Module I, Lecture 04: Quantum Theory of Angular Momentum

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:

$$\begin{array}{lcl} |\psi\rangle \to \hat{T}|\psi\rangle & \Rightarrow & \langle\psi|\hat{T}^{\dagger}\hat{H}\hat{T}|\psi\rangle = \langle\psi|\hat{H}|\psi\rangle \\ |\psi\rangle \to \hat{R}|\psi\rangle & \Rightarrow & \langle\psi|\hat{R}^{\dagger}\hat{H}\hat{R}|\psi\rangle = \langle\psi|\hat{H}|\psi\rangle \end{array} \tag{1}$$

where $\hat{T}$ is a unitary operator that performs coordinate system translation and $\hat{R}$ is the rotation operator, which is also unitary because it preserves norms and angles. 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:

$$\begin{array}{lcl} \hat{T}^{\dagger}\hat{H}\hat{T} = \hat{H} & \Rightarrow \quad \hat{T}^{-1}\hat{H}\hat{T} = \hat{H} & \Rightarrow \quad \left[\hat{H},\hat{T}\right] = 0 \\ \hat{R}^{\dagger}\hat{H}\hat{R} = \hat{H} & \Rightarrow \quad \hat{R}^{-1}\hat{H}\hat{R} = \hat{H} & \Rightarrow \quad \left[\hat{H},\hat{R}\right] = 0 \end{array} \tag{2}$$

This leads to the conservation of the corresponding observables:

$$\begin{array}{l} \dfrac{d}{dt}\langle\psi|\hat{T}|\psi\rangle = ... = i\langle\psi|\left[\hat{H},\hat{T}\right]|\psi\rangle = 0 \\ \dfrac{d}{dt}\langle\psi|\hat{R}|\psi\rangle = ... = i\langle\psi|\left[\hat{H},\hat{R}\right]|\psi\rangle = 0 \end{array} \tag{3}$$

Emmy Noether proved in 1915 that any differentiable symmetry of a physical system leads to a conservation law for the generator of that symmetry. Differentiable symmetries are the subject of Lie group theory.

We will now find out what these observables are. Let us derive the operator performing a rotation by a small angle φ in the XY plane:

$$\begin{cases} \hat{R}(\varphi): x \to x\cos\varphi - y\sin\varphi \\ \hat{R}(\varphi): y \to x\sin\varphi + y\cos\varphi \\ \hat{R}(\varphi): z \to z \end{cases} \tag{4}$$

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

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

$$\hat{R}(\varphi)|\psi\rangle = \hat{R}(0)|\psi\rangle + \left[\frac{\partial}{\partial\varphi}\hat{R}(\varphi)|\psi\rangle\right]_{\varphi=0}\varphi + O(\varphi^2) \tag{5}$$

The derivative in brackets is computed using the composite function differentiation rule:

$$\left[\frac{\partial}{\partial\varphi}\hat{R}(\varphi)|\psi\rangle\right]_{\varphi=0} = \left[\frac{\partial}{\partial\varphi}|\psi(x\cos\varphi - y\sin\varphi, x\sin\varphi + y\cos\varphi, z)\rangle\right]_{\varphi=0} = ... = \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)|\psi\rangle \tag{6}$$

We therefore find the following expression for the operator performing a rotation by an infinitesimal angle $d\varphi$ around the Z axis:

$$\hat{R}(d\varphi)|\psi\rangle = \left[1 - i\hat{L}_Z d\varphi\right]|\psi\rangle \qquad \hat{L}_Z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{7}$$

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

$$\hat{L}_{\mathrm{X}} = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right); \quad \hat{L}_{\mathrm{Y}} = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right) \tag{8}$$

It is easy to see that these operators are *angular momentum operators* – the definition of angular momentum of a point particle with a coordinate vector $\vec{r} = \begin{pmatrix} x & y & z \end{pmatrix}$ and a momentum vector $\vec{p} = \begin{pmatrix} p_{\mathrm{X}} & p_{\mathrm{Y}} & p_{\mathrm{Z}} \end{pmatrix}$ given in classical mechanics is:

$$\vec{L} = \vec{r} \times \vec{p} = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ x & y & z \\ p_{\mathrm{X}} & p_{\mathrm{Y}} & p_{\mathrm{Z}} \end{vmatrix} = \begin{pmatrix} yp_{\mathrm{Z}} - zp_{\mathrm{Y}} \\ zp_{\mathrm{X}} - xp_{\mathrm{Z}} \\ xp_{\mathrm{Y}} - yp_{\mathrm{X}} \end{pmatrix} = \begin{pmatrix} L_{\mathrm{X}} \\ L_{\mathrm{Y}} \\ L_{\mathrm{Z}} \end{pmatrix} \tag{9}$$

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

$$\hat{p}_{\mathrm{X}} = -i\frac{\partial}{\partial x}, \quad \hat{p}_{\mathrm{Y}} = -i\frac{\partial}{\partial y}, \quad \hat{p}_{\mathrm{Z}} = -i\frac{\partial}{\partial z}, \quad \hat{x} = x, \quad \hat{y} = y, \quad \hat{z} = z \tag{10}$$

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

$$\hat{L}_{\mathrm{X}} = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right); \quad \hat{L}_{\mathrm{Y}} = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right); \quad \hat{L}_{\mathrm{Z}} = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \right) \tag{11}$$

We can instantly recognize the infinitesimal rotation operators derived above. They 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 $\hat{L}_{\mathrm{X}}$, $\hat{L}_{\mathrm{Y}}$ and $\hat{L}_{\mathrm{Z}}$:

$$\hat{L}^2 = \hat{L}_{\mathrm{X}}^2 + \hat{L}_{\mathrm{Y}}^2 + \hat{L}_{\mathrm{Z}}^2 \tag{12}$$

It corresponds to the squared norm of the total angular momentum and makes an appearance in systems that undergo rotational diffusion. The other type is raising and lowering operators, defined as:

$$\hat{L}_{+} = \hat{L}_{\mathrm{X}} + i\hat{L}_{\mathrm{Y}} \qquad \hat{L}_{-} = \hat{L}_{\mathrm{X}} - i\hat{L}_{\mathrm{Y}} \tag{13}$$

These are non-Hermitian operators that occur in the construction of the total momentum representation described below – we will use them for manipulation of angular momentum eigenfunctions. It is easy to demonstrate by direct inspection that the following relations hold:

$$\hat{L}^2 = \hat{L}_{-}\hat{L}_{+} + \hat{L}_{\mathrm{Z}}^2 + \hat{L}_{\mathrm{Z}} = \hat{L}_{+}\hat{L}_{-} + \hat{L}_{\mathrm{Z}}^2 - \hat{L}_{\mathrm{Z}}; \qquad \hat{L}_{\mathrm{X}} = \frac{\hat{L}_{+} + \hat{L}_{-}}{2}; \qquad \hat{L}_{\mathrm{Y}} = \frac{\hat{L}_{+} - \hat{L}_{-}}{2i} \tag{14}$$

We can also obtain a differential equation for the *rotation operator* itself and solve it:

$$\begin{gathered} \hat{R}_{\mathrm{Z}}(\varphi + d\varphi) = \hat{R}_{\mathrm{Z}}(d\varphi)\hat{R}_{\mathrm{Z}}(\varphi) = \left[1 - i\hat{L}_{\mathrm{Z}}d\varphi\right]\hat{R}_{\mathrm{Z}}(\varphi) \quad \Rightarrow \\ \frac{\hat{R}_{\mathrm{Z}}(\varphi + d\varphi) - \hat{R}_{\mathrm{Z}}(\varphi)}{d\varphi} = -i\hat{L}_{\mathrm{Z}}\hat{R}_{\mathrm{Z}}(\varphi) \Rightarrow \quad \frac{d\hat{R}_{\mathrm{Z}}(\varphi)}{d\varphi} = -i\hat{L}_{\mathrm{Z}}\hat{R}_{\mathrm{Z}}(\varphi) \quad \Rightarrow \quad \hat{R}_{\mathrm{Z}}(\varphi) = e^{-i\hat{L}_{\mathrm{Z}}\varphi} \end{gathered} \tag{15}$$

The result explains the “rotating frame” name that is commonly given to the interaction representation. The final conclusion is that all rotation operators around a specific axis are exponentials of the angular momentum operator along that axis.

It is important to note that the expressions for the angular momentum operators derived above as well as the conservation laws for the corresponding observables are consequences of just one initial assumption: that physical space is isotropic. These are profound results – all conservation laws stem from symmetries. In the case of infinitesimal translation, linear momentum operators and the associated conservation laws appear in a similar fashion. Time translation symmetry leads to the conservation of energy.

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:

$$[\hat{L},\hat{S}]=\hat{L}\hat{S}-\hat{S}\hat{L} \tag{16}$$

It is easy to prove by direct inspection from the definitions given in Equation (11) the following commutation relations between the angular momentum projection operators:

$$[\hat{L}_{\mathrm{X}},\hat{L}_{\mathrm{Y}}]=i\hat{L}_{\mathrm{Z}},\qquad [\hat{L}_{\mathrm{Y}},\hat{L}_{\mathrm{Z}}]=i\hat{L}_{\mathrm{X}},\qquad [\hat{L}_{\mathrm{Z}},\hat{L}_{\mathrm{X}}]=i\hat{L}_{\mathrm{Y}} \tag{17}$$

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

$$[\hat{L}^2,\hat{L}_{\mathrm{X}}]=0,\qquad [\hat{L}^2,\hat{L}_{\mathrm{Y}}]=0,\qquad [\hat{L}^2,\hat{L}_{\mathrm{Z}}]=0 \tag{18}$$

For commutators involving raising and lowering operators we similarly get:

$$[\hat{L}^2,\hat{L}_{\pm}]=0,\qquad [\hat{L}_{+},\hat{L}_{-}]=2\hat{L}_{\mathrm{Z}},\qquad [\hat{L}_{\mathrm{Z}},\hat{L}_{\pm}]=\pm\hat{L}_{\pm} \tag{19}$$

The commutation relations determine which of the corresponding observables can have a specific value simultaneously. If the uncertainty of a quantum mechanical observable corresponding to a Hermitian operator $\hat{S}$ in a given state $|\psi\rangle$ is defined as:

$$\sigma_S=\sqrt{\langle\hat{S}^2\rangle-\langle\hat{S}\rangle^2}=\sqrt{\langle\psi|\hat{S}^2|\psi\rangle-\langle\psi|\hat{S}|\psi\rangle^2} \tag{20}$$

(note the similarity to the definition of standard deviation) then the *uncertainty relation* states that:

$$\sigma_A\sigma_B\geq\frac{\hbar}{2}\left|\langle[\hat{A},\hat{B}]\rangle\right| \tag{21}$$

The proof is given in standard textbooks. The non-commutation of angular momentum projection operators in Equation (17) leads to the uncertainty relation connecting the corresponding observables. In the case of angular momentum (and in atomic units, where $\hbar=1$) we can see that:

$$[\hat{L}_{\mathrm{X}},\hat{L}_{\mathrm{Y}}]=i\hat{L}_{\mathrm{Z}}\quad\Rightarrow\quad \sigma_{L_{\mathrm{X}}}\sigma_{L_{\mathrm{Y}}}\geq\frac{\langle\psi|\hat{L}_{\mathrm{Z}}|\psi\rangle}{2} \tag{22}$$

and similarly for the other two pairs of projection operators. In practice this means that no two projections of angular momentum can have specific values simultaneously. However, because $\hat{L}^2$ does commute with the projections, it can have a specific value simultaneously with either $\hat{L}_{\mathrm{X}}$, or $\hat{L}_{\mathrm{Y}}$, or $\hat{L}_{\mathrm{Z}}$.

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:

$$\hat{L}^2 = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}, \qquad \hat{L}_Z = -i\frac{\partial}{\partial\varphi} \tag{23}$$

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* $Y_{lm}(\theta,\varphi)$:

$$\begin{cases} \hat{L}^2 Y_{lm}(\theta,\varphi) = l(l+1)Y_{lm}(\theta,\varphi) \\ \hat{L}_Z Y_{lm}(\theta,\varphi) = m Y_{lm}(\theta,\varphi) \end{cases} \qquad l \in \mathbb{N},\ m = -l, -l+1, \ldots, l \tag{24}$$

Their exact definition may be given in terms of spherical Legendre polynomials:

$$\begin{gathered} Y_{lm}(\theta,\varphi) = (-1)^{\frac{m+|m|}{2}} \left(\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right)^{1/2} P_l^m(\cos\theta)e^{im\varphi} \\ P_l^m(x) = (1-x^2)^{|m|/2}\frac{d^{|m|}}{dx^{|m|}}P_l(x) \qquad P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}\left[(x^2-1)^l\right] \end{gathered} \tag{25}$$

After normalization, spherical harmonics are usually labelled with their $\hat{L}_Z$ and $\hat{L}^2$ eigenvalues:

$$Y_{lm}(\theta,\varphi) \xrightarrow{\ \|\ \|\ } |l,m\rangle \qquad \Leftrightarrow \qquad \begin{cases} \hat{L}^2|l,m\rangle = l(l+1)|l,m\rangle \\ \hat{L}_Z|l,m\rangle = m|l,m\rangle \end{cases} \tag{26}$$

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 notch up or down. This is easy to prove:

$$\hat{L}_Z\left(\hat{L}_\pm|l,m\rangle\right) = \left([\hat{L}_Z,\hat{L}_\pm] + \hat{L}_\pm\hat{L}_Z\right)|l,m\rangle = \left(\pm\hat{L}_\pm + \hat{L}_\pm m\right)|l,m\rangle = (m\pm1)\left(\hat{L}_\pm|l,m\rangle\right) \tag{27}$$

It is also easy to show that the l quantum number remains unchanged:

$$\hat{L}^2\left(\hat{L}_\pm|l,m\rangle\right) = \hat{L}_\pm\hat{L}^2|l,m\rangle = \hat{L}_\pm l(l+1)|l,m\rangle = l(l+1)\left(\hat{L}_\pm|l,m\rangle\right) \tag{28}$$

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

$$\hat{L}_\pm|l,m\rangle = \sqrt{l(l+1)-m(m\pm1)}\,|l,m\pm1\rangle \tag{29}$$

Importantly, it is not possible to raise or lower a state beyond the range specified in Equation (24) for the projection quantum number:

$$\hat{L}_+|l,l\rangle = 0 \qquad \hat{L}_-|l,-l\rangle = 0 \tag{30}$$

because the square root in Equation (29) turns into zero.