

# Chapter 8

## Orbital Angular Momentum

Orbital angular momentum is maybe the most intuitive form of angular momentum. In this Chapter we will study the properties of orbital angular momentum, using the general theory we have developed in the previous Chapter.

### 8.1 The Orbital Angular Momentum Operator

Classically, orbital angular momentum is defined as

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}. \quad (8.1.1)$$

In the quantum mechanical setting, we can use the correspondence principle to find the operator equivalent of Eq. (8.1.1). This is achieved promoting dynamical variables to operators  $\mathbf{r} = (x, y, z) \rightarrow \hat{\mathbf{r}} = (\hat{x}, \hat{y}, \hat{z})$ , and similarly for the momentum operator,  $\mathbf{p} = (p_x, p_y, p_z) \rightarrow \hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ . The components of the orbital angular momentum operator  $\hat{\mathbf{L}} = (\hat{L}_x, \hat{L}_y, \hat{L}_z)$  can be found by using the following fact

$$(\vec{a} \times \vec{b})_i = \sum_{jk} \epsilon_{ijk} a_j b_k, \quad (8.1.2)$$

where  $\epsilon_{ijk}$  is the Levi-Civita tensor. Using Eq. (8.1.2) for the orbital angular momentum, we find

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \quad \hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z, \quad \hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x. \quad (8.1.3)$$

We can then compute explicitly commutators between different components of the orbital angular momentum, just using the fundamental commutation relations between positions and momenta. We provide an example with the  $x$  and  $y$  components of the orbital angular momentum operator,

$$\begin{aligned} [\hat{L}_x, \hat{L}_y] &= [\hat{y}\hat{p}_z - \hat{z}\hat{p}_y, \hat{z}\hat{p}_x - \hat{x}\hat{p}_z] = \\ &= [\hat{y}\hat{p}_z, \hat{z}\hat{p}_x] - [\hat{y}\hat{p}_z, \hat{x}\hat{p}_z] - [\hat{z}\hat{p}_y, \hat{z}\hat{p}_x] + [\hat{z}\hat{p}_y, \hat{x}\hat{p}_z] = \\ &= \hat{y}\hat{p}_x[\hat{p}_z, \hat{z}] + \hat{x}\hat{p}_y[\hat{z}, \hat{p}_z] = \\ &= i\hbar(-\hat{y}\hat{p}_x + \hat{x}\hat{p}_y) = \\ &= i\hbar\hat{L}_z. \end{aligned} \quad (8.1.4)$$

In general, we can show that the components of  $\hat{L}$  obey the following commutation relations

$$[\hat{L}_i, \hat{L}_j] = i\hbar\epsilon_{ijk}\hat{L}_k, \quad (8.1.5)$$

where the indices  $i, j, k$  take the values  $x, y, z$ . Thus, the orbital angular momentum operator satisfies the same commutation relations we expect from a general angular momentum operator.

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**Exercise 1.1** Using the commutation relations between the position and momentum operators, show Eq. (8.1.5).

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## 8.2 The Rotation Operator

By explicitly computing the commutator relations of the components of the orbital angular momentum, we have shown that  $\hat{\mathbf{L}}$  satisfies the properties of a rotation operator. We haven't explicitly shown however what *kind* of rotations this operator performs. We will now show that  $\hat{\mathbf{L}}$  is associated to rotations of the coordinate system. Let us consider for example a rotation by an angle  $\theta_z$  around the  $z$  direction, such that the rotation vector reads  $\boldsymbol{\theta} = (0, 0, \theta_z)$ . At the beginning of the previous Chapter, we have recalled that real-space rotations along a certain direction are fully encoded by  $3 \times 3$  matrices. For the case of rotations along the  $z$  axis, we have that this matrix takes the explicit form:

$$\hat{R}(\boldsymbol{\theta}) = \begin{pmatrix} \cos \theta_z & -\sin \theta_z & 0 \\ \sin \theta_z & \cos \theta_z & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (8.2.1)$$

This matrix acts on coordinates, thus we can write rotated eigen-kets of the position operator as

$$|\mathbf{r}'\rangle = \hat{R}(\boldsymbol{\theta}) |\mathbf{r}\rangle = |\cos \theta_z x - \sin \theta_z y, \sin \theta_z x + \cos \theta_z y, z\rangle, \quad (8.2.2)$$

which in the limit of a small rotation angle becomes

$$|\mathbf{r}(\delta\boldsymbol{\theta})\rangle = \hat{R}(\delta\boldsymbol{\theta}) |\mathbf{r}\rangle = |x - \delta\theta_z y, y + \delta\theta_z x, z\rangle, \quad (8.2.3)$$

thus the amplitudes of a quantum state in this rotated frame read:

$$\begin{aligned} \langle \mathbf{r}(\delta\boldsymbol{\theta}) | \psi \rangle &= \psi(x - \delta\theta_z y, y + \delta\theta_z x, z) \\ &= \psi(\mathbf{r}) + \delta\theta_z \left( -y \frac{\partial \psi(\mathbf{r})}{\partial x} + x \frac{\partial \psi(\mathbf{r})}{\partial y} \right) + \dots \end{aligned} \quad (8.2.4)$$

Now, we would like to compare this expression to what we would obtain considering the rotation operator defined in terms of the orbital angular momentum:

$$\hat{D}(\boldsymbol{\theta}) = e^{-i\frac{\hat{L}_z}{\hbar}\theta_z}. \quad (8.2.5)$$

The action of the rotation operator on a basis ket is:

$$|\mathbf{r}'(\boldsymbol{\theta})\rangle = \hat{D}(\boldsymbol{\theta}) |\mathbf{r}\rangle = e^{-i\frac{\hat{L}_z}{\hbar}\theta_z} |\mathbf{r}\rangle, \quad (8.2.6)$$

thus the amplitudes of a given quantum state in this basis (rotated by  $\hat{D}$ ) are:

$$\langle \mathbf{r}'(\boldsymbol{\theta}) | \psi \rangle = \langle \mathbf{r} | e^{i \frac{\hat{L}_z}{\hbar} \theta_z} | \psi \rangle . \quad (8.2.7)$$

Notice that the expression for the amplitudes above can be interpreted in two equivalent ways: either we rotate the basis eigen-kets  $|\mathbf{r}'(\boldsymbol{\theta})\rangle = \hat{D}(\boldsymbol{\theta}) |\mathbf{r}\rangle$  and keep the state  $|\psi\rangle$  unchanged, or we keep the basis eigen-kets unchanged and rotate the state in the opposite direction, thus  $|\psi\rangle \rightarrow \hat{D}^\dagger(-\boldsymbol{\theta}) |\psi\rangle = \hat{D}(\boldsymbol{\theta}) |\psi\rangle$ . In the limit of small angle, the rotation operator  $\hat{D}(\delta\boldsymbol{\theta})$  defined in terms of the  $z$  component on the angular momentum reads:

$$\begin{aligned} e^{i \frac{\hat{L}_z}{\hbar} \delta\theta_z} &= \hat{I} + \frac{i}{\hbar} \delta\theta_z \hat{L}_z + \dots \\ &= \hat{I} + \frac{i}{\hbar} \delta\theta_z (\hat{x} \hat{p}_y - \hat{y} \hat{p}_x) + \dots \\ &= \hat{I} + \delta\theta_z (\hat{x} \partial_y - \hat{y} \partial_x) + \dots \end{aligned} \quad (8.2.8)$$

thus

$$\begin{aligned} \langle \mathbf{r}'(\delta\boldsymbol{\theta}) | \psi \rangle &= \langle \mathbf{r} | e^{i \frac{\hat{L}_z}{\hbar} \delta\theta_z} | \psi \rangle \\ &= \psi(\mathbf{x}) + \delta\theta_z \left( -y \frac{\partial \psi(\mathbf{r})}{\partial x} + x \frac{\partial \psi(\mathbf{r})}{\partial y} \right) , \end{aligned} \quad (8.2.9)$$

which is identical to the expression found using the rotation matrix, also implying that  $|\mathbf{r}'(\delta\boldsymbol{\theta})\rangle = |\mathbf{r}(\delta\boldsymbol{\theta})\rangle$ . We therefore identified rotations of the coordinate system along the  $z$  axis with the action of the operator  $\hat{D}(\boldsymbol{\theta})$  with  $\boldsymbol{\theta} = (0, 0, \theta_z)$  and the orbital angular momentum  $\hat{L}_z$ .

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**Exercise 1.2** Show, by following a very similar procedure, that the  $\hat{L}_x$  and  $\hat{L}_y$  generate rotations in their respective directions by an angle  $\theta_x$  and  $\theta_y$  respectively.

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### 8.3 The Representation in Spherical Coordinates

In order to analyze the eigenfunctions of the orbital angular momentum, it is much more convenient to consider the representation of  $\hat{\mathbf{L}}$  in spherical coordinates  $(r, \theta, \phi)$ , rather than cartesian ones  $(x, y, z)$ . There are several possible conventions for spherical coordinates; here we adopt the following definition:

$$x = r \sin \theta \cos \phi, \quad y = r \sin \theta \sin \phi, \quad z = r \cos \theta . \quad (8.3.1)$$

We can then express the three components of the angular momentum operator in this system. To this end, it is necessary to consider the form of the gradient operator in spherical coordinates. Consider for example derivatives with respect to the angle  $\phi$ , which controls rotations around the  $z$  axis.

$$\begin{aligned} \frac{\partial}{\partial \phi} &= \frac{\partial x}{\partial \phi} \frac{\partial}{\partial x} + \frac{\partial y}{\partial \phi} \frac{\partial}{\partial y} + \frac{\partial z}{\partial \phi} \frac{\partial}{\partial z} = \\ &= -r \sin \theta \sin \phi \frac{\partial}{\partial x} + r \sin \theta \cos \phi \frac{\partial}{\partial y} = \\ &= -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y} . \end{aligned} \quad (8.3.2)$$

On the other hand, we can immediately connect this result to the representation of  $\hat{L}_z$  in cartesian coordinates

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar \left( \hat{x} \frac{\partial}{\partial y} - \hat{y} \frac{\partial}{\partial x} \right) = -i\hbar \frac{\partial}{\partial \phi}. \quad (8.3.3)$$

The  $z$  component of the orbital angular momentum has therefore a very simple expression in terms of gradients with respect to the azimuthal angle, and, in this coordinate system, it closely resembles the action of a linear momentum operator.

Deriving the other components is a straightforward, yet laborious extension of what we have already seen for the  $z$  component. The first step is to consider the gradients in polar coordinates as linear combinations of gradients in cartesian coordinates, differentiating Eq. (8.3.1) we have:

$$\begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial r} & \frac{\partial x}{\partial \theta} & \frac{\partial x}{\partial \phi} \\ \frac{\partial y}{\partial r} & \frac{\partial y}{\partial \theta} & \frac{\partial y}{\partial \phi} \\ \frac{\partial z}{\partial r} & \frac{\partial z}{\partial \theta} & \frac{\partial z}{\partial \phi} \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} \quad (8.3.4)$$

$$= \begin{pmatrix} \sin \theta \cos \phi & \sin \theta \sin \phi & \cos \theta \\ r \cos \theta \cos \phi & r \cos \theta \sin \phi & -r \sin \theta \\ -r \sin \theta \sin \phi & r \sin \theta \cos \phi & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix}. \quad (8.3.5)$$

The second step is to consider the inverse transformation, so to express the cartesian derivatives as a linear combination of the spherical derivatives. This is obtained inverting the  $3 \times 3$  (Jacobian) matrix above, and, after a lengthy and heartless calculation we omit here, we have:

$$\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = \begin{pmatrix} \sin \theta \cos \phi & \frac{\cos \theta \cos \phi}{r} & -\frac{\sin \phi}{r \sin \theta} \\ \sin \theta \sin \phi & \frac{\cos \theta \sin \phi}{r} & \frac{\cos \phi}{r \sin \theta} \\ \cos \theta & -\frac{\sin \theta}{r} & 0 \end{pmatrix} \begin{pmatrix} \frac{\partial}{\partial r} \\ \frac{\partial}{\partial \theta} \\ \frac{\partial}{\partial \phi} \end{pmatrix}. \quad (8.3.6)$$

The third and final step is to express the  $x$  and  $y$  components of the orbital angular momentum in terms of these derivatives, finding

$$\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ &= -i\hbar \left( \hat{y} \frac{\partial}{\partial z} - \hat{z} \frac{\partial}{\partial y} \right) \\ &= -i\hbar r \sin \theta \sin \phi \left( \cos \theta \frac{\partial}{\partial r} - \frac{\sin \theta}{r} \frac{\partial}{\partial \theta} \right) + \\ &\quad + i\hbar r \cos \theta \left( \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{\cos \theta \sin \phi}{r} \frac{\partial}{\partial \theta} + \frac{\cos \phi}{r \sin \theta} \frac{\partial}{\partial \phi} \right) \\ &= i\hbar \left( \sin \phi \frac{\partial}{\partial \theta} + \cot \theta \cos \phi \frac{\partial}{\partial \phi} \right), \end{aligned}$$

for the  $x$  component. With a very similar treatment, we find for the  $y$  component

$$\hat{L}_y = -i\hbar \left( \cos \phi \frac{\partial}{\partial \theta} - \cot \theta \sin \phi \frac{\partial}{\partial \phi} \right). \quad (8.3.7)$$

With these definitions, we can also find explicitly expressions for the ladder operators

$$\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y = \pm\hbar e^{\pm i\phi} \left( \frac{\partial}{\partial\theta} \pm i \cot\theta \frac{\partial}{\partial\phi} \right). \quad (8.3.8)$$

Similarly, using the definition of  $\hat{L}^2$  in terms of the ladder operators:

$$\hat{L}^2 = \hat{L}_z^2 + \frac{1}{2} (\hat{L}_+ \hat{L}_- + \hat{L}_- \hat{L}_+), \quad (8.3.9)$$

and after another lengthy calculation we omit here one gets

$$\hat{L}^2 = -\hbar^2 \left[ \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left( \sin\theta \frac{\partial}{\partial\theta} \right) \right]. \quad (8.3.10)$$

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**Exercise 1.3** Derive the expression of Eq. (8.3.10).

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## 8.4 The Eigenfunctions in the Spherical Coordinates Representation

Armed with the representation of the orbital angular momentum in spherical coordinates, we are now ready to study its eigenstates. As done for the general theory of angular momentum, we consider again common eigenstates of  $\hat{L}_z$  and  $\hat{L}^2$ , such that

$$\hat{L}^2 |l, m\rangle = \hbar^2 l(l+1) |l, m\rangle \quad (8.4.1)$$

$$\hat{L}_z |l, m\rangle = \hbar m |l, m\rangle \quad (8.4.2)$$

As we have seen from their explicit expressions, both operators depend only on the angles  $\theta$  and  $\phi$  and are completely independent on the radial component  $r$ . This implies that also the eigenstates, in polar coordinates, will have a factorized form. At fixed values of  $l$  and  $m$ , the eigenstates of the orbital angular momentum are then the product of a function of  $\theta$  and  $\phi$  times a radial function. They are conventionally written as:

$$\langle r | l, m \rangle = \Phi_m^l(r) Y_m^l(\theta, \phi), \quad (8.4.3)$$

where  $\Phi_m^l(r)$  is a radial function and the functions  $Y_m^l(\theta, \phi)$ , encoding the angular part, are called *spherical harmonics*. The normalization condition that the eigenfunctions satisfy is, in general,

$$\langle l, m | l, m \rangle = \int dr |\Phi_m^l(r)|^2 |Y_m^l(\theta, \phi)|^2 \quad (8.4.4)$$

$$= \left( \int_0^\infty dr |\Phi_m^l(r)|^2 r^2 \right) \times \left( \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin(\theta) |Y_m^l(\theta, \phi)|^2 \right) \quad (8.4.5)$$

$$= N_r^{lm} \times N_{\theta, \phi}^{lm} \quad (8.4.6)$$

$$= 1. \quad (8.4.7)$$

Thus, taking the form of a product of two normalizations, one for the radial part, and one for the angular part. The conventionally adopted choice, which is also quite convenient for all calculations, is to take the two factors identically equal to 1, thus we require

$$\int_0^\infty dr |\Phi_m^l(r)|^2 r^2 = 1, \quad (8.4.8)$$

for the radial part, and the normalization condition for the spherical harmonics is instead

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin(\theta) |Y_m^l(\theta, \phi)|^2 = 1. \quad (8.4.9)$$

Notice that the radial function  $\Phi_m^l(r)$  cannot be determined from the general eigenvalue equations we have written above, and it is thus arbitrary, provided that the normalization condition is verified. In the following, we will concentrate then only on the non-trivial angular part, and study the properties of the spherical harmonics, as well as the associated spectrum of eigenvalues  $l$  and  $m$ .

### 8.4.1 Eigenvalues of $\hat{L}_z$

We start with the case of  $\hat{L}_z$ , for which the eigenvalue equation projected onto spherical coordinates takes the form

$$\langle r | \hat{L}_z | l, m \rangle = \hbar m \langle r | l, m \rangle. \quad (8.4.10)$$

Recalling the representation of the  $\hat{L}_z$  operator in the spherical coordinates representation,

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}, \quad (8.4.11)$$

we have that the spherical harmonics satisfy the following differential equation

$$-i\hbar \frac{\partial}{\partial \phi} \Phi_m^l(r) Y_m^l(\theta, \phi) = \hbar m \Phi_m^l(r) Y_m^l(\theta, \phi), \quad (8.4.12)$$

thus we see that it is independent of the radial part,

$$-i\hbar \frac{\partial}{\partial \phi} Y_m^l(\theta, \phi) = \hbar m Y_m^l(\theta, \phi). \quad (8.4.13)$$

Moreover, this equation does not carry any differential dependence on  $\theta$ , thus it is satisfied by separation of variables

$$Y_m^l(\theta, \phi) = \chi_m^l(\theta) e^{im\phi}. \quad (8.4.14)$$

From this expression we can also make a very important deduction on the possible values taken by  $m$  and  $l$ . The general theory of the angular momentum tells us that  $m$  is either integer or semi-integer and takes values in

$$-l \leq m \leq l. \quad (8.4.15)$$

However, for orbital angular momentum there is a little surprise! If we assume that the eigenfunctions of the angular momentum are single-valued (an assumption which is

essential if we wish to use these functions as a basis in which to expand arbitrary wavefunctions) we must have that

$$Y_m^l(\theta, \phi + 2\pi) = Y_m^l(\theta, \phi), \quad (8.4.16)$$

thus  $e^{im2\pi} = 1$  and  $m$  must be an integer, ruling out the possibility of a semi-integer value. In turn, this implies that  $l$  itself is an integer, and the allowed eigenvalues are

$$m = -l, \dots, -3, -2, -1, 0, 1, 2, 3, \dots, l. \quad (8.4.17)$$

It should be remarked that this spectrum of eigenvalues is in stark contrast with what happens for spins, that instead are allowed to take also semi-integer values of orbital angular momentum and not only integer values. This also explains why the Stern and Gerlach experiment was a “smoking-gun” (direct proof) for the existence of an intrinsic angular momentum, the spin, of the electron as opposed to the orbital angular momentum. The observation of an *even* number of possible values of  $m$  ( $m = \pm 1/2$ , in the SG experiment) indeed is not compatible with orbital angular momentum, that for any value of  $l$  allows only for an *odd* number of  $m$  states.

### 8.4.2 Eigenfunctions of $\hat{L}^2$

The other equation satisfied by the spherical harmonics is the eigenfunction condition for  $\hat{L}^2$ :

$$\langle \theta, \phi | \hat{L}^2 | l, m \rangle = \hbar^2 l(l+1) \langle \theta, \phi | l, m \rangle, \quad (8.4.18)$$

and using the explicit form for  $\hat{L}^2$  in spherical coordinates we get the following differential equation:

$$\frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} Y_m^l(\theta, \phi) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} Y_m^l(\theta, \phi) \right) + l(l+1) Y_m^l(\theta, \phi) = 0. \quad (8.4.19)$$

However, recalling that the  $\phi$  dependence is fixed, we have:

$$\frac{\partial^2}{\partial \phi^2} Y_m^l(\theta, \phi) = im \frac{\partial}{\partial \phi} Y_m^l(\theta, \phi) = -m^2 Y_m^l(\theta, \phi), \quad (8.4.20)$$

thus we can completely remove the  $\phi$  dependence, leading to:

$$\sin \theta \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial}{\partial \theta} \chi_m^l(\theta) \right) + [l(l+1) \sin^2 \theta - m^2] \chi_m^l(\theta) = 0. \quad (8.4.21)$$

This differential equation is equivalent to the associated Legendre equation, and its solution is denoted  $P_m^l(\cos \theta) \equiv \chi_m^l(\theta)$  and can be found in many textbooks. Then, apart from a normalization factor, we have:

$$Y_m^l(\theta, \phi) \propto e^{im\phi} P_m^l(\cos \theta). \quad (8.4.22)$$

The overall normalization can be found recalling the orthonormality conditions:

$$\langle l, m | l', m' \rangle = \delta_{l,l'} \delta_{m,m'}, \quad (8.4.23)$$

implying:

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta Y_m^l(\theta, \phi)^* Y_{m'}^{l'}(\theta, \phi) \sin \theta d\theta d\phi = \delta_{l,l'} \delta_{m,m'}. \quad (8.4.24)$$

This can be used to fix the overall normalization of the spherical harmonics. Furthermore, it is customary in physics literature to take a phase convention such that the spherical harmonics are complex-valued and satisfy:

$$Y_{-m}^l(\theta, \phi) = (-1)^m Y_m^l(\theta, \phi)^*. \quad (9.4.25)$$

Overall, these two conditions fix the final form to be:

$$Y_m^l(\theta, \phi) = (-1)^{(m+|m|)/2} \left[ \frac{(2l+1)(l-|m|)!}{4\pi(l+|m|)!} \right]^{1/2} e^{im\phi} P_m^l(\cos \theta), \quad (8.4.25)$$

where  $P_m^l(\cos \theta)$  are the associated Legendre functions.

We quote some of the first few spherical harmonics, that can be useful in exercises. The lowest spherical harmonic is just a constant,

$$Y_0^0(\theta, \phi) = \frac{1}{\sqrt{4\pi}}, \quad (9.4.27)$$

then for  $l = 1$  we have

$$Y_{\pm 1}^1(\theta, \phi) = \mp \sqrt{\frac{3}{8\pi}} \sin \theta e^{\pm i\phi}, \quad Y_0^1(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad (8.4.26)$$

and for  $l = 2$

$$Y_0^2(\theta, \phi) = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1), \quad (8.4.27)$$

$$Y_{\pm 1}^2(\theta, \phi) = \mp \sqrt{\frac{15}{8\pi}} \sin \theta \cos \theta e^{\pm i\phi}, \quad (8.4.28)$$

$$Y_{\pm 2}^2(\theta, \phi) = \sqrt{\frac{15}{32\pi}} \sin^2 \theta e^{\pm 2i\phi}. \quad (8.4.29)$$

Higher spherical harmonics can be found in books, if necessary.

### 8.4.3 Recursive Relations

An alternative approach to derive explicit expressions for  $\chi_m^l(\theta)$  is based on the ladder operators, similar to what we have already done for the harmonic oscillator. Specifically, we know that for the maximum allowed value of  $m$ , ( $m = l$ ) we must have

$$\hat{L}_+ |l, l\rangle = 0, \quad (8.4.30)$$

thus

$$\begin{aligned} \langle r | \hat{L}_+ |l, l\rangle &= \hbar e^{i\phi} \Phi_m^l(r) \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) \chi_l^l(\theta) e^{il\phi} = \\ &= F_m^l(r, \phi) \left( \frac{\partial}{\partial \theta} \chi_l^l(\theta) - l \cot \theta \chi_l^l(\theta) \right) = 0. \end{aligned} \quad (8.4.31)$$



We then have that the differential equation satisfied by  $\chi_l^l$  is

$$\left( \frac{\partial}{\partial \theta} \chi_l^l(\theta) - l \cot \theta \chi_l^l(\theta) \right) = 0, \quad (8.4.32)$$

which has solution

$$\chi_l^l(\theta) = c_{ll}(\sin \theta)^l, \quad (8.4.33)$$

where  $c_{ll}$  is a normalization constant that can be determined imposing the normalization condition. Omitting the explicit calculation of the normalization constant, the spherical harmonic in this case reads:

$$Y_l^l(\theta, \phi) = c_{ll} e^{il\phi} (\sin \theta)^l. \quad (8.4.34)$$

The spherical harmonics for smaller values of  $m$  can then be found by repeated applications of  $\hat{L}_-$ , since we know from the general theory of angular momentum that

$$\hat{L}_- |l, m\rangle = C_-(l, m) |l, m-1\rangle, \quad (8.4.35)$$

with  $C_-(l, m) = \hbar \sqrt{l(l+1) - m(m-1)}$ . We then find:

$$Y_m^{l-1}(\theta, \phi) = \frac{1}{C_-(l, m)} \times e^{-i\phi} \left( \frac{\partial}{\partial \theta} - i \cot \theta \frac{\partial}{\partial \phi} \right) Y_m^l(\theta, \phi). \quad (8.4.36)$$

$$\chi_m^{l-1}(\theta) = \frac{c_{lm}}{C_-(l, m)} \times \left( \frac{\partial}{\partial \theta} \chi_m^l(\theta) + m \cot \theta \chi_m^l(\theta) \right). \quad (8.4.37)$$

The latter expression is a recursive relation that allows us to systematically compute all the spherical harmonics, starting from the explicit expression we found for  $Y_l^l(\theta, \phi)$ .

#### 8.4.4 Properties of the Spherical Harmonics

While in the previous discussion we have only quoted the final result for the spherical harmonics, since its derivation is not conceptually interesting beyond the mathematical aspect, it is important though to know some general properties of the orbital angular momentum eigenfunctions.

One important property is that spherical harmonics are orthonormal, which implies

$$\int_0^{2\pi} d\phi \int_0^\pi d\theta \sin(\theta) Y_m^l(\theta, \phi) Y_{m'}^{l'}(\theta, \phi)^* = \delta_{ll'} \delta_{mm'}. \quad (8.4.38)$$

and that all functions  $F(\theta, \phi)$  of the solid angles  $\theta$  and  $\phi$  can be written as a linear combination of these basis functions:

$$F(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{lm} Y_m^l(\theta, \phi), \quad (8.4.39)$$

or in ket form

$$\langle \phi, \theta | F \rangle = \sum_{lm} \langle \phi, \theta | l, m \rangle \langle l, m | F \rangle, \quad (8.4.40)$$

thus the coefficients  $c_{lm} = \langle l, m | F \rangle$  read

$$\langle l, m | F \rangle = \int_0^{2\pi} d\phi \int_0^\pi d\theta \sin(\theta) Y_m^l(\theta, \phi)^* F(\theta, \phi). \quad (8.4.41)$$

From the general expressions for the spherical harmonics, we can also immediately notice that spherical harmonics with  $m = 0$  are purely real. This results from the fact that the normalization constant  $c_l$  defined above has an arbitrary phase, which is traditionally fixed in such a way that

$$Y_{-m}^l(\theta, \phi) = (-1)^m Y_m^l(\theta, \phi)^*. \quad (8.4.42)$$

Since the square modulus of the spherical harmonics does not depend on the angle  $\phi$ , a useful way of plotting them is presented in Figure 8.1. From this Figure it can be noticed that  $l = 0$  state, also known as "*s* state", is spherically symmetric, thus it has no preferential angular direction. The  $l = 1$  states, known as "*p* states", instead have different  $\theta$ -dependent shapes. For  $l = 1, m = 0$  for example we can see that there are two lobes, such that they have a zero in the  $xy$  plane.

## 8.5 References and Further Reading

The discussion in this Chapter shows the main conceptual steps required to construct the spherical harmonics, but some more laborious (and less interesting) steps have not been reproduced. Cohen-Tannoudji's book contains, in Chapter 6, a thorough discussion of all these technical aspects. The interested reader is then invited to look in there for more details.

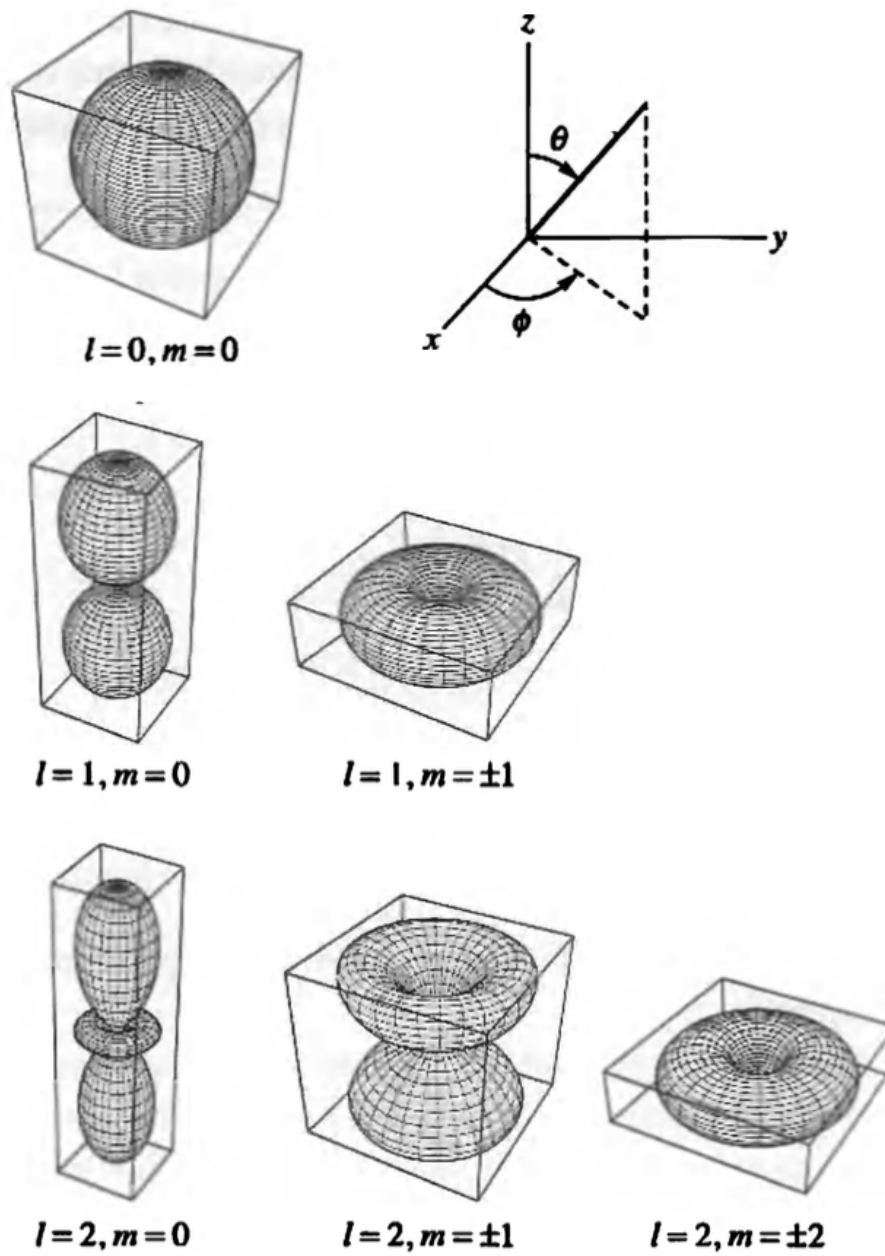


Figure 8.1: Polar Plots of the Spherical Harmonics.