Quantum Mechanics I

PHY 3103

Dr. Mohammad Abdur Rashid

Angular Momentum

Angular momentum

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

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

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

$$L_x = yp_z - zp_y,$$
$$L_y = zp_x - xp_z,$$
$$L_z = xp_y - yp_x.$$

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:

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

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

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

Hermiticity of angular momentum operator

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

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

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

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

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

Spin angular momentum

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

Simultaneous eigenstates of angular momentum

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

$$\hat{L}_x\psi_0 = \lambda_x\psi_0$$
$$\hat{L}_y\psi_0 = \lambda_y\psi_0$$
$$\hat{L}_z\psi_0 = \lambda_z\psi_0$$

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

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

$$\lambda_z = 0.$$

Simultaneous eigenstates of angular momentum

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

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

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

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

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

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

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

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

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

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

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

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

$$e^{i2\pi m} = 1$$

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

Eigenvalues of angular momentum

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

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

$$l = 0, \; 1, \; 2, \; 3, \; \ldots$$

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

$$-\, l \leq m \leq l.$$

Eigenfunctions of angular momentum

Spherical harmonics

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

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

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

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

Eigenfunctions of angular momentum

Spherical harmonics

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

$$\hat{L}_z Y_{lm} = \hbar m Y_{lm},$$

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

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

$$l = 0,\ 1,\ 2,\ 3,\ \ldots$$

$$-\,l \leq m \leq l.$$

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

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

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

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

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

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

Problems

Chapter 5
Angular Momentum

Quantum Mechanics
Nouredine Zettili

Example 5.1, 5.2

Problem 5.9, 5.11

Exercise 5.1 – 5.4

Problem 5.9

Consider a system which is initially in the state

$$\psi(\theta, \varphi) = \frac{1}{\sqrt{5}} Y_{1,-1}(\theta, \varphi) + \sqrt{\frac{3}{5}} Y_{10}(\theta, \varphi) + \frac{1}{\sqrt{5}} Y_{11}(\theta, \varphi).$$

(a) Find $\langle \psi \mid \hat{L}_+ \mid \psi \rangle$.

(b) If $\hat{L}_z$ were measured what values will one obtain and with what probabilities?

(c) If after measuring $\hat{L}_z$ we find $l_z = -\hbar$, calculate the uncertainties ΔL_x and ΔL_y and their product $\Delta L_x \Delta L_y$.

Solution

$$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y.$$

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-), \qquad \hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-);$$

$$[\hat{\vec{J}}^2, \ \hat{J}_\pm] = 0, \qquad [\hat{J}_+, \ \hat{J}_-] = 2\hbar\hat{J}_z, \qquad [\hat{J}_z, \ \hat{J}_\pm] = \pm\hbar\hat{J}_\pm.$$

$$\hat{J}_\pm \mid j, \ m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)} \mid j, \ m\pm 1\rangle$$

$$\langle j, \ m \mid \hat{J}_x \mid j, \ m\rangle = \langle j, \ m \mid \hat{J}_y \mid j, \ m\rangle = 0$$

$$\langle \hat{J}_x^2\rangle = \langle \hat{J}_y^2\rangle = \frac{1}{2}\left[\langle j, \ m \mid \hat{\vec{J}}^2 \mid j, \ m\rangle - \langle j, \ m \mid \hat{J}_z^2 \mid j, \ m\rangle\right] = \frac{\hbar^2}{2}\left[j(j+1) - m^2\right].$$

Solution

(a) Let us use a lighter notation for $|\psi\rangle$: $|\psi\rangle = \frac{1}{\sqrt{5}}|1,\ -1\rangle + \sqrt{\frac{3}{5}}|1,\ 0\rangle + \frac{1}{\sqrt{5}}|1,\ 1\rangle$. From (5.56) we can write $\hat{L}_+ | l,\ m\rangle = \hbar\sqrt{l(l+1) - m(m+1)}\,|l,\ m+1\rangle$; hence the only terms that survive in $\langle\psi | \hat{L}_+ | \psi\rangle$ are

$$\langle\psi | \hat{L}_+ | \psi\rangle = \frac{\sqrt{3}}{5}\langle 1,\ 0|\hat{L}_+ | 1,\ -1\rangle + \frac{\sqrt{3}}{5}\langle 1,\ 1|\hat{L}_+ | 1,\ 0\rangle = \frac{2\sqrt{6}}{5}\hbar, \tag{5.275}$$

since $\langle 1,\ 0|\hat{L}_+ | 1,\ -1\rangle = \langle 1,\ 1|\hat{L}_+ | 1,\ 0\rangle = \sqrt{2}\hbar$.

Solution

(b) If $\hat{L}_z$ were measured, we will find three values $l_z = -\hbar$, 0, and $\hbar$. The probability of finding the value $l_z = -\hbar$ is

$$P_{-1} = |\langle 1,\ -1 \mid \psi\rangle|^2 = \left|\frac{1}{\sqrt{5}}\langle 1,\ -1 \mid 1,\ -1\rangle + \sqrt{\frac{3}{5}}\langle 1,\ -1 \mid 1,\ 0\rangle + \frac{1}{\sqrt{5}}\langle 1,\ -1 \mid 1,\ 1\rangle\right|^2$$
$$= \frac{1}{5}, \tag{5.276}$$

since $\langle 1,\ -1 \mid 1,\ 0\rangle = \langle 1,\ -1 \mid 1,\ 1\rangle = 0$ and $\langle 1,\ -1 \mid 1,\ -1\rangle = 1$. Similarly, we can verify that the probabilities of measuring $l_z = 0$ and $\hbar$ are respectively given by

$$P_0 = |\langle 1,\ 0 \mid \psi\rangle|^2 = \left|\sqrt{\frac{3}{5}}\langle 1,\ 0 \mid 1,\ 0\rangle\right|^2 = \frac{3}{5}, \tag{5.277}$$

$$P_1 = |\langle 1,\ 1 \mid \psi\rangle|^2 = \left|\sqrt{\frac{1}{5}}\langle 1,\ 1 \mid 1,\ 1\rangle\right|^2 = \frac{1}{5}. \tag{5.278}$$

Solution

(c) After measuring $l_z = -\hbar$, the system will be in the eigenstate $|lm\rangle = |\,1,\ -1\rangle$, that is, $\psi(\theta,\ \varphi) = Y_{1,-1}(\theta,\ \varphi)$. We need first to calculate the expectation values of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_x^2$, and $\hat{L}_y^2$ using $|\,1,\ -1\rangle$. Symmetry requires that $\langle 1,\ -1 \mid \hat{L}_x \mid 1,\ -1\rangle = \langle 1,\ -1 \mid \hat{L}_y \mid 1,\ -1\rangle = 0$. The expectation values of $\hat{L}_x^2$ and $\hat{L}_y^2$ are equal, as shown in (5.60); they are given by

$$\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle = \frac{1}{2}[\langle \hat{\vec{L}}^2 \rangle - \langle \hat{L}_z^2 \rangle] = \frac{\hbar^2}{2}\left[l(l+1) - m^2\right] = \frac{\hbar^2}{2}; \tag{5.279}$$

in this relation, we have used the fact that $l = 1$ and $m = -1$. Hence

$$\Delta L_x = \sqrt{\langle \hat{L}_x^2 \rangle} = \frac{\hbar}{\sqrt{2}} = \Delta L_y, \tag{5.280}$$

and the uncertainties product $\Delta L_x \Delta L_y$ is given by

$$\Delta L_x \Delta L_y = \sqrt{\langle \hat{L}_x^2 \rangle \langle \hat{L}_y^2 \rangle} = \frac{\hbar^2}{2}. \tag{5.281}$$