#### Angular Momentum Eigenvalue Picture for Eigenstates

What is  $|l, m\rangle$ ? It is an eigenstate of the commuting operators  $\mathcal{L}^2$  and  $\mathcal{L}_z$ . The quantum numbers l and m are not eigenvalues. The corresponding eigenvalues are  $\hbar^2 l(l+1)$  and  $m\hbar$ . Were we to use eigenvalues in the ket, the eigenstate would look like  $|\hbar^2 l(l+1), m\hbar\rangle$ . But just l and m uniquely identify the state, and that is more economical, so only the quantum numbers are conventionally used. This is essentially the same sort of convenient shorthand used to denote an eigenstate of a SHO  $|n\rangle$ , vice using the eigenvalue  $|(n+\frac{1}{2})\hbar\omega\rangle$ .

Only one quantum number is needed to uniquely identify an eigenstate of a SHO, but two are needed to uniquely identify an eigenstate of angular momentum. Because the angular momentum component operators do not commute, a complete set of commuting observables are needed. Each of the component operators commutes with  $\mathcal{L}^2$ , so we use it and one other, which is  $\mathcal{L}_z$  chosen by convention. One quantum number is needed for each operator in the complete set. Multiple quantum numbers used to identify a ket denote a complete set of commuting observables is needed.

Remember that a system is assumed to exist in a linear combination of all possible eigenstates until we measure. If we measure, what are the possible outcomes? Possible outcomes are the eigenvalues. For a given value of the orbital angular momentum quantum number, the magnetic quantum number can assume integer values ranging from -l to l. The simplest case is  $l = 0 \Rightarrow m = 0$  is the only possible value of the magnetic quantum number. The possible outcomes of a measurement of such a system are eigenvalues of  $\hbar^2(0)(0+1) = 0\hbar^2$  or just 0 for  $\mathcal{L}^2$ , and  $m\hbar = (0)\hbar$  or just 0 for  $\mathcal{L}_z$  as well, corresponding to figure 9–2.a.

Figure 9 – 2.a. l = 0. Figure 9 – 2.b. l = 1. Figure 9 – 2.c. l = 2.

If we somehow knew l = 1, which could be ascertained by a measurement of  $\hbar^2(1)(1+1) = 2\hbar^2$ for  $\mathcal{L}^2$ , the possible values of the magnetic quantum number are m = -1, 0, or 1, so the eigenvalues which could be measured are  $-\hbar$ , 0, or  $\hbar$  for  $\mathcal{L}_z$ , per figure 9–2.b. If we measured  $\hbar^2(2)(2+1) = 6\hbar^2$  for  $\mathcal{L}^2$ , we would know we had l = 2, and the possible values of the magnetic quantum number are m = -2, -1, 0, 1, or 2, so the eigenvalues which could be measured are  $-2\hbar$ ,  $-\hbar$ , 0,  $\hbar$ , or  $2\hbar$  for  $\mathcal{L}_z$ , per figure 9–2.c. Though the magnetic quantum number is bounded by the orbital angular momentum quantum number, the orbital angular momentum quantum number is not bounded, so we can continue indefinitely. Notice there are 2l+1 possible values of m for every value of l.

A semi–classical diagram is often used. A simple interpretation of  $|l, m\rangle$  is that it is a vector quantized in length of

$$\left|\mathcal{L}\right| \rightarrow \left|\mathcal{L}\right| = \sqrt{\mathcal{L}^2} = \hbar \sqrt{l(l+1)}.$$

This vector has values for which the z component is also quantized in units of  $m\hbar$ . These

Figure 9 – 3. Semi – Classical Picture for l = 2.

features are illustrated in figure 9–3 for l = 2. The vectors are free to rotate around the z axis at any azimuthal angle  $\phi$ , but are fixed at polar angles  $\theta$  determined by the fact the projection on the z axis must be  $-2\hbar$ ,  $-\hbar$ , 0,  $\hbar$ , or  $2\hbar$ . Notice there is no information concerning the x or y components other than the square of their sum is fixed. We could express this for  $|\psi(t)\rangle = |l, m\rangle$ by stating the projection on the xy plane will be  $\cos(\omega t)$  or  $\sin(\omega t)$ . In such a case we can determine x and y component expectation values from symmetry alone, *i.e.*,

$$\langle \mathcal{L}_x \rangle = 0, \qquad \langle \mathcal{L}_y \rangle = 0.$$

Finally, what fixes any axis in space? And how do we know which axis is the z axis? The answer is we must introduce some asymmetry. Without an asymmetry of some sort, the axes and their labels are arbitrary. The practical asymmetry to introduce is a magnetic field, and that will establish a component quantization axis which will be the z axis.

# Eigenvalue/Eigenvector Equations for the Raising and Lowering Operators

Using quantum number notation, the fact  $\mathcal{L}_+|\alpha,\beta\rangle$  is and eigenstate of  $\mathcal{L}_z$  would be written

$$\mathcal{L}_{z}\mathcal{L}_{+}|l, m\rangle = (m\hbar + \hbar)\mathcal{L}_{+}|l, m\rangle$$
$$= (m+1)\hbar\mathcal{L}_{+}|l, m\rangle$$
$$= \gamma\mathcal{L}_{z}|l, m+1\rangle,$$

where  $\gamma$  is a proportionality constant. Then

$$\mathcal{L}_{z}\mathcal{L}_{+}|l, m\rangle = \mathcal{L}_{z}\gamma|l, m+1\rangle$$
  
$$\Rightarrow \mathcal{L}_{+}|l, m\rangle = \gamma|l, m+1\rangle,$$

is the eigenvalue/eigenvector equation for the raising operator, where  $\gamma$  is evidently the eigenvalue, and the eigenvector is raised by one element of quantization in the z component. This means if the z component of the state on which the raising operator acts is  $m\hbar$ , the new state has a z component of  $m\hbar + \hbar = (m+1)\hbar$ , and thus the index m+1 is used in the new eigenket. We want to solve for  $\gamma$  and have an equation analogous to the forms of equations (9–28) and (9–29). Forming the adjoint equation,

$$< l, m | \mathcal{L}_{+}^{\dagger} = < l, m + 1 | \gamma^{*} \Rightarrow < l, m | \mathcal{L}_{-} = < l, m + 1 | \gamma^{*},$$

because  $\mathcal{L}_{+}^{\dagger} = \mathcal{L}_{-}$ . Forming a braket with the original equation

$$< l, m | \mathcal{L}_{-} \mathcal{L}_{+} | l, m > = < l, m + 1 | \gamma^* \gamma | l, m + 1 > .$$

Though we did it for  $\beta_{\text{max}}$ , the maximum eigenvalue of  $\mathcal{L}_z$ , the algebra leading to equation (9–22) remains the same for any  $\beta$ , any eigenvalue of  $\mathcal{L}_z$ , so we know

$$\mathcal{L}_{-}\mathcal{L}_{+} = \alpha - \beta^{2} - \hbar\beta = \hbar^{2} l(l+1) - m^{2}\hbar^{2} - m\hbar^{2}$$

Using this in the braket,

$$< l, m \left| \hbar^{2} \left( l(l+1) - m^{2} - m \right) \right| l, m > = < l, m+1 \left| \gamma^{*} \gamma \right| l, m+1 >$$
  

$$\Rightarrow \quad \hbar^{2} \left( l(l+1) - m(m+1) \right) < l, m \left| l, m > = \left| \gamma^{*} \gamma \right| < l, m+1 \left| l, m+1 > \right|$$
  

$$\Rightarrow \quad \hbar^{2} \left( l(l+1) - m(m+1) \right) = \left| \gamma \right|^{2}$$

$$\Rightarrow \quad \gamma = \sqrt{l(l+1) - m(m+1)} \hbar,$$
(9-30)

where we used the orthonormality of eigenstates to arrive at equation (9–30). The eigenvalue/ eigenvector equation is then

$$\mathcal{L}_+ |l, m\rangle = \sqrt{l(l+1) - m(m+1)} \,\hbar |l, m+1\rangle.$$

Were we to do the similar calculation for  $\mathcal{L}_{-}$ , we find

$$\mathcal{L}_{-}|l, m\rangle = \sqrt{l(l+1) - m(m-1)}\hbar|l, m-1\rangle.$$

These are most often expressed as one relation,

$$\mathcal{L}_{\pm}|l, m\rangle = \sqrt{l(l+1) - m(m\pm 1)}\,\hbar|l, m\pm 1\rangle\,.$$
(9-31)

**Example 9–14:** For the eigenstate  $|l, m\rangle = |3, m\rangle$ , what measurements are possible for  $\mathcal{L}^2$  and  $\mathcal{L}_z$ ?

The only measurements that are possible are the eigenvalues. From equation (9–28), the eigenvalue of  $\mathcal{L}^2$  is  $\hbar^2 l(l+1) = \hbar^2 3(3+1) = 12\hbar^2$ .

For l = 3, the possible eigenvalues of  $\mathcal{L}_z$  can range from  $-3\hbar$  to  $3\hbar$  in increments of  $\hbar$ . Explicitly, the measurements that are possible for  $\mathcal{L}_z$  for the eigenstate  $|3, m\rangle$  are  $-3\hbar$ ,  $-2\hbar$ ,  $-\hbar$ , 0,  $\hbar$ ,  $2\hbar$ , or  $3\hbar$ .

**Example 9–15:** What are  $\mathcal{L}_+$  and  $\mathcal{L}_-$  operating on the eigenstate |2, -1>?

Using equation (9-31),

$$\mathcal{L}_{+}|2, -1\rangle = \sqrt{2(2+1) - (-1)((-1)+1)} \hbar |2, -1+1\rangle$$
  
=  $\sqrt{2(3) - (-1)(0)} \hbar |2, 0\rangle$   
=  $\sqrt{6} \hbar |2, 0\rangle$ .  
$$\mathcal{L}_{-}|2, -1\rangle = \sqrt{2(2+1) - (-1)((-1)-1)} \hbar |2, -1-1\rangle$$
  
=  $\sqrt{2(3) - (-1)(-2)} \hbar |2, -2\rangle = \sqrt{6-2} \hbar |2, -2\rangle = \sqrt{4} \hbar |2, -2\rangle$   
=  $2\hbar |2, -2\rangle$ .

#### Possibilities, Probabilities, Expectation Value, Uncertainty, and Time Dependence

Examples 9–16 through 9–21 are intended to interface, apply, and extend calculations developed previously to eigenstates of angular momentum. As indicated earlier, a state vector will be a linear combination of eigenstates, which this development should reinforce. Examples 9–16 through 9–21 all refer to the t = 0 state vector

$$|\psi(t=0)\rangle = A(|2, 1\rangle + 3|1, -1\rangle)$$
 (9-32)

is a linear combination of two eigenstates.

**Example 9–16:** Normalize the state vector of equation (9–32).

There are two eigenstates, so we can work in a two dimensional subspace. We can model the first eigenstate  $\begin{pmatrix} 1\\0 \end{pmatrix}$  and the second  $\begin{pmatrix} 0\\1 \end{pmatrix}$ . Then the state vector can be written  $|\psi(0)\rangle = A\left[\begin{pmatrix} 1\\0 \end{pmatrix} + 3\begin{pmatrix} 0\\1 \end{pmatrix}\right] = A\begin{pmatrix} 1\\3 \end{pmatrix}.$ 

Another way to look at it is the state vector is two dimensional with one part the first eigenstate and three parts the second eigenstate. This technique makes the normalization calculation, and a number of others, particularly simple.

$$(1,3)A^*A\begin{pmatrix}1\\3\end{pmatrix} = |A|^2(1+9) = 10|A|^2 = 1$$
  
$$\Rightarrow A = \frac{1}{\sqrt{10}} \Rightarrow |\psi(0)\rangle = \frac{1}{\sqrt{10}}\begin{pmatrix}1\\3\end{pmatrix} = \frac{1}{\sqrt{10}}(|2,1\rangle + 3|1,-1\rangle).$$

**Example 9–17:** What are the possibilities and probabilities of a measurement of  $\mathcal{L}^2$ ?

The possibilities are the eigenvalues. There are two eigenstates, each with its own eigenvalue. If we measure and put the system into the first eigenstate, we measure the state corresponding to the quantum number l = 2, which has the eigenvalue  $\hbar^2 l(l+1) = \hbar^2 2(2+1) = 6\hbar^2$ . If

we measure and place the state vector into the second eigenstate corresponding to the quantum number l = 1, the eigenvalue measured is  $\hbar^2 l(l+1) = \hbar^2 1(1+1) = 2\hbar^2$ .

Since the state function is normalized,

$$P(\mathcal{L}^2 = 6\hbar^2) = \left| \langle \psi | \psi_i \rangle \right|^2 = \left| \frac{1}{\sqrt{10}} (1, 3) \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right|^2 = \frac{1}{10} |1+0|^2 = \frac{1}{10}.$$
$$P(\mathcal{L}^2 = 2\hbar^2) = \left| \langle \psi | \psi_i \rangle \right|^2 = \left| \frac{1}{\sqrt{10}} (1, 3) \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right|^2 = \frac{1}{10} |0+3|^2 = \frac{9}{10}.$$

**Example 9–18:** What are the possibilities and probabilities of a measurement of  $\mathcal{L}_z$ ?

For exactly the same reasons, the possible results of a measurement are  $m = 1 \implies \hbar$  is the first eigenvalue and  $m = -1 \implies -\hbar$  is the second possible eigenvalue. Using exactly the same math,

$$P(\mathcal{L}_z = \hbar) = \frac{1}{10}, \qquad P(\mathcal{L}_z = -\hbar) = \frac{9}{10}.$$

**Example 9–19:** What is the expectation value of  $\mathcal{L}^2$ ?

$$\langle \mathcal{L}^2 \rangle = \sum P(\alpha_i)\alpha_i = \frac{1}{10}6\hbar^2 + \frac{9}{10}2\hbar^2 = \frac{6}{10}\hbar^2 + \frac{18}{10}\hbar^2 = \frac{24}{10}\hbar^2 = 2.4\hbar^2.$$

**Example 9–20:** What is the uncertainty of  $\mathcal{L}^2$ ?

$$\Delta \mathcal{L}^2 = \sqrt{\sum P(\alpha_i) (\alpha_i - \langle \mathcal{L}^2 \rangle)^2} = \left[ \frac{1}{10} (6\hbar^2 - 2.4\hbar^2)^2 + \frac{9}{10} (2\hbar^2 - 2.4\hbar^2)^2 \right]^{1/2}$$
$$= \hbar^2 \left[ \frac{1}{10} (3.6)^2 + \frac{9}{10} (-0.4)^2 \right]^{1/2} = \hbar^2 [1.296 + 0.144]^{1/2} = \hbar^2 \sqrt{1.44}$$
$$= 1.2\hbar^2.$$

**Example 9–21:** What is the time dependent state vector?

$$\begin{aligned} |\psi(t)\rangle &= \sum |j\rangle \langle j|\psi(0)\rangle e^{-iE_jt/\hbar} \\ &= \begin{pmatrix} 1\\0 \end{pmatrix} \begin{pmatrix} 1, 0 \end{pmatrix} \frac{1}{\sqrt{10}} \begin{pmatrix} 1\\3 \end{pmatrix} e^{-iE_1t/\hbar} + \begin{pmatrix} 0\\1 \end{pmatrix} \begin{pmatrix} 0, 1 \end{pmatrix} \frac{1}{\sqrt{10}} \begin{pmatrix} 1\\3 \end{pmatrix} e^{-iE_2t/\hbar} \\ &= \frac{1}{\sqrt{10}} \begin{pmatrix} 1\\0 \end{pmatrix} e^{-iE_1t/\hbar} + \frac{3}{\sqrt{10}} \begin{pmatrix} 0\\1 \end{pmatrix} e^{-iE_2t/\hbar} \\ &= \frac{1}{\sqrt{10}} |2, 1\rangle e^{-iE_1t/\hbar} + \frac{3}{\sqrt{10}} |1, -1\rangle e^{-iE_2t/\hbar} \end{aligned}$$

which is as far as we can go with the given information. We need a specific system and an energy operator, a Hamiltonian, to attain specific  $E_i$ .

#### Angular Momentum Operators in Spherical Coordinates

The conservation of angular momentum, or rotational invariance, implies circular or spherical symmetry. We want to examine spherical symmetry, because spherical symmetry is often a reasonable assumption for simple physical systems. We will assume a hydrogen atom is spherically symmetric, for instance. Remember in spherical coordinates,

$$x = r \sin \theta \cos \phi, \qquad r = (x^2 + y^2 + z^2)^{1/2}$$
  

$$y = r \sin \theta \sin \phi, \qquad \theta = \tan^{-1} \left( \sqrt{x^2 + y^2} / z \right)$$
  

$$z = r \cos \theta, \qquad \phi = \tan^{-1} \left( y / x \right).$$

From these it follows that position space representations in spherical coordinates are

$$\mathcal{L}_{x} = i\hbar \left( \sin \phi \, \frac{\partial}{\partial \theta} + \cos \phi \, \cot \theta \, \frac{\partial}{\partial \phi} \right),$$
  
$$\mathcal{L}_{y} = i\hbar \left( -\cos \phi \, \frac{\partial}{\partial \theta} + \sin \phi \, \cot \theta \, \frac{\partial}{\partial \phi} \right),$$
  
$$\mathcal{L}_{z} = -i\hbar \frac{\partial}{\partial \phi},$$
 (9-32)

$$\mathcal{L}^{2} = -\hbar^{2} \left( \frac{\partial^{2}}{\partial \theta^{2}} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial \phi^{2}} \right), \qquad (9-33)$$

$$\mathcal{L}_{\pm} = \pm \hbar \, e^{\pm i\phi} \left( \frac{\partial}{\partial \theta} \pm i \cot \theta \frac{\partial}{\partial \phi} \right). \tag{9-34}$$

**Example 9–22:** Derive equation (9–32).

From equation (9-2),

$$\mathcal{L}_z = i\hbar \left( -x\frac{\partial}{\partial y} + y\frac{\partial}{\partial x} \right).$$

We can develop the desired partial differentials from the relation between azimuthal angle and position coordinates, or

$$\phi = \tan^{-1} (y/x) \implies y = x \tan \phi$$
$$\Rightarrow \quad \frac{\partial y}{\partial \phi} = x \,\partial \big(\tan \phi\big) = x \sec^2 \phi = \frac{x}{\cos^2 \phi}$$
$$\Rightarrow \quad \partial y = \frac{x \,\partial \phi}{\cos^2 \phi}.$$

The same relation gives us

$$x = \frac{y}{\tan \phi} = y \frac{\cos \phi}{\sin \phi} = y \cos \phi \, \sin^{-1} \phi$$
$$\Rightarrow \quad \frac{\partial x}{\partial \phi} = y \left( -\sin \phi \, \sin^{-1} \phi + \cos \phi \, (-1) \, \sin^{-2} \phi \cos \phi \right)$$

$$= -y\left(1 + \frac{\cos^2\phi}{\sin^2\phi}\right) = -y\left(\frac{\sin^2\phi + \cos^2\phi}{\sin^2\phi}\right) = -\frac{y}{\sin^2\phi}$$
$$\Rightarrow \quad \partial x = -\frac{y\,\partial\phi}{\sin^2\phi}.$$

Using the partial differentials in the Cartesian formulation for the z component of angular momentum,

$$\mathcal{L}_{z} = i\hbar \left( -x \cos^{2} \frac{\partial}{x \partial \phi} + y \left( -\sin^{2} \phi \frac{\partial x}{y \partial \phi} \right) \right)$$
$$= -i\hbar (\cos^{2} \phi + \sin^{2} \phi) \frac{\partial}{\partial \phi}$$
$$= -i\hbar \frac{\partial}{\partial \phi}.$$

**Example 9–23:** Given the spherical coordinate representations of  $\mathcal{L}_x$  and  $\mathcal{L}_y$ , show equation (9–34) is true for  $\mathcal{L}_+$ .

$$\begin{split} \mathcal{L}_{+} &= \mathcal{L}_{x} + i\mathcal{L}_{y} \\ &= i\hbar \left( \sin \phi \, \frac{\partial}{\partial \theta} + \cos \phi \, \cot \theta \, \frac{\partial}{\partial \phi} \right) + i \left[ i\hbar \left( -\cos \phi \, \frac{\partial}{\partial \theta} + \sin \phi \, \cot \theta \, \frac{\partial}{\partial \phi} \right) \right] \\ &= \hbar \left[ i \sin \phi \, \frac{\partial}{\partial \theta} + i \cos \phi \, \cot \theta \, \frac{\partial}{\partial \phi} + \cos \phi \, \frac{\partial}{\partial \theta} - \sin \phi \, \cot \theta \, \frac{\partial}{\partial \phi} \right] \\ &= \hbar \left[ (\cos \phi + i \sin \phi) \, \frac{\partial}{\partial \theta} + (i \cos \phi - \sin \phi) \, \cot \theta \, \frac{\partial}{\partial \phi} \right] \\ &= \hbar \left[ (\cos \phi + i \sin \phi) \, \frac{\partial}{\partial \theta} + i \, (\cos \phi + i \sin \phi) \, \cot \theta \, \frac{\partial}{\partial \phi} \right] \\ &= \hbar \left[ (e^{i\phi}) \, \frac{\partial}{\partial \theta} + i \, (e^{i\phi}) \, \cot \theta \, \frac{\partial}{\partial \phi} \right] \\ &= \hbar^{2} e^{i\phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \, \frac{\partial}{\partial \phi} \right). \end{split}$$

An outline of the derivations of the all components and square of angular momentum in spherical coordinates is included in Ziock<sup>5</sup>. These calculations can be "messy" by practical standards.

## Special Functions Used for the Hydrogen Atom

Two special functions are particularly useful in describing a hydrogen atom assumed to have spherical symmetry. These are **spherical harmonics** and **Associated Laguerre functions**. The plan will be to separate the Schrodinger equation into radial and angular equations. The solutions to the radial equation can be expressed in terms of associated Laguerre polynomials, which we will examine in the next chapter. The solutions to the angular equation can be expressed in terms of spherical harmonic functions, which we will examine in the next section. Spherical harmonics are closely related to a third special function, **Legendre functions**. They are so closely related, the spherical harmonics can be expressed in terms of **associated Legendre polynomials**.

<sup>&</sup>lt;sup>5</sup> Ziock Basic Quantum Mechanics (John Wiley & Sons, New York, 1969), pp. 91–94

The name spherical harmonic comes from the geometry the functions naturally describe, spherical, and the fact any solution of Laplace's equation is known as harmonic. Picture a ball. The surface may be smooth, which is likely the first picture you form. Put a rubber band around the center, and you get a minima at the center and bulges, or maxima, in the top and bottom half. Put rubber bands on the circumference, like lines of longitude, and you get a different pattern of maxima and minima. We could imagine other, more complex patterns of maxima and minima. When these maxima and minima are symmetric with respect to an origin, the center of the ball, Legendre functions, associated Legendre functions, and spherical harmonics provide useful descriptions.

Properties that makes these special functions particularly useful is they are orthogonal and complete. Any set that is orthogonal can be made orthonormal. We have used orthonormality in a number of calculations, and the property of orthonormality continues to be a practical necessity. They are also complete in the sense any phenomenon can be described by an appropriate linear combination. Other complete sets of orthonormal functions we have encountered are sines and cosines for the square well, and Hermite polynomials for the SHO. A set of complete, orthonormal functions is equivalent to a linear vector space; these special functions are different manifestations of a complex linear vector space.

## Spherical Harmonics

The ket  $|l, m\rangle$  is an eigenstate of the commuting operators  $\mathcal{L}^2$  and  $\mathcal{L}_z$ , but it is an abstract eigenstate. That  $|l, m\rangle$  is abstract is irrelevant for the eigenvalues, since eigenvalues are properties of the operators. We would, however, like a representation useful for description for the eigenvectors. Per chapter 4, we can form an inner product with an abstract vector to attain a representation. Using a guided choice, the angles of spherical coordinate system will yield an appropriate representation. Just as  $\langle x|g \rangle = g(x)$ , we will write

$$<\theta, \phi | l, m > = Y_{l,m}(\theta, \phi).$$

The functions of polar and azimuthal angles,  $Y_{l,m}(\theta, \phi)$ , are the spherical harmonics.

The spherical harmonics are related so strongly to the geometry of the current problem, they can be derived from the spherical coordinate form of the eigenvalue/eigenvector equation (9–29),  $\mathcal{L}_z|l, m\rangle = m\hbar|l, m\rangle$ , and use of the raising/lowering operator equation (9–31).

Using the spherical coordinate system form of the operator and the functional forms of the eigenstates, equation (9-29) is

$$-i\hbar\frac{\partial}{\partial\phi}Y_{l,m}(\theta,\phi) = m\hbar Y_{l,m}(\theta,\phi).$$

We are going to assume the spherical harmonics are separable, that they can be expressed as a product of a function of  $\theta$  and a second function of  $\phi$ , or

$$Y_{l,m}(\theta,\phi) = f_{l,m}(\theta) g_{l,m}(\phi).$$

Using this in the differential equation,

$$-i\hbar \frac{\partial}{\partial \phi} f_{l,m}(\theta) g_{l,m}(\phi) = m\hbar f_{l,m}(\theta) g_{l,m}(\phi)$$

$$\Rightarrow -i f_{l,m}(\theta) \frac{\partial}{\partial \phi} g_{l,m}(\phi) = m f_{l,m}(\theta) g_{l,m}(\phi)$$

$$\Rightarrow -i \frac{\partial}{\partial \phi} g_{l,m}(\phi) = m g_{l,m}(\phi)$$

$$\Rightarrow \frac{\partial g_{l,m}(\phi)}{g_{l,m}(\phi)} = im \partial \phi$$

$$\Rightarrow \ln g_{l,m}(\phi) = im \phi$$

$$\Rightarrow g_{l,m}(\phi) = e^{im\phi}.$$

Notice the exponential has no dependence on l, so we can write

$$g_m(\phi) = e^{im\phi},\tag{9-35}$$

which is the azimuthal dependence.

Remember that there is a top and bottom to the ladder for a given l. The top of the ladder is at m = l. If we act on an eigenstate on the top of the ladder, we get zero, meaning

$$\mathcal{L}_+|l,\,l>=0,$$

Using the spherical coordinate forms of the raising operator and separated eigenstate including equation (9–35), this is

$$\begin{split} \hbar e^{i\phi} \left[ \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right] f_{l,l}(\theta) e^{il\phi} &= 0 \\ \Rightarrow \quad e^{il\phi} \frac{\partial}{\partial \theta} f_{l,l}(\theta) + i f_{l,l}(\theta) \cot \theta (il) e^{il\phi} &= 0 \\ \Rightarrow \quad \frac{\partial}{\partial \theta} f_{l,l}(\theta) - l f_{l,l}(\theta) \cot \theta &= 0. \end{split}$$

The solution to this is  $f_{l,l}(\theta) = A(\sin \theta)^l$ . To see that it is a solution,

$$\frac{\partial}{\partial \theta} f_{l,l}(\theta) = \frac{\partial}{\partial \theta} A \left( \sin \theta \right)^l = A l \left( \sin \theta \right)^{l-1} \cos \theta,$$

and substituting this in the differential equation,

$$A l \left(\sin \theta\right)^{l-1} \cos \theta - l \left[A \left(\sin \theta\right)^{l}\right] \frac{\cos \theta}{\sin \theta} = A l \left(\sin \theta\right)^{l-1} \left[\cos \theta - \sin \theta \frac{\cos \theta}{\sin \theta}\right] = 0.$$

So the unnormalized form of the m = l spherical harmonics is

$$Y_{l,m}(\theta,\phi) = A\left(\sin\theta\right)^l e^{im\phi}.$$
(9-36)

Example 9–24 derives  $Y_{1,1}(\theta, \phi)$  starting with equation (9–36).

So how do we get the spherical harmonics for which  $m \neq l$ ? The answer is to attain a  $Y_{l,l}(\theta, \phi)$  and operate on it with the lowering operator. Example 9–25 derives  $Y_{1,0}(\theta, \phi)$  in this manner.

One comment before we proceed. The spherical harmonics of equation (9–36) can be made orthonormal, so we need to calculate the normalization constants, A for each  $Y_{l,m}(\theta, \phi)$ . Having selected a representation, this is most easily approached by the appropriate form of integration. The appropriate form of integration for spherical angles is with respect to solid angle,  $d\Omega = \sin \theta d\theta d\phi$ , or

$$\int Y_{l,m}^*(\theta,\phi) Y_{l,m}(\theta,\phi) d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta |Y_{l,m}(\theta,\phi)|^2 = 1$$

which will also be illustrated in examples 9–24 and 9–25. These and other special functions are addressed in most mathematical physics texts including Arken<sup>6</sup> and Mathews and Walker<sup>7</sup>.

A list of the first few spherical harmonics is

$$\begin{split} Y_{0,0}(\theta,\phi) &= \frac{1}{4\pi} & Y_{2,0}(\theta,\phi) = \sqrt{\frac{5}{16\pi}} \left( 3\cos^2 \theta - 1 \right) \\ Y_{1,\pm 1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}} \sin \theta \, e^{\pm i\phi} & Y_{3,\pm 3}(\theta,\phi) = \sqrt{\frac{35}{64\pi}} \sin^3 \theta \, e^{\pm 3i\phi} \\ Y_{1,0}(\theta,\phi) &= \sqrt{\frac{3}{4\pi}} \cos \theta & Y_{3,\pm 2}(\theta,\phi) = \sqrt{\frac{105}{32\pi}} \sin^2 \theta \, \cos \theta \, e^{\pm 2i\phi} \\ Y_{2,\pm 2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}} \sin^2 \theta \, e^{\pm 2i\phi} & Y_{3,\pm 1}(\theta,\phi) = \sqrt{\frac{21}{64\pi}} \sin \theta \, \left( 5\cos^2 \theta - 1 \right) e^{\pm i\phi} \\ Y_{2,\pm 1}(\theta,\phi) &= \sqrt{\frac{15}{8\pi}} \sin \theta \, \cos \theta \, e^{\pm i\phi} & Y_{3,0}(\theta,\phi) = \sqrt{\frac{7}{16\pi}} \left( 5\cos^3 \theta - 3\cos \theta \right) \\ \text{Table } 9 - 1. \text{ The First Sixteen Spherical Harmonic Functions.} \end{split}$$

A few comments about the list are appropriate. First, notice the symmetry about m = 0. For example,  $Y_{2,1}$  and  $Y_{2,-1}$  are exactly the same except for the sign of the argument of the exponential. Second, notice the  $Y_{l,0}$  are independent of  $\phi$ . When m = 0, the spherical harmonic functions are constant with respect to azimuthal angle. Next, per the previous sentences, it is common to refer to spherical harmonic functions without explicitly indicating that the arguments are polar and azimuthal angles. Finally, and most significantly, some texts will use a negative sign leading the spherical harmonic functions for which m < 0. This is a different choice of phase. We will use the convention denoted in table 9–1, where all spherical harmonics are positive. Used consistently, either choice is reasonable and both choices have advantages and disadvantages.

Figure 9–2 illustrates the functional form of the first 16 spherical harmonic functions. Note that the radial coordinate has not yet been addressed. Angular distribution is all that is being

<sup>&</sup>lt;sup>6</sup> Arfken Mathematical Methods for Physicists (Academic Press, New York, 1970), 2nd ed., chapters 9–13.

<sup>&</sup>lt;sup>7</sup> Mathews and Walker *Mathematical Methods of Physics* (The Benjamin/Cummings Publishing Co., Menlo Park, California, 1970), 2nd ed., chapter 7.

illustrated. The radial coordinate will be examined in the next chapter. The size of any of the individual pictures in figure 9–2 is arbitrary; they could be very large or very small. We assume a radius of one unit to draw the sketches. In other words, you can look at the smooth sphere of  $Y_{0,0}$  as having radius one unit, and the relative sizes of other spherical harmonic functions are comparable on the same radial scale.

Figure 9-2. Illustrations of the First Sixteen Spherical Harmonic Functions.

There is a technique here we want to exploit when we address radial functions. The spherical harmonics are orthonormal so are normalized. The figures represent spherical harmonics of magnitude one, multiplied by one, so remain orthonormal. We want the radial functions to be orthonormal, or individually to have magnitude one. Just as we have assumed a one unit radius to draw the figures here, if we multiply two quantities of magnitude one, we attain a product of magnitude one. If the angular function and radial function are individually normalized, the product function will be normalized as well.

**Example 9–24:** Show  $Y_{l,l} = A(\sin\theta)^l e^{im\phi}$  yields the normalized  $Y_{1,1}$  of table 9–1.  $Y_{1,1} = A(\sin\theta)^1 e^{i(1)\phi} = A\sin\theta e^{i\phi}.$ 

To normalize this,

$$\begin{split} 1 &= \int (Y_{1,1})^* Y_{1,1} \, d\Omega = \int A^* \sin \theta \, e^{-i\phi} \, A \sin \theta \, e^{i\phi} \, d\Omega \\ &= |A|^2 \int \sin^2 \theta \, e^0 \, d\Omega = |A|^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, \sin^2 \theta \, \sin \theta \\ &= |A|^2 \int_0^{\pi} d\theta \, \sin^3 \theta \int_0^{2\pi} d\phi = 2\pi |A|^2 \int_0^{\pi} d\theta \, \sin^3 \theta \\ &= 2\pi |A|^2 \left[ -\frac{1}{3} \cos \theta \left( \sin^2 \theta + 2 \right) \right]_0^{\pi} = \frac{2\pi}{3} |A|^2 \left[ \cos \theta \left( \sin^2 \theta + 2 \right) \right]_{\pi}^0 \\ &= \frac{2\pi}{3} |A|^2 \left[ \cos(0) \left( \sin^2(0) + 2 \right) - \cos(\pi) \left( \sin^2(\pi) + 2 \right) \right] \\ &= \frac{2\pi}{3} |A|^2 \left[ (1)(2) - (-1)(2) \right] = \frac{2\pi}{3} |A|^2 [4] \\ &\Rightarrow \quad \frac{8\pi}{3} |A|^2 = 1 \quad \Rightarrow \quad A = \sqrt{\frac{3}{8\pi}} \\ &\Rightarrow \quad Y_{1,1} = \sqrt{\frac{3}{8\pi}} \sin \theta \, e^{i\phi}, \end{split}$$

which is identical to  $Y_{1,1}$  in table 9–1.

**Example 9–25:** Derive  $Y_{1,0}$  from the result of the previous example using the lowering operator.

A lowering operator acting on an abstract eigenstate is  $\mathcal{L}_{-}|l, m\rangle = B|l, m-1\rangle$ , where B is a proportionality constant. Using the spherical angle representation on the eigenstate  $Y_{1,1}$ , this eigenvalue/eigenvector equation is

$$-\hbar e^{-i\phi} \left(\frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi}\right) Y_{1,1} = B Y_{1,0},$$

where B is the eigenvalue. Using the unnormalized form of  $Y_{1,1}$ , we have

$$BY_{1,0} = -\hbar e^{-i\phi} \left( \frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right) A \sin \theta e^{i\phi}$$
$$= -A\hbar e^{-i\phi} \left( e^{i\phi} \frac{\partial}{\partial \theta} \sin \theta - i \cot \theta \sin \theta \frac{\partial}{\partial \phi} e^{i\phi} \right)$$
$$= -A\hbar e^{-i\phi} \left( e^{i\phi} \cos \theta - i \frac{\cos \theta}{\sin \theta} \sin \theta(i) e^{i\phi} \right)$$
$$= -A\hbar (\cos \theta + \cos \theta) = -2A\hbar (\cos \theta)$$

$$\Rightarrow Y_{1,0} = C \cos \theta,$$

where all constants have been combined to form C, which becomes simply a normalization constant. We normalize this using the same procedure as the previous example,

$$\begin{split} 1 &= \int C^* \cos \theta \, C \cos \theta \, d\Omega = \left| C \right|^2 \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \, \cos^2 \theta \, \sin \theta \\ &= 2\pi |C|^2 \int_0^{\pi} d\theta \, \cos^2 \theta \, \sin \theta = 2\pi |C|^2 \Big[ -\frac{\cos^3 \theta}{3} \Big]_0^{\pi} = \frac{2\pi}{3} |C|^2 \Big[ \cos^3 \theta \Big]_{\pi}^0 \\ &= \frac{2\pi}{3} |C|^2 \Big[ \cos^3(0) - \cos^3(\pi) \Big] = \frac{2\pi}{3} |C|^2 \Big[ 1 - (-1) \Big] = \frac{2\pi}{3} |C|^2 \Big[ 2 \Big] \\ &\Rightarrow \quad \frac{4\pi}{3} |C|^2 = 1 \quad \Rightarrow \quad C = \sqrt{\frac{3}{4\pi}} \\ &\Rightarrow \quad Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos \theta, \end{split}$$

which is identical to  $Y_{1,0}$  as listed in table 9–1.

# **Generating Function for Spherical Harmonics**

A generating functions for higher index spherical harmonics is

$$Y_{l,m}(\theta,\phi) = (-1)^m \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_{l,m}(\cos\theta) e^{im\phi}, \qquad m \ge 0,$$

and

$$Y_{l,-m}(\theta,\phi) = Y_{l,m}^*(\theta,\phi), \qquad m < 0,$$

where the  $P_{l,m}(\cos \theta)$  are associated Legendre polynomials. Associated Legendre polynomials can be generated from Legendre polynomials using

$$P_{l,m}(u) = (-1)^m \sqrt{(1-u^2)^m} \frac{d^m}{du^m} P_l(u),$$

where the  $P_l(u)$  are Legendre polynomials. Legendre polynomials can be generated using

$$P_l(u) = \frac{(-1)^l}{2^l l!} \frac{d^l}{du^l} (1 - u^2)^l.$$

Notice the generating function for spherical harmonics contains the restriction  $m \ge 0$ . Our strategy to attain spherical harmonics with m < 0 will be to form them from the adjoint of the corresponding spherical harmonic with m > 0 as indicated. The advantage of this strategy is we do not need to consider associated Legendre polynomials with m < 0, though those also have meaning and can be attained using

$$P_{l,-m}(u) = \frac{(l-m)!}{(l+m)!} P_{l,m}(u),$$

in our phase scheme.

**Example 9–26:** Derive  $Y_{2,1}$  and  $Y_{2,-1}$  using the generating functions.

$$P_2(u) = \frac{(-1)^2}{2^2 \cdot 2!} \frac{d^2}{du^2} (1-u^2)^2 = \frac{1}{4 \cdot 2} \frac{d}{du} \Big[ 2(1-u^2)(-2u) \Big] = \frac{1}{2} \frac{d}{du} (u^3-u) = \frac{1}{2} (3u^2-1),$$

is the appropriate Legendre polynomial. The appropriate associated Legendre polynomial is

$$P_{2,1}(u) = (-1)^1 \sqrt{(1-u^2)^1} \frac{d^1}{du^1} P_2(u) = -\sqrt{(1-u^2)} \frac{d}{du} \frac{1}{2} (3u^2 - 1)$$
$$= -\frac{1}{2} \sqrt{(1-u^2)} (6u) = -3u \sqrt{(1-u^2)}.$$

The spherical harmonic in terms of this associated Legendre polynomial is

$$Y_{2,1}(\theta,\phi) = (-1)^1 \sqrt{\frac{(2\cdot 2+1)(2-1)!}{4\pi(2+1)!}} P_{2,1}(\cos\theta) e^{i(1)\phi}$$
  
=  $-\sqrt{\frac{(5)(1)!}{4\pi(3)!}} \Big( -3\cos\theta\sqrt{(1-\cos^2\theta)} \Big) e^{i\phi}$   
=  $3\sqrt{\frac{5}{4\pi\cdot 3\cdot 2}}\cos\theta\sin\theta e^{i\phi} = \sqrt{\frac{3^2\cdot 5}{4\pi\cdot 3\cdot 2}}\cos\theta\sin\theta e^{i\phi}$   
=  $\sqrt{\frac{15}{8\pi}}\cos\theta\sin\theta e^{i\phi}$ ,

which is identical to  $Y_{2,1}$  in table 9–1. Then,

$$Y_{2,-1}(\theta,\phi) = Y_{2,1}^*(\theta,\phi) \implies Y_{2,-1}(\theta,\phi) = \sqrt{\frac{15}{8\pi}}\cos\theta\,\sin\theta\,e^{-i\phi},$$

also identical to the listing in table 9–1.