19.3 Multiplets of Angular Momentum

In our first encounter with angular momentum in chapter 10, we learned that there are angular wave functions $Y_{\ell m}(\theta, \phi)$, called spherical harmonics, that are eigenfunctions of the differential operators $\hat{L}_z$ and $\hat{\mathbf{L}}^2$ (see (10.5.32)):

$$\begin{aligned} \hat{\mathbf{L}}^2\, Y_{\ell m} &= \hbar^2\, \ell(\ell+1)\, Y_{\ell m}, \quad \ell=0,1,\ldots \\ \hat{L}_z\, Y_{\ell m} &= \hbar m\, Y_{\ell m}, \qquad\qquad m=-\ell,\ldots,\ell. \end{aligned} \tag{19.3.1}$$

For any fixed integer value of ℓ, there are $2\ell + 1$ spherical harmonics, as the index m quantifying the z-component of angular momentum varies from $-\ell$ to ℓ in integer steps. These wave functions can be thought of as eigenstates of the operators $\hat{L}_z$ and $\hat{\mathbf{L}}^2$. They form a *multiplet*, a collection of $2\ell + 1$ states that have a common value of $\hat{\mathbf{L}}^2$.

In fact, the theory of spin one-half angular momentum supplies two basis states $|\pm\rangle$ that also form a multiplet. For this recall that

$$\hat{S}_z|\pm\rangle = \pm\tfrac{\hbar}{2}|\pm\rangle, \tag{19.3.2}$$

suggesting that the states correspond to $m=\pm\frac{1}{2}$ in the notation we used for orbital angular momentum. But how about the $\hat{\mathbf{S}}^2$ eigenvalue? Recalling that $\hat{S}_i=\frac{\hbar}{2}\sigma_i$, with σ_i the Pauli matrices, we see that

$$\hat{\mathbf{S}}^2 = \hat{S}_1^2+\hat{S}_2^2+\hat{S}_3^2 = \tfrac{1}{4}\hbar^2(\sigma_1^2+\sigma_2^2+\sigma_3^2). \tag{19.3.3}$$

Since all Pauli matrices square to the 2×2 identity matrix, we have

$$\hat{\mathbf{S}}^2 = \tfrac{3}{4}\hbar^2\mathbb{1}. \tag{19.3.4}$$

It follows that acting on the $|\pm\rangle$ states and writing $\frac{3}{4}=\frac{1}{2}\frac{3}{2}$ we get

$$\begin{aligned} \hat{\mathbf{S}}^2|\pm\rangle &= \hbar^2\tfrac{1}{2}\tfrac{3}{2}|\pm\rangle, \\ \hat{S}_z|\pm\rangle &= \pm\tfrac{\hbar}{2}|\pm\rangle, \end{aligned} \tag{19.3.5}$$

where we copied (19.3.2) on the second line. In analogy to (19.3.1), for spin operators and associated states $|s, m_s\rangle$ we write

$$\begin{aligned} \hat{\mathbf{S}}^2\,|s,m_s\rangle &= \hbar^2\, s(s+1)\,|s,m_s\rangle, \\ \hat{S}_z\,|s,m_s\rangle &= \hbar m_s\,|s,m_s\rangle. \end{aligned} \tag{19.3.6}$$

Comparing with (19.3.5), we see that the states $|\pm\rangle$ correspond to $s=\frac{1}{2}$. Moreover, we deduce that $m_s=\pm\frac{1}{2}$ and identify

$$|\pm\rangle = |s=\tfrac{1}{2}, m_s=\pm\tfrac{1}{2}\rangle. \tag{19.3.7}$$

In fact, the rule we had for orbital multiplets seems to hold here as well: $m_s = -s, \ldots, s$ in integer steps. In this example, $s=\frac{1}{2}$, and there are two states. Note that orbital angular momentum does not allow ℓ to be equal to $\frac{1}{2}$. We do not have spherical harmonics corresponding to fractional values of ℓ. It is perhaps not too surprising that orbital angular momentum and spin angular momentum can have different kinds of eigenstates. After all, the orbital operators are built from position and momenta, while spin operators cannot be built this way.

A general understanding of angular momentum requires learning what multiplets are *allowed*. For this we want to use only the algebra of angular momentum so the results will apply to orbital angular momentum, spin one-half angular momentum, and any other angular momentum that may exist. In order to speak generally of angular momentum operators, we do not call them $\hat{L}_i$ or $\hat{S}_i$ but rather use the new symbol $\hat{J}_i$, with $i = 1, 2, 3$. The operator-valued vector is denoted as $\hat{\mathbf{J}}$.

Any triplet of *Hermitian* operators $\hat{\mathbf{J}} = (\hat{J}_1, \hat{J}_2, \hat{J}_3) = (\hat{J}_x, \hat{J}_y, \hat{J}_z)$ is said to satisfy the algebra of angular momentum if the following commutation relations hold:

$$\boxed{\text{Algebra of angular momentum:} \quad [\hat{J}_i, \hat{J}_j] = i\hbar\,\epsilon_{ijk}\hat{J}_k.} \tag{19.3.8}$$

All the properties of the $\hat{L}_i$ operators derived earlier using only the algebra of angular momentum clearly hold for $\hat{J}_i$ operators, which satisfy the same algebra. Thus, on account of (19.2.14) we have

$$[\hat{J}_i, \hat{\mathbf{J}}^2\,] = 0. \tag{19.3.9}$$

It is useful to begin our work by considering an alternative rewriting of the algebra of angular momentum.

Rewriting the algebra of angular momentum Recall that in the harmonic oscillator the Hermitian operators $\hat{x}$ and $\hat{p}$ could be traded for the non-Hermitian operators $\hat{a}$ and $\hat{a}^\dagger$ that are in fact Hermitian conjugates of each other. We do something analogous here. We will define two non-Hermitian operators $\hat{J}_\pm$ starting from the Hermitian operators $\hat{J}_x$ and $\hat{J}_y$:

$$\begin{aligned} \hat{J}_+ &\equiv \hat{J}_x + i\hat{J}_y, \\ \hat{J}_- &\equiv \hat{J}_x - i\hat{J}_y. \end{aligned} \tag{19.3.10}$$

The two operators are Hermitian conjugates of each other:

$$(\hat{J}_+)^\dagger = \hat{J}_-. \tag{19.3.11}$$

Note that both $\hat{J}_x$ and $\hat{J}_y$ can be solved for in terms of $\hat{J}_+$ and $\hat{J}_-$. We can now compute the algebra of the operators $\hat{J}_+$, $\hat{J}_-$, and $\hat{J}_z$. This is, again, the algebra of angular momentum, in terms of redefined operators. We begin by computing the product $\hat{J}_+\hat{J}_-$:

$$\hat{J}_+\hat{J}_- = \hat{J}_x^2 + \hat{J}_y^2 - i[\hat{J}_x, \hat{J}_y] = \hat{J}_x^2 + \hat{J}_y^2 + \hbar\hat{J}_z. \tag{19.3.12}$$

Together with the product in the opposite order, we have

$$\begin{aligned} \hat{J}_+\hat{J}_- &= \hat{J}_x^2 + \hat{J}_y^2 + \hbar\hat{J}_z, \\ \hat{J}_-\hat{J}_+ &= \hat{J}_x^2 + \hat{J}_y^2 - \hbar\hat{J}_z, \end{aligned} \tag{19.3.13}$$

which can be summarized as

$$\hat{J}_\pm\hat{J}_\mp = \hat{J}_x^2 + \hat{J}_y^2 \pm \hbar\hat{J}_z. \tag{19.3.14}$$

From (19.3.13) we can quickly get the commutator:

$$[\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z. \tag{19.3.15}$$

We also compute the commutator of $\hat{J}_\pm$ with $\hat{J}_z$:

$$[\hat{J}_z, \hat{J}_+] = [\hat{J}_z, \hat{J}_x] + i[\hat{J}_z, \hat{J}_y] = i\hbar\hat{J}_y + i(-i\hbar\hat{J}_x) = \hbar(\hat{J}_x + i\hat{J}_y) = \hbar\hat{J}_+. \tag{19.3.16}$$

Similarly, $[\hat{J}_z, \hat{J}_-] = -\hbar\hat{J}_-$, and therefore, all in all,

$$[\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm. \tag{19.3.17}$$

This is similar to our harmonic oscillator commutators $[\hat{N}, \hat{a}^\dagger] = \hat{a}^\dagger$ and $[N, \hat{a}] = -\hat{a}$, if we identify $\hat{N}$ with $\hat{J}_z$, $\hat{a}^\dagger$ with $\hat{J}_+$, and $\hat{a}$ with $\hat{J}_-$. For the oscillator they taught us that, acting on states, $\hat{a}^\dagger$ raises the $\hat{N}$ eigenvalue by one unit, while $\hat{a}$ decreases it by one unit. As we will see, $\hat{J}_+$ adds $\hbar$ to the $\hat{J}_z$ eigenvalue, and $\hat{J}_-$ subtracts $\hbar$ from the $\hat{J}_z$ eigenvalue. We collect our results to emphasize that we can take the algebra of angular momentum to be the following:

$$\boxed{\text{Algebra of angular momentum:} \quad [\hat{J}_+, \hat{J}_-] = 2\hbar\hat{J}_z, \quad [\hat{J}_z, \hat{J}_\pm] = \pm\hbar\hat{J}_\pm.} \tag{19.3.18}$$

If one views the above as *the* definition of the algebra of angular momentum, one must also state that $(\hat{J}_\pm)^\dagger = \hat{J}_\mp$ and that $\hat{J}_z$ is Hermitian. You can then convince yourself that defining $\hat{J}_x$ and $\hat{J}_y$, consistent with (19.3.10), is as follows:

$$\hat{J}_x = \tfrac{1}{2}(\hat{J}_+ + \hat{J}_-), \quad \hat{J}_y = \tfrac{1}{2i}(\hat{J}_+ - \hat{J}_-) \tag{19.3.19}$$

results in Hermitian $\hat{J}_x$ and $\hat{J}_y$. These operators, together with $\hat{J}_z$, satisfy the original angular momentum algebra (19.3.8) on account of (19.3.18).

We also write $\hat{\mathbf{J}}^2$ in a nice way beginning from (19.3.13), which gives two expressions for $\hat{J}_x^2 + \hat{J}_y^2$:

$$\hat{J}_x^2 + \hat{J}_y^2 = \hat{J}_+\hat{J}_- - \hbar\hat{J}_z = \hat{J}_-\hat{J}_+ + \hbar\hat{J}_z. \tag{19.3.20}$$

Adding $\hat{J}_z^2$ to both sides of the equation, we find that

$$\boxed{\hat{\mathbf{J}}^2 = \hat{J}_+\hat{J}_- + \hat{J}_z^2 - \hbar\hat{J}_z = \hat{J}_-\hat{J}_+ + \hat{J}_z^2 + \hbar\hat{J}_z.} \tag{19.3.21}$$

Of course, since $\hat{J}_i$ and $\hat{\mathbf{J}}^2$ commute,

$$[\hat{J}_\pm, \hat{\mathbf{J}}^2] = 0. \tag{19.3.22}$$

Multiplets of angular momentum Our analysis will only use the algebra of the operators $\hat{J}_i$ and their Hermiticity to discuss the allowed angular momentum multiplets. Since $\hat{\mathbf{J}}^2$ and $\hat{J}_z$ are Hermitian and commute, they can be simultaneously diagonalized. In fact, there are no more operators in the angular momentum algebra that can be added to this list of simultaneously diagonalizable operators. Our work in section 15.7 shows that the common eigenstates form an orthonormal basis for the vector space the operators act on. We thus introduce eigenstates $|j, m\rangle$, with $j, m \in \mathbb{R}$, where the first label relates to the $\hat{\mathbf{J}}^2$ eigenvalue and the second label to the $\hat{J}_z$ eigenvalue:

$$\begin{aligned} \hat{\mathbf{J}}^2 |j,m\rangle &= \hbar^2 j(j+1)\,|j,m\rangle\,, \\ \hat{J}_z\,|j,m\rangle &= \hbar m\,|j,m\rangle. \end{aligned} \tag{19.3.23}$$

A multiplet of angular momentum is a special collection of linearly independent states, or vectors. It is useful to think of the multiplet as the vector space V generated as the span of these vectors. This vector space V must be invariant under the action of the angular momentum operators: $\hat{J}_i$: $V \to V$, for $i = 1, 2, 3$. Multiplets, moreover, are *irreducible*, meaning there is no proper subspace of V that is invariant under the action of the angular momentum operators. The set of states that generate a multiplet thus mix completely under the action of the angular momentum operators. In summary, a **multiplet of angular momentum** is a vector space that is irreducible and invariant under the action of the angular momentum operators. In general, if we have a vector space W on which angular momentum operators act, W can be written as a direct sum of multiplets—that is, a direct sum of the corresponding vector spaces.

As we can anticipate from our examples and our previous experience, the states $|j, m\rangle$ that generate a multiplet would be defined by an allowed, *fixed* value of j and a set of associated values of m. We will see below that no operator in the algebra of angular momentum can change the value of j. States with different eigenvalues of Hermitian operators must be orthogonal; therefore, we can assume that the states generating a multiplet are orthogonal:

$$\langle j, m' | j, m\rangle = \delta_{m',m}. \tag{19.3.24}$$

We assume that we do not have to deal with continuous values of j, m that would require delta function normalization (this will be confirmed below). Since j and m are real, the eigenvalues of the Hermitian operators are real, as they have to be.

The value of j in (19.3.23) is constrained by a positivity condition. Indeed, $\hbar^2 j(j + 1)$ must be nonnegative:

$$\hbar^2 j(j+1) = \langle j,m|\hat{\mathbf{J}}^2|j,m\rangle = \sum_{i=1}^{3}\langle j,m|\hat{J}_i\hat{J}_i|j,m\rangle = \sum_{i=1}^{3}||\hat{J}_i|j,m\rangle||^2 \geq 0, \tag{19.3.25}$$

where in the first step we used the eigenvalue definition and orthonormality. Therefore, the condition

$$j(j+1) \geq 0 \tag{19.3.26}$$

is the only a priori condition on the values of j. Since what matters is the eigenvalue of $\hat{\mathbf{J}}^2$, to label the state we can use any of the two j's that give a particular value of $j(j + 1)$. As shown in figure 19.1, the positivity of $j(j + 1)$ requires $j \geq 0$ or $j \leq -1$. We will use $j \geq 0$:

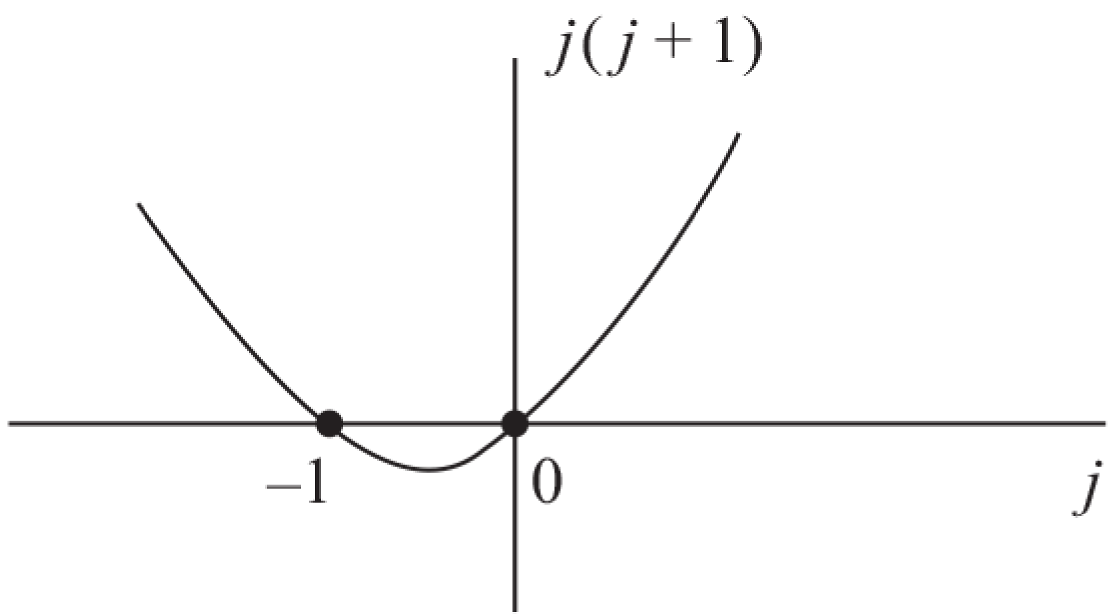

Figure 19.1
Since $j(j + 1) \geq 0$, for consistency we can label the states $|j, m\rangle$ using $j \geq 0$.

$$\text{States are labeled as } |j,m\rangle \text{ with } j \geq 0. \tag{19.3.27}$$

You should not think there are two different states, with two different j's associated with the eigenvalue $\hbar j(j + 1)$. It is just one state, labeled in an unusual way.

Just as we did for the case of the simple harmonic oscillator, we will assume that a state $|j, m\rangle$ of norm one exists and find out what the algebra of angular momentum implies for the existence of additional states and the possible values of j and m that have no inconsistencies. As in the harmonic oscillator case, an inconsistency would be the appearance of negative norm states.

Let us now investigate what the operators $\hat{J}_\pm$ do when acting on $|j, m\rangle$. Since they commute with $\hat{\mathbf{J}}^2$, the operators $\hat{J}_+$ or $\hat{J}_-$ do not change the j value of a state:

$$\hat{\mathbf{J}}^2(\hat{J}_\pm|j,m\rangle) = \hat{J}_\pm\hat{\mathbf{J}}^2|j,m\rangle = \hbar j(j+1)(\hat{J}_\pm|j,m\rangle) \tag{19.3.28}$$

so that we must have

$$\hat{J}_\pm|j,m\rangle \propto |j,m'_\pm\rangle, \quad \text{for some } m'_\pm. \tag{19.3.29}$$

Since $\hat{J}_z$ also commutes with $\hat{\mathbf{J}}^2$, this operator also does not change the value of j, so as mentioned earlier, no operator in the algebra of angular momentum can change the value of j. On the other hand, as anticipated above, the $\hat{J}_\pm$ operators change the value of m:

$$\begin{aligned}
\hat{J}_z(\hat{J}_\pm|j,m\rangle) &= ([\hat{J}_z, J_\pm] + J_\pm\hat{J}_z)|j,m\rangle \\
&= (\pm\hbar J_\pm + \hbar m J_\pm)|j,m\rangle \\
&= \hbar(m\pm 1)\, J_\pm|j,m\rangle,
\end{aligned} \tag{19.3.30}$$

from which we learn that

$$\hat{J}_\pm|j,m\rangle = C_\pm(j,m)|j,m\pm 1\rangle, \tag{19.3.31}$$

where $C_\pm(j, m)$ is a constant to be determined. Indeed, $\hat{J}_+$ raises the m eigenvalue by one unit, while $\hat{J}_-$ lowers the m eigenvalue by one unit. To determine $C_\pm(j, m)$, we first take the adjoint of the above equation:

$$\langle j,m|\hat{J}_\mp = \langle j,m\pm 1|C_\pm(j,m)^*, \tag{19.3.32}$$

and then form the overlap

$$\langle j,m|\hat{J}_\mp\hat{J}_\pm|j,m\rangle = |C_\pm(j,m)|^2. \tag{19.3.33}$$

To evaluate the left-hand side, use (19.3.21) in the form $\hat{J}_\mp\hat{J}_\pm = \hat{\mathbf{J}}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z$:

$$|C_\pm(j,m)|^2 = \langle j,m|(\hat{\mathbf{J}}^2 - \hat{J}_z^2 \mp \hbar\hat{J}_z)|j,m\rangle = \hbar^2 j(j+1) - \hbar^2 m^2 \mp \hbar^2 m. \tag{19.3.34}$$

We thus find that

$$\boxed{|C_\pm(j,m)|^2 \;=\; \hbar^2\left(j(j+1) - m(m\pm 1)\right) \;=\; ||\hat{J}_\pm|j,m\rangle||^2.} \tag{19.3.35}$$

Because the norm $||\hat{J}_\pm\,|j,\,m\rangle||$ is nonnegative, we can take $C_\pm(j,\,m)$ to be real and equal to the positive square root of the middle term:

$$C_\pm(j,m) \;=\; \hbar\sqrt{j(j+1) - m(m\pm 1)}. \tag{19.3.36}$$

We have thus obtained, in (19.3.31),

$$\boxed{\hat{J}_\pm|j,m\rangle \;=\; \hbar\sqrt{j(j+1) - m(m\pm 1)}\;|j,m\pm 1\rangle.} \tag{19.3.37}$$

Given a consistent state $|j,\,m\rangle$, how far can we raise or lower the value of m? Our classical intuition is that $|\hat{J}_z| \leq |\mathbf{J}|$. So we should get something like $|m| \leq \sqrt{j(j+1)}$. We analyze the situation in two steps:

1. For the raised state to be consistent, we must have $||J_+|j,\,m\rangle||^2 \geq 0$, and therefore,

$$j(j+1) - m(m+1) \geq 0 \quad \Rightarrow \quad m(m+1) \leq j(j+1). \tag{19.3.38}$$

The solution to this inequality is obtained using figure 19.2:

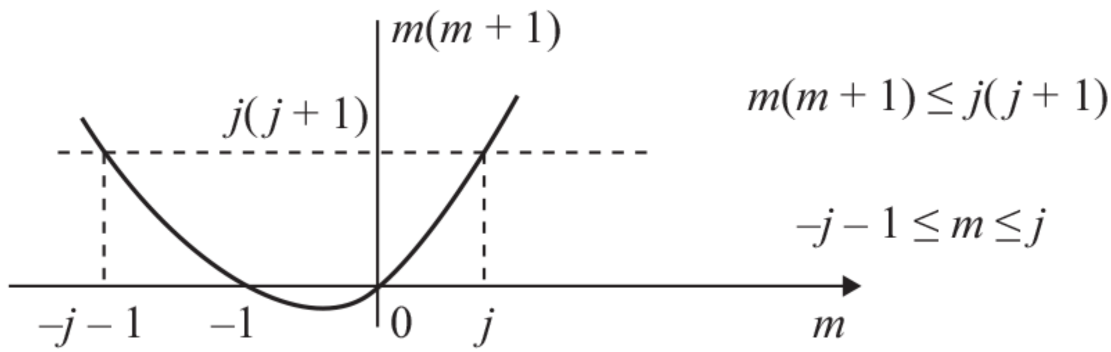

Figure 19.2
Solving the inequality $m(m+1) \leq j(j+1)$.

$$-j-1 \;\leq m \;\leq j. \tag{19.3.39}$$

Since we are raising m, we can focus on the troubles that raising can give because $m \leq j$. Assume $m = j - \beta$ with $0 < \beta < 1$ so that the inequality (19.3.39) is satisfied, and m is less than one unit below j. Then raising once gives us a state with $m' = m + 1 > j$, and since the inequality is now violated, $J_+|j, m'\rangle$ is an inconsistent state. To prevent such inconsistency, the process of raising must terminate: there must be a state on which raising gives no state (the zero state). That happens only if $m = j$, since then $C_+(j, j) = 0$:

$$\hat{J}_+|j,j\rangle = 0. \tag{19.3.40}$$

2. For the lowered state to be consistent, we must have $\|\hat{J}_-|j, m\rangle\|^2 \geq 0$, and therefore,

$$-j \leq m \leq j+1. \tag{19.3.42}$$

The solution to this inequality is obtained using figure 19.3:

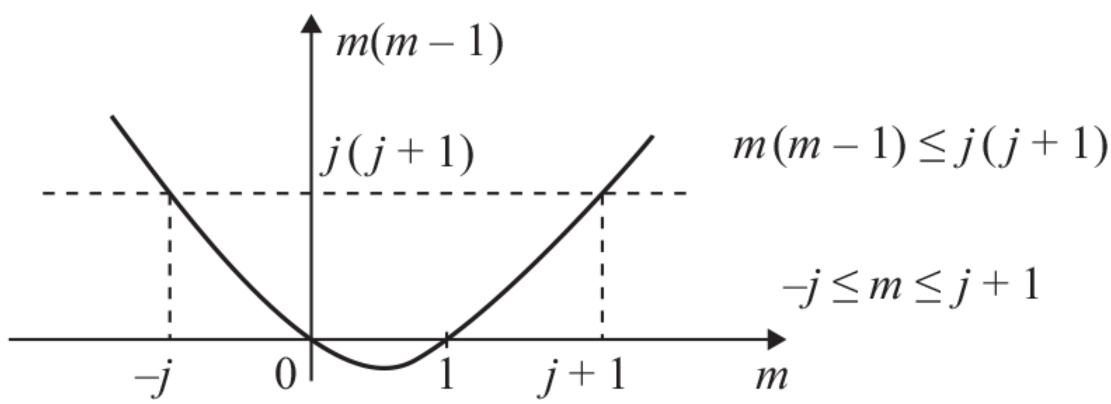

Figure 19.3
Solving the inequality $m(m-1) \leq j(j-1)$.

$$-j \leq m \leq j+1. \tag{19.3.42}$$

This time we can focus on $m \geq -j$ and the complications due to lowering. Assume $m = -j + \beta$ with $0 < \beta < 1$ so the constraint (19.3.42) is satisfied, and m is less than one unit above $-j$. Then lowering once gives us a state with $m' = m - 1 < -j$, and since the inequality is now violated, the state $\hat{J}_-|j, m'\rangle$ is an inconsistent state. To prevent such inconsistency, the process of lowering must terminate: there must be a state on which lowering gives no state (the zero state). That happens only if $m = -j$ since then $C_{-}(j, -j) = 0$:

$$\hat{J}_{-}|j, -j\rangle = 0. \tag{19.3.43}$$

The above analysis shows that for consistency the starting state $|j, m\rangle$ must have m in the range

$$-j \leq m \leq j, \tag{19.3.44}$$

which is the condition that combines (19.3.39) *and* (19.3.42). Additionally, m must be such that as it is increased by unit steps it reaches j and as it is decreased by unit steps it reaches $-j$. It follows that the distance $2j$ between j and $-j$ must be an integer:

$$\boxed{2j \in \mathbb{Z} \quad \Rightarrow \quad j \in \mathbb{Z}/2, \quad \Rightarrow \quad j = 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, \ldots.} \tag{19.3.45}$$

This is the fundamental quantization of angular momentum. Angular momentum can be integral or half integral. For any allowed value of j, the m values will be $j, j - 1, \ldots, -j$. Thus, the multiplet with angular momentum j is a vector space with the following $2j + 1$ orthonormal basis states:

$$\text{Multiplet of angular momentum } j: \quad \begin{array}{l} |j, j\rangle, \\ |j, j-1\rangle. \\ \quad \vdots \\ |j, -j+1\rangle, \\ |j, -j\rangle. \end{array} \tag{19.3.46}$$

For $j = 0$ there is just one state, the **singlet** with $m = 0$: $|0, 0\rangle$. The multiplet is then a one-dimensional vector space. For $j = \frac{1}{2}$, we have a **doublet**—that is, two basis states, one with $m = \frac{1}{2}$, the other with $m = -\frac{1}{2}$:

$$\text{Multiplet of angular momentum } j = \tfrac{1}{2}: \quad |\tfrac{1}{2}, \tfrac{1}{2}\rangle, \ |\tfrac{1}{2}, -\tfrac{1}{2}\rangle. \tag{19.3.47}$$

As we discussed below equation (19.3.5), when $\hat{\mathbf{J}}$ is the spin angular momentum $\hat{\mathbf{S}}$ these are basis states of a spin one-half particle, the conventional $|\pm\rangle$ states with $\hat{S}_z = \pm\frac{\hbar}{2}$. The multiplet is the state space $\mathbb{C}^2$ for spin states. For $j = 1$ we have three states, a **triplet**:

$$\text{Multiplet of angular momentum } j=1: \quad |1,\ 1\rangle,\ \ |1,\ 0\rangle,\ \ |1,-1\rangle. \tag{19.3.48}$$

If $\hat{\mathbf{J}}$ is orbital angular momentum $\hat{L}$, these would be the $\ell = 1$ spherical harmonics with $m = 1, 0, -1$ (see (19.3.1)). If $\hat{\mathbf{J}}$ is spin angular momentum $\hat{\mathbf{S}}$, the above states would be the basis vectors on which 3×3 spin matrices act, obeying the algebra of angular momentum. We would be describing a spin one particle. The details of the matrix construction are given below in example 19.1 and explored further in problem 19.2. For $j = 3/2$, we have four states:

$$\text{Multiplet of angular momentum } j=\tfrac{3}{2}: \quad |\tfrac{3}{2},\ \tfrac{3}{2}\rangle,\ \ |\tfrac{3}{2},\ \tfrac{1}{2}\rangle,\ \ |\tfrac{3}{2},-\tfrac{1}{2}\rangle,\ \ |\tfrac{3}{2},-\tfrac{3}{2}\rangle. \tag{19.3.49}$$

This cannot arise from orbital angular momentum but does arise from spin angular momentum. It corresponds to spin $\frac{3}{2}$. The above basis states allow a construction of the spin operators as 4×4 matrices.

On any state of a multiplet with angular momentum j, the eigenvalue J^2 of $\hat{\mathbf{J}}^2$ can be used to define the “magnitude” J of the angular momentum. We have

$$J^2 \ = \ \hbar^2 j(j+1) \quad \Rightarrow \quad \tfrac{1}{\hbar} J \ = \ \sqrt{j(j+1)}. \tag{19.3.50}$$

In the limit as j is large: $\frac{1}{\hbar}J = j\sqrt{1+\frac{1}{j}} \simeq j + \frac{1}{2} + \mathcal{O}(1/j)$.

Example 19.1. *Matrix construction of angular momentum operators for j = 1.*

For a $j = 1$ multiplet, we have the three basis states listed in (19.3.48). We order them as follows: $|1\rangle \equiv |1,\ 1\rangle$, $|2\rangle \equiv |1,\ 0\rangle$, $|3\rangle \equiv |1,\ -1\rangle$. In this basis the operator $\hat{J}_z$ is diagonal, and since $\hat{J}_z|1,\ m\rangle = \hbar m|1,\ m\rangle$, we have

$$\hat{J}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{19.3.51}$$

The matrices for $\hat{J}_x$ and $\hat{J}_y$ are obtained by first calculating the matrices for $\hat{J}_+$ and $\hat{J}_-$. Equation (19.3.37) with $j = 1$ gives $\hat{J}_+|1,m\rangle = \hbar\sqrt{2-m(m+1)}|1,m+1\rangle$. This means that

$$\hat{J}_+|1,1\rangle = 0, \quad \hat{J}_+|1,0\rangle = \hbar\sqrt{2}\,|1,1\rangle, \quad \hat{J}_+|1,-1\rangle = \hbar\sqrt{2}\,|1,0\rangle, \tag{19.3.52}$$

or equivalently, $\hat{J}_+|1\rangle = 0$, $\hat{J}_+|1\rangle = 0, \hat{J}_+|2\rangle = \hbar\sqrt{2}\,|1\rangle$, and $\hat{J}_+|3\rangle = \hbar\sqrt{2}\,|2\rangle$. This is all we need to build the matrix for $\hat{J}_+$:

$$\hat{J}_+ = \hbar\sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \hat{J}_- = \hbar\sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \tag{19.3.53}$$

where the matrix for $\hat{J}_-$ is the Hermitian conjugate of that for $\hat{J}_+$, given that $\hat{J}_- = \hat{J}_+^\dagger$. The matrices for $\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-)$ and $\hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-)$ now follow immediately:

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \tag{19.3.54}$$

The above matrices are Hermitian, as expected for Hermitian operators. It is a good check of our arithmetic that the above matrices satisfy $[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z$ and the other relations in the algebra of angular momentum. The matrices for $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ represent the operators as they act on a three-dimensional complex vector space $\mathbb{C}^3$, itself identified as the vector space of the $j = 1$ multiplet.

□

Exercise 19.10. *Show that tr $\hat{J}_i = 0$, for all $i = 1, 2, 3$, on any multiplet of angular momentum. Note that for $\hat{J}_3$ this follows quickly from the matrix representation.*

Relation to spherical harmonics The states we have found are described abstractly by (19.3.23). If $\mathbf{j}$ refers to orbital angular momentum, we would write

$$\begin{aligned} \hat{\mathbf{L}}^2|\ell,m\rangle &= \hbar^2\,\ell(\ell+1)\,|\ell,m\rangle\,, \\ \hat{L}_z\,|\ell,m\rangle &= \hbar m\,|\ell,m\rangle. \end{aligned} \tag{19.3.55}$$

Here the form of the operators is not specified, and the states are not described concretely. We can compare these to the relations (19.3.1)

$$\begin{aligned}\hat{\mathcal{L}}^2\, Y_{\ell m}(\theta,\phi) &= \hbar^2\,\ell(\ell+1)\, Y_{\ell m}(\theta,\phi),\\ \hat{\mathcal{L}}_z\, Y_{\ell m}(\theta,\phi) &= \hbar m\, Y_{\ell m}(\theta,\phi),\end{aligned} \tag{19.3.56}$$

where we have rewritten the operators $\hat{L}^2$ and $\hat{L}^z$ with calligraphic symbols to emphasize that here they are differential operators that satisfy the algebra of the abstract operators and act on the spherical harmonics. The correspondence between the two sets of relations can be established with the help of some formal notation. In one dimension, $\psi(x) = \langle x|\psi\rangle$ expresses a wave function in terms of a state and position eigenstates. Here, we introduce angular position eigenstates $|\theta\phi\rangle$. To make their definition more concrete, these states satisfy an orthogonality relation analogous to the one-dimensional $\langle x|x'\rangle = \delta(x-x')$:

$$\langle\theta\phi|\theta'\phi'\rangle = \delta(\cos\theta - \cos\theta')\delta(\phi-\phi'). \tag{19.3.57}$$

The delta functions to the right are the natural ones in spherical coordinates. Moreover, the completeness of these position states, in analogy to $\int dx|x\rangle\langle x| = \mathbb{1}$, would read

$$\int d\Omega\, |\theta\phi\rangle\langle\theta\phi| = \mathbb{1}, \qquad \int d\Omega = \int_{-1}^{1} d(\cos\theta) \int_0^{2\pi} d\phi. \tag{19.3.58}$$

The integral is over solid angle. Equipped with angular position states, we now write

$$Y_{\ell m}(\theta,\phi) \equiv \langle\theta\phi|\ell, m\rangle, \tag{19.3.59}$$

identifying the spherical harmonics as the wave functions associated to the $|\ell, m\rangle$ states! To see how this relation is used, we now derive the completeness and orthogonality relations for spherical harmonics from the completeness and orthogonality relations of the $|\ell, m\rangle$ states:

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} |\ell, m\rangle\langle\ell, m| \;=\; \mathbb{1}, \qquad \langle\ell', m'|\ell, m\rangle \;=\; \delta_{\ell',\ell}\delta_{m',m}. \tag{19.3.60}$$

Start with the orthogonality relation, and introduce a complete set of position states:

$$\int d\Omega\, \langle\ell', m'|\theta\phi\rangle\langle\theta\phi|\ell, m\rangle \;=\; \delta_{\ell',\ell}\delta_{m',m}. \tag{19.3.61}$$

This is, in fact, the familiar orthogonality property of the spherical harmonics:

$$\int d\Omega\, Y^*_{\ell' m'}(\theta,\phi)\, Y_{\ell m}(\theta,\phi) \;=\; \delta_{\ell',\ell}\delta_{m',m}. \tag{19.3.62}$$

Analogously, acting with $\langle\theta'\phi'|$ from the left and $|\theta\phi\rangle$ from the right on the completeness relation (19.3.60) gives us

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} \langle\theta'\phi'|\ell,m\rangle\langle\ell,m|\theta\phi\rangle \;=\; \delta(\cos\theta-\cos\theta')\delta(\phi-\phi'). \tag{19.3.63}$$

This expresses the completeness of the spherical harmonics. After taking complex conjugates, it reads

$$\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} Y^*_{\ell m}(\theta',\phi')Y_{\ell m}(\theta,\phi) \;=\; \delta(\cos\theta-\cos\theta')\delta(\phi-\phi'). \tag{19.3.64}$$

We can elaborate on the wave function/state correspondence. For the case of wave functions in one dimension, we have the following relations:

$$\begin{aligned} \hat{p}\,|p\rangle &= p\,|p\rangle, \\ \frac{\hbar}{i}\frac{\partial}{\partial x}\,\langle x|p\rangle &= p\,\langle x|p\rangle, \end{aligned} \tag{19.3.65}$$

where $\frac{\hbar}{i}\frac{\partial}{\partial x}$ is the differential operator that represents momentum in coordinate space. These two relations were used in section 14.10 to demonstrate the interplay between the operator and its differential representation for any general state $|\psi\rangle$:

$$\langle x|\hat{p}|\psi\rangle = \frac{\hbar}{i}\frac{\partial}{\partial x}\,\langle x|\psi\rangle. \tag{19.3.66}$$

Similarly, the two relations

$$\begin{aligned} \hat{\mathbf{L}}^2|\ell,m\rangle \;&=\; \hbar^2\,\ell(\ell+1)\,|\ell,m\rangle\,, \\ \hat{\mathcal{L}}^2\,Y_{\ell m}(\theta,\phi) \;&=\; \hbar^2\,\ell(\ell+1)Y_{\ell,m}(\theta,\phi) \end{aligned} \tag{19.3.67}$$

can be used to show that for any angular state $|F\rangle$,

$$\langle\theta\phi|\hat{\mathbf{L}}^2|F\rangle = \hat{\mathcal{L}}^2\,\langle\theta\phi|F\rangle. \tag{19.3.68}$$

To do this, start from the left-hand side, and introduce a complete set of angular momentum states:

$$\langle\theta\phi|\hat{\mathbf{L}}^2|F\rangle = \sum_{\ell,m}\langle\theta\phi|\ell,m\rangle\langle\ell,m|\hat{\mathbf{L}}^2|F\rangle = \sum_{\ell,m}\hbar^2\ell(\ell+1)Y_{\ell m}(\theta,\phi)\langle\ell,m|F\rangle, \tag{19.3.69}$$

where $\hat{\mathbf{L}}^2$ acted on the bra using the first equation of (19.3.67). Now we use the second equation there to find

$$\langle\theta\phi|\hat{\mathbf{L}}^2|F\rangle = \sum_{\ell,m}(\hat{\mathcal{L}}^2 Y_{\ell m}(\theta,\phi))\,\langle\ell,m|F\rangle = \hat{\mathcal{L}}^2\sum_{\ell,m}Y_{\ell m}(\theta,\phi)\langle\ell,m|F\rangle, \tag{19.3.70}$$

where the operator $\hat{\mathcal{L}}^2$ can be brought out of the sum since $\langle\ell, m|F\rangle$ has no angular dependence. Rewriting the $Y_{\ell m}$ again in terms of bra-kets, we show that

$$\langle\theta\phi|\hat{\mathbf{L}}^2|F\rangle = \hat{\mathcal{L}}^2\sum_{\ell,m}\langle\theta\phi|\ell,m\rangle\langle\ell,m|F\rangle = \hat{\mathcal{L}}^2\langle\theta\phi|F\rangle, \tag{19.3.71}$$

as we wanted. For $|F\rangle = |\ell, m\rangle$ this relation gives $\langle\theta\phi|\hat{\mathbf{L}}^2|\ell, m\rangle = \hat{\mathcal{L}}^2 Y_{\ell m}$. An analogous derivation results in the relation $\langle\theta\phi|\hat{L}_z|F\rangle = \hat{\mathcal{L}}_z\langle\theta\phi|F\rangle$.

Example 19.2. *Spherical harmonics from lowering operators.*
We want to confirm that

$$Y_{\ell 0}(\theta,\phi) = \frac{1}{\sqrt{(2\ell)!}}\Big(\frac{\hat{L}_-}{\hbar}\Big)^{\ell}Y_{\ell\ell}(\theta,\phi). \tag{19.3.72}$$

This equation makes precise the relation $Y_{\ell 0} \sim (\hat{L}_-)^\ell Y_{\ell\ell}$, which we expect to hold because each $\hat{L}_-$ lowers the value of the m quantum number by one unit. The above formula can be used in practice to calculate spherical harmonics. The expression for $Y_{\ell\ell}$ is given in (10.5.35), and the angular form of $\hat{L}_-$ is in (19.2.21).

To prove (19.3.72) we recall (19.3.37), which for orbital angular momentum reads

$$\hat{L}_-|\ell,m\rangle = \hbar\sqrt{\ell(\ell+1)-m(m-1)}\,|\ell,m-1\rangle\,. \tag{19.3.73}$$

For spherical harmonics, and factorizing the expression inside the square root, we have

$$\frac{\hat{L}_-}{\hbar} Y_{\ell,m} = \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell,m-1}\,. \tag{19.3.74}$$

We thus see that

$$\begin{aligned}
\frac{\hat{L}_-}{\hbar} Y_{\ell\ell} &= \sqrt{2\ell\cdot 1}\quad Y_{\ell,\ell-1}\,,\\
\frac{\hat{L}_-}{\hbar} Y_{\ell,\ell-1} &= \sqrt{(2\ell-1)\,2}\, Y_{\ell,\ell-2}\,,\\
\vdots \qquad & \qquad \vdots\\
\frac{\hat{L}_-}{\hbar} Y_{\ell,1} &= \sqrt{(\ell+1)\ell}\, Y_{\ell,0}.
\end{aligned} \tag{19.3.75}$$

If you look inside the square root prefactors, you will see that they include all integers from 1 to 2ℓ. Therefore,

$$\left(\frac{\hat{L}_-}{\hbar}\right)^{\ell} Y_{\ell\ell} = \sqrt{(2\ell)!}\, Y_{\ell 0}, \tag{19.3.76}$$

which is indeed the relation we wanted to prove.

□

Example 19.3. *Wave functions for p orbitals.*
A p orbital is a state with angular momentum $\ell = 1$. This terminology is commonly used to describe states of electrons in atoms. With three possible values of the m quantum number, $m = -1, 0, 1$, there are three p orbitals. The p_z orbital is defined as the $\hat{L}_z = 0$ state $|1, 0\rangle$. Thus, the angular wave function $\psi_{p_z}(\theta, \phi)$ for this orbital is

$$\psi_{p_z}(\theta,\phi) = \langle\theta\phi|1,0\rangle = Y_{1,0}(\theta,\phi) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\,\frac{z}{r}, \tag{19.3.77}$$

where we read the spherical harmonic from (10.5.33). The p_x orbital is defined as the $\ell = 1$ state with $\hat{L}_x = 0$. Using the matrix representation (19.3.54) in the standard $(\hat{\mathbf{L}}^2, \hat{L}_z)$ basis, we see that $\hat{L}_x$ kills the vector $(1, 0, -1)$:

$$\hat{L}_x \begin{pmatrix} 1\\ 0\\ -1\end{pmatrix} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}\begin{pmatrix} 1\\ 0\\ -1\end{pmatrix} = 0, \tag{19.3.78}$$

confirming that the normalized state $|\psi_{p_x}\rangle$ with $\hat{L}_x = 0$ is

$$|\psi_{p_x}\rangle = \frac{1}{\sqrt{2}}(|1,1\rangle - |1,-1\rangle) \quad \Rightarrow \quad \psi_{p_x} = \frac{1}{\sqrt{2}}(Y_{1,1} - Y_{1,-1}). \tag{19.3.79}$$

This quickly gives

$$\begin{aligned} \psi_{p_x} &= -\sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi = -\sqrt{\frac{3}{4\pi}}\,\frac{x}{r}, \\ \psi_{p_y} &= -i\sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi = -i\sqrt{\frac{3}{4\pi}}\,\frac{y}{r}, \end{aligned} \tag{19.3.80}$$

where we included the p_y orbital that, with $\hat{L}_y = 0$, is the state $\frac{1}{\sqrt{2}}(|1,1\rangle + |1,-1\rangle)$. The three orbitals $|\psi_{p_x}\rangle$, $|\psi_{p_y}\rangle$, and $|\psi_{p_z}\rangle$ form an orthonormal basis for the $\ell = 1$ multiplet. Note the nice symmetry between their wave functions, made manifest in the plots in figure 19.4. These orbitals are useful in atomic physics because they represent the choices made by electrons in multielectron atoms as they fill $\ell = 1$ spaces (example 21.5).

□

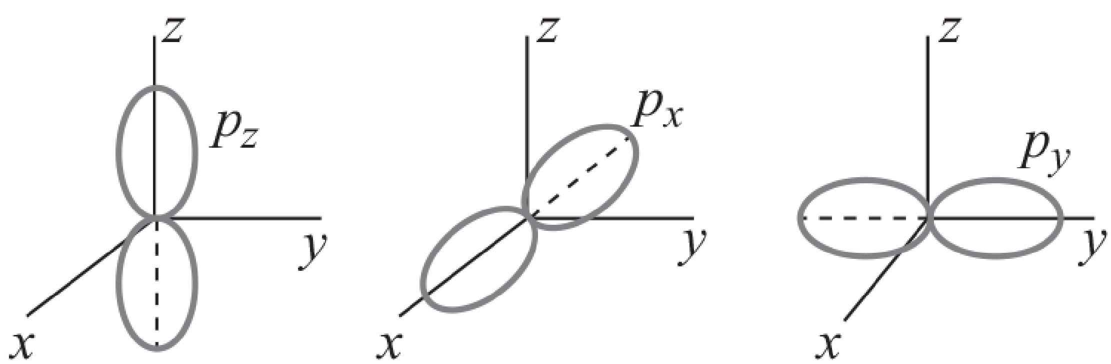

Figure19.4
From left to right, the angular behavior of the p_z, p_x, and p_y orbitals.