Chapter 5

Angular Momentum

5.1 Introduction

After treating one-dimensional problems in Chapter 4, we now should deal with three-dimensional problems. However, the study of three-dimensional systems such as atoms cannot be undertaken unless we first cover the formalism of angular momentum. The current chapter, therefore, serves as an essential prelude to Chapter 6.

Angular momentum is as important in classical mechanics as in quantum mechanics. It is particularly useful for studying the dynamics of systems that move under the influence of *spherically symmetric*, or *central*, potentials, $V(\vec{r}) = V(r)$, for the orbital angular momenta of these systems are *conserved*. For instance, as mentioned in Chapter 1, one of the cornerstones of Bohr's model of the hydrogen atom (where the electron moves in the proton's Coulomb potential, a central potential) is based on the quantization of angular momentum. Additionally, angular momentum plays a critical role in the description of molecular rotations, the motion of electrons in atoms, and the motion of nucleons in nuclei. The quantum theory of angular momentum is thus a prerequisite for studying molecular, atomic, and nuclear systems.

In this chapter we are going to consider the general formalism of angular momentum. We will examine the various properties of the angular momentum operator, and then focus on determining its eigenvalues and eigenstates. Finally, we will apply this formalism to the determination of the eigenvalues and eigenvectors of the spin and orbital angular momenta.

5.2 Orbital Angular Momentum

In classical physics the angular momentum of a particle with momentum $\vec{p}$ and position $\vec{r}$ is defined by

$$\vec{L} = \vec{r} \times \vec{p} = (yp_z - zp_y)\vec{i} + (zp_x - xp_z)\vec{j} + (xp_y - yp_x)\vec{k}. \tag{5.1}$$

The orbital angular momentum operator $\hat{\vec{L}}$ can be obtained at once by replacing $\vec{r}$ and $\vec{p}$ by the corresponding operators in the position representation, $\hat{\vec{R}}$ and $\hat{\vec{P}} = -i\hbar\vec{\nabla}$:

$$\boxed{\hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}} = -i\hbar\hat{\vec{R}} \times \vec{\nabla}\ .} \tag{5.2}$$

The Cartesian components of $\hat{\vec{L}}$ are

$$\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y = -i\hbar\left(\hat{Y}\frac{\partial}{\partial z} - \hat{Z}\frac{\partial}{\partial y}\right), \tag{5.3}$$

$$\hat{L}_y = \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z = -i\hbar\left(\hat{Z}\frac{\partial}{\partial x} - \hat{X}\frac{\partial}{\partial z}\right), \tag{5.4}$$

$$\hat{L}_z = \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x = -i\hbar\left(\hat{X}\frac{\partial}{\partial y} - \hat{Y}\frac{\partial}{\partial x}\right). \tag{5.5}$$

Clearly, angular momentum does not exist in a one-dimensional space. We should mention that the components $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, and the square of $\hat{\vec{L}}$,

$$\hat{\vec{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2, \tag{5.6}$$

are all Hermitian.

Commutation relations

Since $\hat{X}$, $\hat{Y}$, and $\hat{Z}$ mutually commute and so do $\hat{P}_x$, $\hat{P}_y$, and $\hat{P}_z$, and since $[\hat{X}, \hat{P}_x] = i\hbar$, $[\hat{Y}, \hat{P}_y] = i\hbar$, $[\hat{Z}, \hat{P}_z] = i\hbar$, we have

$$\begin{aligned}
[\hat{L}_x, \hat{L}_y] &= [\hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y,\ \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] \\
&= [\hat{Y}\hat{P}_z, \hat{Z}\hat{P}_x] - [\hat{Y}\hat{P}_z, \hat{X}\hat{P}_z] - [\hat{Z}\hat{P}_y, \hat{Z}\hat{P}_x] + [\hat{Z}\hat{P}_y, \hat{X}\hat{P}_z] \\
&= \hat{Y}[\hat{P}_z, \hat{Z}]\hat{P}_x + \hat{X}[\hat{Z}, \hat{P}_z]\hat{P}_y = i\hbar(\hat{X}\hat{P}_y - \hat{Y}\hat{P}_x) \\
&= i\hbar\hat{L}_z.
\end{aligned} \tag{5.7}$$

A similar calculation yields the other two commutation relations; but it is much simpler to infer them from (5.7) by means of a *cyclic permutation* of the xyz components, $x \to y \to z \to x$:

$$\boxed{[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z, \qquad [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x, \qquad [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y.} \tag{5.8}$$

As mentioned in Chapter 3, since $\hat{L}_x$, $\hat{L}_y$, and $\hat{L}_z$ do not commute, we cannot measure them simultaneously to arbitrary accuracy.

Note that the commutation relations (5.8) were derived by expressing the orbital angular momentum in the *position representation*, but since these are operator relations, they must be valid in any representation. In the following section we are going to consider the general formalism of angular momentum, a formalism that is restricted to no particular representation.

Example 5.1

(a) Calculate the commutators $[\hat{X},\ \hat{L}_x]$, $[\hat{X},\ \hat{L}_y]$, and $[\hat{X},\ \hat{L}_z]$.

(b) Calculate the commutators: $[\hat{P}_x,\ \hat{L}_x]$, $[\hat{P}_x,\ \hat{L}_y]$, and $[\hat{P}_x,\ \hat{L}_z]$.

(c) Use the results of (a) and (b) to calculate $[\hat{X},\ \hat{\vec{L}}^2]$ and $[\hat{P}_x,\ \hat{\vec{L}}^2]$.

Solution

(a) The only nonzero commutator which involves $\hat{X}$ and the various components of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ is $[\hat{X}, \hat{P}_x] = i\hbar$. Having stated this result, we can easily evaluate the needed commutators. First, since $\hat{L}_x = \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y$ involves no $\hat{P}_x$, the operator $\hat{X}$ commutes separately with $\hat{Y}$, $\hat{P}_z$, $\hat{Z}$, and $\hat{P}_y$; hence

$$[\hat{X}, \hat{L}_x] = [\hat{X}, \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y] = 0. \tag{5.9}$$

The evaluation of the other two commutators is straightforward:

$$[\hat{X}, \hat{L}_y] = [\hat{X}, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = [\hat{X}, \hat{Z}\hat{P}_x] = \hat{Z}[\hat{X}, \hat{P}_x] = i\hbar\hat{Z}, \tag{5.10}$$

$$[\hat{X}, \hat{L}_z] = [\hat{X}, \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x] = -[\hat{X}, \hat{Y}\hat{P}_x] = -\hat{Y}[\hat{X}, \hat{P}_x] = -i\hbar\hat{Y}. \tag{5.11}$$

(b) The only commutator between $\hat{P}_x$ and the components of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ that survives is again $[\hat{P}_x, \hat{X}] = -i\hbar$. We may thus infer

$$[\hat{P}_x, \hat{L}_x] = [\hat{P}_x, \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y] = 0, \tag{5.12}$$

$$[\hat{P}_x, \hat{L}_y] = [\hat{P}_x, \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z] = -[\hat{P}_x, \hat{X}\hat{P}_z] = -[\hat{P}_x, \hat{X}]\hat{P}_z = i\hbar\hat{P}_z, \tag{5.13}$$

$$[\hat{P}_x, \hat{L}_z] = [\hat{P}_x, \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x] = [\hat{P}_x, \hat{X}\hat{P}_y] = [\hat{P}_x, \hat{X}]\hat{P}_y = -i\hbar\hat{P}_y. \tag{5.14}$$

(c) Using the commutators derived in (a) and (b), we infer

$$\begin{aligned}
[\hat{X}, \hat{\vec{L}}^2] &= [\hat{X}, \hat{L}_x^2] + [\hat{X}, \hat{L}_y^2] + [\hat{X}, \hat{L}_z^2] \\
&= 0 + \hat{L}_y[\hat{X}, \hat{L}_y] + [\hat{X}, \hat{L}_y]\hat{L}_y + \hat{L}_z[\hat{X}, \hat{L}_z] + [\hat{X}, \hat{L}_z]\hat{L}_z \\
&= i\hbar(\hat{L}_y\hat{Z} + \hat{Z}\hat{L}_y - \hat{L}_z\hat{Y} - \hat{Y}\hat{L}_y),
\end{aligned} \tag{5.15}$$

$$\begin{aligned}
[\hat{P}_x, \hat{\vec{L}}^2] &= [\hat{P}_x, \hat{L}_x^2] + [\hat{P}_x, \hat{L}_y^2] + [\hat{P}_x, \hat{L}_z^2] \\
&= 0 + \hat{L}_y[\hat{P}_x, \hat{L}_y] + [\hat{P}_x, \hat{L}_y]\hat{L}_y + \hat{L}_z[\hat{P}_x, \hat{L}_z] + [\hat{P}_x, \hat{L}_z]\hat{L}_z \\
&= i\hbar(\hat{L}_y\hat{P}_z + \hat{P}_z\hat{L}_y - \hat{L}_z\hat{P}_y - \hat{P}_y\hat{L}_y).
\end{aligned} \tag{5.16}$$

5.3 General Formalism of Angular Momentum

Let us now introduce a more general angular momentum operator $\hat{\vec{J}}$ that is defined by its three components $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$, which satisfy the following commutation relations:

$$\boxed{[\hat{J}_x, \hat{J}_y] = i\hbar\hat{J}_z, \qquad [\hat{J}_y, \hat{J}_z] = i\hbar\hat{J}_x, \qquad [\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y,} \tag{5.17}$$

or equivalently by

$$\hat{\vec{J}} \times \hat{\vec{J}} = i\hbar\hat{\vec{J}}. \tag{5.18}$$

Since $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ do not mutually commute, they cannot be simultaneously diagonalized; that is, they do not possess common eigenstates. The square of the angular momentum,

$$\hat{\vec{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \tag{5.19}$$

is a scalar operator; hence it commutes with $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$:

$$[\hat{\vec{J}}^2, \hat{J}_k] = 0, \tag{5.20}$$

where k stands for x, y, and z. For instance, in the the case $k = x$ we have

$$\begin{aligned} [\hat{\vec{J}}^2, \hat{J}_x] &= [\hat{J}_x^2, \hat{J}_x] + \hat{J}_y[\hat{J}_y, \hat{J}_x] + [\hat{J}_y, \hat{J}_x]\hat{J}_y + \hat{J}_z[\hat{J}_z, \hat{J}_x] + [\hat{J}_z, \hat{J}_x]\hat{J}_z \\ &= \hat{J}_y(-i\hbar\hat{J}_z) + (-i\hbar\hat{J}_z)\hat{J}_y + \hat{J}_z(i\hbar\hat{J}_y) + (i\hbar\hat{J}_y)\hat{J}_z \\ &= 0, \end{aligned} \tag{5.21}$$

because $[\hat{J}_x^2, \hat{J}_x] = 0$, $[\hat{J}_y, \hat{J}_x] = -i\hbar\hat{J}_z$, and $[\hat{J}_z, \hat{J}_x] = i\hbar\hat{J}_y$. We should note that the operators $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$, and $\hat{\vec{J}}^2$ are all Hermitian; their eigenvalues are real.

Eigenstates and eigenvalues of the angular momentum operator

Since $\hat{\vec{J}}^2$ commutes with $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$, each component of $\vec{J}$ can be separately diagonalized (hence it has simultaneous eigenfunctions) with $\hat{\vec{J}}^2$. But since the components $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ do not mutually commute, we can choose only one of them to be simultaneously diagonalized with $\hat{\vec{J}}^2$. By convention we choose $\hat{J}_z$. There is nothing special about the z-direction; we can just as well take $\hat{\vec{J}}^2$ and $\hat{J}_x$ or $\hat{\vec{J}}^2$ and $\hat{J}_y$.

Let us now look for the joint eigenstates of $\hat{\vec{J}}^2$ and $\hat{J}_z$ and their corresponding eigenvalues. Denoting the joint eigenstates by $\mid \alpha,\ \beta\rangle$ and the eigenvalues of $\hat{\vec{J}}^2$ and $\hat{J}_z$ by $\hbar^2\alpha$ and $\hbar\beta$, respectively, we have

$$\hat{\vec{J}}^2 \mid \alpha,\ \beta\rangle = \hbar^2\alpha \mid \alpha,\ \beta\rangle, \tag{5.22}$$

$$\hat{J}_z \mid \alpha,\ \beta\rangle = \hbar\beta \mid \alpha,\ \beta\rangle. \tag{5.23}$$

The factor $\hbar$ is introduced so that α and β are dimensionless; recall that the angular momentum has the dimensions of $\hbar$ and that the physical dimensions of $\hbar$ are: $[\hbar]$ = energy × time. For simplicity, we will assume that these eigenstates are orthonormal:

$$\langle\alpha',\ \beta' \mid \alpha,\ \beta\rangle = \delta_{\alpha',\alpha}\delta_{\beta',\beta}. \tag{5.24}$$

Now we need to introduce *raising* and *lowering* operators $\hat{J}_+$ and $\hat{J}_-$, just as we did when we studied the harmonic oscillator in Chapter 4:

$$\boxed{\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y.} \tag{5.25}$$

This leads to

$$\hat{J}_x = \frac{1}{2}(\hat{J}_+ + \hat{J}_-), \qquad \hat{J}_y = \frac{1}{2i}(\hat{J}_+ - \hat{J}_-); \tag{5.26}$$

hence

$$\hat{J}_x^2 = \frac{1}{4}(\hat{J}_+^2 + \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ + \hat{J}_-^2), \qquad \hat{J}_y^2 = -\frac{1}{4}(\hat{J}_+^2 - \hat{J}_+\hat{J}_- - \hat{J}_-\hat{J}_+ + \hat{J}_-^2). \tag{5.27}$$

Using (5.17) we can easily obtain the following commutation relations:

$$[\hat{\vec{J}}^2,\ \hat{J}_\pm] = 0, \qquad [\hat{J}_+,\ \hat{J}_-] = 2\hbar\hat{J}_z, \qquad [\hat{J}_z,\ \hat{J}_\pm] = \pm\hbar\hat{J}_\pm. \tag{5.28}$$

In addition, $\hat{J}_+$ and $\hat{J}_-$ satisfy

$$\hat{J}_+\hat{J}_- = \hat{J}_x^2 + \hat{J}_y^2 + \hbar\hat{J}_z = \hat{\vec{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z, \tag{5.29}$$

$$\hat{J}_-\hat{J}_+ = \hat{J}_x^2 + \hat{J}_y^2 - \hbar\hat{J}_z = \hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z. \tag{5.30}$$

These relations lead to

$$\boxed{\hat{\vec{J}}^2 = \hat{J}_\pm\hat{J}_\mp + \hat{J}_z^2 \mp \hbar\hat{J}_z,} \tag{5.31}$$

which in turn yield

$$\boxed{\hat{\vec{J}}^2 = \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_z^2.} \tag{5.32}$$

Let us see how $\hat{J}_\pm$ operate on $\mid \alpha,\ \beta\rangle$. First, since $\hat{J}_\pm$ do not commute with $\hat{J}_z$, the kets $\mid \alpha,\ \beta\rangle$ are not eigenstates of $\hat{J}_\pm$. Using the relations (5.28) we have

$$\hat{J}_z(\hat{J}_\pm \mid \alpha,\ \beta\rangle) = (\hat{J}_\pm\hat{J}_z\ \pm\ \hbar\hat{J}_\pm) \mid \alpha,\ \beta\rangle = \hbar(\beta \pm 1)(\hat{J}_\pm \mid \alpha,\ \beta\rangle); \tag{5.33}$$

hence the ket $(\hat{J}_\pm \mid \alpha,\ \beta\rangle)$ is an eigenstate of $\hat{J}_z$ with eigenvalues $\hbar(\beta \pm 1)$. Now since $\hat{J}_z$ and $\hat{\vec{J}}^2$ commute, $(\hat{J}_\pm \mid \alpha,\ \beta\rangle)$ must also be an eigenstate of $\hat{\vec{J}}^2$. The eigenvalue of $\hat{\vec{J}}^2$ when acting on $\hat{J}_\pm \mid \alpha,\ \beta\rangle$ can be determined by making use of the commutator $[\hat{\vec{J}}^2, \hat{J}_\pm] = 0$. The state $(\hat{J}_\pm \mid \alpha,\ \beta\rangle)$ is also an eigenstate of $\hat{\vec{J}}^2$ with eigenvalue $\hbar^2\alpha$:

$$\hat{\vec{J}}^2(\hat{J}_\pm \mid \alpha,\ \beta\rangle) = \hat{J}_\pm\hat{\vec{J}}^2 \mid \alpha,\ \beta\rangle = \hbar^2\alpha(\hat{J}_\pm \mid \alpha,\ \beta\rangle). \tag{5.34}$$

From (5.33) and (5.34) we infer that when $\hat{J}_\pm$ acts on $\mid \alpha,\ \beta\rangle$, it does not affect the first quantum number α, but it raises or lowers the second quantum number β by one unit. That is, $J_\pm \mid \alpha,\ \beta\rangle$ is proportional to $\mid \alpha,\ \beta \pm 1\rangle$:

$$\hat{J}_\pm \mid \alpha,\ \beta\rangle = C_{\alpha\beta}^\pm \mid \alpha,\ \beta \pm 1\rangle. \tag{5.35}$$

We will determine the constant $C_{\alpha\beta}^\pm$ later on.

Note that, for a given eigenvalue α of $\hat{\vec{J}}^2$, there exists an *upper limit* for the quantum number β. This is due to the fact that the operator $\hat{\vec{J}}^2 - \hat{J}_z^2$ is positive, since the matrix elements of $\hat{\vec{J}}^2 - \hat{J}_z^2 = \hat{J}_x^2 + \hat{J}_y^2$ are ≥ 0; we can therefore write

$$\langle\alpha,\ \beta \mid \hat{\vec{J}}^2 - \hat{J}_z^2 \mid \alpha,\ \beta\rangle = \hbar^2(\alpha - \beta^2) \geq 0, \quad \Longrightarrow \quad \alpha \geq \beta^2. \tag{5.36}$$

Since β has an upper limit β_{max}, there must exist a state $\mid \alpha,\ \beta_{max}\rangle$ which cannot be raised further:

$$\hat{J}_+ \mid \alpha,\ \beta_{max}\rangle = 0. \tag{5.37}$$

Using this relation along with $\hat{J}_-\hat{J}_+ = \hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z$, we see that $\hat{J}_-\hat{J}_+ \mid \alpha,\ \beta_{max}\rangle = 0$ or

$$(\hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z) \mid \alpha,\ \beta_{max}\rangle = \hbar^2(\alpha - \beta_{max}^2 - \beta_{max}) \mid \alpha,\ \beta_{max}\rangle; \tag{5.38}$$

hence

$$\alpha = \beta_{max}(\beta_{max} + 1). \tag{5.39}$$

After n successive applications of $\hat{J}_-$ on $| \alpha, \beta_{max}\rangle$, we must be able to reach a state $| \alpha, \beta_{min}\rangle$ which cannot be lowered further:

$$\hat{J}_- \mid \alpha, \beta_{min}\rangle = 0. \tag{5.40}$$

Using $\hat{J}_+\hat{J}_- = \hat{\vec{J}}^2 - \hat{J}_z^2 + \hbar\hat{J}_z$, and by analogy with (5.38) and (5.39), we infer that

$$\alpha = \beta_{min}(\beta_{min} - 1). \tag{5.41}$$

Comparing (5.39) and (5.41) we obtain

$$\beta_{max} = -\beta_{min}. \tag{5.42}$$

Since β_{min} was reached by n applications of $\hat{J}_-$ on $| \alpha, \beta_{max}\rangle$, it follows that

$$\beta_{max} = \beta_{min} + n, \tag{5.43}$$

and since $\beta_{min} = -\beta_{max}$ we conclude that

$$\beta_{max} = \frac{n}{2}. \tag{5.44}$$

Hence β_{max} can be integer or half-odd-integer, depending on n being even or odd.

It is now appropriate to introduce the notation j and m to denote β_{max} and β, respectively:

$$j = \beta_{max} = \frac{n}{2}, \qquad m = \beta; \tag{5.45}$$

hence the eigenvalue of $\hat{\vec{J}}^2$ is given by

$$\alpha = j(j+1). \tag{5.46}$$

Now since $\beta_{min} = -\beta_{max}$, and with n positive, we infer that the allowed values of m lie between $-j$ and $+j$:

$$\boxed{-j \le m \le j.} \tag{5.47}$$

The results obtained thus far can be summarized as follows: the eigenvalues of $\hat{\vec{J}}^2$ and J_z corresponding to the joint eigenvectors $| j, m\rangle$ are given, respectively, by $\hbar^2 j(j+1)$ and $\hbar m$:

$$\boxed{\hat{\vec{J}}^2 \mid j, m\rangle = \hbar^2 j(j+1) \mid j, m\rangle \quad \text{and} \quad \hat{J}_z \mid j, m\rangle = \hbar m \mid j, m\rangle,} \tag{5.48}$$

where $j = 0, 1/2, 1, 3/2, \ldots$ and $m = -j, -(j-1), \ldots, j-1, j$. So for each j there are $2j+1$ values of m. For example, if $j = 1$ then m takes the three values $-1, 0, 1$; and if $j = 5/2$ then m takes the six values $-5/2, -3/2, -1/2, 1/2, 3/2, 5/2$. The values of j are either integer or half-integer. We see that the spectra of the angular momentum operators $\hat{\vec{J}}^2$ and $\hat{J}_z$ are discrete. Since the eigenstates corresponding to different angular momenta are orthogonal, and since the angular momentum spectra are discrete, the orthonormality condition is

$$\boxed{\langle j', m' \mid j, m\rangle = \delta_{j', j}\delta_{m', m}.} \tag{5.49}$$

Let us now determine the eigenvalues of $\hat{J}_\pm$ within the $\{| j, m\rangle\}$ basis; $| j, m\rangle$ is not an eigenstate of $\hat{J}_\pm$. We can rewrite equation (5.35) as

$$\hat{J}_\pm | j, m\rangle = C^{\pm}_{jm} | j, m \pm 1\rangle. \tag{5.50}$$

We are going to derive $C^{+}_{j\,m}$ and then infer $C^{-}_{j\,m}$. Since $| j, m\rangle$ is normalized, we can use (5.50) to obtain the following two expressions:

$$\begin{aligned}(\hat{J}_+ | j, m\rangle)^\dagger (\hat{J}_+ | j, m\rangle) &= |C^{+}_{jm}|^2 \langle j, m+1 | j, m+1\rangle = |C^{+}_{j\,m}|^2, && (5.51)\\ \left|C^{+}_{jm}\right|^2 &= \langle j, m|\hat{J}_-\hat{J}_+ | j, m\rangle. && (5.52)\end{aligned}$$

But since $\hat{J}_-\hat{J}_+$ is equal to $(\hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z)$, and assuming the arbitrary phase of $C^{+}_{j\,m}$ to be zero, we conclude that

$$C^{+}_{jm} = \sqrt{\langle j, m|\hat{\vec{J}}^2 - \hat{J}_z^2 - \hbar\hat{J}_z | j, m\rangle} = \hbar\sqrt{j(j+1) - m(m+1)}. \tag{5.53}$$

By analogy with $C^{+}_{j\,m}$ we can easily infer the expression for $C^{-}_{j\,m}$:

$$C^{-}_{jm} = \hbar\sqrt{j(j+1) - m(m-1)}. \tag{5.54}$$

Thus, the eigenvalue equations for $\hat{J}_+$ and $\hat{J}_-$ are given by

$$\boxed{\hat{J}_\pm | j, m\rangle = \hbar\sqrt{j(j+1) - m(m\pm 1)}\ | j, m\pm 1\rangle} \tag{5.55}$$

or

$$\boxed{\hat{J}_\pm | j, m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}\ | j, m\pm 1\rangle,} \tag{5.56}$$

which in turn leads to the two relations:

$$\begin{aligned}\hat{J}_x | j, m\rangle &= \frac{1}{2}(\hat{J}_+ + \hat{J}_-) | j, m\rangle\\ &= \frac{\hbar}{2}\left[\sqrt{(j-m)(j+m+1)}\ | j, m+1\rangle + \sqrt{(j+m)(j-m+1)}\ | j, m-1\rangle\right],\end{aligned} \tag{5.57}$$

$$\begin{aligned}\hat{J}_y | j, m\rangle &= \frac{1}{2i}(\hat{J}_+ - \hat{J}_-) | j, m\rangle\\ &= \frac{\hbar}{2i}\left[\sqrt{(j-m)(j+m+1)}\ | j, m+1\rangle - \sqrt{(j+m)(j-m+1)}\ | j, m-1\rangle\right].\end{aligned} \tag{5.58}$$

The expectation values of $\hat{J}_x$ and $\hat{J}_y$ are therefore zero:

$$\langle j, m | \hat{J}_x | j, m\rangle = \langle j, m | \hat{J}_y | j, m\rangle = 0 \tag{5.59}$$

We will show later in (5.208) that the expectation values $\langle j, m | \hat{J}_x^2 | j, m\rangle$ and $\langle j, m | \hat{J}_y^2 | j, m\rangle$ are equal and given by

$$\boxed{\langle\hat{J}_x^2\rangle = \langle\hat{J}_y^2\rangle = \frac{1}{2}\left[\langle j, m | \hat{\vec{J}}^2 | j, m\rangle - \langle j, m | \hat{J}_z^2 | j, m\rangle\right] = \frac{\hbar^2}{2}\left[j(j+1) - m^2\right].} \tag{5.60}$$

Example 5.2

Calculate $[\hat{J}_x^2,\ \hat{J}_y]$, $[\hat{J}_z^2,\ \hat{J}_y]$, and $[\hat{\vec{J}}^2,\ \hat{J}_y]$; then show $\langle j,\ m \mid \hat{J}_x^2 \mid j,\ m\rangle = \langle j,\ m \mid \hat{J}_y^2 \mid j,\ m\rangle$.

Solution

Since $[\hat{J}_x,\ \hat{J}_y] = i\hbar\hat{J}_z$ and $[\hat{J}_z,\ \hat{J}_x] = i\hbar\hat{J}_y$, we have

$$[\hat{J}_x^2,\ \hat{J}_y] = \hat{J}_x[\hat{J}_x,\ \hat{J}_y] + [\hat{J}_x,\ \hat{J}_y]\hat{J}_x = i\hbar(\hat{J}_x\hat{J}_z + \hat{J}_z\hat{J}_x) = i\hbar(2\hat{J}_x\hat{J}_z + i\hbar\hat{J}_y). \tag{5.61}$$

Similarly, since $[\hat{J}_z,\ \hat{J}_y] = -i\hbar\hat{J}_x$ and $[\hat{J}_z,\ \hat{J}_x] = i\hbar\hat{J}_y$, we have

$$[\hat{J}_z^2,\ \hat{J}_y] = \hat{J}_z[\hat{J}_z,\ \hat{J}_y] + [\hat{J}_z,\ \hat{J}_y]\hat{J}_z = -i\hbar(\hat{J}_z\hat{J}_x + \hat{J}_x\hat{J}_z) = -i\hbar(2\hat{J}_x\hat{J}_z + i\hbar\hat{J}_y). \tag{5.62}$$

The previous two expressions yield

$$\begin{aligned}[\hat{\vec{J}}^2,\ \hat{J}_y] &= [\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2,\ \hat{J}_y] = [\hat{J}_x^2,\ \hat{J}_y] + [\hat{J}_z^2,\ \hat{J}_y] \\ &= i\hbar(2\hat{J}_x\hat{J}_z + i\hbar\hat{J}_y) - i\hbar(2\hat{J}_x\hat{J}_z + i\hbar\hat{J}_y) = 0.\end{aligned} \tag{5.63}$$

Since we have

$$\hat{J}_x^2 = \frac{1}{4}(\hat{J}_+^2 + \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ + J_-^2), \qquad \hat{J}_y^2 = -\frac{1}{4}(\hat{J}_+^2 - \hat{J}_+\hat{J}_- - \hat{J}_-\hat{J}_+ + J_-^2), \tag{5.64}$$

and since $\langle j,\ m \mid \hat{J}_+^2 \mid j,\ m\rangle = \langle j,\ m \mid \hat{J}_-^2 \mid j,\ m\rangle = 0$, we can write

$$\langle j,\ m \mid \hat{J}_x^2 \mid j,\ m\rangle = \frac{1}{4}\langle j,\ m \mid \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ \mid j,\ m\rangle = \langle j,\ m \mid \hat{J}_y^2 \mid j,\ m\rangle. \tag{5.65}$$

5.4 Matrix Representation of Angular Momentum

The formalism of the previous section is general and independent of any particular representation. There are many ways to represent the angular momentum operators and their eigenstates. In this section we are going to discuss the matrix representation of angular momentum where eigenkets and operators will be represented by column vectors and square matrices, respectively. This is achieved by expanding states and operators in a discrete basis. We will see later how to represent the orbital angular momentum in the position representation.

Since $\hat{\vec{J}}^2$ and $\hat{J}_z$ commute, the set of their common eigenstates $\{\mid j,\ m\rangle\}$ can be chosen as a basis; this basis is discrete, orthonormal, and complete. For a given value of j, the orthonormalization condition for this base is given by (5.49), and the completeness condition is expressed by

$$\sum_{m=-j}^{+j} \mid j,\ m\rangle\langle j,\ m \mid = \hat{I}, \tag{5.66}$$

where $\hat{I}$ is the unit matrix. The operators $\hat{\vec{J}}^2$ and $\hat{J}_z$ are diagonal in the basis given by their joint eigenstates

$$\langle j',\ m' \mid \hat{\vec{J}}^2 \mid j,\ m\rangle = \hbar^2 j(j+1)\delta_{j',\,j}\delta_{m',\,m}, \tag{5.67}$$

$$\langle j',\ m' \mid \hat{J}_z \mid j,\ m\rangle = \hbar m\delta_{j',\,j}\delta_{m',\,m}. \tag{5.68}$$

Thus, the matrices representing $\hat{\vec{J}}^2$ and $\hat{J}_z$ in the $\{| \ j, \ m\rangle\}$ eigenbasis are diagonal, their diagonal elements being equal to $\hbar^2 j(j+1)$ and $\hbar m$, respectively.

Now since the operators $\hat{J}_\pm$ do not commute with $\hat{J}_z$, they are represented in the $\{| \ j, \ m\rangle\}$ basis by matrices that are not diagonal:

$$\boxed{\langle j', \ m' \mid \ \hat{J}_\pm \ \mid j, \ m\rangle = \hbar\sqrt{j(j+1) - m(m \pm 1)}\ \delta_{j',\,j}\delta_{m',\,m\pm 1}.} \tag{5.69}$$

We can infer the matrices of $\hat{J}_x$ and $\hat{J}_y$ from (5.57) and (5.58):

$$\begin{aligned}\langle j', \ m' \mid \hat{J}_x \mid j, \ m\rangle &= \frac{\hbar}{2}\Big[\sqrt{j(j+1) - m(m+1)}\delta_{m',\,m+1} \\ &\quad + \sqrt{j(j+1) - m(m-1)}\delta_{m',\,m-1}\Big]\delta_{j',\,j},\end{aligned} \tag{5.70}$$

$$\begin{aligned}\langle j', \ m' | \hat{J}_y \mid j, \ m\rangle &= \frac{\hbar}{2i}\Big[\sqrt{j(j+1) - m(m+1)}\delta_{m',\,m+1} \\ &\quad - \sqrt{j(j+1) - m(m-1)}\delta_{m',\,m-1}\Big]\delta_{j',\,j}.\end{aligned} \tag{5.71}$$

Example 5.3 (Angular momentum $j = 1$)

Consider the case where $j = 1$.

(a) Find the matrices representing the operators $\hat{\vec{J}}^2$, $\hat{J}_z$, $\hat{J}_\pm$, $\hat{J}_x$, and $\hat{J}_y$.

(b) Find the joint eigenstates of $\hat{\vec{J}}^2$ and $\hat{J}_z$ and verify that they form an orthonormal and complete basis.

(c) Use the matrices of $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$ to calculate $[\hat{J}_x, \ \hat{J}_y]$, $[\hat{J}_y, \ \hat{J}_z]$, and $[\hat{J}_z, \ \hat{J}_x]$.

(d) Verify that $\hat{J}_z^3 = \hbar^2 \hat{J}_z$ and $\hat{J}_\pm^3 = 0$.

Solution

(a) For $j = 1$ the allowed values of m are -1, 0, 1. The joint eigenstates of $\hat{\vec{J}}^2$ and $\hat{J}_z$ are $| \ 1, \ -1\rangle$, $| \ 1, \ 0\rangle$, and $| \ 1, \ 1\rangle$. The matrix representations of the operators $\hat{\vec{J}}^2$ and $\hat{J}_z$ can be inferred from (5.67) and (5.68):

$$\begin{aligned}\hat{\vec{J}}^2 &= \begin{pmatrix} \langle 1, \ 1 \mid \hat{\vec{J}}^2 \mid 1, \ 1\rangle & \langle 1, \ 1 \mid \hat{\vec{J}}^2 \mid 1, \ 0\rangle & \langle 1, \ 1 \mid \hat{\vec{J}}^2 \mid 1, \ -1\rangle \\ \langle 1, \ 0 \mid \hat{\vec{J}}^2 \mid 1, \ 1\rangle & \langle 1, \ 0 \mid \hat{\vec{J}}^2 \mid 1, \ 0\rangle & \langle 1, \ 0 \mid \hat{\vec{J}}^2 \mid 1, \ -1\rangle \\ \langle 1, \ -1 \mid \hat{\vec{J}}^2 \mid 1, \ 1\rangle & \langle 1, \ -1 \mid \hat{\vec{J}}^2 \mid 1, \ 0\rangle & \langle 1, \ -1 \mid \hat{\vec{J}}^2 \mid 1, \ -1\rangle \end{pmatrix} \\ &= 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\end{aligned} \tag{5.72}$$

$$\hat{J}_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{5.73}$$

Similarly, using (5.69), we can ascertain that the matrices of $\hat{J}_+$ and $\hat{J}_-$ are given by

$$\hat{J}_- = \hbar\sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \hat{J}_+ = \hbar\sqrt{2} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}. \tag{5.74}$$

The matrices for $\hat{J}_x$ and $\hat{J}_y$ in the $\{|\ j,\ m\rangle\}$ basis result immediately from the relations $\hat{J}_x = (\hat{J}_+ + \hat{J}_-)/2$ and $\hat{J}_y = i(\hat{J}_- - \hat{J}_+)/2$:

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \qquad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \tag{5.75}$$

(b) The joint eigenvectors of $\hat{\vec{J}}^2$ and $\hat{J}_z$ can be obtained as follows. The matrix equation of $\hat{J}_z \mid j,\ m\rangle = m\hbar \mid j,\ m\rangle$ is

$$\hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = m\hbar\begin{pmatrix} a \\ b \\ c \end{pmatrix} \quad \Longrightarrow \quad \begin{array}{c} \hbar a = m\hbar a \\ 0 = m\hbar b \\ -\hbar c = m\hbar c \end{array}. \tag{5.76}$$

The normalized solutions to these equations for $m = 1, 0, -1$ are respectively given by $a = 1$, $b = c = 0$; $a = 0, b = 1, c = 0$; and $a = b = 0, c = 1$; that is,

$$\mid 1,\ 1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \qquad \mid 1,\ 0\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \qquad \mid 1,\ -1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \tag{5.77}$$

We can verify that these vectors are orthonormal:

$$\langle 1,\ m' \mid 1,\ m\rangle = \delta_{m',\,m} \qquad (m', m = -1, 0, 1). \tag{5.78}$$

We can also verify that they are complete:

$$\begin{aligned} \sum_{m=-1}^{1} \mid 1,\ m\rangle\langle 1,\ m| &= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}(0\ 0\ 1) + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}(0\ 1\ 0) + \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}(1\ 0\ 0) \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \end{aligned} \tag{5.79}$$

(c) Using the matrices (5.75) we have

$$\hat{J}_x\hat{J}_y = \frac{\hbar^2}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} = \frac{\hbar^2}{2}\begin{pmatrix} i & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & -i \end{pmatrix}, \tag{5.80}$$

$$\hat{J}_y\hat{J}_x = \frac{\hbar^2}{2}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = \frac{\hbar^2}{2}\begin{pmatrix} -i & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & i \end{pmatrix}; \tag{5.81}$$

hence

$$\hat{J}_x\hat{J}_y - \hat{J}_y\hat{J}_x = \frac{\hbar^2}{2}\begin{pmatrix} 2i & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2i \end{pmatrix} = i\hbar^2\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = i\hbar J_z, \tag{5.82}$$

where the matrix of $\hat{J}_z$ is given by (5.73). A similar calculation leads to $[\hat{J}_y,\ \hat{J}_z] = i\hbar\hat{J}_x$ and $[\hat{J}_z,\ \hat{J}_x] = i\hbar\hat{J}_y$.

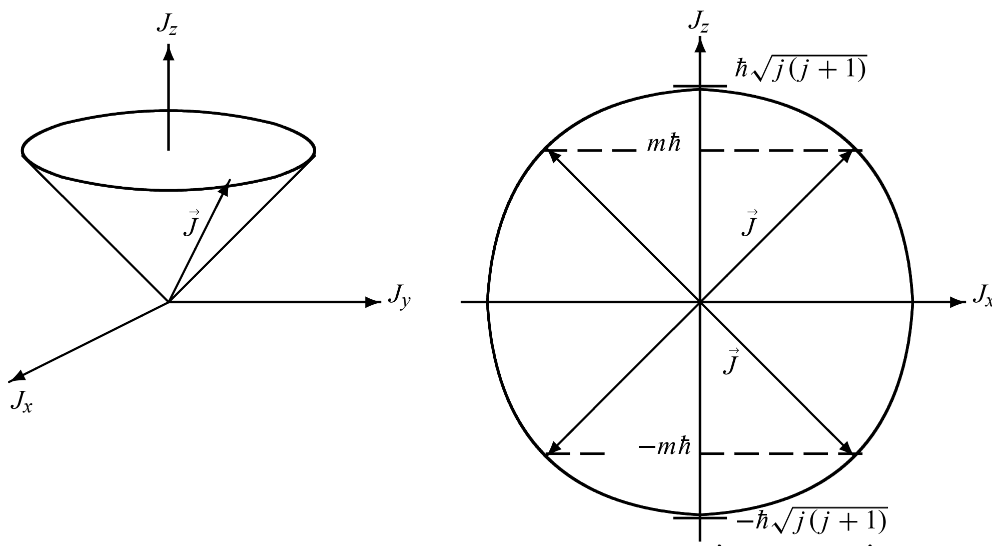

Figure 5.1 Geometrical representation of the angular momentum $\hat{\vec{J}}$: the vector $\hat{\vec{J}}$ rotates along the surface of a cone about its axis; the cone's height is equal to $m\hbar$, the projection of $\hat{\vec{J}}$ on the cone's axis. The tip of $\hat{\vec{J}}$ lies, within the $J_z J_{xy}$ plane, on a circle of radius $\hbar\sqrt{j(j+1)}$.

(d) The calculation of $\hat{J}_z^3$ and $\hat{J}_\pm^3$ is straightforward:

$$\hat{J}_z^3 = \hbar^3 \left[\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \right]^3 = \hbar^3 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \hbar^2 \hat{J}_z, \tag{5.83}$$

$$\hat{J}_+^3 = 2\hbar^3\sqrt{2} \left[\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \right]^3 = 2\hbar^3\sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0, \tag{5.84}$$

and

$$\hat{J}_-^3 = 2\hbar^3\sqrt{2} \left[\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \right]^3 = 2\hbar^3\sqrt{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = 0. \tag{5.85}$$

5.5 Geometrical Representation of Angular Momentum

At issue here is the relationship between the angular momentum and its z-component; this relation can be represented geometrically as follows. For a fixed value of j, the total angular momentum $\hat{\vec{J}}$ may be represented by a vector whose length, as displayed in Figure 5.1, is given by $\sqrt{\langle \hat{\vec{J}}^2 \rangle} = \hbar\sqrt{j(j+1)}$ and whose z-component is $\langle \hat{J}_z \rangle = \hbar m$. Since $\hat{J}_x$ and $\hat{J}_y$ are separately undefined, only their sum $\hat{J}_x^2 + \hat{J}_y^2 = \vec{J}^2 - \hat{J}_z^2$, which lies within the xy plane, is well defined.

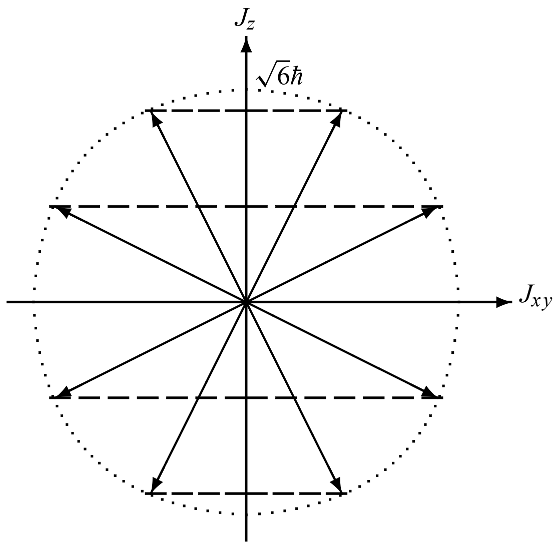

Figure 5.2 Graphical representation of the angular momentum $j = 2$ for the state $\mid 2,\ m\rangle$ with $m = -2, -1, 0, 1, 2$. The radius of the circle is $\hbar\sqrt{2(2+1)} = \sqrt{6}\hbar$.

In classical terms, we can think of $\vec{J}$ as representable graphically by a vector, whose endpoint lies on a circle of radius $\hbar\sqrt{j(j+1)}$, rotating along the surface of a cone of half-angle

$$\theta = \cos^{-1}\left(\frac{m}{\sqrt{j(j+1)}}\right), \tag{5.86}$$

such that its projection along the z-axis is always $m\hbar$. Notice that, as the values of the quantum number m are limited to $m = -j, -j+1, \ldots, j-1, j$, the angle θ is quantized; the only possible values of θ consist of a discrete set of $2j+1$ values:

$$\begin{aligned} \theta \quad = \quad & \cos^{-1}\left(\frac{-j}{\sqrt{j(j+1)}}\right),\ \cos^{-1}\left(\frac{-j+1}{\sqrt{j(j+1)}}\right),\ \ldots,\ \cos^{-1}\left(\frac{j-1}{\sqrt{j(j+1)}}\right), \\ & \cos^{-1}\left(\frac{j}{\sqrt{j(j+1)}}\right). \end{aligned} \tag{5.87}$$

Since all orientations of $\hat{\vec{J}}$ on the surface of the cone are equally likely, the projection of $\hat{\vec{J}}$ on both the x and y axes average out to zero:

$$\langle \hat{J}_x \rangle = \langle \hat{J}_y \rangle = 0, \tag{5.88}$$

where $\langle \hat{J}_x \rangle$ stands for $\langle j,\ m \mid \hat{J}_x \mid j,\ m\rangle$.

As an example, Figure 5.2 shows the graphical representation for the $j = 2$ case. As specified in (5.87), θ takes only a discrete set of values. In this case where $j = 2$, the angle θ takes only five values corresponding respectively to $m = -2,\ -1,\ 0,\ 1,\ 2$; they are given by

$$\theta = -35.26^\circ,\ -65.91^\circ,\ 90^\circ,\ 65.91^\circ,\ 35.26^\circ. \tag{5.89}$$

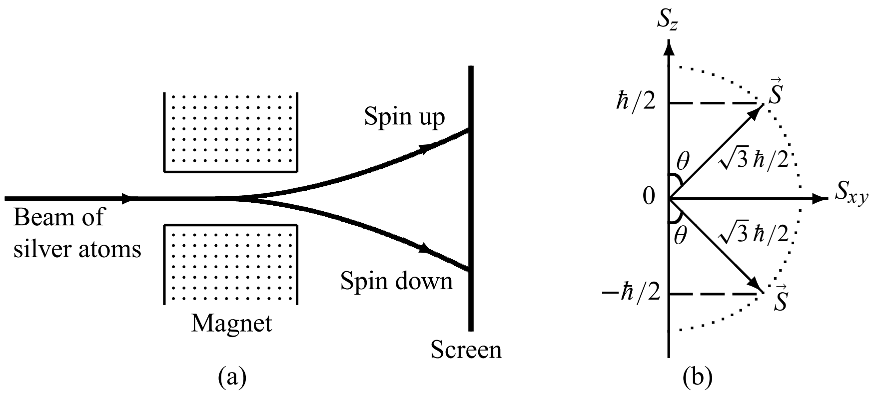

Figure 5.3 (a) Stern–Gerlach experiment: when a beam of silver atoms passes through an inhomogeneous magnetic field, it splits into two distinct components corresponding to spin-up and spin-down. (b) Graphical representation of spin $\frac{1}{2}$: the tip of $\vec{S}$ lies on a circle of radius $|\vec{S}| = \sqrt{3}\hbar/2$ so that its projection on the z-axis takes only two values, $\pm\hbar/2$, with $\theta = 54.73°$.

5.6 Spin Angular Momentum

5.6.1 Experimental Evidence of the Spin

The existence of spin was confirmed experimentally by Stern and Gerlach in 1922 using silver (Ag) atoms. Silver has 47 electrons; 46 of them form a spherically symmetric charge distribution and the 47th electron occupies a 5s orbital. If the silver atom were in its ground state, its total orbital angular momentum would be zero: $l = 0$ (since the fifth shell electron would be in a 5s state). In the Stern–Gerlach experiment, a beam of silver atoms passes through an inhomogeneous (nonuniform) magnetic field. If, for argument's sake, the field were along the z-direction, we would expect classically to see on the screen a *continuous* band that is symmetric about the undeflected direction, $z = 0$. According to Schrödinger's wave theory, however, if the atoms had an orbital angular momentum l, we would expect the beam to split into an *odd* (*discrete*) number of $2l + 1$ components. Suppose the beam's atoms were in their ground state $l = 0$, there would be only one spot on the screen, and if the fifth shell electron were in a 5p state ($l = 1$), we would expect to see three spots. Experimentally, however, the beam behaves according to the predictions of neither classical physics nor Schrödinger's wave theory. Instead, *it splits into two distinct components* as shown in Figure 5.3a. This result was also observed for hydrogen atoms in their ground state ($l = 0$), where no splitting is expected.

To solve this puzzle, Goudsmit and Uhlenbeck postulated in 1925 that, in addition to its orbital angular momentum, the electron possesses an *intrinsic* angular momentum which, unlike the orbital angular momentum, has nothing to do with the spatial degrees of freedom. By analogy with the motion of the Earth, which consists of an orbital motion around the Sun and an internal rotational or *spinning* motion about its axis, the electron or, for that matter, any other microscopic particle may also be considered to have some sort of internal or intrinsic spinning motion. This intrinsic degree of freedom was given the suggestive name of *spin* angular momentum. One has to keep in mind, however, that the electron remains thus far a structureless or pointlike particle; hence caution has to be exercised when trying to link the electron's spin to an internal spinning motion. The spin angular momentum of a particle does not depend on

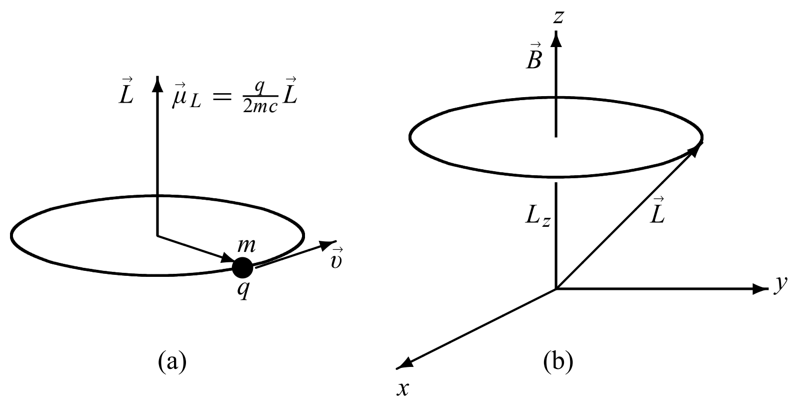

Figure 5.4 (a) Orbital magnetic dipole moment of a positive charge q. (b) When an external magnetic field is applied, the orbital magnetic moment precesses about it.

its spatial degrees of freedom. The spin, an intrinsic degree of freedom, is a purely quantum mechanical concept with no classical analog. Unlike the orbital angular momentum, *the spin cannot be described by a differential operator*.

From the classical theory of electromagnetism, an *orbital magnetic dipole moment* is generated with the orbital motion of a particle of charge q:

$$\vec{\mu}_L = \frac{q}{2mc}\vec{L}, \tag{5.90}$$

where $\vec{L}$ is the orbital angular momentum of the particle, m is its mass, and c is the speed of light. As shown in Figure 5.4a, if the charge q is positive, $\vec{\mu}_L$ and $\vec{L}$ will be in the same direction; for a negative charge such as an electron ($q = -e$), the magnetic dipole moment $\vec{\mu}_L = -e\vec{L}/(2m_e c)$ and the orbital angular momentum will be in opposite directions. Similarly, if we follow a classical analysis and picture the electron as a spinning spherical charge, then we obtain an intrinsic or *spin magnetic dipole moment* $\vec{\mu}_S = -e\vec{S}/(2m_e c)$. This classical derivation of $\vec{\mu}_S$ is quite erroneous, since the electron cannot be viewed as a spinning sphere; in fact, it turns out that the electron's spin magnetic moment is twice its classical expression. Although the spin magnetic moment cannot be derived classically, as we did for the orbital magnetic moment, it can still be postulated by analogy with (5.90):

$$\vec{\mu}_S = -g_s \frac{e}{2m_e c}\vec{S}, \tag{5.91}$$

where g_s is called the Landé factor or the gyromagnetic ratio of the electron; its experimental value is $g_s \simeq 2$ (this factor can be calculated using Dirac's relativistic theory of the electron).

When the electron is placed in a magnetic field $\vec{B}$ and if the field is inhomogeneous, a force will be exerted on the electron's intrinsic dipole moment; the direction and magnitude of the force depend on the relative orientation of the field and the dipole. This force tends to align $\vec{\mu}_S$ along $\vec{B}$, producing a precessional motion of $\vec{\mu}_S$ around $\vec{B}$ (Figure 5.4b). For instance, if $\vec{\mu}_S$ is parallel to $\vec{B}$, the electron will move in the direction in which the field increases; conversely, if $\vec{\mu}_S$ is antiparallel to $\vec{B}$, the electron will move in the direction in which the field decreases. For hydrogen-like atoms (such as silver) that are in the ground state, the orbital angular momentum will be zero; hence the dipole moment of the atom will be entirely due to the spin of the electron.

The atomic beam will therefore deflect according to the orientation of the electron's spin. Since, experimentally, the beam splits into two components, the electron's spin must have only two possible orientations relative to the magnetic field, either parallel or antiparallel.

By analogy with the orbital angular momentum of a particle, which is characterized by two quantum numbers—the orbital number l and the azimuthal number m_l (with $m_l = -l, -l+1, \ldots, l-1, l$)—the spin angular momentum is also characterized by two quantum numbers, the spin s and its projection m_s on the z-axis (the direction of the magnetic field), where $m_s = -s, -s+1, \ldots, s-1, s$. Since only two components were observed in the Stern–Gerlach experiment, we must have $2s + 1 = 2$. The quantum numbers for the electron must then be given by $s = \frac{1}{2}$ and $m_s = \pm\frac{1}{2}$.

In nature it turns out that every fundamental particle has a specific spin. Some particles have integer spins $s = 0, 1, 2, \ldots$ (the pi mesons have spin $s = 0$, the photons have spin $s = 1$, and so on) and others have half-odd-integer spins $s = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$ (the electrons, protons, and neutrons have spin $s = \frac{1}{2}$, the deltas have spin $s = \frac{3}{2}$, and so on). We will see in Chapter 8 that particles with *half-odd-integer* spins are called *fermions* (quarks, electrons, protons, neutrons, etc.) and those with *integer* spins are called *bosons* (pions, photons, gravitons, etc.).

Besides confirming the existence of spin and measuring it, the Stern–Gerlach experiment offers a number of other important uses to quantum mechanics. First, by showing that a beam splits into a *discrete* set of components rather than a continuous band, it provides additional confirmation for the quantum hypothesis on the discrete character of the microphysical world. The Stern–Gerlach experiment also turns out to be an invaluable technique for preparing a quantum state. Suppose we want to prepare a beam of spin-up atoms; we simply pass an unpolarized beam through an inhomogeneous magnet, then collect the desired component and discard (or block) the other. The Stern–Gerlach experiment can also be used to determine the total angular momentum of an atom which, in the case where $l \neq 0$, is given by the sum of the orbital and spin angular momenta: $\vec{J} = \vec{L} + \vec{S}$. The addition of angular momenta is covered in Chapter 7.

5.6.2 General Theory of Spin

The theory of spin is identical to the general theory of angular momentum (Section 5.3). By analogy with the vector angular momentum $\hat{\vec{J}}$, the spin is also represented by a vector operator $\hat{\vec{S}}$ whose components $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$ obey the same commutation relations as $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$:

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z, \qquad [\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x, \qquad [\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y. \tag{5.92}$$

In addition, $\hat{\vec{S}}^2$ and $\hat{S}_z$ commute; hence they have common eigenvectors:

$$\hat{\vec{S}}^{\,2} \mid s,\ m_s\rangle = \hbar^2 s(s+1) \mid s,\ m_s\rangle, \qquad \hat{S}_z \mid s,\ m_s\rangle = \hbar m_s \mid s,\ m_s\rangle, \tag{5.93}$$

where $m_s = -s, -s+1, \ldots, -s+1, s$. Similarly, we have

$$\hat{S}_\pm \mid s,\ m_s\rangle = \hbar\sqrt{s(s+1) - m_s(m_s \pm 1)}\ \mid s,\ m_s \pm 1\rangle, \tag{5.94}$$

where $\hat{S}_\pm = \hat{S}_x \pm i\hat{S}_y$, and

$$\langle \hat{S}_x^2\rangle = \langle \hat{S}_y^2\rangle = \frac{1}{2}(\langle \hat{\vec{S}}^2\rangle - \langle \hat{S}_z^2\rangle) = \frac{\hbar^2}{2}\left[s(s+1) - m_s^2\right], \tag{5.95}$$

where $\langle \hat{A} \rangle$ denotes $\langle \hat{A} \rangle = \langle s,\ m_s | \hat{A} \mid s,\ m_s \rangle$.

The spin states form an orthonormal and complete basis

$$\langle s',\ m'_s \mid s,\ m_s \rangle = \delta_{s',\,s}\delta_{m'_s,\,m_s}, \qquad \sum_{m_s=-s}^{s} \mid s,\ m_s \rangle \langle s,\ m_s \mid = I, \tag{5.96}$$

where I is the unit matrix.

5.6.3 Spin $1/2$ and the Pauli Matrices

For a particle with spin $\frac{1}{2}$ the quantum number m_s takes only two values: $m_s = -\frac{1}{2}$ and $\frac{1}{2}$. The particle can thus be found in either of the following two states: $\mid s,\ m_s \rangle = \left| \frac{1}{2},\ \frac{1}{2} \right\rangle$ and $\left| \frac{1}{2},\ -\frac{1}{2} \right\rangle$. The eigenvalues of $\hat{\vec{S}}^{\,2}$ and $\hat{S}_z$ are given by

$$\hat{\vec{S}}^2 \left| \frac{1}{2},\ \pm\frac{1}{2} \right\rangle = \frac{3}{4}\hbar^2 \left| \frac{1}{2},\ \pm\frac{1}{2} \right\rangle, \qquad \hat{S}_z \left| \frac{1}{2},\ \pm\frac{1}{2} \right\rangle = \pm\frac{\hbar}{2} \left| \frac{1}{2},\ \pm\frac{1}{2} \right\rangle. \tag{5.97}$$

Hence the spin may be represented graphically, as shown in Figure 5.3b, by a vector of length $|\vec{S}| = \sqrt{3}\hbar/2$, whose endpoint lies on a circle of radius $\sqrt{3}\hbar/2$, rotating along the surface of a cone with half-angle

$$\theta = \cos^{-1}\left(\frac{|m_s|}{\sqrt{s(s+1)}}\right) = \cos^{-1}\left(\frac{\hbar/2}{\sqrt{3}\hbar/2}\right) = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right) = 54.73^\circ. \tag{5.98}$$

The projection of $\hat{\vec{S}}$ on the z-axis is restricted to two values only: $\pm\hbar/2$ corresponding to spin-up and spin-down.

Let us now study the matrix representation of the spin $s = \frac{1}{2}$. Using (5.67) and (5.68) we can represent the operators $\hat{\vec{S}}^2$ and $\hat{S}_z$ within the $\{|s,\ m_s\rangle\}$ basis by the following matrices:

$$\hat{\vec{S}}^2 = \begin{pmatrix} \langle \frac{1}{2},\ \frac{1}{2} \mid \hat{\vec{S}}^2 \mid \frac{1}{2},\ \frac{1}{2} \rangle & \langle \frac{1}{2},\ \frac{1}{2} \mid \hat{\vec{S}}^2 \mid \frac{1}{2},\ -\frac{1}{2} \rangle \\ \langle \frac{1}{2},\ -\frac{1}{2} \mid \hat{\vec{S}}^2 \mid \frac{1}{2},\ \frac{1}{2} \rangle & \langle \frac{1}{2},\ -\frac{1}{2} \mid \hat{\vec{S}}^2 | \frac{1}{2},\ -\frac{1}{2} \rangle \end{pmatrix} = \frac{3\hbar^2}{4}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{5.99}$$

$$\hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.100}$$

The matrices of $\hat{S}_+$ and $\hat{S}_-$ can be inferred from (5.69):

$$\hat{S}_+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad \hat{S}_- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{5.101}$$

and since $\hat{S}_x = \frac{1}{2}(\hat{S}_+ + \hat{S}_-)$ and $\hat{S}_y = \frac{i}{2}(\hat{S}_- - \hat{S}_+)$, we have

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{5.102}$$

The joint eigenvectors of $\hat{\vec{S}}^2$ and $\hat{S}_z$ are expressed in terms of two-element column matrices, known as *spinors*:

$$\left| \frac{1}{2},\ \frac{1}{2} \right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad \left| \frac{1}{2},\ -\frac{1}{2} \right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{5.103}$$

It is easy to verify that these eigenvectors form a basis that is complete,

$$\sum_{m_s=-\frac{1}{2}}^{\frac{1}{2}} \left|\frac{1}{2},\ m_s\right\rangle\left\langle\frac{1}{2},\ m_s\right| = \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0\ \ 1) + \begin{pmatrix} 1 \\ 0 \end{pmatrix}(1\ \ 0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{5.104}$$

and orthonormal,

$$\left\langle\frac{1}{2},\ \frac{1}{2}\ \middle|\ \frac{1}{2},\ \frac{1}{2}\right\rangle = (1\ \ 0)\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 1, \tag{5.105}$$

$$\left\langle\frac{1}{2},\ -\frac{1}{2}\ \middle|\ \frac{1}{2},\ -\frac{1}{2}\right\rangle = (0\ \ 1)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 1, \tag{5.106}$$

$$\left\langle\frac{1}{2},\ \frac{1}{2}\ \middle|\ \frac{1}{2},\ -\frac{1}{2}\right\rangle = \left\langle\frac{1}{2},\ -\frac{1}{2}\ \middle|\ \frac{1}{2},\ \frac{1}{2}\right\rangle = 0. \tag{5.107}$$

Let us now find the eigenvectors of $\hat{S}_x$ and $\hat{S}_y$. First, note that the basis vectors $|s,\ m_s\rangle$ are eigenvectors of neither $\hat{S}_x$ nor $\hat{S}_y$; their eigenvectors can, however, be expressed in terms of $|s,\ m_s\rangle$ as follows:

$$|\ \psi_x\rangle_\pm = \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\ \frac{1}{2}\right\rangle \pm \left|\frac{1}{2},\ -\frac{1}{2}\right\rangle\right], \tag{5.108}$$

$$|\ \psi_y\rangle_\pm = \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2},\ \frac{1}{2}\right\rangle \pm i\left|\frac{1}{2},\ -\frac{1}{2}\right\rangle\right]. \tag{5.109}$$

The eigenvalue equations for $\hat{S}_x$ and $\hat{S}_y$ are thus given by

$$\hat{S}_x\ |\ \psi_x\rangle_\pm = \pm\frac{\hbar}{2}\ |\ \psi_x\rangle_\pm, \qquad \hat{S}_y\ |\ \psi_y\rangle_\pm = \pm\frac{\hbar}{2}\ |\ \psi_y\rangle_\pm. \tag{5.110}$$

Pauli matrices

When $s = \frac{1}{2}$ it is convenient to introduce the *Pauli matrices* σ_x, σ_y, σ_z, which are related to the spin vector as follows:

$$\hat{\vec{S}} = \frac{\hbar}{2}\vec{\sigma}. \tag{5.111}$$

Using this relation along with (5.100) and (5.102), we have

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.112}$$

These matrices satisfy the following two properties:

$$\sigma_j^2 = \hat{I} \qquad (j = x, y, z), \tag{5.113}$$

$$\sigma_j\sigma_k + \sigma_k\sigma_j = 0 \qquad (j \neq k), \tag{5.114}$$

where the subscripts j and k refer to x, y, z, and $\hat{I}$ is the 2×2 unit matrix. These two equations are equivalent to the anticommutation relation

$$\left\{\sigma_j, \sigma_k\right\} = 2\hat{I}\delta_{j,k}. \tag{5.115}$$

We can verify that the Pauli matrices satisfy the commutation relations

$$[\sigma_j, \sigma_k] = 2i\, \varepsilon_{jkl}\sigma_l, \tag{5.116}$$

where ε_{jkl} is the antisymmetric tensor (also known as the Levi–Civita tensor)

$$\varepsilon_{jkl} = \begin{cases} 1 & \text{if } jkl \text{ is an even permutation of } x, y, z, \\ -1 & \text{if } jkl \text{ is an odd permutation of } x, y, z, \\ 0 & \text{if any two indices among } j, k, l \text{ are equal.} \end{cases} \tag{5.117}$$

We can condense the relations (5.113), (5.114), and (5.116) into

$$\sigma_j \sigma_k = \delta_{j,k} + i \sum_l \varepsilon_{jkl}\sigma_l. \tag{5.118}$$

Using this relation we can verify that, for any two vectors $\vec{A}$ and $\vec{B}$ which commute with $\vec{\sigma}$, we have

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = (\vec{A} \cdot \vec{B})\hat{I} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B}), \tag{5.119}$$

where $\hat{I}$ is the unit matrix. The Pauli matrices are Hermitian, traceless, and have determinants equal to -1:

$$\sigma_j^\dagger = \sigma_j, \qquad \text{Tr}(\sigma_j) = 0, \qquad \det(\sigma_j) = -1 \qquad (j = x,\ y,\ z). \tag{5.120}$$

Using the relation $\sigma_x \sigma_y = i\sigma_z$ along with $\sigma_z^2 = \hat{I}$, we obtain

$$\sigma_x \sigma_y \sigma_z = i\hat{I}. \tag{5.121}$$

From the commutation relations (5.116) we can show that

$$e^{i\alpha\sigma_j} = I\cos\alpha + i\sigma_j \sin\alpha \qquad (j = x, y, z), \tag{5.122}$$

where I is the unit matrix and α is an arbitrary real constant.

Remarks

- Since the spin does not depend on the spatial degrees of freedom, the components $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_z$ of the spin operator commute with all the spatial operators, notably the orbital angular momentum $\hat{\vec{L}}$, the position and the momentum operators $\hat{\vec{R}}$ and $\hat{\vec{P}}$:

$$[\hat{S}_j,\ \hat{L}_k] = 0, \qquad [\hat{S}_j,\ \hat{R}_k] = 0, \qquad [\hat{S}_j,\ \hat{P}_k] = 0 \qquad (j, k = x, y, z). \tag{5.123}$$

- The total wave function $\mid \Psi\rangle$ of a system with spin consists of a product of two parts: a spatial part $\psi(\vec{r})$ and a spin part $\mid s,\ m_s\rangle$:

$$\mid \Psi\rangle = \mid \psi\rangle \mid s,\ m_s\rangle. \tag{5.124}$$

  This product of the space and spin degrees of freedom is not a product in the usual sense, but a direct or tensor product as discussed in Chapter 7. We will show in Chapter 6 that the four quantum numbers n, l, m_l, and m_s are required to completely describe the state of an electron moving in a central field; its wave function is

$$\Psi_{nlm_lm_s}(\vec{r}) = \psi_{nlm_l}(\vec{r}) \mid s,\ m_s\rangle. \tag{5.125}$$

Since the spin operator does not depend on the spatial degrees of freedom, it acts only on the spin part $\mid s,\ m_s\rangle$ and leaves the spatial wave function, $\psi_{nlm_l}(\vec{r})$, unchanged; conversely, the spatial operators $\hat{\vec{L}}$, $\hat{\vec{R}}$, and $\hat{\vec{P}}$ act on the spatial part and not on the spin part. For spin $\frac{1}{2}$ particles, the total wave function corresponding to spin-up and spin-down cases are respectively expressed in terms of the spinors:

$$\Psi_{nlm_l\frac{1}{2}}(\vec{r}) = \psi_{nlm_l}(\vec{r})\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \psi_{nlm_l}(\vec{r}) \\ 0 \end{pmatrix}, \tag{5.126}$$

$$\Psi_{nlm_l-\frac{1}{2}}(\vec{r}) = \psi_{nlm_l}(\vec{r})\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ \psi_{nlm_l}(\vec{r}) \end{pmatrix}. \tag{5.127}$$

Example 5.4
Find the energy levels of a spin $s = \frac{3}{2}$ particle whose Hamiltonian is given by

$$\hat{H} = \frac{\alpha}{\hbar^2}(\hat{S}_x^2 + \hat{S}_y^2 - 2\hat{S}_z^2) - \frac{\beta}{\hbar}\hat{S}_z;$$

α and β are constants. Are these levels degenerate?

Solution
Rewriting $\hat{H}$ in the form,

$$\hat{H} = \frac{\alpha}{\hbar^2}\left(\hat{\vec{S}}^2 - 3\hat{S}_z^2\right) - \frac{\beta}{\hbar}\hat{S}_z, \tag{5.128}$$

we see that $\hat{H}$ is diagonal in the $\{|s,\ m\rangle\}$ basis:

$$E_m = \langle s,\ m \mid \hat{H} \mid s,\ m\rangle = \frac{\alpha}{\hbar^2}\left[\hbar^2 s(s+1) - 3\hbar^2 m^2\right] - \frac{\beta}{\hbar}\hbar m = \frac{15}{4}\alpha - m(3\alpha m + \beta), \tag{5.129}$$

where the quantum number m takes any of the four values $m = -\frac{3}{2},\ -\frac{1}{2},\ \frac{1}{2},\ \frac{3}{2}$. Since E_m depends on m, the energy levels of this particle are nondegenerate.

5.7 Eigenfunctions of Orbital Angular Momentum

We now turn to the coordinate representation of the angular momentum. In this section, we are going to work within the spherical coordinate system. Let us denote the joint eigenstates of $\hat{\vec{L}}^2$ and $\hat{L}_z$ by $\mid l,\ m\rangle$:

$$\boxed{\hat{\vec{L}}^2 \mid l,\ m\rangle = \hbar^2 l(l+1) \mid l,\ m\rangle,} \tag{5.130}$$

$$\boxed{\hat{L}_z \mid l,\ m\rangle = \hbar m \mid l,\ m\rangle.} \tag{5.131}$$

The operators $\hat{L}_z$, $\hat{\vec{L}}^2$, $\hat{L}_\pm$, whose Cartesian components are listed in Eqs (5.3) to (5.5), can be expressed in terms of spherical coordinates (Appendix B) as follows:

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}, \tag{5.132}$$

$$\hat{\vec{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right], \tag{5.133}$$

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y = \pm\hbar e^{\pm i\varphi}\left[\frac{\partial}{\partial\theta}\pm i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right]. \tag{5.134}$$

Since the operators $\hat{L}_z$ and $\hat{\vec{L}}$ depend only on the angles θ and φ, their eigenstates depend only on θ and φ. Denoting their joint eigenstates by

$$\boxed{\langle\theta\varphi \mid l,\ m\rangle = Y_{lm}(\theta,\varphi),} \tag{5.135}$$

where[1] $Y_{lm}(\theta,\varphi)$ are continuous functions of θ and φ, we can rewrite the eigenvalue equations (5.130) and (5.131) as follows:

$$\boxed{\hat{\vec{L}}^2 Y_{lm}(\theta,\varphi) = \hbar^2 l(l+1)Y_{lm}(\theta,\varphi),} \tag{5.136}$$

$$\boxed{\hat{L}_z Y_{lm}(\theta,\varphi) = m\hbar Y_{lm}(\theta,\varphi).} \tag{5.137}$$

Since $\hat{L}_z$ depends only on φ, as shown in (5.132), the previous two equations suggest that the eigenfunctions $Y_{lm}(\theta,\varphi)$ are separable:

$$Y_{lm}(\theta,\varphi) = \Theta_{lm}(\theta)\Phi_m(\varphi). \tag{5.138}$$

We ascertain that

$$\boxed{\hat{L}_\pm Y_{lm}(\theta,\varphi) = \hbar\sqrt{l(l+1)-m(m\pm 1)}\ Y_{l\ m\pm1}(\theta,\varphi).} \tag{5.139}$$

5.7.1 Eigenfunctions and Eigenvalues of $\hat{L}_z$

Inserting (5.138) into (5.137) we obtain $\hat{L}_z\Theta_{lm}(\theta)\Phi_m(\varphi) = m\hbar\Theta_{lm}(\theta)\Phi_m(\varphi)$. Now since $\hat{L}_z = -i\hbar\partial/\partial\varphi$, we have

$$-i\hbar\Theta_{lm}(\theta)\frac{\partial\Phi_m(\varphi)}{\partial\varphi} = m\hbar\Theta_{lm}(\theta)\Phi_m(\varphi), \tag{5.140}$$

which reduces to

$$-i\frac{\partial\Phi_m(\varphi)}{\partial\varphi} = m\Phi_m(\varphi). \tag{5.141}$$

The normalized solutions of this equation are given by

$$\Phi_m(\varphi) = \frac{1}{\sqrt{2\pi}}e^{im\varphi}, \tag{5.142}$$

[1] For notational consistency throughout this text, we will insert a comma between l and m in $Y_{lm}(\theta,\varphi)$ whenever m is negative.

where $1/\sqrt{2\pi}$ is the normalization constant,

$$\int_0^{2\pi} d\varphi\, \Phi^*_{m'}(\varphi)\Phi_m(\varphi) = \delta_{m',\,m}. \tag{5.143}$$

For $\Phi_m(\varphi)$ to be single-valued, it must be periodic in φ with period 2π, $\Phi_m(\varphi+2\pi) = \Phi_m(\varphi)$; hence

$$e^{im(\varphi+2\pi)} = e^{im\varphi}. \tag{5.144}$$

This relation shows that the expectation value of $\hat{L}_z$, $l_z = \langle l,\ m \mid \hat{L}_z \mid l\ m\rangle$, is restricted to a *discrete* set of values

$$l_z = m\hbar, \qquad m = 0, \pm 1, \pm 2, \pm 3, \ldots. \tag{5.145}$$

Thus, the values of m vary from $-l$ to l:

$$m = -l, -(l-1), -(l-2), \ldots, 0, 1, 2, \ldots, l-2, l-1, l. \tag{5.146}$$

Hence the quantum number l must also be an integer. This is expected since the orbital angular momentum must have integer values.

5.7.2 Eigenfunctions of $\hat{\vec{L}}^2$

Let us now focus on determining the eigenfunctions $\Theta_{lm}(\theta)$ of $\hat{\vec{L}}^2$. We are going to follow two methods. The first method involves differential equations and gives $\Theta_{lm}(\theta)$ in terms of the well-known associated Legendre functions. The second method is algebraic; it deals with the operators $\hat{L}_\pm$ and enables an explicit construction of $Y_{lm}(\theta, \varphi)$, the spherical harmonics.

5.7.2.1 First Method for Determining the Eigenfunctions of $\hat{\vec{L}}^2$

We begin by applying $\hat{\vec{L}}^2$ of (5.133) to the eigenfunctions

$$Y_{lm}(\theta, \varphi) = \frac{1}{\sqrt{2\pi}}\Theta_{lm}(\theta)e^{im\varphi}. \tag{5.147}$$

This gives

$$\begin{aligned}\hat{\vec{L}}^2 Y_{lm}(\theta, \varphi) &= \frac{-\hbar^2}{\sqrt{2\pi}}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]\Theta_{lm}(\theta)e^{im\varphi}\\ &= \frac{\hbar^2 l(l+1)}{\sqrt{2\pi}}\Theta_{lm}(\theta)e^{im\varphi},\end{aligned} \tag{5.148}$$

which, after eliminating the φ-dependence, reduces to

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta_{lm}(\theta)}{d\theta}\right) + \left[l(l+1) - \frac{m^2}{\sin^2\theta}\right]\Theta_{lm}(\theta) = 0. \tag{5.149}$$

This equation is known as the *Legendre differential equation*. Its solutions can be expressed in terms of the *associated Legendre functions* $P_l^m(\cos\theta)$:

$$\Theta_{lm}(\theta) = C_{lm}P_l^m(\cos\theta), \tag{5.150}$$

which are defined by

$$P_l^m(x) = (1-x^2)^{|m|/2}\frac{d^{|m|}}{dx^{|m|}}P_l(x). \tag{5.151}$$

This shows that

$$P_l^{-m}(x) = P_l^m(x), \tag{5.152}$$

where $P_l(x)$ is the lth *Legendre polynomial* which is defined by the *Rodrigues formula*

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l. \tag{5.153}$$

We can obtain at once the first few Legendre polynomials:

$$P_0(x) = 1, \qquad P_1(x) = \frac{1}{2}\frac{d(x^2-1)}{dx} = x, \tag{5.154}$$

$$P_2(x) = \frac{1}{8}\frac{d^2(x^2-1)^2}{dx^2} = \frac{1}{2}(3x^2-1), \qquad P_3(x) = \frac{1}{48}\frac{d^3(x^2-1)^3}{dx^3} = \frac{1}{2}(5x^3-3x), \tag{5.155}$$

$$P_4(x) = \frac{1}{8}(35x^4-30x^2+3), \qquad P_5(x) = \frac{1}{8}(63x^5-70x^3+15x). \tag{5.156}$$

The Legendre polynomials satisfy the following closure or completeness relation:

$$\frac{1}{2}\sum_{l=0}^{\infty}(2l+1)P_l(x')P_l(x) = \delta(x-x'). \tag{5.157}$$

From (5.153) we can infer at once

$$P_l(-x) = (-1)^l P_l(x). \tag{5.158}$$

A similar calculation leads to the first few associated Legendre functions:

$$P_1^1(x) = \sqrt{1-x^2}, \tag{5.159}$$

$$P_2^1(x) = 3x\sqrt{1-x^2}, \qquad P_2^2(x) = 3(1-x^2), \tag{5.160}$$

$$P_3^1(x) = \frac{3}{2}(5x^2-1)\sqrt{1-x^2}, \quad P_3^2(x) = 15x(1-x^2), \quad P_3^3(x) = 15(1-x^2)^{3/2}, \tag{5.161}$$

where $P_l^0(x) = P_l(x)$, with $l = 0, 1, 2, 3, \ldots$. The first few expressions for the associated Legendre functions and the Legendre polynomials are listed in Table 5.1. Note that

$$P_l^m(-x) = (-1)^{l+m}P_l^m(x). \tag{5.162}$$

The constant C_{lm} of (5.150) can be determined from the orthonormalization condition

$$\langle l',\ m' \mid l,\ m\rangle = \int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\ \sin\theta \langle l', m'|\theta\,\varphi\rangle\langle\theta\varphi \mid l,\ m\rangle = \delta_{l',l}\delta_{m',m}, \tag{5.163}$$

which can be written as

$$\boxed{\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\ \sin\theta\, Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi) = \delta_{l',l}\delta_{m',m}.} \tag{5.164}$$

Table 5.1 First few Legendre polynomials and associated Legendre functions.

Legendre polynomials	Associated Legendre functions
$P_0(\cos\theta) = 1$	$P_1^1(\cos\theta) = \sin\theta$
$P_1(\cos\theta) = \cos\theta$	$P_2^1(\cos\theta) = 3\cos\theta\sin\theta$
$P_2(\cos\theta) = \frac{1}{2}(3\cos^2\theta - 1)$	$P_2^2(\cos\theta) = 3\sin^2\theta$
$P_3(\cos\theta) = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$	$P_3^1(\cos\theta) = \frac{3}{2}\sin\theta(5\cos^2\theta - 1)$
$P_4(\cos\theta) = \frac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 3)$	$P_3^2(\cos\theta) = 15\sin^2\theta\cos\theta$
$P_5(\cos\theta) = \frac{1}{8}(63\cos^5\theta - 70\cos^3\theta + 15\cos\theta)$	$P_3^3(\cos\theta) = 15\sin^3\theta$

This relation is known as the normalization condition of spherical harmonics. Using the form (5.147) for $Y_{lm}(\theta, \varphi)$, we obtain

$$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta\ \sin\theta\,|Y_{lm}(\theta,\varphi)|^2 = \frac{|C_{lm}|^2}{2\pi}\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta |P_l^m(\cos\theta)|^2 = 1. \quad (5.165)$$

From the theory of associated Legendre functions, we have

$$\int_0^{\pi} d\theta\ \sin\theta P_l^m(\cos\theta) P_{l'}^m(\cos\theta) = \frac{2}{2l+1}\frac{(l+m)!}{(l-m)!}\delta_{l,\,l'}, \quad (5.166)$$

which is known as the normalization condition of associated Legendre functions. A combination of the previous two relations leads to an expression for the coefficient C_{lm}:

$$C_{lm} = (-1)^m \sqrt{\left(\frac{2l+1}{2}\right)\frac{(l-m)!}{(l+m)!}} \qquad (m \geq 0). \quad (5.167)$$

Inserting this equation into (5.150), we obtain the eigenfunctions of $\hat{\vec{L}}^2$:

$$\Theta_{lm}(\theta) = (-1)^m \sqrt{\left(\frac{2l+1}{2}\right)\frac{(l-m)!}{(l+m)!}}\ P_l^m(\cos\theta). \quad (5.168)$$

Finally, the joint eigenfunctions, $Y_{lm}(\theta, \varphi)$, of $\hat{\vec{L}}^2$ and $\hat{J}_z$ can be obtained by substituting (5.142) and (5.168) into (5.138):

$$\boxed{Y_{lm}(\theta,\varphi) = (-1)^m \sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l-m)!}{(l+m)!}} P_l^m(\cos\theta) e^{im\varphi} \qquad (m \geq 0).} \quad (5.169)$$

These are called the *normalized spherical harmonics*.

5.7.2.2 Second Method for Determining the Eigenfunctions of $\hat{\vec{L}}^2$

The second method deals with a direct construction of $Y_{lm}(\theta, \varphi)$; it starts with the case $m = l$ (this is the maximum value of m). By analogy with the general angular momentum algebra developed in the previous section, the action of $\hat{L}_+$ on Y_{ll} gives zero,

$$\langle\theta\ \varphi|\hat{L}_+ \mid l,\ l\rangle = \hat{L}_+ Y_{ll}(\theta,\varphi) = 0, \quad (5.170)$$

since Y_{ll} cannot be raised further as $Y_{ll} = Y_{lm_{max}}$.

Using the expression (5.134) for $\hat{L}_+$ in the spherical coordinates, we can rewrite (5.170) as follows:

$$\frac{\hbar e^{i\varphi}}{\sqrt{2\pi}}\left[\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi}\right]\Theta_{ll}(\theta)e^{i\,l\varphi} = 0, \tag{5.171}$$

which leads to

$$\frac{1}{\Theta_{ll}}\frac{\partial\Theta_{ll}(\theta)}{\partial\theta} = l\cot\theta. \tag{5.172}$$

The solution to this differential equation is of the form

$$\Theta_{ll}(\theta) = C_l\sin^l\theta, \tag{5.173}$$

where C_l is a constant to be determined from the normalization condition (5.164) of $Y_{ll}(\theta, \varphi)$:

$$Y_{ll}(\theta,\varphi) = \frac{C_l}{\sqrt{2\pi}}e^{il\varphi}\sin^l\theta. \tag{5.174}$$

We can ascertain that C_l is given by

$$C_l = \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!}{2}}. \tag{5.175}$$

The action of $\hat{L}_-$ on $Y_{ll}(\theta, \varphi)$ is given, on the one hand, by

$$\hat{L}_- Y_{ll}(\theta,\varphi) = \hbar\sqrt{2l}\,Y_{l,l-1}(\theta,\varphi) \tag{5.176}$$

and, on the other hand, by

$$\hat{L}_- Y_{ll}(\theta,\varphi) = \hbar\frac{(-1)^l}{2^l\,l!}\sqrt{\frac{(2l+1)!}{4\pi}}e^{i(l-1)\varphi}(\sin\theta)^{1-l}\frac{d}{d(\cos\theta)}[(\sin\theta)^{2l}], \tag{5.177}$$

where we have used the spherical coordinate form (5.134).

Similarly, we can show that the action of $\hat{L}_-^{l-m}$ on $Y_{ll}(\theta, \varphi)$ is given, on the one hand, by

$$\hat{L}_-^{l-m} Y_{ll}(\theta,\varphi) = \hbar^{l-m}\sqrt{\frac{(2l)!(l+m)!}{(l-m)!}}Y_{lm}(\theta,\varphi) \tag{5.178}$$

and, on the other hand, by

$$\hat{L}_-^{l-m} Y_{ll}(\theta,\varphi) = \hbar^{l-m}\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l)!(2l+1)!}{4\pi}}e^{im\varphi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l}, \tag{5.179}$$

where $m \geq 0$. Equating the previous two relations, we obtain the expression of the spherical harmonic $Y_{lm}(\theta, \varphi)$ for $m \geq 0$:

$$\boxed{Y_{lm}(\theta,\varphi) = \frac{(-1)^l}{2^l l!}\sqrt{\left(\frac{2l+1}{4\pi}\right)\frac{(l+m)!}{(l-m)!}}e^{im\varphi}\frac{1}{\sin^m\theta}\frac{d^{l-m}}{d(\cos\theta)^{l-m}}(\sin\theta)^{2l}.} \tag{5.180}$$

5.7.3 Properties of the Spherical Harmonics

Since the spherical harmonics $Y_{lm}(\theta, \varphi)$ are joint eigenfunctions of $\hat{\vec{L}}^2$ and $\hat{L}_z$ and are orthonormal (5.164), they constitute an orthonormal basis in the Hilbert space of square-integrable functions of θ and φ. The completeness relation is given by

$$\sum_{m=-l}^{l} \mid l,\ m\rangle\langle l,\ m \mid = 1 \tag{5.181}$$

or

$$\begin{aligned}\sum_{m}\langle\theta\varphi \mid l,\ m\rangle\langle l,\ m \mid \theta'\varphi'\rangle &= \sum_{m} Y^*_{l\,m}(\theta', \varphi')Y_{lm}(\theta, \varphi) = \delta(\cos\theta - \cos\theta')\delta(\varphi - \varphi') \\ &= \frac{\delta(\theta - \theta')}{\sin\theta}\delta(\varphi - \varphi').\end{aligned} \tag{5.182}$$

Let us mention some essential properties of the spherical harmonics. First, the spherical harmonics are complex functions; their complex conjugate is given by

$$\boxed{[Y_{lm}(\theta, \varphi)]^* = (-1)^m Y_{l,-m}(\theta, \varphi).} \tag{5.183}$$

We can verify that $Y_{lm}(\theta, \varphi)$ is an eigenstate of the parity operator $\hat{\mathcal{P}}$ with an eigenvalue $(-1)^l$:

$$\hat{\mathcal{P}}Y_{lm}(\theta, \varphi) = Y_{lm}(\pi - \theta, \varphi + \pi) = (-1)^l Y_{lm}(\theta, \varphi), \tag{5.184}$$

since a spatial reflection about the origin, $\vec{r}\,' = -\vec{r}$, corresponds to $r' = r$, $\theta' = \pi - \theta$, and $\varphi' = \pi + \varphi$, which leads to $P_l^m(\cos\theta') = P_l^m(-\cos\theta) = (-1)^{l+m}P_l^m(\cos\theta)$ and $e^{im\varphi'} = e^{im\pi}e^{im\varphi} = (-1)^m e^{im\varphi}$.

We can establish a connection between the spherical harmonics and the Legendre polynomials by simply taking $m = 0$. Then equation (5.180) yields

$$Y_{l0}(\theta, \varphi) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{4\pi}}\frac{d^l}{d(\cos\theta)^l}(\sin\theta)^{2l} = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta), \tag{5.185}$$

with

$$P_l(\cos\theta) = \frac{1}{2^l l!}\frac{d^l}{d(\cos\theta)^l}(\cos^2\theta - 1)^l. \tag{5.186}$$

From the expression of Y_{lm}, we can verify that

$$Y_{lm}(0, \varphi) = \sqrt{\frac{2l+1}{4\pi}}\delta_{m,\,0}. \tag{5.187}$$

The expressions for the spherical harmonics corresponding to $l = 0$, $l = 1$, and $l = 2$ are listed in Table 5.2.

Spherical harmonics in Cartesian coordinates

Note that $Y_{lm}(\theta, \varphi)$ can also be expressed in terms of the Cartesian coordinates. For this, we need only to substitute

$$\sin\theta\cos\varphi = \frac{x}{r}, \qquad \sin\theta\sin\varphi = \frac{y}{r}, \qquad \cos\theta = \frac{z}{r} \tag{5.188}$$

Table 5.2 Spherical harmonics and their expressions in Cartesian coordinates.

$Y_{lm}(\theta, \varphi)$	$Y_{lm}(x, y, z)$
$Y_{00}(\theta, \varphi) = \frac{1}{\sqrt{4\pi}}$	$Y_{00}(x, y, z) = \frac{1}{\sqrt{4\pi}}$
$Y_{10}(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta$	$Y_{10}(x, y, z) = \sqrt{\frac{3}{4\pi}} \frac{z}{r}$
$Y_{1,\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{3}{8\pi}} e^{\pm i\varphi} \sin\theta$	$Y_{1,\pm 1}(x, y, z) = \mp\sqrt{\frac{3}{8\pi}} \frac{x\pm iy}{r}$
$Y_{20}(\theta, \varphi) = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$	$Y_{20}(x, y, z) = \sqrt{\frac{5}{16\pi}} \frac{3z^2-r^2}{r^2}$
$Y_{2,\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{15}{8\pi}} e^{\pm i\varphi} \sin\theta\cos\theta$	$Y_{2,\pm 1}(x, y, z) = \mp\sqrt{\frac{15}{8\pi}} \frac{(x\pm iy)z}{r^2}$
$Y_{2,\pm 2}(\theta, \varphi) = \sqrt{\frac{15}{32\pi}} e^{\pm 2i\varphi} \sin^2\theta$	$Y_{2,\pm 2}(x, y, z) = \sqrt{\frac{15}{32\pi}} \frac{x^2-y^2\pm 2ixy}{r^2}$

in the expression for $Y_{lm}(\theta, \varphi)$.

As an illustration, let us show how to derive the Cartesian expressions for Y_{10} and $Y_{1,\pm 1}$. Substituting $\cos\theta = z/r$ into $Y_{10}(\theta, \varphi) = \sqrt{3/4\pi}\cos\theta\ Y_{10}$, we have

$$Y_{10}(x, y, z) = \sqrt{\frac{3}{4\pi}}\frac{z}{r} = \sqrt{\frac{3}{4\pi}}\frac{z}{\sqrt{x^2 + y^2 + z^2}}. \tag{5.189}$$

Using $\sin\theta\cos\varphi = x/r$ and $\sin\theta\sin\varphi = y/r$, we obtain

$$\frac{x \pm iy}{r} = \sin\theta\cos\varphi \pm i\sin\theta\sin\varphi = \sin\theta\, e^{\pm i\varphi}, \tag{5.190}$$

which, when substituted into $Y_{1\pm 1}(\theta, \varphi) = \mp\sqrt{3/8\pi}\sin\theta\, e^{\pm i\varphi}$, leads to

$$Y_{1,\pm 1}(x, y, z) = \mp\sqrt{\frac{3}{8\pi}}\frac{x \pm iy}{r}. \tag{5.191}$$

Following the same procedure, we can derive the Cartesian expressions of the remaining harmonics; for a listing, see Table 5.2.

Example 5.5 (Application of ladder operators to spherical harmonics)

(a) Use the relation $Y_{l0}(\theta, \varphi) = \sqrt{(2l+1)/4\pi}\, P_l(\cos\theta)$ to find the expression of $Y_{30}(\theta, \varphi)$.

(b) Find the expression of Y_{30} in Cartesian coordinates.

(c) Use the expression of $Y_{30}(\theta, \varphi)$ to infer those of $Y_{3,\pm 1}(\theta, \varphi)$.

Solution

(a) From Table 5.1 we have $P_3(\cos\theta) = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$; hence

$$Y_{30}(\theta, \varphi) = \sqrt{\frac{7}{4\pi}}P_3(\cos\theta) = \sqrt{\frac{7}{16\pi}}(5\cos^3\theta - 3\cos\theta). \tag{5.192}$$

(b) Since $\cos\theta = z/r$, we have $5\cos^3\theta - 3\cos\theta = 5\cos\theta(5\cos^2\theta - 3) = z(5z^2 - 3r^2)/r^3$; hence

$$Y_{30}(x, y, z) = \sqrt{\frac{7}{16\pi}}\frac{z}{r^3}(5z^2 - 3r^2). \tag{5.193}$$

(c) To find Y_{31} from Y_{30}, we need to apply the ladder operator $\hat{L}_+$ on Y_{30} in two ways: first, algebraically

$$\hat{L}_+ Y_{30} = \hbar\sqrt{3(3+1) - 0}\, Y_{31} = 2\hbar\sqrt{3}\, Y_{31} \tag{5.194}$$

and hence

$$Y_{31} = \frac{1}{2\hbar\sqrt{3}}\hat{L}_+ Y_{30}; \tag{5.195}$$

then we use the differential form (5.134) of $\hat{L}_+$:

$$\begin{aligned} \hat{L}_+ Y_{30}(\theta, \varphi) &= \hbar e^{i\varphi}\left[\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right] Y_{30}(\theta, \varphi) \\ &= \hbar\sqrt{\frac{7}{16\pi}}e^{i\varphi}\left[\frac{\partial}{\partial\theta} + i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right](5\cos^3\theta - 3\cos\theta) \\ &= -3\hbar\sqrt{\frac{7}{16\pi}}\sin\theta(5\cos^2\theta - 1)e^{i\varphi}. \end{aligned} \tag{5.196}$$

Inserting (5.196) into (5.195) we end up with

$$Y_{31} = \frac{1}{2\hbar\sqrt{3}}\hat{L}_+ Y_{30} = -\sqrt{\frac{21}{64\pi}}\sin\theta(5\cos^2\theta - 1)e^{i\varphi}. \tag{5.197}$$

Now, to find $Y_{3,-1}$ from Y_{30}, we also need to apply $\hat{L}_-$ on Y_{30} in two ways:

$$\hat{L}_- Y_{30} = \hbar\sqrt{3(3+1) - 0}Y_{3,-1} = 2\hbar\sqrt{3}Y_{3,-1} \tag{5.198}$$

and hence

$$Y_{3,-1} = \frac{1}{2\hbar\sqrt{3}}\hat{L}_- Y_{30}; \tag{5.199}$$

then we use the differential form (5.134) of $\hat{L}_-$:

$$\begin{aligned} \hat{L}_- Y_{30}(\theta, \varphi) &= -\hbar e^{-i\varphi}\left[\frac{\partial}{\partial\theta} - i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right] Y_{30}(\theta, \varphi) \\ &= -\hbar\sqrt{\frac{7}{16\pi}}e^{-i\varphi}\left[\frac{\partial}{\partial\theta} - i\frac{\cos\theta}{\sin\theta}\frac{\partial}{\partial\varphi}\right](5\cos^3\theta - 3\cos\theta) \\ &= 3\hbar\sqrt{\frac{7}{16\pi}}\sin\theta(5\cos^2\theta - 1)e^{-i\varphi}. \end{aligned} \tag{5.200}$$

Inserting (5.200) into (5.199), we obtain

$$Y_{3,-1} = \frac{1}{2\hbar\sqrt{3}}\hat{L}_- Y_{30} = \sqrt{\frac{21}{64\pi}}\sin\theta(5\cos^2\theta - 1)e^{-i\varphi}. \tag{5.201}$$

5.8 Solved Problems

Problem 5.1

(a) Show that $\Delta J_x \Delta J_y = \hbar^2[j(j+1)-m^2]/2$, where $\Delta J_x = \sqrt{\langle \hat{J}_x^2\rangle - \langle \hat{J}_x\rangle^2}$ and the same for ΔJ_y.

(b) Show that this relation is consistent with $\Delta J_x \Delta J_y \geq (\hbar/2)\,|\langle \hat{J}_z\rangle| = \hbar^2 m/2$.

Solution

(a) First, note that $\langle \hat{J}_x\rangle$ and $\langle \hat{J}_y\rangle$ are zero, since

$$\langle \hat{J}_x\rangle = \frac{1}{2}\langle j,\ m \mid \hat{J}_+ \mid j,\ m\rangle + \frac{1}{2}\langle j,\ m \mid \hat{J}_- \mid j,\ m\rangle = 0. \tag{5.202}$$

As for $\langle \hat{J}_x^2\rangle$ and $\langle \hat{J}_y^2\rangle$, they are given by

$$\langle \hat{J}_x^2\rangle = \frac{1}{4}\langle(\hat{J}_+ + \hat{J}_-)^2\rangle = \frac{1}{4}\langle \hat{J}_+^2 + \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+ + J_-^2\rangle, \tag{5.203}$$

$$\langle \hat{J}_y^2\rangle = \frac{1}{4}\langle(\hat{J}_+ - \hat{J}_-)^2\rangle = -\frac{1}{4}\langle \hat{J}_+^2 - \hat{J}_+\hat{J}_- - \hat{J}_-\hat{J}_+ + J_-^2\rangle. \tag{5.204}$$

Since $\langle \hat{J}_+^2\rangle = \langle \hat{J}_-^2\rangle = 0$, we see that

$$\langle \hat{J}_x^2\rangle = \frac{1}{4}\langle \hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+\rangle = \langle \hat{J}_y^2\rangle. \tag{5.205}$$

Using the fact that

$$\langle \hat{J}_x^2\rangle + \langle \hat{J}_y^2\rangle = \langle \hat{\vec{J}}^2\rangle - \langle \hat{J}_z^2\rangle \tag{5.206}$$

along with $\langle \hat{J}_x^2\rangle = \langle \hat{J}_y^2\rangle$, we see that

$$\langle \hat{J}_x^2\rangle = \langle \hat{J}_y^2\rangle = \frac{1}{2}[\langle \hat{\vec{J}}^2\rangle - \langle \hat{J}_z^2\rangle]. \tag{5.207}$$

Now, since $\mid j,\ m\rangle$ is a joint eigenstate of $\hat{\vec{J}}^{\,2}$ and $\hat{J}_z$ with eigenvalues $j(j+1)\hbar^2$ and $m\hbar$, we can easily see that the expressions of $\langle \hat{J}_x^2\rangle$ and $\langle \hat{J}_y^2\rangle$ are given by

$$\boxed{\langle \hat{J}_x^2\rangle = \langle \hat{J}_y^2\rangle = \frac{1}{2}[\langle \hat{\vec{J}}^2\rangle - \langle \hat{J}_z^2\rangle] = \frac{\hbar^2}{2}\left[j(j+1) - m^2\right].} \tag{5.208}$$

Hence $\Delta J_x \Delta J_y$ is given by

$$\Delta J_x \Delta J_y = \sqrt{\langle \hat{J}_x^2\rangle\langle \hat{J}_y^2\rangle} = \frac{\hbar^2}{2}[j(j+1) - m^2]. \tag{5.209}$$

(b) Since $j \geq m$ (because $m = -j, -j+1, \ldots, j-1, j$), we have

$$j(j+1) - m^2 \geq m(m+1) - m^2 = m, \tag{5.210}$$

from which we infer that $\Delta J_x \Delta J_y \geq \hbar^2 m/2$, or

$$\Delta J_x \Delta J_y \geq \frac{\hbar}{2}|\langle \hat{J}_z\rangle|. \tag{5.211}$$

Problem 5.2
Find the energy levels of a particle which is free except that it is constrained to move on the surface of a sphere of radius r.

Solution
This system consists of a particle that is constrained to move on the surface of a sphere but free from the influence of any other potential; it is called a *rigid rotator*. Since $V = 0$ the energy of this system is purely kinetic; the Hamiltonian of the rotator is

$$\hat{H} = \frac{\hat{\vec{L}}^2}{2I}, \tag{5.212}$$

where $I = mr^2$ is the moment of inertia of the particle with respect to the origin. In deriving this relation, we have used the fact that $H = p^2/2m = (rp)^2/2mr^2 = L^2/2I$, since $L = |\vec{r} \times \vec{p}| = rp$.

The wave function of the system is clearly independent of the radial degree of freedom, for it is constant. The Schrödinger equation is thus given by

$$\hat{H}\psi(\theta, \varphi) = \frac{\hat{\vec{L}}^2}{2I}\psi(\theta, \varphi) = E\psi(\theta, \varphi). \tag{5.213}$$

Since the eigenstates of $\hat{\vec{L}}^2$ are the spherical harmonics $Y_{lm}(\theta, \varphi)$, the corresponding energy eigenvalues are given by

$$E_l = \frac{\hbar^2}{2I}l(l+1), \qquad l = 0, 1, 2, 3, \ldots, \tag{5.214}$$

and the Schrödinger equation by

$$\frac{\hat{\vec{L}}^2}{2I}Y_{lm}(\theta, \varphi) = \frac{\hbar^2}{2I}l(l+1)Y_{lm}(\theta, \varphi). \tag{5.215}$$

Note that the energy levels do not depend on the azimuthal quantum number m. This means that there are $(2l + 1)$ eigenfunctions $Y_{l\,-l}, Y_{l\,-l+1}, \ldots, Y_{l\,l-1}, Y_{ll}$ corresponding to the same energy. Thus, every energy level E_l is $(2l + 1)$-fold degenerate. This is due to the fact that the rotator's Hamiltonian, $\hat{\vec{L}}^2/2I$, commutes with $\hat{\vec{L}}$. That is, the Hamiltonian is independent of the orientation of $\hat{\vec{L}}$ in space; hence the energy spectrum does not depend on the component of $\hat{\vec{L}}$ in any particular direction.

Problem 5.3
Find the rotational energy levels of a diatomic molecule.

Solution
Consider two molecules of masses m_1 and m_2 separated by a constant distance $\vec{r}$. Let r_1 and r_2 be their distances from the center of mass, i.e., $m_1 r_1 = m_2 r_2$. The moment of inertia of the diatomic molecule is

$$I = m_1 r_1^2 + m_2 r_2^2 \equiv \mu r^2, \tag{5.216}$$

where $r = |\vec{r}_1 - \vec{r}_2|$ and where μ is their reduced mass, $\mu = m_1 m_2/(m_1 + m_2)$. The total angular momentum is given by

$$|\hat{\vec{L}}\,| = m_1 r_1 r_1 \omega + m_2 r_2 r_2 \omega = I\omega = \mu r^2 \omega \tag{5.217}$$

and the Hamiltonian by

$$\hat{H} = \frac{\hat{\vec{L}}^2}{2I} = \frac{\hat{\vec{L}}^2}{2\mu r^2}. \tag{5.218}$$

The corresponding eigenvalue equation

$$\hat{H} \mid l,\; m\rangle = \frac{\hat{\vec{L}}^2}{2\mu r^2} \mid l,\; m\rangle = \frac{l(l+1)\hbar^2}{2\mu r^2} \mid l,\; m\rangle, \tag{5.219}$$

shows that the eigenenergies are $(2l+1)$-fold degenerate and given by

$$E_l = \frac{l(l+1)\hbar^2}{2\mu r^2}. \tag{5.220}$$

Problem 5.4

(a) Find the eigenvalues and eigenstates of the spin operator $\vec{S}$ of an electron in the direction of a unit vector $\vec{n}$; assume that $\vec{n}$ lies in the xz plane.

(b) Find the probability of measuring $\hat{S}_z = +\hbar/2$.

Solution

(a) In this question we want to solve

$$\vec{n} \cdot \vec{S}|\lambda\rangle = \frac{\hbar}{2}\lambda|\lambda\rangle, \tag{5.221}$$

where $\vec{n}$ is given by $\vec{n} = (\sin\theta\,\vec{i} + \cos\theta\,\vec{k})$, because it lies in the xz plane, with $0 \le \theta \le \pi$. We can thus write

$$\vec{n} \cdot \vec{S} = (\sin\theta\,\vec{i} + \cos\theta\,\vec{k}) \cdot (S_x\vec{i} + S_y\vec{j} + S_z\vec{k}) = S_x \sin\theta + S_z \cos\theta. \tag{5.222}$$

Using the spin matrices

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{S}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{S}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5.223}$$

we can write (5.222) in the following matrix form:

$$\vec{n} \cdot \vec{S} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\sin\theta + \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\cos\theta = \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{5.224}$$

The diagonalization of this matrix leads to the following secular equation:

$$-\frac{\hbar^2}{4}(\cos\theta - \lambda)(\cos\theta + \lambda) - \frac{\hbar^2}{4}\sin^2\theta = 0, \tag{5.225}$$

which in turn leads as expected to the eigenvalues $\lambda = \pm 1$.

The eigenvector corresponding to $\lambda = 1$ can be obtained from

$$\frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}. \tag{5.226}$$

This matrix equation can be reduced to a single equation

$$a \sin\frac{1}{2}\theta = b\cos\frac{1}{2}\theta. \tag{5.227}$$

Combining this equation with the normalization condition $|a|^2 + |b|^2 = 1$, we infer that $a = \cos\frac{1}{2}\theta$ and $b = \sin\frac{1}{2}\theta$; hence the eigenvector corresponding to $\lambda = 1$ is

$$|\lambda_+\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}. \tag{5.228}$$

Proceeding in the same way, we can easily obtain the eigenvector for $\lambda = -1$:

$$|\lambda_-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ \cos(\theta/2) \end{pmatrix}. \tag{5.229}$$

(b) Let us write $|\lambda_\pm\rangle$ of (5.228) and (5.229) in terms of the spin-up and spin-down eigenvectors, $\left|\frac{1}{2}, \frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$:

$$|\lambda_+\rangle = \cos\frac{1}{2}\theta\left|\frac{1}{2}, \frac{1}{2}\right\rangle + \sin\frac{1}{2}\theta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \tag{5.230}$$

$$|\lambda_-\rangle = -\sin\frac{1}{2}\theta\left|\frac{1}{2}, \frac{1}{2}\right\rangle + \cos\frac{1}{2}\theta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle. \tag{5.231}$$

We see that the probability of measuring $\hat{S}_z = +\hbar/2$ is given by

$$\left|\left\langle\frac{1}{2}, \frac{1}{2}\right|\lambda_+\right\rangle\right|^2 = \cos^2\frac{1}{2}\theta. \tag{5.232}$$

Problem 5.5

(a) Find the eigenvalues and eigenstates of the spin operator $\vec{S}$ of an electron in the direction of a unit vector $\vec{n}$, where $\vec{n}$ is *arbitrary*.

(b) Find the probability of measuring $\hat{S}_z = -\hbar/2$.

(c) Assuming that the eigenvectors of the spin calculated in (a) correspond to $t = 0$, find these eigenvectors at time t.

Solution

(a) We need to solve

$$\vec{n}\cdot\vec{S}|\lambda\rangle = \frac{\hbar}{2}\lambda|\lambda\rangle, \tag{5.233}$$

where $\vec{n}$, a unit vector pointing along an *arbitrary* direction, is given in spherical coordinates by

$$\vec{n} = (\sin\theta\cos\varphi)\vec{i} + (\sin\theta\sin\varphi)\vec{j} + (\cos\theta)\vec{k}, \tag{5.234}$$

with $0 \le \theta \le \pi$ and $0 \le \varphi \le 2\pi$. We can thus write

$$\begin{aligned}\vec{n}\cdot\vec{S} &= (\sin\theta\cos\varphi\,\vec{i} + \sin\theta\sin\varphi\,\vec{j} + \cos\theta\,\vec{k})\cdot(S_x\vec{i} + S_y\vec{j} + S_z\vec{k}) \\ &= S_x\sin\theta\cos\varphi + S_y\sin\theta\sin\varphi + S_z\cos\theta.\end{aligned} \tag{5.235}$$

Using the spin matrices, we can write this equation in the following matrix form:

$$\begin{aligned}\vec{n}\cdot\vec{S} &= \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\sin\theta\cos\varphi + \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\sin\theta\sin\varphi + \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\cos\theta \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta\,(\cos\varphi - i\sin\varphi) \\ \sin\theta\,(\cos\varphi + i\sin\varphi) & -\cos\theta \end{pmatrix} \\ &= \frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}.\end{aligned} \tag{5.236}$$

Diagonalization of this matrix leads to the secular equation

$$-\frac{\hbar^2}{4}(\cos\theta - \lambda)(\cos\theta + \lambda) - \frac{\hbar^2}{4}\sin^2\theta = 0, \tag{5.237}$$

which in turn leads to the eigenvalues $\lambda = \pm 1$.

The eigenvector corresponding to $\lambda = 1$ can be obtained from

$$\frac{\hbar}{2}\begin{pmatrix} \cos\theta & e^{-i\varphi}\sin\theta \\ e^{i\varphi}\sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} a \\ b \end{pmatrix}, \tag{5.238}$$

which leads to

$$a\cos\theta + be^{-i\varphi}\sin\theta = a \tag{5.239}$$

or

$$a(1 - \cos\theta) = be^{-i\varphi}\sin\theta. \tag{5.240}$$

Using the relations $1 - \cos\theta = 2\sin^2\frac{1}{2}\theta$ and $\sin\theta = 2\cos\frac{1}{2}\theta\sin\frac{1}{2}\theta$, we have

$$b = a\tan\frac{1}{2}\theta e^{i\varphi}. \tag{5.241}$$

Combining this equation with the normalization condition $|a|^2 + |b|^2 = 1$, we obtain $a = \cos\frac{1}{2}\theta$ and $b = e^{i\varphi}\sin\frac{1}{2}\theta$. Thus, the eigenvector corresponding to $\lambda = 1$ is

$$|\lambda_+\rangle = \begin{pmatrix} \cos(\theta/2) \\ e^{i\varphi}\sin(\theta/2) \end{pmatrix}. \tag{5.242}$$

A similar treatment leads to the eigenvector for $\lambda = -1$:

$$|\lambda_-\rangle = \begin{pmatrix} -\sin(\theta/2) \\ e^{i\varphi}\cos(\theta/2) \end{pmatrix}. \tag{5.243}$$

(b) Write $|\lambda_-\rangle$ of (5.243) in terms of $\left|\frac{1}{2}, \frac{1}{2}\right\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\left|\frac{1}{2}, -\frac{1}{2}\right\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$:

$$|\lambda_+\rangle = \cos\frac{1}{2}\theta\left|\frac{1}{2}, \frac{1}{2}\right\rangle + e^{i\varphi}\sin\frac{1}{2}\theta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \tag{5.244}$$

$$|\lambda_-\rangle = -\sin\frac{1}{2}\theta\left|\frac{1}{2}, \frac{1}{2}\right\rangle + e^{i\varphi}\cos\frac{1}{2}\theta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle. \tag{5.245}$$

We can then obtain the probability of measuring $\hat{S}_z = -\hbar/2$:

$$\left|\left\langle\frac{1}{2}, -\frac{1}{2}\right|\lambda_-\right\rangle\right|^2 = \cos^2\frac{1}{2}\theta. \tag{5.246}$$

(c) The spin's eigenstates at time t are given by

$$|\lambda_+(t)\rangle = e^{-iE_+t/\hbar}\cos\frac{1}{2}\theta\left|\frac{1}{2}, \frac{1}{2}\right\rangle + e^{i(\varphi-E_-t/\hbar)}\sin\frac{1}{2}\theta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \tag{5.247}$$

$$|\lambda_-(t)\rangle = -e^{-iE_+t/\hbar}\sin\frac{1}{2}\theta\left|\frac{1}{2}, \frac{1}{2}\right\rangle + e^{i(\varphi-E_-t/\hbar)}\cos\frac{1}{2}\theta\left|\frac{1}{2}, -\frac{1}{2}\right\rangle, \tag{5.248}$$

where $E_\pm$ are the energy eigenvalues corresponding to the spin-up and spin-down states, respectively.

Problem 5.6

The Hamiltonian of a system is $\hat{H} = \varepsilon\vec{\sigma}\cdot\vec{n}$, where ε is a constant having the dimensions of energy, $\vec{n}$ is an arbitrary unit vector, and σ_x, σ_y, and σ_z are the Pauli matrices.

(a) Find the energy eigenvalues and normalized eigenvectors of $\hat{H}$.

(b) Find a transformation matrix that diagonalizes $\hat{H}$.

Solution

(a) Using the Pauli matrices $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ and the expression of an arbitrary unit vector in spherical coordinates $\vec{n} = (\sin\theta\cos\varphi)\vec{i} + (\sin\theta\sin\varphi)\vec{j} + (\cos\theta)\vec{k}$, we can rewrite the Hamiltonian

$$\hat{H} = \varepsilon\vec{\sigma}\cdot\vec{n} = \varepsilon\left(\sigma_x\sin\theta\cos\varphi + \sigma_y\sin\theta\sin\varphi + \sigma_z\cos\theta\right) \tag{5.249}$$

in the following matrix form:

$$\hat{H} = \varepsilon\begin{pmatrix} \cos\theta & \exp(-i\varphi)\sin\theta \\ \exp(i\varphi)\sin\theta & -\cos\theta \end{pmatrix}. \tag{5.250}$$

The eigenvalues of $\hat{H}$ are obtained by solving the secular equation $\det(H - E) = 0$, or

$$(\varepsilon\cos\theta - E)(-\varepsilon\cos\theta - E) - \varepsilon^2\sin^2\theta = 0, \tag{5.251}$$

which yields two eigenenergies $E_1 = \varepsilon$ and $E_2 = -\varepsilon$.

The energy eigenfunctions are obtained from

$$\varepsilon\begin{pmatrix} \cos\theta & \exp(-i\varphi)\sin\theta \\ \exp(i\varphi)\sin\theta & -\cos\theta \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = E\begin{pmatrix} x \\ y \end{pmatrix}. \tag{5.252}$$

For the case $E = E_1 = \varepsilon$, this equation yields

$$(\cos\theta - 1)x + y\sin\theta\exp(-i\varphi) = 0, \tag{5.253}$$

which in turn leads to

$$\frac{x}{y} = \frac{\sin\theta\exp(-i\varphi)}{1-\cos\theta} = \frac{\cos\theta/2\exp(-i\varphi/2)}{\sin\theta/2\exp(i\varphi/2)}; \tag{5.254}$$

hence

$$\begin{pmatrix} x_1 \\ y_1 \end{pmatrix} = \begin{pmatrix} \exp(-i\varphi/2)\cos(\theta/2) \\ \exp(i\varphi/2)\sin(\theta/2) \end{pmatrix}; \tag{5.255}$$

this vector is normalized. Similarly, in the case where $E = E_2 = -\varepsilon$, we can show that the second normalized eigenvector is

$$\begin{pmatrix} x_2 \\ y_2 \end{pmatrix} = \begin{pmatrix} -\exp(-i\varphi/2)\sin(\theta/2) \\ \exp(i\varphi/2)\cos(\theta/2) \end{pmatrix}. \tag{5.256}$$

(b) A transformation $\hat{U}$ that diagonalizes $\hat{H}$ can be obtained from the two eigenvectors obtained in part (a): $U_{11} = x_1$, $U_{21} = y_1$, $U_{12} = x_2$, $U_{22} = y_2$. That is,

$$U = \begin{pmatrix} \exp(-i\varphi/2)\cos(\theta/2) & -\exp(-i\varphi/2)\sin(\theta/2) \\ \exp(i\varphi/2)\sin(\theta/2) & \exp(i\varphi/2)\cos(\theta/2) \end{pmatrix}. \tag{5.257}$$

Note that this matrix is unitary, since $U^\dagger = U^{-1}$ and $\det(U) = 1$. We can ascertain that

$$\hat{U}\hat{H}\hat{U}^\dagger = \begin{pmatrix} \varepsilon & 0 \\ 0 & -\varepsilon \end{pmatrix}. \tag{5.258}$$

Problem 5.7

Consider a system of total angular momentum $j = 1$. As shown in (5.73) and (5.75), the operators $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ are given by

$$\hat{J}_x = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \hat{J}_y = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \hat{J}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{5.259}$$

(a) What are the possible values when measuring $\hat{J}_x$?

(b) Calculate $\langle\hat{J}_z\rangle$, $\langle\hat{J}_z^2\rangle$, and ΔJ_z if the system is in the state $j_x = -\hbar$.

(c) Repeat (b) for $\langle\hat{J}_y\rangle$, $\langle\hat{J}_y^2\rangle$, and ΔJ_y.

(d) If the system were initially in state $|\,\psi\rangle = \frac{1}{\sqrt{14}}\begin{pmatrix} -\sqrt{3} \\ 2\sqrt{2} \\ \sqrt{3} \end{pmatrix}$, what values will one obtain when measuring $\hat{J}_x$ and with what probabilities?

Solution

(a) According to Postulate 2 of Chapter 3, the results of the measurements are given by the eigenvalues of the measured quantity. Here the eigenvalues of $\hat{J}_x$, which are obtained by diagonalizing the matrix J_x, are $j_x = -\hbar$, 0, and $\hbar$; the respective (normalized) eigenstates are

$$|-1\rangle = \frac{1}{2}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix}, \qquad |0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \qquad |1\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}. \tag{5.260}$$

(b) If the system is in the state $j_x = -\hbar$, its eigenstate is given by $|-1\rangle$. In this case $\langle \hat{J}_z \rangle$ and $\langle \hat{J}_z^2 \rangle$ are given by

$$\langle -1|\hat{J}_z|-1\rangle = \frac{\hbar}{4}\begin{pmatrix} -1 & \sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix} = 0, \tag{5.261}$$

$$\langle -1|\hat{J}_z^2|-1\rangle = \frac{\hbar^2}{4}\begin{pmatrix} -1 & \sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix} = \frac{\hbar^2}{2}. \tag{5.262}$$

Thus, the uncertainty ΔJ_z is given by

$$\Delta J_z = \sqrt{\langle -1|\hat{J}_z^2|-1\rangle - \langle -1|\hat{J}_z|-1\rangle^2} = \sqrt{\frac{\hbar^2}{2}} = \frac{\hbar}{\sqrt{2}}. \tag{5.263}$$

(c) Following the same procedure in (b), we have

$$\langle -1|\hat{J}_y|-1\rangle = \frac{\hbar}{4\sqrt{2}}\begin{pmatrix} -1 & \sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix} = 0, \tag{5.264}$$

$$\langle -1|\hat{J}_y^2|-1\rangle = \frac{\hbar^2}{8}\begin{pmatrix} -1 & \sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 1 \end{pmatrix}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix} = \frac{\hbar^2}{2}; \tag{5.265}$$

hence

$$\Delta J_y = \sqrt{\langle -1|\hat{J}_y^2|-1\rangle - \langle -1|\hat{J}_y|-1\rangle^2} = \frac{\hbar}{\sqrt{2}}. \tag{5.266}$$

(d) We can express $|\,\psi\rangle = \frac{1}{\sqrt{14}}\begin{pmatrix} -\sqrt{3} \\ 2\sqrt{2} \\ \sqrt{3} \end{pmatrix}$ in terms of the eigenstates (5.260) as

$$\frac{1}{\sqrt{14}}\begin{pmatrix} -\sqrt{3} \\ 2\sqrt{2} \\ \sqrt{3} \end{pmatrix} = \sqrt{\frac{2}{7}}\frac{1}{2}\begin{pmatrix} -1 \\ \sqrt{2} \\ -1 \end{pmatrix} + \sqrt{\frac{3}{7}}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} + \sqrt{\frac{2}{7}}\frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \tag{5.267}$$

or

$$|\,\psi\rangle = \sqrt{\frac{2}{7}}|-1\rangle + \sqrt{\frac{3}{7}}|0\rangle + \sqrt{\frac{2}{7}}|1\rangle. \tag{5.268}$$

A measurement of $\hat{J}_x$ on a system initially in the state (5.268) yields a value $j_x = -\hbar$ with probability

$$P_{-1} = |\langle -1 \mid \psi\rangle|^2 = \left|\sqrt{\frac{2}{7}}\langle -1| -1\rangle + \sqrt{\frac{3}{7}}\langle -1|0\rangle + \sqrt{\frac{2}{7}}\langle -1|1\rangle\right|^2 = \frac{2}{7}, \tag{5.269}$$

since $\langle -1|0\rangle = \langle -1|1\rangle = 0$ and $\langle -1| -1\rangle = 1$, and the values $j_x = 0$ and $j_x = \hbar$ with the respective probabilities

$$P_0 = |\langle 0 \mid \psi\rangle|^2 = \left|\sqrt{\frac{3}{7}}\langle 0|0\rangle\right|^2 = \frac{3}{7}, \qquad P_1 = |\langle 1 \mid \psi\rangle|^2 = \left|\sqrt{\frac{2}{7}}\langle 1|1\rangle\right|^2 = \frac{2}{7}. \tag{5.270}$$

Problem 5.8
Consider a particle of total angular momentum $j = 1$. Find the matrix for the component of $\vec{J}$ along a unit vector with arbitrary direction $\vec{n}$. Find its eigenvalues and eigenvectors.

Solution
Since $\vec{J} = J_x\vec{i} + J_y\vec{j} + J_z\vec{k}$ and $\vec{n} = (\sin\theta\cos\varphi)\vec{i} + (\sin\theta\sin\varphi)\vec{j} + (\cos\theta)\vec{k}$, the component of $\vec{J}$ along $\vec{n}$ is

$$\vec{n}\cdot\vec{J} = J_x\sin\theta\cos\varphi + J_y\sin\theta\sin\varphi + J_z\cos\theta, \tag{5.271}$$

with $0 \le \theta \le \pi$ and $0 \le \varphi \le 2\pi$; the matrices of $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ are given by (5.259). We can therefore write this equation in the following matrix form:

$$\begin{aligned}\vec{n}\cdot\vec{J} &= \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}\sin\theta\cos\varphi + \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}\sin\theta\sin\varphi \\ &+ \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}\cos\theta = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} \sqrt{2}\cos\theta & e^{-i\varphi}\sin\theta & 0 \\ e^{i\varphi}\sin\theta & 0 & e^{-i\varphi}\sin\theta \\ 0 & e^{i\varphi}\sin\theta & -\sqrt{2}\cos\theta \end{pmatrix}.\end{aligned} \tag{5.272}$$

The diagonalization of this matrix leads to the eigenvalues $\lambda_1 = -\hbar$, $\lambda_2 = 0$, and $\lambda_3 = \hbar$; the corresponding eigenvectors are given by

$$|\lambda_1\rangle = \frac{1}{2}\begin{pmatrix} (1-\cos\theta)e^{-i\varphi} \\ -\frac{2}{\sqrt{2}}\sin\theta \\ (1+\cos\theta)e^{i\varphi} \end{pmatrix}, \qquad |\lambda_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} -e^{-i\varphi}\sin\theta \\ \sqrt{2}\cos\theta \\ e^{i\varphi}\sin\theta \end{pmatrix}, \tag{5.273}$$

$$|\lambda_3\rangle = \frac{1}{2}\begin{pmatrix} (1+\cos\theta)e^{-i\varphi} \\ \frac{2}{\sqrt{2}}\sin\theta \\ (1-\cos\theta)e^{i\varphi} \end{pmatrix}. \tag{5.274}$$

Problem 5.9
Consider a system which is initially in the state

$$\psi(\theta,\ \varphi) = \frac{1}{\sqrt{5}}Y_{1,-1}(\theta,\ \varphi) + \sqrt{\frac{3}{5}}Y_{10}(\theta,\ \varphi) + \frac{1}{\sqrt{5}}Y_{11}(\theta,\ \varphi).$$

(a) Find $\langle \psi \mid \hat{L}_+ \mid \psi \rangle$.
(b) If $\hat{L}_z$ were measured what values will one obtain and with what probabilities?
(c) If after measuring $\hat{L}_z$ we find $l_z = -\hbar$, calculate the uncertainties ΔL_x and ΔL_y and their product $\Delta L_x \Delta L_y$.

Solution

(a) Let us use a lighter notation for $\mid \psi\rangle$: $\mid \psi\rangle = \frac{1}{\sqrt{5}} \mid 1,\ -1\rangle + \sqrt{\frac{3}{5}} \mid 1,\ 0\rangle + \frac{1}{\sqrt{5}} \mid 1,\ 1\rangle$. From (5.56) we can write $\hat{L}_+ \mid l,\ m\rangle = \hbar\sqrt{l(l+1) - m(m+1)}\ |l,\ m+1\rangle$; hence the only terms that survive in $\langle \psi \mid \hat{L}_+ \mid \psi\rangle$ are

$$\langle \psi \mid \hat{L}_+ \mid \psi\rangle = \frac{\sqrt{3}}{5}\langle 1,\ 0|\hat{L}_+ \mid 1,\ -1\rangle + \frac{\sqrt{3}}{5}\langle 1,\ 1|\hat{L}_+ \mid 1,\ 0\rangle = \frac{2\sqrt{6}}{5}\hbar, \tag{5.275}$$

since $\langle 1,\ 0|\hat{L}_+ \mid 1,\ -1\rangle = \langle 1,\ 1|\hat{L}_+ \mid 1,\ 0\rangle = \sqrt{2}\hbar$.

(b) If $\hat{L}_z$ were measured, we will find three values $l_z = -\hbar$, 0, and $\hbar$. The probability of finding the value $l_z = -\hbar$ is

$$\begin{aligned} P_{-1} &= |\langle 1,\ -1 \mid \psi\rangle|^2 = \left| \frac{1}{\sqrt{5}}\langle 1,\ -1 \mid 1,\ -1\rangle + \sqrt{\frac{3}{5}}\langle 1,\ -1 \mid 1,\ 0\rangle + \frac{1}{\sqrt{5}}\langle 1,\ -1 \mid 1,\ 1\rangle \right|^2 \\ &= \frac{1}{5}, \end{aligned} \tag{5.276}$$

since $\langle 1,\ -1 \mid 1,\ 0\rangle = \langle 1,\ -1 \mid 1,\ 1\rangle = 0$ and $\langle 1,\ -1 \mid 1,\ -1\rangle = 1$. Similarly, we can verify that the probabilities of measuring $l_z = 0$ and $\hbar$ are respectively given by

$$P_0 = |\langle 1,\ 0 \mid \psi\rangle|^2 = \left| \sqrt{\frac{3}{5}}\langle 1,\ 0 \mid 1,\ 0\rangle \right|^2 = \frac{3}{5}, \tag{5.277}$$

$$P_1 = |\langle 1,\ 1 \mid \psi\rangle|^2 = \left| \sqrt{\frac{1}{5}}\langle 1,\ 1 \mid 1,\ 1\rangle \right|^2 = \frac{1}{5}. \tag{5.278}$$

(c) After measuring $l_z = -\hbar$, the system will be in the eigenstate $|lm\rangle = \mid 1,\ -1\rangle$, that is, $\psi(\theta,\ \varphi) = Y_{1,-1}(\theta,\ \varphi)$. We need first to calculate the expectation values of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_x^2$, and $\hat{L}_y^2$ using $\mid 1,\ -1\rangle$. Symmetry requires that $\langle 1,\ -1 \mid \hat{L}_x \mid 1,\ -1\rangle = \langle 1,\ -1 \mid \hat{L}_y \mid 1,\ -1\rangle = 0$. The expectation values of $\hat{L}_x^2$ and $\hat{L}_y^2$ are equal, as shown in (5.60); they are given by

$$\langle \hat{L}_x^2\rangle = \langle \hat{L}_y^2\rangle = \frac{1}{2}[\langle \hat{\vec{L}}^2\rangle - \langle \hat{L}_z^2\rangle] = \frac{\hbar^2}{2}\left[l(l+1) - m^2\right] = \frac{\hbar^2}{2}; \tag{5.279}$$

in this relation, we have used the fact that $l = 1$ and $m = -1$. Hence

$$\Delta L_x = \sqrt{\langle \hat{L}_x^2\rangle} = \frac{\hbar}{\sqrt{2}} = \Delta L_y, \tag{5.280}$$

and the uncertainties product $\Delta L_x \Delta L_y$ is given by

$$\Delta L_x \Delta L_y = \sqrt{\langle \hat{L}_x^2\rangle\langle \hat{L}_y^2\rangle} = \frac{\hbar^2}{2}. \tag{5.281}$$

Problem 5.10
Find the angle between the angular momentum $l = 4$ and the z-axis for all possible orientations.

Solution
Since $m_l = 0, \pm 1, \pm 2, \ldots, \pm l$ and the angle between the orbital angular momentum l and the z-axis is $\cos\theta_{m_l} = m_l/\sqrt{l(l+1)}$ we have

$$\theta_{m_l} = \cos^{-1}\left[\frac{m_l}{\sqrt{l(l+1)}}\right] = \cos^{-1}\left[\frac{m_l}{2\sqrt{5}}\right]; \tag{5.282}$$

hence

$$\theta_0 = \cos^{-1}(0) = 90^\circ, \tag{5.283}$$

$$\theta_1 = \cos^{-1}\left[\frac{1}{2\sqrt{5}}\right] = 77.08^\circ, \qquad \theta_2 = \cos^{-1}\left[\frac{2}{2\sqrt{5}}\right] = 63.43^\circ, \tag{5.284}$$

$$\theta_3 = \cos^{-1}\left[\frac{3}{2\sqrt{5}}\right] = 47.87^\circ, \qquad \theta_4 = \cos^{-1}\left[\frac{4}{2\sqrt{5}}\right] = 26.57^\circ. \tag{5.285}$$

The angles for the remaining quantum numbers $m_4 = -1, -2, -3, -4$ can be inferred at once from the relation

$$\theta_{-m_l} = 180^\circ - \theta_{m_l}, \tag{5.286}$$

hence

$$\theta_{-1} = 180^\circ - 77.08^\circ = 102.92^\circ, \qquad \theta_{-2} = 180^\circ - 63.43^\circ = 116.57^\circ, \tag{5.287}$$

$$\theta_{-3} = 180^\circ - 47.87^\circ = 132.13^\circ, \qquad \theta_{-4} = 180^\circ - 26.57^\circ = 153.43^\circ. \tag{5.288}$$

Problem 5.11
Using $[\hat{X},\ \hat{P}] = i\hbar$, calculate the various commutation relations between the following operators[2]

$$\hat{T}_1 = \frac{1}{4}(\hat{P}^2 - \hat{X}^2), \qquad \hat{T}_2 = \frac{1}{4}(\hat{X}\hat{P} + \hat{P}\hat{X}), \qquad \hat{T}_3 = \frac{1}{4}(\hat{P}^2 + \hat{X}^2).$$

Solution
The operators $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$ can be viewed as describing some sort of *collective* vibrations; $\hat{T}_3$ has the structure of a harmonic oscillator Hamiltonian. The first commutator can be calculated as follows:

$$[\hat{T}_1,\ \hat{T}_2] = \frac{1}{4}[\hat{P}^2 - \hat{X}^2,\ \hat{T}_2] = \frac{1}{4}[\hat{P}^2,\ \hat{T}_2] - \frac{1}{4}[\hat{X}^2,\ \hat{T}_2], \tag{5.289}$$

where, using the commutation relation $[\hat{X},\ \hat{P}] = i\hbar$, we have

$$\begin{aligned}
[\hat{P}^2,\ \hat{T}_2] &= \frac{1}{4}[\hat{P}^2,\ \hat{X}\hat{P}] + \frac{1}{4}[\hat{P}^2,\ \hat{P}\hat{X}] \\
&= \frac{1}{4}\hat{P}[\hat{P},\ \hat{X}\hat{P}] + \frac{1}{4}[\hat{P},\ \hat{X}\hat{P}]\hat{P} + \frac{1}{4}\hat{P}[\hat{P},\ \hat{P}\hat{X}] + \frac{1}{4}[\hat{P},\ \hat{P}\hat{X}]\hat{P} \\
&= \frac{1}{4}\hat{P}[\hat{P},\ \hat{X}]\hat{P} + \frac{1}{4}[\hat{P},\ \hat{X}]\hat{P}^2 + \frac{1}{4}\hat{P}^2[\hat{P},\ \hat{X}] + \frac{1}{4}\hat{P}[\hat{P},\ \hat{X}]\hat{P}
\end{aligned}$$

[2] N. Zettili and F. Villars, *Nucl. Phys.*, **A469**, 77 (1987).

$$= -\frac{i\hbar}{4}\hat{P}^2 - \frac{i\hbar}{4}\hat{P}^2 - \frac{i\hbar}{4}\hat{P}^2 - \frac{i\hbar}{4}\hat{P}^2 = -i\hbar\hat{P}^2, \tag{5.290}$$

$$\begin{aligned}
[\hat{X}^2,\ \hat{T}_2] &= \frac{1}{4}[\hat{X}^2,\ \hat{X}\hat{P}] + \frac{1}{4}[\hat{X}^2,\ \hat{P}\hat{X}] \\
&= \frac{1}{4}\hat{X}[\hat{X},\ \hat{X}\hat{P}] + \frac{1}{4}[\hat{X},\ \hat{X}\hat{P}]\hat{X} + \frac{1}{4}\hat{X}[\hat{X},\ \hat{P}\hat{X}] + \frac{1}{4}[\hat{X},\ \hat{P}\hat{X}]\hat{X} \\
&= \frac{1}{4}\hat{X}^2[\hat{X},\ \hat{P}] + \frac{1}{4}\hat{X}[\hat{X},\ \hat{P}]\hat{X} + \frac{1}{4}\hat{X}[\hat{X},\ \hat{P}]\hat{X} + \frac{1}{4}[\hat{X},\ \hat{P}]\hat{X}^2 \\
&= \frac{i\hbar}{4}\hat{X}^2 + \frac{i\hbar}{4}\hat{X}^2 + \frac{i\hbar}{4}\hat{X}^2 + \frac{i\hbar}{4}\hat{X}^2 = i\hbar\hat{X}^2;
\end{aligned} \tag{5.291}$$

hence

$$[\hat{T}_1,\ \hat{T}_2] = \frac{1}{4}[\hat{P}^2 - \hat{X}^2,\ \hat{T}_2] = -\frac{1}{4}(i\hbar\hat{P}^2 + i\hbar\hat{X}^2) = -i\hbar\hat{T}_3. \tag{5.292}$$

The second commutator is calculated as follows:

$$[\hat{T}_2,\ \hat{T}_3] = \frac{1}{4}[\hat{T}_2,\ \hat{P}^2 + \hat{X}^2] = \frac{1}{4}[\hat{T}_2,\ \hat{P}^2] + \frac{1}{4}[\hat{T}_2,\ \hat{X}^2], \tag{5.293}$$

where $[\hat{T}_2,\ \hat{P}^2]$ and $[\hat{T}_2,\ \hat{X}^2]$ were calculated in (5.290) and (5.291):

$$[\hat{T}_2,\ \hat{P}^2] = i\hbar\hat{P}^2, \qquad [\hat{T}_2,\ \hat{X}^2] = -i\hbar\hat{X}^2. \tag{5.294}$$

Thus, we have

$$[\hat{T}_2,\ \hat{T}_3] = \frac{1}{4}(i\hbar\hat{P}^2 - i\hbar\hat{X}^2) = i\hbar\hat{T}_1. \tag{5.295}$$

The third commutator is

$$[\hat{T}_3,\ \hat{T}_1] = \frac{1}{4}[\hat{T}_3,\ \hat{P}^2 - \hat{X}^2] = \frac{1}{4}[\hat{T}_3,\ \hat{P}^2] - \frac{1}{4}[\hat{T}_3,\ \hat{X}^2], \tag{5.296}$$

where

$$\begin{aligned}
[\hat{T}_3,\ \hat{P}^2] &= \frac{1}{4}[\hat{P}^2,\ \hat{P}^2] + \frac{1}{4}[\hat{X}^2,\ \hat{P}^2] = \frac{1}{4}[\hat{X}^2,\ \hat{P}^2] = \frac{1}{4}\hat{X}[\hat{X},\ \hat{P}^2] + \frac{1}{4}[\hat{X},\ \hat{P}^2]\hat{X} \\
&= \frac{1}{4}\hat{X}\hat{P}[\hat{X},\ \hat{P}] + \frac{1}{4}\hat{X}[\hat{X},\ \hat{P}]\hat{P} + \frac{1}{4}\hat{P}[\hat{X},\ \hat{P}]\hat{X} + \frac{1}{4}[\hat{X},\ \hat{P}]\hat{P}\hat{X} \\
&= \frac{i\hbar}{4}(2\hat{X}\hat{P} + 2\hat{P}\hat{X}) = \frac{i\hbar}{2}(\hat{X}\hat{P} + \hat{P}\hat{X}),
\end{aligned} \tag{5.297}$$

$$[\hat{T}_3,\ \hat{X}^2] = \frac{1}{4}[\hat{P}^2,\ \hat{X}^2] + \frac{1}{4}[\hat{X}^2,\ \hat{X}^2] = \frac{1}{4}[\hat{P}^2,\ \hat{X}^2] = -\frac{i\hbar}{2}(\hat{X}\hat{P} + \hat{P}\hat{X}); \tag{5.298}$$

hence

$$\begin{aligned}
[\hat{T}_3,\ \hat{T}_1] &= \frac{1}{4}[\hat{T}_3,\ \hat{P}^2] - \frac{1}{4}[\hat{T}_3,\ \hat{X}^2] = \frac{i\hbar}{8}(\hat{X}\hat{P} + \hat{P}\hat{X}) + \frac{i\hbar}{8}(\hat{X}\hat{P} + \hat{P}\hat{X}) \\
&= \frac{i\hbar}{4}(\hat{X}\hat{P} + \hat{P}\hat{X}) = i\hbar\hat{T}_2.
\end{aligned} \tag{5.299}$$

In sum, the commutation relations between $\hat{T}_1$, $\hat{T}_2$, and $\hat{T}_3$ are

$$[\hat{T}_1, \hat{T}_2] = -i\hbar\hat{T}_3, \qquad [\hat{T}_2, \hat{T}_3] = i\hbar\hat{T}_1, \qquad [\hat{T}_3, \hat{T}_1] = i\hbar\hat{T}_2. \tag{5.300}$$

These relations are similar to those of ordinary angular momentum, save for the minus sign in $[\hat{T}_1, \hat{T}_2] = -i\hbar\hat{T}_3$.

Problem 5.12
Consider a particle whose wave function is

$$\psi(x, y, z) = \frac{1}{4\sqrt{\pi}} \frac{2z^2 - x^2 - y^2}{r^2} + \sqrt{\frac{3}{\pi}} \frac{xz}{r^2}.$$

(a) Calculate $\hat{\vec{L}}^2 \psi(x, y, z)$ and $\hat{L}_z \psi(x, y, z)$. Find the total angular momentum of this particle.

(b) Calculate $\hat{L}_+ \psi(x, y, z)$ and $\langle \psi \mid \hat{L}_+ \mid \psi \rangle$.

(c) If a measurement of the z-component of the orbital angular momentum is carried out, find the probabilities corresponding to finding the results 0, $\hbar$, and $-\hbar$.

(d) What is the probability of finding the particle at the position $\theta = \pi/3$ and $\varphi = \pi/2$ within $d\theta = 0.03$ rad and $d\varphi = 0.03$ rad?

Solution

(a) Since $Y_{20}(x, y, z) = \sqrt{5/16\pi}(3z^2 - r^2)/r^2$ and $Y_{2,\pm1}(x, y, z) = \mp\sqrt{15/8\pi}(x \pm iy)z/r^2$, we can write

$$\frac{2z^2 - x^2 - y^2}{r^2} = \frac{3z^2 - r^2}{r^2} = \sqrt{\frac{16\pi}{5}}\, Y_{20} \qquad \text{and} \qquad \frac{xz}{r^2} = \sqrt{\frac{2\pi}{15}}\, (Y_{2,-1} - Y_{21}); \quad (5.301)$$

hence

$$\psi(x, y, z) = \frac{1}{4\sqrt{\pi}} \sqrt{\frac{16\pi}{5}} Y_{20} + \sqrt{\frac{3}{\pi}} \sqrt{\frac{2\pi}{15}} \left(Y_{2,-1} - Y_{21}\right) = \frac{1}{\sqrt{5}} Y_{20} + \sqrt{\frac{2}{5}} \left(Y_{2,-1} - Y_{21}\right). \quad (5.302)$$

Having expressed ψ in terms of the spherical harmonics, we can now easily write

$$\hat{\vec{L}}^2 \psi(x, y, z) = \frac{1}{\sqrt{5}} \hat{\vec{L}}^2 Y_{20} + \sqrt{\frac{2}{5}} \hat{\vec{L}}^2 \left(Y_{2,-1} - Y_{21}\right) = 6\hbar^2 \psi(x, y, z) \quad (5.303)$$

and

$$\hat{L}_z \psi(x, y, z) = \frac{1}{\sqrt{5}} \hat{L}_z Y_{20} + \sqrt{\frac{2}{5}} \hat{L}_z \left(Y_{2,-1} - Y_{21}\right) = -\hbar \sqrt{\frac{2}{5}} \hat{L}_z \left(Y_{2,-1} + Y_{21}\right). \quad (5.304)$$

This shows that $\psi(x, y, z)$ is an eigenstate of $\hat{\vec{L}}^2$ with eigenvalue $6\hbar^2$; $\psi(x, y, z)$ is, however, not an eigenstate of $\hat{L}_z$. Thus the total angular momentum of the particle is

$$\sqrt{\langle \psi \mid \hat{\vec{L}}^2 \mid \psi \rangle} = \sqrt{6}\hbar. \quad (5.305)$$

(b) Using the relation $\hat{L}_+ Y_{lm} = \hbar\sqrt{l(l+1) - m(m+1)}\, Y_{l\, m+1}$, we have

$$\hat{L}_+ \psi(x, y, z) = \frac{1}{\sqrt{5}} \hat{L}_+ Y_{20} + \sqrt{\frac{2}{5}} \hat{L}_+ \left(Y_{2,-1} - Y_{21}\right) = \hbar \sqrt{\frac{6}{5}} Y_{21} + \hbar \sqrt{\frac{2}{5}} \left(\sqrt{6} Y_{20} - 2Y_{22}\right); \quad (5.306)$$

hence

$$\begin{aligned}\langle \psi \mid \hat{L}_+ \mid \psi \rangle &= \left[\frac{1}{\sqrt{5}} \langle 2,\ 0| + \sqrt{\frac{2}{5}} \left(\langle 2,\ -1| - \langle 2,\ 1| \right) \right] \\ &\quad \times \left[\hbar \sqrt{\frac{6}{5}} Y_{21} + \hbar \sqrt{\frac{2}{5}} \left(\sqrt{6} Y_{20} - 2Y_{22} \right) \right] \\ &= 0. \end{aligned} \tag{5.307}$$

(c) Since $| \psi \rangle = (1/\sqrt{5}) Y_{20} + \sqrt{2/5}(Y_{2,-1} - Y_{21})$, a calculation of $\langle \psi \mid \hat{L}_z \mid \psi \rangle$ yields

$$\langle \psi \mid \hat{L}_z \mid \psi \rangle = 0, \qquad \text{with probability} \qquad P_0 = \frac{1}{5}, \tag{5.308}$$

$$\langle \psi \mid \hat{L}_z \mid \psi \rangle = -\hbar, \qquad \text{with probability} \qquad P_{-1} = \frac{2}{5}, \tag{5.309}$$

$$\langle \psi \mid \hat{L}_z \mid \psi \rangle = \hbar, \qquad \text{with probability} \qquad P_1 = \frac{2}{5}. \tag{5.310}$$

(d) Since $\psi(x, y, z) = (1/4\sqrt{\pi})(2z^2 - x^2 - y^2)/r^2 + \sqrt{3/\pi}\, xz/r^2$ can be written in terms of the spherical coordinates as

$$\psi(\theta, \varphi) = \frac{1}{4\sqrt{\pi}} (3 \cos \theta^2 - 1) + \sqrt{\frac{3}{\pi}} \sin \theta \cos \theta \cos \varphi, \tag{5.311}$$

the probability of finding the particle at the position θ and φ is

$$P(\theta, \varphi) = |\psi(\theta, \varphi)|^2 \sin \theta d\theta d\varphi = \left[\frac{1}{4\sqrt{\pi}} (3 \cos^2 \theta - 1) + \sqrt{\frac{3}{\pi}} \sin \theta \cos \theta \cos \varphi \right]^2 \sin \theta d\theta d\varphi; \tag{5.312}$$

hence

$$P\left(\frac{\pi}{3}, \frac{\pi}{2}\right) = \left[\frac{1}{4\sqrt{\pi}} \left(3 \cos^2 \frac{\pi}{3} - 1 \right) + 0 \right]^2 (0.03)^2 \sin \frac{\pi}{3} = 9.7 \times 10^{-7}. \tag{5.313}$$

Problem 5.13

Consider a particle of spin $s = 3/2$.

(a) Find the matrices representing the operators $\hat{S}_z$, $\hat{S}_x$, $\hat{S}_y$, $\hat{S}_x^2$, and $\hat{S}_y^2$ within the basis of $\hat{S}^2$ and $\hat{S}_z$.

(b) Find the energy levels of this particle when its Hamiltonian is given by

$$\hat{H} = \frac{\varepsilon_0}{\hbar^2} (\hat{S}_x^2 - \hat{S}_y^2) - \frac{\varepsilon_0}{\hbar} \hat{S}_z,$$

where ε_0 is a constant having the dimensions of energy. Are these levels degenerate?

(c) If the system was initially in an eigenstate $|\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$, find the state of the system at time t.

Solution

(a) Following the same procedure that led to (5.73) and (5.75), we can verify that for $s = \frac{3}{2}$ we have

$$S_z = \frac{\hbar}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}, \tag{5.314}$$

$$\hat{S}_- = \hbar\begin{pmatrix} 0 & 0 & 0 & 0 \\ \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \qquad \hat{S}_+ = \hbar\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{5.315}$$

which, when combined with $\hat{S}_x = (\hat{S}_+ + \hat{S}_-)/2$ and $\hat{S}_y = i(\hat{S}_- - \hat{S}_+)/2$, lead to

$$\hat{S}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}, \qquad \hat{S}_y = \frac{i\hbar}{2}\begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}. \tag{5.316}$$

Thus, we have

$$\hat{S}_x^2 = \frac{\hbar^2}{4}\begin{pmatrix} 3 & 0 & 2\sqrt{3} & 0 \\ 0 & 7 & 0 & 2\sqrt{3} \\ 2\sqrt{3} & 0 & 7 & 0 \\ 0 & 2\sqrt{3} & 0 & 3 \end{pmatrix}, \quad \hat{S}_y^2 = \frac{\hbar^2}{4}\begin{pmatrix} 3 & 0 & -2\sqrt{3} & 0 \\ 0 & 7 & 0 & -2\sqrt{3} \\ -2\sqrt{3} & 0 & 7 & 0 \\ 0 & -2\sqrt{3} & 0 & 3 \end{pmatrix}. \tag{5.317}$$

(b) The Hamiltonian is then given by

$$H = \frac{\varepsilon_0}{\hbar^2}(\hat{S}_x^2 - \hat{S}_y^2) - \frac{\varepsilon_0}{\hbar}\hat{S}_z = \frac{1}{2}\varepsilon_0\begin{pmatrix} -3 & 0 & 2\sqrt{3} & 0 \\ 0 & -1 & 0 & 2\sqrt{3} \\ 2\sqrt{3} & 0 & 1 & 0 \\ 0 & 2\sqrt{3} & 0 & 3 \end{pmatrix}. \tag{5.318}$$

The diagonalization of this Hamiltonian yields the following energy values:

$$E_1 = -\frac{5}{2}\varepsilon_0, \qquad E_2 = -\frac{3}{2}\varepsilon_0, \qquad E_3 = \frac{3}{2}\varepsilon_0, \qquad E_4 = \frac{5}{2}\varepsilon_0. \tag{5.319}$$

The corresponding normalized eigenvectors are given by

$$|1\rangle = \frac{1}{2}\begin{pmatrix} -\sqrt{3} \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |2\rangle = \frac{1}{2}\begin{pmatrix} 0 \\ -\sqrt{3} \\ 0 \\ 1 \end{pmatrix}, \quad |3\rangle = \frac{1}{\sqrt{12}}\begin{pmatrix} \sqrt{3} \\ 0 \\ 3 \\ 0 \end{pmatrix}, \quad |4\rangle = \frac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 0 \\ \sqrt{3} \end{pmatrix}. \tag{5.320}$$

None of the energy levels is degenerate.

(c) Since the initial state $|\,\psi_0\rangle$ can be written in terms of the eigenvectors (5.320) as follows:

$$|\,\psi_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = -\frac{\sqrt{3}}{2}\,|\,1\rangle + \frac{1}{2}\,|\,3\rangle; \tag{5.321}$$

the eigenfunction at a later time t is given by

$$\begin{aligned} \mid \psi(t)\rangle &= -\frac{\sqrt{3}}{2} \mid 1\rangle e^{-iE_1 t/\hbar} + \frac{1}{2} \mid 3\rangle e^{-iE_3 t/\hbar} \\ &= -\frac{\sqrt{3}}{4} \begin{pmatrix} -\sqrt{3} \\ 0 \\ 1 \\ 0 \end{pmatrix} \exp\left[\frac{5i\varepsilon_0 t}{2\hbar}\right] + \frac{1}{2\sqrt{12}} \begin{pmatrix} \sqrt{3} \\ 0 \\ 3 \\ 0 \end{pmatrix} \exp\left[-\frac{3i\varepsilon_0 t}{2\hbar}\right]. \end{aligned} \tag{5.322}$$

5.9 Exercises

Exercise 5.1

(a) Show the following commutation relations:

$$[\hat{Y},\ \hat{L}_y] = 0, \qquad [\hat{Y},\ \hat{L}_z] = i\hbar\hat{X}, \qquad [\hat{Y},\ \hat{L}_x] = -i\hbar\hat{Z},$$

$$[\hat{Z},\ \hat{L}_z] = 0, \qquad [\hat{Z},\ \hat{L}_x] = i\hbar\hat{Y}, \qquad [\hat{Z},\ \hat{L}_y] = -i\hbar\hat{X}.$$

(b) Using a cyclic permutation of xyz, apply the results of (a) to infer expressions for $[\hat{X},\ \hat{L}_x]$, $[\hat{X},\ \hat{L}_y]$, and $[\hat{X},\ \hat{L}_z]$.

(c) Use the results of (a) and (b) to calculate $[\hat{R}^2,\ \hat{L}_x]$, $[\hat{R}^2,\ \hat{L}_y]$, and $[\hat{R}^2,\ \hat{L}_x]$, where $\hat{R}^2 = \hat{X}^2 + \hat{Y}^2 + \hat{Z}^2$.

Exercise 5.2

(a) Show the following commutation relations:

$$[\hat{P}_y,\ \hat{L}_y] = 0, \qquad [\hat{P}_y,\ \hat{L}_z] = i\hbar\hat{P}_x, \qquad [\hat{P}_y,\ \hat{L}_x] = -i\hbar\hat{P}_z,$$

$$[\hat{P}_z,\ \hat{L}_z] = 0, \qquad [\hat{P}_z,\ \hat{L}_x] = i\hbar\hat{P}_y, \qquad [\hat{P}_z,\ \hat{L}_y] = -i\hbar\hat{P}_x.$$

(b) Use the results of (a) to infer by means of a cyclic permutation the expressions for $[\hat{P}_x,\ \hat{L}_x]$, $[\hat{P}_x,\ \hat{L}_y]$, and $[\hat{P}_x,\ \hat{L}_z]$.

(c) Use the results of (a) and (b) to calculate $[\hat{P}^2,\ \hat{L}_x]$, $[\hat{P}^2,\ \hat{L}_y]$, and $[\hat{P}^2,\ \hat{L}_z]$, where $\hat{P}^2 = \hat{P}_x^2 + \hat{P}_y^2 + \hat{P}_z^2$.

Exercise 5.3

If $\hat{L}_\pm$ and $\hat{R}_\pm$ are defined by $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ and $\hat{R}_\pm = \hat{X} \pm i\hat{Y}$, prove the following commutators: (a) $[\hat{L}_\pm,\ \hat{R}_\pm] = \pm 2\hbar\hat{Z}$ and (b) $[\hat{L}_\pm,\ \hat{R}_\mp] = 0$.

Exercise 5.4

If $\hat{L}_\pm$ and $\hat{R}_\pm$ are defined by $\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ and $\hat{R}_\pm = \hat{X} \pm i\hat{Y}$, prove the following commutators: (a) $[\hat{L}_\pm,\ \hat{Z}] = \mp\hbar\hat{R}_\pm$, (b) $[\hat{L}_z,\ \hat{R}_\pm] = \pm\hbar\hat{R}_\pm$, and (c) $[\hat{L}_z,\ \hat{Z}] = 0$.

Exercise 5.5

Prove the following two relations: $\hat{\vec{R}} \cdot \hat{\vec{L}} = 0$ and $\hat{\vec{P}} \cdot \hat{\vec{L}} = 0$.

Exercise 5.6
The Hamiltonian due to the interaction of a particle of spin $\vec{S}$ with a magnetic field $\vec{B}$ is given by $\hat{H} = -\vec{S} \cdot \vec{B}$ where $\vec{S}$ is the spin. Calculate the commutator $[\vec{S},\ \hat{H}]$.

Exercise 5.7
Prove the following relation:

$$[\hat{L}_z,\ \cos\varphi] = i\hbar \sin\varphi,$$

where φ is the azimuthal angle.

Exercise 5.8
Prove the following relation:

$$[\hat{L}_z,\ \sin(2\varphi)] = 2i\hbar \left(\sin^2\varphi - \cos^2\varphi\right),$$

where φ is the azimuthal angle. *Hint:* $[\hat{A},\ \hat{B}\hat{C}] = \hat{B}[\hat{A},\ \hat{C}] + [\hat{A},\ \hat{B}]\hat{C}$.

Exercise 5.9
Using the properties of $\hat{J}_+$ and $\hat{J}_-$, calculate $|j,\ \pm j\rangle$ and $|j,\ \pm m\rangle$ as functions of the action of $\hat{J}_\pm$ on the states $|j,\ \pm m\rangle$ and $|j,\ \pm j\rangle$, respectively.

Exercise 5.10
Consider the operator $\hat{A} = \frac{1}{2}(\hat{J}_x\hat{J}_y + \hat{J}_y\hat{J}_x)$.

(a) Calculate the expectation value of $\hat{A}$ and $\hat{A}^2$ with respect to the state $|\ j,\ m\rangle$.

(b) Use the result of (a) to find an expression for $\hat{A}^2$ in terms of: $\hat{\vec{J}}^4$, $\hat{\vec{J}}^2$, $\hat{J}_z^2$, $\hat{J}_+^4$, $\hat{J}_-^4$.

Exercise 5.11
Consider the wave function

$$\psi(\theta, \varphi) = 3\sin\theta\cos\theta e^{i\varphi} - 2(1-\cos^2\theta)e^{2i\varphi}.$$

(a) Write $\psi(\theta, \varphi)$ in terms of the spherical harmonics.

(b) Write the expression found in (a) in terms of the Cartesian coordinates.

(c) Is $\psi(\theta, \varphi)$ an eigenstate of $\hat{\vec{L}}^2$ or $\hat{L}_z$?

(d) Find the probability of measuring $2\hbar$ for the z-component of the orbital angular momentum.

Exercise 5.12
Show that $\hat{L}_z(\cos^2\varphi - \sin^2\varphi + 2i\sin\varphi\cos\varphi) = 2\hbar^{2i\varphi}$, where φ is the azimuthal angle.

Exercise 5.13
Find the expressions for the spherical harmonics $Y_{30}(\theta, \varphi)$ and $Y_{3,\pm 1}(\theta, \varphi)$,

$$Y_{30}(\theta, \varphi) = \sqrt{7/16\pi}\,(5\cos^3\theta - 3\cos\theta), \quad Y_{3,\pm 1}(\theta, \varphi) = \mp\sqrt{21/64\pi}\,\sin\theta(5\cos^2\theta - 1)e^{\pm i\varphi},$$

in terms of the Cartesian coordinates x, y, z.

Exercise 5.14
(a) Show that the following expectation values between $|lm\rangle$ states satisfy the relations $\langle\hat{L}_x\rangle = \langle\hat{L}_y\rangle = 0$ and $\langle\hat{L}_x^2\rangle = \langle\hat{L}_y^2\rangle = \frac{1}{2}\left[l(l+1)\hbar^2 - m^2\hbar^2\right]$.

(b) Verify the inequality $\Delta L_x \Delta L_y \geq \hbar^2 m/2$, where $\Delta L_x = \sqrt{\langle L_x^2\rangle - \langle L_x\rangle^2}$.

Exercise 5.15
A particle of mass m is fixed at one end of a rigid rod of negligible mass and length R. The other end of the rod rotates in the xy plane about a bearing located at the origin, whose axis is in the z-direction.

(a) Write the system's total energy in terms of its angular momentum L.

(b) Write down the time-independent Schrödinger equation of the system. *Hint:* In spherical coordinates, only φ varies.

(c) Solve for the possible energy levels of the system, in terms of m and the moment of inertia $I = mR^2$.

(d) Explain why there is no zero-point energy.

Exercise 5.16
Consider a system which is described by the state

$$\psi(\theta,\ \varphi) = \sqrt{\frac{3}{8}} Y_{11}(\theta,\ \varphi) + \sqrt{\frac{1}{8}} Y_{10}(\theta,\ \varphi) + A Y_{1,-1}(\theta,\ \varphi),$$

where A is a real constant

(a) Calculate A so that $\mid \psi\rangle$ is normalized.

(b) Find $\hat{L}_+ \psi(\theta,\ \varphi)$.

(c) Calculate the expectation values of $\hat{L}_x$ and $\hat{\vec{L}}^2$ in the state $\mid \psi\rangle$.

(d) Find the probability associated with a measurement that gives zero for the z-component of the angular momentum.

(e) Calculate $\langle \Phi | \hat{L}_z \mid \psi\rangle$ and $\langle \Phi | \hat{L}_- \mid \psi\rangle$ where

$$\Phi(\theta,\ \varphi) = \sqrt{\frac{8}{15}} Y_{11}(\theta,\ \varphi) + \sqrt{\frac{4}{15}} Y_{10}(\theta,\ \varphi) + \sqrt{\frac{3}{15}} Y_{2,-1}(\theta,\ \varphi).$$

Exercise 5.17

(a) Using the commutation relations of angular momentum, verify the validity of the (Jacobi) identity: $[\hat{J}_x,\ [\hat{J}_y,\ \hat{J}_z]] + [\hat{J}_y,\ [\hat{J}_z,\ \hat{J}_x]] + [\hat{J}_z,\ [\hat{J}_x,\ \hat{J}_y]] = 0$.

(b)Prove the following identity: $[\hat{J}_x^2,\ \hat{J}_y^2] = [\hat{J}_y^2,\ \hat{J}_z^2] = [\hat{J}_z^2,\ \hat{J}_x^2]$.

(c) Calculate the expressions of $\hat{L}_-\hat{L}_+ Y_{lm}(\theta,\ \varphi)$ and $\hat{L}_+\hat{L}_- Y_{lm}(\theta,\ \varphi)$, and then infer the commutator $[\hat{L}_+\hat{L}_-,\ \hat{L}_-\hat{L}_+] Y_{lm}(\theta,\ \varphi)$.

Exercise 5.18
Consider a particle whose wave function is given by $\psi(x, y, z) = A[(x+z)y + z^2]/r^2 - A/3$, where A is a constant.

(a) Is ψ an eigenstate of $\hat{\vec{L}}^{\,2}$? If yes, what is the corresponding eigenvalue? Is it also an eigenstate of $\hat{L}_z$?

(b) Find the constant A so that ψ is normalized.

(c) Find the relative probabilities for measuring the various values of $\hat{L}_z$ and $\hat{\vec{L}}^{\,2}$, and then calculate the expectation values of $\hat{L}_z$ and $\hat{\vec{L}}^{\,2}$.

(d) Calculate $\hat{L}_\pm \mid \psi\rangle$ and then infer $\langle \psi \mid \hat{L}_\pm \mid \psi\rangle$.

Exercise 5.19
Consider a system which is in the state

$$\psi(\theta,\ \varphi) = \sqrt{\frac{2}{13}} Y_{3,-3} + \sqrt{\frac{3}{13}} Y_{3,-2} + \sqrt{\frac{3}{13}} Y_{30} + \sqrt{\frac{3}{13}} Y_{3,2} + \sqrt{\frac{2}{13}} Y_{33}.$$

(a) If $\hat{L}_z$ were measured, what values will one obtain and with what probabilities?

(b) If after a measurement of $\hat{L}_z$ we find $l_z = 2\hbar$, calculate the uncertainties ΔL_x and ΔL_y and their product $\Delta L_x \Delta L_y$.

(c) Find $\langle \psi \mid \hat{L}_x \mid \psi \rangle$ and $\langle \psi \mid \hat{L}_y \mid \psi \rangle$.

Exercise 5.20

(a) Calculate the energy eigenvalues of an axially symmetric rotator and find the degeneracy of each energy level (i.e., for each value of the azimuthal quantum number m, find how many states $|l\ m\rangle$ correspond to the same energy). We may recall that the Hamiltonian of an axially symmetric rotator is given by

$$\hat{H} = \frac{\hat{L}_x^2 + \hat{L}_y^2}{2I_1} + \frac{\hat{L}_z^2}{2I_2},$$

where I_1 and I_2 are the moments of inertia.

(b) From part (a) infer the energy eigenvalues for the various levels of $l = 3$.

(c) In the case of a rigid rotator (i.e., $I_1 = I_2 = I$), find the energy expression and the corresponding degeneracy relation.

(d) Calculate the orbital quantum number l and the corresponding energy degeneracy for a rigid rotator where the magnitude of the total angular momentum is $\sqrt{56}\hbar$.

Exercise 5.21

Consider a system of total angular momentum $j = 1$. We are interested here in the measurement of $\hat{J}_y$; its matrix is given by

$$\hat{J}_y = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

(a) What are the possible values will we obtain when measuring $\hat{J}_y$?

(b) Calculate $\langle \hat{J}_z \rangle$, $\langle \hat{J}_z^2 \rangle$, and ΔJ_z if the system is in the state $j_y = \hbar$.

(c) Repeat (b) for $\langle \hat{J}_x \rangle$, $\langle \hat{J}_x^2 \rangle$, and ΔJ_x.

Exercise 5.22

Calculate $Y_{3,\pm 2}(\theta, \varphi)$ by applying the ladder operators $\hat{L}_\pm$ on $Y_{3,\pm 1}(\theta, \varphi)$.

Exercise 5.23

Consider a system of total angular momentum $j = 1$. We want to carry out measurements on

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

(a) What are the possible values will we obtain when measuring $\hat{J}_z$?

(b) Calculate $\langle \hat{J}_x \rangle$, $\langle \hat{J}_x^2 \rangle$, and ΔJ_x if the system is in the state $j_z = -\hbar$.

(c) Repeat (b) for $\langle \hat{J}_y \rangle$, $\langle \hat{J}_y^2 \rangle$, and ΔJ_y.

Exercise 5.24

Consider a system which is in the state

$$\psi(x, y, z) = \frac{1}{4\sqrt{\pi}} \frac{z}{r} + \frac{1}{\sqrt{3\pi}} \frac{x}{r}.$$

(a) Express $\psi(x, y, z)$ in terms of the spherical harmonics then calculate $\hat{\vec{L}}^2\psi(x, y, z)$ and $\hat{L}_z\psi(x, y, z)$. Is $\psi(x, y, z)$ an eigenstate of $\hat{\vec{L}}^2$ or $\hat{L}_z$?

(b) Calculate $\hat{L}_\pm\psi(x, y, z)$ and $\langle\psi \mid \hat{L}_\pm \mid \psi\rangle$.

(c) If a measurement of the z-component of the orbital angular momentum is carried out, find the probabilities corresponding to finding the results 0, $\hbar$, and $-\hbar$.

Exercise 5.25

Consider a system whose wave function is given by

$$\psi(\theta, \varphi) = \frac{1}{2}Y_{00}(\theta, \varphi) + \frac{1}{\sqrt{3}}Y_{11}(\theta, \varphi) + \frac{1}{2}Y_{1,-1}(\theta, \varphi) + \frac{1}{\sqrt{6}}Y_{22}(\theta, \varphi).$$

(a) Is $\psi(\theta, \varphi)$ normalized?

(b) Is $\psi(\theta, \varphi)$ an eigenstate of $\hat{\vec{L}}^2$ or $\hat{L}_z$?

(c) Calculate $\hat{L}_\pm\psi(\theta, \varphi)$ and $\langle\psi \mid \hat{L}_\pm \mid \psi\rangle$.

(d) If a measurement of the z-component of the orbital angular momentum is carried out, find the probabilities corresponding to finding the results 0, $\hbar$, $-\hbar$, and $2\hbar$.

Exercise 5.26

Using the expression of $\hat{L}_-$ in spherical coordinates, prove the following two commutators: $[\hat{L}_-,\ e^{-i\varphi}\sin\theta] = 0$ and $[\hat{L}_-,\ \cos\theta] = \hbar e^{-i\varphi}\sin\theta$.

Exercise 5.27

Consider a particle whose angular momentum is $l = 1$.

(a) Find the eigenvalues and eigenvectors, $|1,\ m_x\rangle$, of $\hat{L}_x$.

(b) Express the state $|1,\ m_x = 1\rangle$ as a linear superposition of the eigenstates of $\hat{L}_z$. *Hint:* you need first to find the eigenstates of L_x and find which of them corresponds to the eigenvalue $m_x = 1$; this eigenvector will be expanded in the z basis.

(c) What is the probability of measuring $m_z = 1$ when the particle is in the eigenstate $|1,\ m_x = 1\rangle$? What about the probability corresponding to measuring $m_z = 0$?

(d) Suppose that a measurement of the z-component of angular momentum is performed and that the result $m_z = 1$ is obtained. Now we measure the x-component of angular momentum. What are the possible results and with what probabilities?

Exercise 5.28

Consider a system which is given in the following angular momentum eigenstates $\mid l,\ m\rangle$:

$$\mid\psi\rangle = \frac{1}{\sqrt{7}} \mid 1,\ -1\rangle + A \mid 1,\ 0\rangle + \sqrt{\frac{2}{7}}|1,\ 1\rangle,$$

where A is a real constant

(a) Calculate A so that $\mid\psi\rangle$ is normalized.

(b) Calculate the expectation values of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, and $\hat{\vec{L}}^2$ in the state $\mid\psi\rangle$.

(c) Find the probability associated with a measurement that gives $1\hbar$ for the z-component of the angular momentum.

(d) Calculate $\langle 1,\ m|\hat{L}_+^2 \mid \psi\rangle$ and $\langle 1,\ m|\hat{L}_-^2 \mid \psi\rangle$.

Exercise 5.29
Consider a particle of angular momentum $j = 3/2$.

(a) Find the matrices representing the operators $\hat{\vec{J}}^2$, $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$ in the $\{|\frac{3}{2},\ m\rangle\}$ basis.
(b) Using these matrices, show that $\hat{J}_x$, $\hat{J}_y$, $\hat{J}_z$ satisfy the commutator $[\hat{J}_x,\ \hat{J}_y] = i\hbar\hat{J}_z$.
(c) Calculate the mean values of $\hat{J}_x$ and $\hat{J}_x^2$ with respect to the state $\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$.
(d) Calculate $\Delta J_x \Delta J_y$ with respect to the state

$$\begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

and verify that this product satisfies Heisenberg's uncertainty principle.

Exercise 5.30
Consider the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

(a) Verify that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = I$, where I is the unit matrix

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

(b) Calculate the commutators $[\sigma_x, \sigma_y]$, $[\sigma_x, \sigma_z]$, and $[\sigma_y, \sigma_z]$.
(c) Calculate the anticommutator $\sigma_x\sigma_y + \sigma_y\sigma_x$.
(d) Show that $e^{i\theta\sigma_y} = I\cos\theta + i\sigma_y \sin\theta$, where I is the unit matrix.
(e) Derive an expression for $e^{i\theta\sigma_z}$ by analogy with the one for σ_y.

Exercise 5.31
Consider a spin $\frac{3}{2}$ particle whose Hamiltonian is given by

$$\hat{H} = \frac{\varepsilon_0}{\hbar^2}(\hat{S}_x^2 - \hat{S}_y^2) - \frac{\varepsilon_0}{\hbar^2}\hat{S}_z^2,$$

where ε_0 is a constant having the dimensions of energy.

(a) Find the matrix of the Hamiltonian and diagonalize it to find the energy levels.
(b) Find the eigenvectors and verify that the energy levels are doubly degenerate.

Exercise 5.32
Find the energy levels of a spin $\frac{5}{2}$ particle whose Hamiltonian is given by

$$\hat{H} = \frac{\varepsilon_0}{\hbar^2}(\hat{S}_x^2 + \hat{S}_y^2) + \frac{\varepsilon_0}{\hbar}\hat{S}_z,$$

where ε_0 is a constant having the dimensions of energy. Are the energy levels degenerate?

Exercise 5.33
Consider an electron whose spin direction is located in the xy plane.

(a) Find the eigenvalues (call them λ_1, λ_2) and eigenstates ($| \lambda_1\rangle$, $| \lambda_2\rangle$) of the electron's spin operator $\vec{S}$.

(b) Assuming that the initial state of the electron is given by

$$| \psi_0\rangle = \frac{1}{3} | \lambda_1\rangle + \frac{2\sqrt{2}}{3} | \lambda_2\rangle,$$

find the probability of obtaining a value of $\hat{S} = -\hbar/2$ after measuring the spin of the electron.

Exercise 5.34
(a) Find the eigenvalues (call them λ_1, λ_2) and eigenstates ($| \lambda_1\rangle$, $| \lambda_2\rangle$) of the spin operator $\vec{S}$ of an electron when $\vec{S}$ is pointing along an arbitrary unit vector $\vec{n}$ that lies within the yz plane.

(b) Assuming that the initial state of the electron is given by

$$| \psi_0\rangle = \frac{1}{2} | \lambda_1\rangle + \frac{\sqrt{3}}{2} | \lambda_2\rangle,$$

find the probability of obtaining a value of $\hat{S} = \hbar/2$ after measuring the spin of the electron.

Exercise 5.35
Consider a particle of spin $\frac{3}{2}$. Find the matrix for the component of the spin along a unit vector with arbitrary direction $\vec{n}$. Find its eigenvalues and eigenvectors. *Hint:*

$$\vec{n} = (\sin\theta\cos\varphi)\vec{i} + (\sin\theta\sin\varphi)\vec{j} + (\cos\theta)\vec{k}.$$

Exercise 5.36
Show that $[\hat{J}_x\hat{J}_y,\ \hat{J}_z] + [\hat{J}_x,\ \hat{J}_y\hat{J}_z] = i\hbar\left(\hat{J}_x^2 - 2\hat{J}_y^2 + \hat{J}_z^2\right)$.

Exercise 5.37
Find the eigenvalues of the operators $\hat{\vec{L}}^2$ and $\hat{L}_z$ for each of the following states:

(a) $Y_{21}(\theta, \varphi)$,
(b) $Y_{3,-2}(\theta, \varphi)$,
(c) $\frac{1}{\sqrt{2}}\left[Y_{33}(\theta, \varphi) + Y_{3,-3}(\theta, \varphi)\right]$, and
(d) $Y_{40}(\theta, \varphi)$.

Exercise 5.38
Use the following general relations:

$$| \psi_x\rangle_\pm = \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2}, \frac{1}{2}\right\rangle \pm \left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right], \qquad | \psi_y\rangle_\pm = \frac{1}{\sqrt{2}}\left[\left|\frac{1}{2}, \frac{1}{2}\right\rangle \pm i\left|\frac{1}{2}, -\frac{1}{2}\right\rangle\right]$$

to verify the following eigenvalue equations:

$$\hat{S}_x | \psi_x\rangle_\pm = \pm\frac{\hbar}{2} |\psi_x\rangle_\pm \qquad \text{and} \qquad \hat{S}_y | \psi_y\rangle_\pm = \pm\frac{\hbar}{2} |\psi_y\rangle_\pm .$$