat{L}_y = (-i\hbar) \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$$

$$\hat{L}_z = (-i\hbar) \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$$

$$[\hat{L}_x, \hat{L}_y] f = (-i\hbar)^2 \left[\left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) - \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \right] f$$

($f \in C^1(x,y,z)$)

$$= (-i\hbar)^2 \left[\left\{ y \frac{\partial}{\partial z} z \frac{\partial f}{\partial x} - y \frac{\partial}{\partial z} x \frac{\partial f}{\partial z} - z \frac{\partial}{\partial y} z \frac{\partial f}{\partial x} + z \frac{\partial}{\partial y} x \frac{\partial f}{\partial z} \right\} - \left\{ z \frac{\partial}{\partial x} y \frac{\partial f}{\partial z} - z \frac{\partial}{\partial x} z \frac{\partial f}{\partial y} - x \frac{\partial}{\partial z} y \frac{\partial f}{\partial z} + x \frac{\partial}{\partial z} z \frac{\partial f}{\partial y} \right\} \right]$$

$$= (-i\hbar)^2 \left(y \frac{\partial}{\partial z} - x \frac{\partial}{\partial y} \right) f$$

$$= -(-i\hbar) (-i\hbar) \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) f$$

$$[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$$

$$\begin{aligned} & z^2 \frac{\partial^2 f}{\partial x \partial y} \\ & \uparrow \\ & z^2 \frac{\partial^2 f}{\partial x \partial z} - z \frac{\partial}{\partial x} z \frac{\partial f}{\partial y} \\ & \quad \downarrow \\ & -x \frac{\partial}{\partial z} y \frac{\partial f}{\partial z} + x \frac{\partial}{\partial z} z \frac{\partial f}{\partial y} \\ & \quad \downarrow \\ & -z y \frac{\partial^2 f}{\partial x \partial z} \\ & \quad \downarrow \\ & x y^2 \frac{\partial^2 f}{\partial z^2} \\ & \quad \downarrow \\ & -x \frac{\partial f}{\partial y} - x z \frac{\partial^2 f}{\partial z \partial y} \end{aligned}$$

$$\begin{aligned} [\hat{L}_x, \hat{L}_y] &= i\hbar \hat{L}_z \\ [\hat{L}_x, \hat{L}_z] &= -i\hbar \hat{L}_y \\ [\hat{L}_z, \hat{L}_x] &= i\hbar \hat{L}_y \end{aligned}$$

$\hat{L}_x \hat{L}_y$

$$[\hat{L}_x, \hat{L}_z] = [\hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \hat{L}_z]$$

$$= [\hat{L}_x^2, \hat{L}_z] + [\hat{L}_y^2, \hat{L}_z] + \cancel{[\hat{L}_z^2, \hat{L}_z]}$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$$

$$[A \neq B, C] = [A, C] + [B, C]$$

$$[\hat{L}_x, \hat{L}_z] = 0 \rightarrow$$

$$[\hat{L}_x, \hat{L}_x] = 0$$

$$\begin{aligned} [\hat{L}_x^2, \hat{L}_z] &= \hat{L}_x^2 \hat{L}_z - \hat{L}_z \hat{L}_x^2 \\ &= \hat{L}_x^2 \hat{L}_z - \hat{L}_x \hat{L}_y \hat{L}_x + \hat{L}_x \hat{L}_z \hat{L}_x - \hat{L}_z \hat{L}_x^2 \\ &= \underbrace{\hat{L}_x (\hat{L}_x \hat{L}_z - \hat{L}_z \hat{L}_x)}_{(-i\hbar) \hat{L}_y} + \underbrace{(\hat{L}_x \hat{L}_z - \hat{L}_z \hat{L}_x) \hat{L}_x}_{(-i\hbar) \hat{L}_y} = (-i\hbar) \{ \hat{L}_x \hat{L}_y + \hat{L}_y \hat{L}_x \} \quad \dots \textcircled{1} \\ &\quad \textcircled{1} + \textcircled{2} \end{aligned}$$

$$\begin{aligned} [\hat{L}_y^2, \hat{L}_z] &= \hat{L}_y^2 \hat{L}_z - \hat{L}_z \hat{L}_y^2 \\ &= \hat{L}_y^2 \hat{L}_z - \hat{L}_y \hat{L}_z \hat{L}_y + \hat{L}_y \hat{L}_z \hat{L}_y - \hat{L}_z \hat{L}_y^2 \\ &= \underbrace{\hat{L}_y (\hat{L}_y \hat{L}_z - \hat{L}_z \hat{L}_y)}_{i\hbar \hat{L}_x} + \underbrace{(\hat{L}_y \hat{L}_z - \hat{L}_z \hat{L}_y) \hat{L}_y}_{i\hbar \hat{L}_x} = (i\hbar) (\hat{L}_y \hat{L}_x + \hat{L}_x \hat{L}_y) \quad \dots \textcircled{2} \end{aligned}$$

$$\hat{H} = -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] \right\} - \frac{e^2}{4\pi\epsilon_0 r}$$

$\hat{L}^2 = -\hbar^2 \left(\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right)$

Operator
for the square
of the angular
momentum

$$\hat{H} = -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right\} + \frac{\hat{L}^2}{2\mu r^2} - \frac{e^2}{4\pi\epsilon_0 r}$$

K. E due
to radial
motion

$$\left. \begin{aligned} [\hat{H}, \hat{L}^2] &= 0 \\ [\hat{L}^2, \hat{L}_z] &= 0 \\ [\hat{H}, \hat{L}_z] &= 0 \end{aligned} \right\} \text{Common set of eigen functions}$$

$\hat{L}_z = -i\hbar \frac{\partial}{\partial\phi}$ (check)

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r) \underbrace{\Theta(\theta)}_{l|m|} \underbrace{\Phi(\phi)}_{-m}$$

$\gamma_{lm}(\theta, \phi) \rightarrow \text{Spherical Harmonics}$

$$\hat{L}^2 \psi_{nlm}(r, \theta, \phi) = \hat{L}^2 R_{nl}(r) Y_{lm}(\theta, \phi) = R_{nl}(r) \hat{L}^2 Y_{lm}(\theta, \phi)$$

no θ, ϕ dependence

Not difficult
to show

Recall

$$\left\{ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \left(l(l+1) - \frac{m^2}{\sin^2 \theta} \right) \right\} \Theta(\theta) = 0$$

$$\frac{d^2 \Phi}{d\phi^2} = -m^2 \Phi$$

Orbital angular momentum

$$\hat{L}^2 Y_{lm}(\theta, \phi) = \underbrace{l(l+1)}_{\text{Eigen value}} \hbar^2 Y_{lm}(\theta, \phi)$$

$\sqrt{l(l+1)} \hbar^2 \rightarrow$ length or
the magnitude
of angular momentum

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

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$[\hat{L}_z \Phi_m(\phi)] = \frac{1}{\sqrt{2\pi}} (-i\hbar) \frac{\partial}{\partial \phi} e^{im\phi}$$

$$= (-i\hbar) \frac{1}{\sqrt{2\pi}} im |e^{im\phi}|$$

$$= m\hbar \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

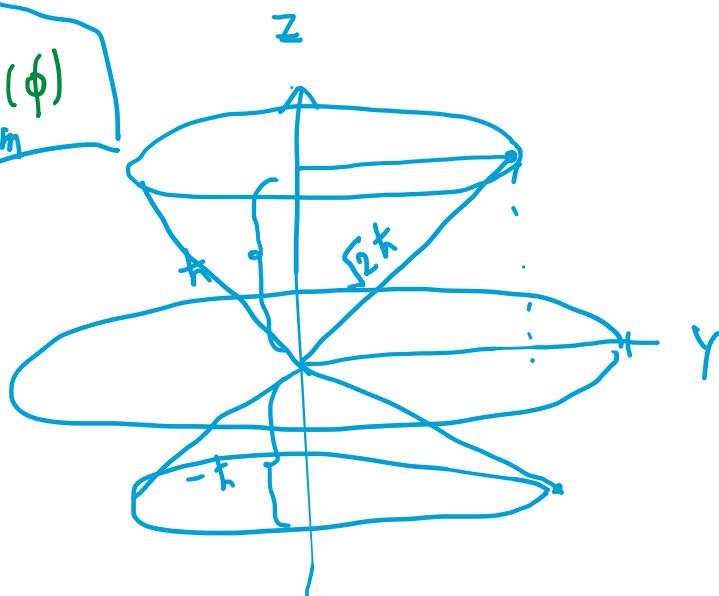
$m = 0, \pm 1, \pm 2, \dots$

$\ell = 1 (\dagger)$

$$[\hat{L}_z \Phi_m(\phi)] = m\hbar \Phi_m(\phi)$$

$$[\hat{L}_x, \hat{L}_y] \neq 0$$

$$[\hat{L}_x, \hat{L}_z] \neq 0$$



$$\sqrt{\ell(\ell+1)}\hbar = \sqrt{2}\hbar$$

$m = 0, 1, -1$

$$\begin{aligned} m\hbar &= 0 \\ &= \hbar \\ &= -\hbar \end{aligned}$$

$\ell = 2 (\dagger)$