

I. Angular momentum

Up to this point, we have been dealing primarily with one dimensional systems. In practice, of course, most of the systems we deal with live in three dimensions and 1D quantum mechanics is at best a useful *model*. In this section, we will focus in particular on the quantum mechanics of 3D systems. Many of the elements we discovered for one dimensional problems will carry over directly to higher dimensions; however, we will encounter certain effects that are qualitatively new, and we will spend most of our time exploring these new phenomena.

The first change comes in how we associate operators with classical observables. In one dimension, we had

$$x \rightarrow \hat{x} \quad p \rightarrow \hat{p} = -i \frac{\partial}{\partial x}$$

In three dimensions the position and momentum are vectors and so we must substitute vector calculus for the single variable results:

$$\mathbf{r} \rightarrow \hat{\mathbf{r}} \quad \mathbf{p} \rightarrow \hat{\mathbf{p}} = -i\hbar \nabla \equiv -i\hbar \left(\mathbf{i} \frac{\partial}{\partial x} + \mathbf{j} \frac{\partial}{\partial y} + \mathbf{k} \frac{\partial}{\partial z} \right)$$

Where \mathbf{r} is the position vector and vector quantities will always be indicated in **bold face**. Note that the operators \hat{x}, \hat{y} and \hat{z} commute with one another.

a. Rotations

The first difference between 3D and 1D is the possibility of performing a rotation of our system about one of the three axes. Let us denote a rotation of an angle θ about a unit vector \mathbf{n} by $\mathbf{R}_{\mathbf{n}}(\theta)$. Clearly, $\mathbf{R}_{\mathbf{n}}(\theta)$ is a matrix (it transforms vectors to vectors). Further, it is clear that $\mathbf{R}_{\mathbf{n}}(\theta)\mathbf{R}_{\mathbf{m}}(\theta) \neq \mathbf{R}_{\mathbf{m}}(\theta)\mathbf{R}_{\mathbf{n}}(\theta)$ (rotations about different axes do not commute). Note that this has nothing to do with quantum mechanics and everything to do with geometry!

It is easy to verify that the rotation operators associated with the three Cartesian axes are:

$$\mathbf{R}_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix}$$

$$\mathbf{R}_y(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix}$$

$$\mathbf{R}_z(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Note that the relations for x and y can be obtained from the z result by cyclic permutations (i.e. $\mathbf{x} \rightarrow \mathbf{y}, \mathbf{y} \rightarrow \mathbf{z}, \mathbf{z} \rightarrow \mathbf{x}$). This **must always** be the case, because our labeling of the x,y and z axes is totally arbitrary! The only thing we must be careful of is that the “triple product” $\mathbf{z} \cdot (\mathbf{x} \times \mathbf{y})$ is always +1. This defines the handedness, or chirality, of our coordinates. Cyclic permutations preserve the handedness while a simple interchange of two axes (i.e. $\mathbf{x} \leftrightarrow \mathbf{y}$) will flip the sign of the triple product, reverse the handedness of our coordinates and give us the wrong answer (try it and see). This cyclic invariance is very important because it reduces the work we need to do by a factor of 3, but we must be careful to apply it correctly. In the future, we can therefore state the result for the z axis and then infer the results for x and y by cyclic permutations.

These rotations are unitary (i.e. $\mathbf{R}^T \mathbf{R} = \mathbf{1}$) and like many unitary transformations they can be written in the form $e^{-i\theta J / \hbar}$ where J is called a *generator*. For example, the generator of rotations about the z axis is

$$J_z = \hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

This can be verified by actually computing $e^{i\theta J_z / \hbar}$ and checking that it gives the rotation operator discussed earlier.

b. Commutation Relations

We now wish to compute the commutator between J_x and J_y :

$$J_x J_y = \hbar^2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} = \hbar^2 \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$-J_y J_x = -\hbar^2 \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} = \hbar^2 \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\boxed{\Rightarrow [J_x, J_y] = i\hbar J_z}$$

As discussed previously, all other commutators between the elementary generators of rotations can be deduced from the above relation by cyclic permutations of the indices. These are the **fundamental** commutation relations for angular momentum. In fact, they are so fundamental that we will use them to **define** angular momentum: any three transformations that obey these commutation relations will be associated with some form of angular momentum.

It is also useful to define the vector $\mathbf{J} \equiv J_x \mathbf{i} + J_y \mathbf{j} + J_z \mathbf{k}$ and the scalar $\mathbf{J}^2 = \mathbf{J} \cdot \mathbf{J} = J_x^2 + J_y^2 + J_z^2$. It is easy to show that while the elementary generators **do not** commute with \mathbf{J} they do commute with \mathbf{J}^2 :

$$[J_z, \mathbf{J}^2] = [J_z, J_x^2] + [J_z, J_y^2] = [J_z, J_x]J_x + J_x [J_z, J_x] + [J_z, J_y]J_y + J_y [J_z, J_y]$$

$$= (-i\hbar J_y)J_x + J_x(-i\hbar J_y) + (i\hbar J_x)J_y + J_y(i\hbar J_x)$$

$$= 0$$

Note that these \mathbf{J} matrices are **not quantum operators** – they are simply transformations of 3D space.

However, we can use this as a definition of angular momentum in the quantum case. Specifically, we assume that the quantum operators (which act in Hilbert space) obey the same commutation rules as the classical transformations (which act in real space). Hence, quantum angular momentum operators obey $[\hat{J}_x, \hat{J}_y] = i\hbar \hat{J}_z$ and cyclic permutations thereof. This seems strange at first, but momentarily

we will show that this rule for associating operators with classical variables is *consistent* with our definitions of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$, which strongly supports the new quantization rule. Further, we will later see that the same commutation rules apply to a particle's intrinsic spin angular momentum, which cannot be described as some function of $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$. Hence the commutation relation above actually *generalizes* the standard quantization rules.

Classically, angular momentum is given by $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$. Using our standard prescription, this means the corresponding quantum operator should be $\hat{\mathbf{L}} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$. We proceed to verify that the components of $\hat{\mathbf{L}}$ obey the expected commutation relations.

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

c. Eigenstates

Since $\hat{\mathbf{J}}^2$ and \hat{J}_z commute, they share common eigenstates. We will denote the eigenvalues of $\hat{\mathbf{J}}^2$ and \hat{J}_z by α and β , respectively so that:

$$\hat{\mathbf{J}}^2|\alpha, \beta\rangle = \alpha|\alpha, \beta\rangle \quad \hat{J}_z|\alpha, \beta\rangle = \beta|\alpha, \beta\rangle$$

It is convenient to define the raising and lowering operators (note the similarity to the Harmonic oscillator!):

$$\hat{J}_{\pm} \equiv \hat{J}_x \pm i\hat{J}_y$$

Which satisfy the commutation relations:

$$[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z \quad [\hat{J}_z, \hat{J}_{\pm}] = \pm\hbar\hat{J}_{\pm} \quad [\hat{J}_{\pm}, \hat{\mathbf{J}}^2] = 0$$

The raising and lowering operators have a peculiar effect on the eigenvalue of \hat{J}_z :

$$\hat{J}_z(\hat{J}_{\pm}|\alpha, \beta\rangle) = ([\hat{J}_z, \hat{J}_{\pm}] + \hat{J}_{\pm}\hat{J}_z)|\alpha, \beta\rangle = (\beta \pm \hbar)(\hat{J}_{\pm}|\alpha, \beta\rangle)$$

Thus, \hat{J}_+ (\hat{J}_-) raises (lowers) the eigenvalue of \hat{J}_z by \hbar , hence the names. Since the raising and lowering operators commute with $\hat{\mathbf{J}}^2$ they do not change the value of α and so we can write

$$\hat{J}_\pm |\alpha, \beta\rangle \propto |\alpha, \beta \pm \hbar\rangle$$

and so the eigenvalues of \hat{J}_z are evenly spaced.

What are the limits on this ladder of eigenvalues? Recall that for the harmonic oscillator, we found that there was a minimum eigenvalue and the eigenstates could be created by successive applications of the raising operator to the lowest state. There is also a minimum eigenvalue in this case. To see this, note that:

$$\begin{aligned} (\alpha - \beta^2) \langle \alpha, \beta | \hat{\mathbf{J}}^2 - \hat{J}_z^2 | \alpha, \beta \rangle &= \frac{1}{2} \langle \alpha, \beta | (\hat{J}_+ \hat{J}_- + \hat{J}_- \hat{J}_+) | \alpha, \beta \rangle \\ &= \frac{1}{2} \langle \alpha, \beta | (\hat{J}_+ \hat{J}_+^\dagger + \hat{J}_+^\dagger \hat{J}_+) | \alpha, \beta \rangle \\ &= \frac{1}{2} \left(\langle \alpha, \beta | \hat{J}_+ | \alpha, \beta \rangle \right)^2 + \frac{1}{2} \left(\langle \alpha, \beta | \hat{J}_+ | \alpha, \beta \rangle \right)^2 \geq 0 \end{aligned}$$

Hence $\beta^2 \leq \alpha$ and therefore $-\sqrt{\alpha} \leq \beta \leq \sqrt{\alpha}$. Which means that there are both *maximum* and *minimum* values that β can take on for a given α . If we denote these values by β_{\max} and β_{\min} , respectively, then it is clear that

$$\hat{J}_+ |\alpha, \beta_{\max}\rangle = 0 \quad \hat{J}_- |\alpha, \beta_{\min}\rangle = 0.$$

We can then use this knowledge and a trick to determine the relationship between α and β_{\max} (or β_{\min}):

$$\begin{aligned} &\Rightarrow \hat{J}_- \hat{J}_+ |\alpha, \beta_{\max}\rangle = 0 \quad \hat{J}_+ \hat{J}_- |\alpha, \beta_{\min}\rangle = 0 \\ \Rightarrow \left(\hat{J}_x^2 + \hat{J}_y^2 - i(\hat{J}_y \hat{J}_x - \hat{J}_x \hat{J}_y) \right) |\alpha, \beta_{\max}\rangle &= 0 \quad \left(\hat{J}_x^2 + \hat{J}_y^2 + i(\hat{J}_y \hat{J}_x - \hat{J}_x \hat{J}_y) \right) |\alpha, \beta_{\min}\rangle = 0 \\ \Rightarrow \left(\hat{\mathbf{J}}^2 - \hat{J}_z^2 - \hbar \hat{J}_z \right) |\alpha, \beta_{\max}\rangle &= 0 \quad \left(\hat{\mathbf{J}}^2 - \hat{J}_z^2 + \hbar \hat{J}_z \right) |\alpha, \beta_{\min}\rangle = 0 \\ \Rightarrow \left(\alpha - \beta_{\max}^2 - \hbar \beta_{\max} \right) &= 0 \quad \left(\alpha - \beta_{\min}^2 + \hbar \beta_{\min} \right) = 0 \\ \Rightarrow \alpha &= \beta_{\max} (\beta_{\max} + \hbar) = \beta_{\min} (\beta_{\min} - \hbar) \\ \Rightarrow \beta_{\max} &= -\beta_{\min} \equiv \hbar j \end{aligned}$$

So we have that $-\hbar j \leq \beta \leq \hbar j$. Further, since we can get from the lowest to the highest eigenvalue in increments of \hbar by successive applications of the raising operator, it is clear that the difference

between the highest and lowest values $[\hbar j - (-\hbar j) = 2\hbar j]$ must be an integer multiple of \hbar . Thus, j itself must either be an integer or a half-integer.

Putting all these facts together, we conclude (Define $m \equiv b/\hbar$):

and

$\hat{\mathbf{J}}^2 j, m\rangle = \hbar^2 j(j+1) j, m\rangle \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots$
$\hat{J}_z j, m\rangle = m\hbar j, m\rangle \quad m = -j, -j+1, \dots, j-1, j$

where in the first equation, we have noted that $0 \leq \langle \hat{\mathbf{J}}^2 \rangle = \hbar^2 j(j+1)$ implies $j \geq 0$. These are the fundamental eigenvalue equations for all forms of angular momentum.

The other matrix elements we might be interested in are those of the raising and lowering operators. As we saw before $\hat{J}_\pm |j, m\rangle \propto |j, m \pm 1\rangle$ and so

$$\langle j', m' | \hat{J}_\pm |j, m\rangle = C_{j,m}^\pm \delta_{j,j} \delta_{m,m \pm 1}$$

and one only needs to determine the value of $C_{j,m}^\pm$. To this end,

$$\begin{aligned} |\hat{J}_\pm |j, m\rangle|^2 &= \langle j, m | \hat{J}_\pm^\dagger \hat{J}_\pm |j, m\rangle = \langle j, m | \hat{J}_\mp \hat{J}_\pm |j, m\rangle = \langle j, m | \hat{\mathbf{J}}^2 - \hat{J}_z^2 \mp \hbar \hat{J}_z |j, m\rangle \\ &= \hbar^2 [j(j+1) - m^2 \mp m] = |C_{j,m}^\pm|^2 \end{aligned}$$

the phase of $C_{j,m}^\pm$ is undetermined, because the phase of the eigenstate $|j, m\rangle$ is arbitrary. We will choose the phase of $|j, m\rangle$ so that $C_{j,m}^\pm$ is real and positive which leads to:

$\langle j', m' \hat{J}_\pm j, m\rangle = \hbar \sqrt{j(j+1) - m(m \mp 1)} \delta_{j,j} \delta_{m,m \pm 1}.$
