Angular momentum in quantum mechanics

It stands to reason that, in the absence of external fields and perturbations, the result of an experiment on a physical system should not depend on the choice of coordinates. In other words, it is reasonable to assume that space itself is uniform and isotropic. In particular, the energy of a physical system should not be changed by static coordinate translations and rotations:

\[
\begin{aligned}
|\psi\rangle \rightarrow \hat{T}|\psi\rangle & \Rightarrow \langle \psi | \hat{T}^\dagger \hat{H} \hat{T} | \psi \rangle = \langle \psi | \hat{H} | \psi \rangle \\
|\psi\rangle \rightarrow \hat{R}|\psi\rangle & \Rightarrow \langle \psi | \hat{R}^\dagger \hat{H} \hat{R} | \psi \rangle = \langle \psi | \hat{H} | \psi \rangle 
\end{aligned}
\]

(1)

where \( \hat{T} \) is an operator that performs coordinate system translation and \( \hat{R} \) is a rotation operator. Because the relations above hold for any wavefunction, they must hold for the corresponding operators. Therefore, both \( \hat{T} \) and \( \hat{R} \) commute with the Hamiltonian:

\[
\begin{aligned}
\hat{T}^\dagger \hat{H} \hat{T} = \hat{H} & \Rightarrow \hat{T}^\dagger \hat{H} \hat{T} = \hat{H} \\
\hat{R}^\dagger \hat{H} \hat{R} = \hat{H} & \Rightarrow \hat{R}^\dagger \hat{H} \hat{R} = \hat{H}
\end{aligned}
\]

\[
\begin{bmatrix}
\hat{H}, \hat{T} \\
\hat{H}, \hat{R}
\end{bmatrix} = 0
\]

(2)

This leads to the conservation of the corresponding observables:

\[
\frac{d}{dt} \langle \psi | \hat{T} | \psi \rangle = \ldots = i \langle \psi | [\hat{H}, \hat{T}] | \psi \rangle = 0
\]

(3)

We will now find out what these observables are. Let us derive the operator for a positive (counter clockwise) rotation of the wavefunction (not the coordinate system) by a small angle \( \varphi \) in the XY plane:

\[
\begin{aligned}
\hat{R}(\varphi): x & \rightarrow +x \cos \varphi + y \sin \varphi \\
\hat{R}(\varphi): y & \rightarrow -x \sin \varphi + y \cos \varphi \\
\hat{R}(\varphi): z & \rightarrow z
\end{aligned}
\]

(4)

\[
\hat{R}(\varphi)|\psi(x, y, z)\rangle = |\psi(x \cos \varphi + y \sin \varphi, -x \sin \varphi + y \cos \varphi, z)\rangle
\]

Because the angle \( \varphi \) is small, we can use a Taylor expansion to second term around \( \varphi = 0 \):

\[
\hat{R}(\varphi)|\psi\rangle = \hat{R}(0)|\psi\rangle + \left[ \frac{\partial}{\partial \varphi} \hat{R}(\varphi)|\psi\rangle \right]_{\varphi=0} + O(\varphi^2)
\]

(5)

The derivative in the square brackets is computed using the chain rule:

\[
\left[ \frac{\partial}{\partial \varphi} \hat{R}(\varphi)|\psi\rangle \right]_{\varphi=0} = \left[ \frac{\partial}{\partial \varphi} \langle \psi | x \cos \varphi + y \sin \varphi, -x \sin \varphi + y \cos \varphi, z \rangle \right]_{\varphi=0} = \ldots = \left( y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right)|\psi\rangle
\]

(6)

We therefore find the following expression for the operator performing a rotation by an infinitesimal angle \( d\varphi \) around the Z axis:
\[
\hat{R}(d\varphi)|\psi\rangle = \left[1 - i\hat{L}_z d\varphi\right]|\psi\rangle \quad \hat{L}_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)
\] (7)

A similar treatment can demonstrate that small rotations in the YZ and XZ planes are performed by:

\[
\hat{L}_x = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right); \quad \hat{L}_y = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)
\] (8)

These operators are actually **angular momentum operators** – the definition of angular momentum of a point particle with a coordinate vector \(\vec{r} = (x, y, z)\) and a momentum vector \(\vec{p} = (p_x, p_y, p_z)\) given in classical mechanics is:

\[
\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix}
\hat{i} & \hat{j} & \hat{k} \\
x & y & z \\
p_x & p_y & p_z
\end{vmatrix} = \begin{pmatrix}
y p_z - z p_y \\
z p_x - x p_z \\
x p_y - y p_x
\end{pmatrix} = \begin{pmatrix}
L_x \\
L_y \\
L_z
\end{pmatrix}
\] (9)

The quantization procedure in this case amounts to replacing all quantities in this definition with the corresponding quantum mechanical operators, which are:

\[
\hat{p}_x = -i\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\frac{\partial}{\partial y}, \quad \hat{p}_z = -i\frac{\partial}{\partial z}, \quad \hat{x} = x, \quad \hat{y} = y, \quad \hat{z} = z
\] (10)

with the result that the operators corresponding to the three components of the angular momentum vector become:

\[
\hat{L}_x = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right); \quad \hat{L}_y = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right); \quad \hat{L}_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)
\] (11)

These operators make an appearance whenever a physical system has rotational dynamics or symmetry.

Two more types of angular momentum operators will be useful later. One is the **total momentum operator** – the sum of squares of \(\hat{L}_x\), \(\hat{L}_y\) and \(\hat{L}_z\):

\[
\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2
\] (12)

It corresponds to the squared norm of the total angular momentum. The other type is raising and lowering operators, defined as:

\[
\hat{L}_+ = \hat{L}_x + i\hat{L}_y \quad \hat{L}_- = \hat{L}_x - i\hat{L}_y
\] (13)

These are non-Hermitian operators that we will use for manipulating angular momentum eigenfunctions.

It is easy to demonstrate by direct inspection that the following relations also hold:

\[
\hat{L}^2 = \hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+ + \hat{L}_z^2 - \hat{L}_z; \quad \hat{L}_x = \frac{\hat{L}_+ + \hat{L}_-}{2}; \quad \hat{L}_y = \frac{\hat{L}_+ - \hat{L}_-}{2i}
\] (14)

**Commutation and uncertainty relations**

Many equations that we will encounter later in the course involve operator commutators, *i.e.* combinations of the following general form:

\[
[\hat{L}, \hat{S}] = \hat{L}\hat{S} - \hat{S}\hat{L}
\] (15)

One can prove by direct inspection from the definitions given in Equation (11) the following commutation relations between the angular momentum projection operators:
\[ [\hat{L}_X, \hat{L}_Y] = i\hat{L}_Z, \quad [\hat{L}_Y, \hat{L}_Z] = i\hat{L}_X, \quad [\hat{L}_Z, \hat{L}_X] = i\hat{L}_Y \]  

(16)

One can also show that the total momentum operator commutes with all projection operators:

\[ [\hat{L}_Z, \hat{L}_X] = 0, \quad [\hat{L}_Z, \hat{L}_Y] = 0, \quad [\hat{L}_Z, \hat{L}_Z] = 0 \]  

(17)

For commutators involving raising and lowering operators we similarly get:

\[ [\hat{L}_+, \hat{L}_-] = 0, \quad [\hat{L}_+, \hat{L}_z] = 2\hat{L}_z, \quad [\hat{L}_-, \hat{L}_z] = \pm \hat{L}_z \]  

(18)

Angular momentum eigenfunctions

Because the angular momentum operators derived above correspond to three-dimensional rotations, it is natural to seek their eigenfunctions in spherical coordinates. After the transformation from Cartesian to spherical coordinates, the total momentum operator and the Z projection operator become:

\[
\hat{L}_Z = -i \frac{\partial}{\partial \varphi}, \quad \hat{L}_Z^2 = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \right) - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2},
\]

(19)

The simultaneous diagonalization problem for these operators is analytically cumbersome and we shall simply state here that the eigenfunctions exist and are known as spherical harmonics \( Y_{lm}(\theta, \varphi) \):

\[
\begin{align*}
\hat{L}_Z Y_{lm}(\theta, \varphi) &= i(l + 1)Y_{lm}(\theta, \varphi) \\
\hat{L}_Z Y_{lm}(\theta, \varphi) &= mY_{lm}(\theta, \varphi)
\end{align*}
\]

(20)

Spherical harmonics are usually labelled with their \( \hat{L}_z \) and \( \hat{L}^2 \) eigenvalues:

\[
\begin{align*}
[\hat{L}^2 |l, m\rangle &= l(l+1)|l, m\rangle \\
[\hat{L}_z |l, m\rangle &= m|l, m\rangle
\end{align*}
\]

(21)

and only addressed in terms of their properties under the action of specific operators – the explicit trigonometric form of these functions is rarely required in practice. In the angular momentum research jargon, the \( l \) quantum number is called total momentum and \( m \) is known as projection.

Raising and lowering operators got their names because they shift the projection quantum number of a given angular momentum eigenfunction \( |l, m\rangle \) one click up or down:

\[
\hat{L}_Z \{ [\hat{L}_+ \hat{L}_-] |l, m\rangle = (\hat{L}_+ \hat{L}_- + \hat{L}_- \hat{L}_+) |l, m\rangle = (\pm \hat{L}_z + \hat{L}_x m)|l, m\rangle = (m \pm 1)(\hat{L}_z |l, m\rangle)
\]

(22)

At the same time, the \( l \) quantum number remains unchanged:

\[
\hat{L}^2 \{ \hat{L}_\pm \hat{L}_\mp |l, m\rangle = \hat{L}_\pm \hat{L}_\mp \hat{L}^2 |l, m\rangle = \hat{L}_\pm l(l+1)|l, m\rangle = l(l+1)(\hat{L}_\pm |l, m\rangle)
\]

(23)

More specifically (the coefficient may be derived from the properties of spherical harmonics):

\[
\hat{L}_\pm |l, m\rangle = \sqrt{l(l+1) - m(m \pm 1)} |l, m \pm 1\rangle
\]

(24)

It is not possible to raise or lower a state beyond the range specified in Equation (20) for the projection quantum number:

\[
\hat{L}_\pm |l, l\rangle = 0 \quad \hat{L}_\pm |l, -l\rangle = 0
\]

(25)

because the square root in Equation (24) becomes zero.