Quantum Mechanics I

PHY 3103

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Angular Momentum

Angular momentum

In classical physics the angular momentum of a particle with momentum **p** and position **r** is defined by

$$\boxed{\mathbf{L} = \mathbf{r} \times \mathbf{p}.}$$

Hence the components of $\mathbf{L} = (L_x, L_y, L_z)$ are given by

$$\begin{aligned} L_x &= yp_z - zp_y, \\ L_y &= zp_x - xp_z, \\ L_z &= xp_y - yp_x. \end{aligned}$$

Angular momentum operator

The angular momentum operator $\hat{\mathbf{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$ can be obtained by replacing $\mathbf{r}$ and $\mathbf{p}$ by the corresponding operators in the position representation:

$$\boxed{\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned}}$$

Hermiticity of angular momentum operator

$$(\hat{L}_x)^\dagger = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y)^\dagger$$

$$= (\hat{y}\hat{p}_z)^\dagger - (\hat{z}\hat{p}_y)^\dagger$$

$$= (\hat{p}_z)^\dagger(\hat{y})^\dagger - (\hat{p}_y)^\dagger(\hat{z})^\dagger$$

$$= \hat{p}_z\hat{y} - \hat{p}_y\hat{z}$$

$$= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$

$$= \hat{L}_x$$

$$\boxed{(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger}$$

$$\boxed{\hat{L}_x^\dagger = \hat{L}_x, \qquad \hat{L}_y^\dagger = \hat{L}_y, \qquad \hat{L}_z^\dagger = \hat{L}_z.}$$

Commutation relations

$$
\begin{aligned}
[\hat{L}_x,\ \hat{L}_y] &= [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y,\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] \\
&= [\hat{y}\hat{p}_z,\ \hat{z}\hat{p}_x] - [\hat{y}\hat{p}_z,\ \hat{x}\hat{p}_z] - [\hat{z}\hat{p}_y,\ \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y,\ \hat{x}\hat{p}_z] \\
&= [\hat{y}\hat{p}_z,\ \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y,\ \hat{x}\hat{p}_z] \\
&= \hat{y}[\hat{p}_z,\ \hat{z}]\hat{p}_x + \hat{x}[\hat{z},\ \hat{p}_z]\hat{p}_y \\
&= \hat{y}(-i\hbar)\hat{p}_x + \hat{x}(i\hbar)\hat{p}_y \\
&= i\hbar(\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) \\
&= i\hbar\hat{L}_z.
\end{aligned}
$$

Commutation relations

Orbital angular momentum

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

Spin angular momentum

$$\boxed{[\hat{S}_x,\, \hat{S}_y] = i\hbar\hat{S}_z, \qquad [\hat{S}_y,\, \hat{S}_z] = i\hbar\hat{S}_x, \qquad [\hat{S}_z,\, \hat{S}_x] = i\hbar\hat{S}_y.}$$

Simultaneous eigenstates of angular momentum

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

$$\begin{aligned}
\hat{L}_x\psi_0 &= \lambda_x\psi_0 \\
\hat{L}_y\psi_0 &= \lambda_y\psi_0 \\
\hat{L}_z\psi_0 &= \lambda_z\psi_0
\end{aligned}$$

$$\begin{aligned}
i\hbar\hat{L}_z\psi_0 &= [\hat{L}_x, \hat{L}_y]\psi_0 \\
&= \hat{L}_x\hat{L}_y\psi_0 - \hat{L}_y\hat{L}_x\psi_0 \\
&= \hat{L}_x\lambda_y\psi_0 - \hat{L}_y\lambda_x\psi_0 \\
&= (\lambda_x\lambda_y - \lambda_y\lambda_x)\psi_0 \\
&= 0
\end{aligned}$$

$$\boxed{\hat{L}_x\psi_0 = \hat{L}_y\psi_0 = \hat{L}_z\psi_0 = 0.}$$

$$\boxed{\lambda_z = 0.}$$

Simultaneous eigenstates of angular momentum

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

$$\begin{aligned}
[\hat{L}_z,\, \hat{\mathbf{L}}^2] &= [\hat{L}_z,\, \hat{L}_x\hat{L}_x + \hat{L}_y\hat{L}_y + \hat{L}_z\hat{L}_z] \\
&= [\hat{L}_z,\, \hat{L}_x\hat{L}_x + \hat{L}_y\hat{L}_y] \\
&= [\hat{L}_z,\, \hat{L}_x]\hat{L}_x + \hat{L}_x[\hat{L}_z,\, \hat{L}_x] + [\hat{L}_z,\, \hat{L}_y]\hat{L}_y + \hat{L}_y[\hat{L}_z,\, \hat{L}_y] \\
&= i\hbar\hat{L}_y\hat{L}_x + i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_x\hat{L}_y - i\hbar\hat{L}_y\hat{L}_x \\
&= 0.
\end{aligned}$$

Angular momentum in spherical coordinates

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

$$y = r\sin\theta\sin\phi, \qquad \theta = \cos^{-1}\left(\frac{z}{r}\right),$$

$$z = r\cos\theta, \qquad \phi = \tan^{-1}\left(\frac{y}{x}\right).$$

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

Angular momentum in spherical coordinates

$$\begin{aligned}\frac{\partial}{\partial \phi} &= \frac{\partial x}{\partial \phi}\frac{\partial}{\partial x} + \frac{\partial y}{\partial \phi}\frac{\partial}{\partial y} + \frac{\partial z}{\partial \phi}\frac{\partial}{\partial z} \\ &= -y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y} + 0 \\ &= x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x},\end{aligned}$$

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

Angular momentum in spherical coordinates

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

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

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

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

Eigenvalues of angular momentum

$$\hat{L}_z\,\psi_{lm}(\theta,\phi) = \hbar m\,\psi_{lm}(\theta,\phi), \qquad m \in \mathbb{R}$$

$$\hat{\mathbf{L}}^2\,\psi_{lm}(\theta,\phi) = \hbar^2\,l(l+1)\,\psi_{lm}(\theta,\phi), \qquad l \in \mathbb{R}.$$

$$\begin{aligned}(\psi,\,\hat{\mathbf{L}}^2\psi) &= (\psi,\,\hat{L}_x^2\psi) + (\psi,\,\hat{L}_y^2\psi) + (\psi,\,\hat{L}_z^2\psi)\\ &= (\hat{L}_x\psi,\,\hat{L}_x\psi) + (\hat{L}_y\psi,\,\hat{L}_y\psi) + (\hat{L}_z\psi,\,\hat{L}_z\psi) \geq 0\end{aligned}$$

Eigenvalues of angular momentum

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

$$-i\hbar\frac{\partial\psi_{lm}}{\partial\phi} = \hbar m\,\psi_{lm}$$

$$\frac{\partial\psi_{lm}}{\partial\phi} = im\,\psi_{lm}$$

$$\psi_{lm}(\theta,\phi) = e^{im\phi}\,P_l^m(\theta)$$

$$\boxed{\psi_{lm}(\theta,\phi+2\pi) = \psi_{lm}(\theta,\phi).}$$

$$e^{im(\phi+2\pi)} = e^{im\phi}$$

$$e^{i2\pi m} = 1 \qquad \boxed{m\in\mathbb{Z}}$$

Eigenvalues of angular momentum

$$\hat{L}_z \, \psi_{lm}(\theta, \phi) = \hbar m \, \psi_{lm}(\theta, \phi),$$

$$\hat{\mathbf{L}}^2 \, \psi_{lm}(\theta, \phi) = \hbar^2 \, l(l+1) \, \psi_{lm}(\theta, \phi),$$

$$\boxed{l = 0,\ 1,\ 2,\ 3,\ \ldots}$$

$$\boxed{m \in \mathbb{Z}}$$

$$\boxed{-\,l \le m \le l.}$$

Eigenfunctions of angular momentum

Spherical harmonics

$$\boxed{Y_{lm}(\theta,\phi) = (-1)^m \sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\phi}, \qquad (m \geq 0).}$$

Here $P_l^m(\cos\theta)$ is the associated Legendre functions. $m < 0$, we use

$$Y_{l,m}(\theta,\phi) = (-1)^m [Y_{l,-m}(\theta,\phi)]^*.$$

$$\boxed{\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta\, \sin\theta\, Y^*_{l'm'}(\theta,\phi)\, Y_{lm}(\theta,\phi) = (Y^*_{l'm'},\, Y_{lm}) = \delta_{l'l}\,\delta_{m'm}.}$$

Eigenfunctions of angular momentum

Spherical harmonics

$$\boxed{Y_{lm}(\theta,\phi) = (-1)^m \sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l-m)!}{(l+m)!}}\, P_l^m(\cos\theta)\, e^{im\phi}, \qquad (m \geq 0).}$$

$$\boxed{\begin{aligned} \hat{L}_z Y_{lm} &= \hbar m Y_{lm}, \\ \hat{\mathbf{L}}^2 Y_{lm} &= \hbar^2 l(l+1) Y_{lm}, \end{aligned}}$$

$$\boxed{m \in \mathbb{Z}}$$

$$\boxed{l = 0,\ 1,\ 2,\ 3,\ \ldots}$$

$$\boxed{-\,l \leq m \leq l.}$$

Eigenfunctions of angular momentum

$Y_{lm}(\theta,\varphi)$	$Y_{lm}(x,y,z)$
$Y_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}}$	$Y_{00}(x,y,z) = \frac{1}{\sqrt{4\pi}}$
$Y_{10}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}}\cos\theta$	$Y_{10}(x,y,z) = \sqrt{\frac{3}{4\pi}}\frac{z}{r}$
$Y_{1,\pm1}(\theta,\varphi) = \mp\sqrt{\frac{3}{8\pi}}e^{\pm i\varphi}\sin\theta$	$Y_{1,\pm1}(x,y,z) = \mp\sqrt{\frac{3}{8\pi}}\frac{x\pm iy}{r}$
$Y_{20}(\theta,\varphi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$	$Y_{20}(x,y,z) = \sqrt{\frac{5}{16\pi}}\frac{3z^2-r^2}{r^2}$
$Y_{2,\pm1}(\theta,\varphi) = \mp\sqrt{\frac{15}{8\pi}}e^{\pm i\varphi}\sin\theta\cos\theta$	$Y_{2,\pm1}(x,y,z) = \mp\sqrt{\frac{15}{8\pi}}\frac{(x\pm iy)z}{r^2}$
$Y_{2,\pm2}(\theta,\varphi) = \sqrt{\frac{15}{32\pi}}e^{\pm 2i\varphi}\sin^2\theta$	$Y_{2,\pm2}(x,y,z) = \sqrt{\frac{15}{32\pi}}\frac{x^2-y^2\pm 2ixy}{r^2}$

Central potential

Consider a particle represented by a three-dimensional wave function $\psi(x, y, z)$ moving in a three dimensional potential V (**r**). The Schrödinger equation takes the form

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r}).}$$

We have a **central potential** if $V(\mathbf{r}) = V(r)$.

In spherical coordinates, the Laplacian is

$$\nabla^2\psi = (\nabla\cdot\nabla)\psi = \left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi.$$

The Schrödinger equation

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

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

$$\boxed{-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)\psi(\mathbf{r})+\frac{\hat{\mathbf{L}}^2}{2mr^2}\psi(\mathbf{r})+V(r)\psi(\mathbf{r})=E\psi(\mathbf{r}).}$$