5.5: Angular Momentum

The Spherical Harmonics are involved in a number of problems where **angular momentum** is important (including the Rigid Rotor problem, the H-atom problem and anything else where spherical symmetry is involved.) Angular momentum is a vector quantity that is given by the cross product of position and momentum.

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

This quantity can be calculated from the following determinant.

$$\begin{aligned}\overrightarrow{\mathbf{L}} &= \overrightarrow{\mathbf{r}} \times \overrightarrow{\mathbf{p}} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \\ &= (yp_z - zp_y)\,\mathbf{i} + (zp_x - xp_z)\,\mathbf{j} + (xp_y - yp_x)\,\mathbf{k}\end{aligned}$$

Substituting the operators for the components of linear momentum, the operators that correspond to the three components of angular momentum are

$$\begin{aligned}\widehat{L_x} &= -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \widehat{L_y} &= -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \widehat{L_z} &= -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\end{aligned}$$

These can be used to determine the square of the angular momentum, which is given by the dot product of $\overrightarrow{\mathbf{L}}$ with itself.

$$\overrightarrow{\mathbf{L}} \cdot \overrightarrow{\mathbf{L}} = L^2 = L_x^2 + L_y^2 + L_z^2$$

Similarly, the operator for the square of the angular momentum is given by

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

In spherical polar coordinates, the angular momentum operators are given by the expressions

$$\begin{aligned}\hat{L}_x &= -i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) \\ \hat{L}_y &= -i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \\ \hat{L}_z &= -i\hbar\frac{\partial^2}{\partial\phi^2}\end{aligned}$$

And the angular momentum squared operator is given by

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

For the Rigid-Rotator problem, it is interesting to note that the Hamiltonian is very closely related to the angular momentum squared operator.

$$\begin{aligned}\hat{H} &= -\frac{\hbar^2}{2\mu r^2}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \\ &= \frac{1}{2I}\hat{L}^2\end{aligned}$$

The eigenfunctions of the $\hat{L}^2$ operator are the Spherical Harmonics, $Y_l^{m_1}(\theta, \phi)$. These functions have the important properties that

$$\hat{H}Y_l^{m_l}(\theta,\phi)=\frac{\hbar^2 l(l+1)}{2\mu r^2}Y_l^{m_l}(\theta,\phi)$$
$$\hat{L}^2 Y_l^{m_l}(\theta,\phi)=\hbar^2 l(l+1)Y_l^{m_l}(\theta,\phi)$$
$$\hat{L}_z Y_l^{m_l}(\theta,\phi)=\hbar m_l Y_l^{m_l}(\theta,\phi)$$

Seeing as the spherical harmonics are eigenfunctions of all three of these operators, what is implied about the commutator of these two operators?

There are important relationships between the angular momentum operators. Each of the operators corresponding to the components of angular momentum commutes with the $\hat{L}^2$ operator, but they do not commute with one another. This implies that one can measure the squared angular momentum and only one component of angular momentum. This is generally taken as the z-axis component of angular momentum as the z-axis has special properties due to the manner in which the spherical polar coordinates have been defined.

$$\left[\hat{L}^2,\hat{L}_x\right]=\left[\hat{L}^2,\hat{L}_y\right]=\left[\hat{L}^2,\hat{L}_z\right]=0$$
$$\left[\hat{L}_x,\hat{L}_y\right]\neq 0;\left[\hat{L}_y,\hat{L}_z\right]\neq 0;\left[\hat{L}_x,\hat{L}_z\right]\neq 0$$

The commutators involving two components of angular momentum are particularly interesting. Consider the commutator between and $\hat{L}_x$ and $\hat{L}_y$.

$$\left|\hat{L}_x,\hat{L}_y\right|=\hat{L}_x\hat{L}_y-\hat{L}_y\hat{L}_x$$

Let’s define each term separately and then take the difference.

$$\begin{aligned}\hat{L}_x\hat{L}_y &=(-i\hbar)^2\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\\ &=-\hbar^2\left(y\frac{\partial}{\partial z}z\frac{\partial}{\partial x}-y\frac{\partial}{\partial z}x\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}z\frac{\partial}{\partial x}+z\frac{\partial}{\partial y}x\frac{\partial}{\partial z}\right)\end{aligned}$$

The second, third and fourth terms are easy to simplify as the derivatives do not affect the x or z variables. The first term, however, requires some application of the chain rule.

$$\hat{L}_x\hat{L}_y=-\hbar^2\left(\left\{y\frac{\partial}{\partial x}+yz\frac{\partial^2}{\partial x\partial z}\right\}-xy\frac{\partial^2}{\partial z^2}-z^2\frac{\partial^2}{\partial x\partial y}+xz\frac{\partial^2}{\partial y\partial z}\right)$$

Similarly,

$$\begin{aligned}\hat{L}_y\hat{L}_x &=(-i\hbar)^2\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\\ &=-\hbar^2\left(z\frac{\partial}{\partial x}y\frac{\partial}{\partial z}-z\frac{\partial}{\partial x}z\frac{\partial}{\partial y}-x\frac{\partial}{\partial z}y\frac{\partial}{\partial z}+x\frac{\partial}{\partial z}z\frac{\partial}{\partial y}\right)\\ &=-\hbar^2\left(zy\frac{\partial^2}{\partial x\partial z}-z^2\frac{\partial^2}{\partial x\partial y}-xy\frac{\partial^2}{\partial z^2}+\left\{x\frac{\partial}{\partial y}+xz\frac{\partial^2}{\partial z\partial y}\right\}\right)\end{aligned}$$

Taking the difference will cancel all of the second derivative terms, leaving only the first derivative terms behind.

$$\begin{aligned}\hat{L}_x\hat{L}_y-\hat{L}_y\hat{L}_x &=-\hbar^2\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\\ &=i\hbar\hat{L}_z\end{aligned}$$

Similarly, it can be shown that

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