Chapter 15. Orbital Angular Momentum

§ 1 *Introduction.* So far we have defined angular momentum through the commutation relations. The results obtained are valid for the orbital angular momentum of a moving particle and for the intrinsic angular momentum (spin). This chapter specializes the results to orbital angular momentum.

Our main achievement is to find the expression of $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, and $\hat{L}^2$ in coordinate representation and derive some properties of the angular momentum for a particle moving under the action of a force that does not depend on angles (central force).

§ 2 *Classical orbital angular momentum.* You might have noticed by now that one of the recipes for generating quantum dynamics is to take a classical formula and replace the classical quantities with the corresponding operators.

The classical angular momentum is

$$\vec{L} = \vec{r} \times \vec{p} \tag{1}$$

where $\vec{r}$ is the position of the particle *in a Cartesian coordinate system* and $\vec{p}$ is the momentum in the same system. If the system has N particles, the total angular momentum is

$$\vec{L} = \sum_{i=1}^{N} \vec{r}_i \times \vec{p}_i \tag{2}$$

where $\vec{r}_i$ and $\vec{p}_i$ are the position and the momentum of the i-th particle. If no torque[1] acts on the particles, then $\vec{L}$ is time-independent. Moreover, the energy of the rotational motion is proportional to $\vec{L}^2$.

These results can be derived from Newton's equations. They are true for a rotating rigid body and also for a swarm of particles that interacts with forces that depend only on the distance between them (no torque). No matter how they move, whether the swarm expands or the particles come together, their total angular momentum stays the same. We expect this conservation law to also hold in quantum mechanics.

§ **3** *Quantum definition.* We define the orbital angular momentum of one particle as

$$\hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}} \tag{3}$$

If we expand the cross product, the components of $\hat{\vec{L}}$ are

$$\begin{aligned} \hat{L}_x &= \hat{y}\hat{p}_z - \hat{z}\hat{p}_y && (4) \\ \hat{L}_y &= \hat{z}\hat{p}_x - \hat{x}\hat{p}_z && (5) \\ \hat{L}_z &= \hat{x}\hat{p}_y - \hat{y}\hat{p}_x && (6) \end{aligned}$$

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[1] The torque is $\sum_{i=1}^{N} \vec{r}_i \times \vec{F}_i$ where $\vec{F}_i$ is the force acting on the i-th particle.

Note that the components of the position operator and of the momentum operator involved in these expressions commute. For example, $\hat{y}\hat{p}_z - \hat{p}_z\hat{y} = 0$. Because of this, we can translate the classical expression $yp_z - p_y z$ into the operator $\hat{y}\hat{p}_z - \hat{z}\hat{p}_y$ without concern about the order of the operators. It is easy to show that $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ are Hermitian operators, as they must be.

§ **4** *Angular momentum in coordinate representation.* To represent $\hat{O}|\psi\rangle$, where $\hat{O}$ is an arbitrary operator and $|\psi\rangle$ is an arbitrary ket, we calculate

$$\langle x, y, z \,|\, \hat{O} \,|\, \psi\rangle$$

We can do this for the angular momentum because we know that

$$\langle x, y, z \,|\, \hat{y} \,|\, \psi\rangle = y\langle x, y, z \,|\, \psi\rangle \tag{7}$$

and

$$\langle x, y, z \,|\, \hat{p}_z \,|\, \psi\rangle = \frac{\hbar}{\mathrm{i}}\frac{\partial}{\partial z}\langle x, y, z \,|\, \psi\rangle \tag{8}$$

Similar equations hold for the other operators. Also, we often write

$$\langle x, y, z \,|\, \psi\rangle \equiv \psi(x, y, z) \tag{9}$$

Applying these rules, we find that

$$\langle x, y, z \,|\, \hat{L}_x \,|\, \psi\rangle = \frac{\hbar}{\mathrm{i}}\left(y\,\frac{\partial\psi(x,y,z)}{\partial z} - z\,\frac{\partial\psi(x,y,z)}{\partial y}\right) \tag{10}$$

$$\langle x, y, z \,|\, \hat{L}_y \,|\, \psi\rangle = \frac{\hbar}{\mathrm{i}}\left(z\,\frac{\partial\psi(x,y,z)}{\partial x} - x\,\frac{\partial\psi(x,y,z)}{\partial z}\right) \tag{11}$$

$$\langle x, y, z \,|\, \hat{L}_z \,|\, \psi\rangle = \frac{\hbar}{\mathrm{i}}\left(x\,\frac{\partial\psi(x,y,z)}{\partial y} - y\,\frac{\partial\psi(x,y,z)}{\partial x}\right) \tag{12}$$

§ 5 *Commutators.* The definition in Eq. 3 is acceptable only if the components of the angular momentum satisfy the commutation relations

$$[\hat{L}_x, \hat{L}_y] = \mathrm{i}\hbar\hat{L}_z \tag{13}$$

$$[\hat{L}_y, \hat{L}_z] = \mathrm{i}\hbar\hat{L}_x \tag{14}$$

$$[\hat{L}_z, \hat{L}_x] = \mathrm{i}\hbar\hat{L}_y \tag{15}$$

It is a simple but tedious exercise to test that $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ given by Eqs. 10–12 satisfy these commutation relations. Because the orbital angular momenta satisfy the commutation relations, they inherit all the general properties of the angular momentum derived in Chapter 13.

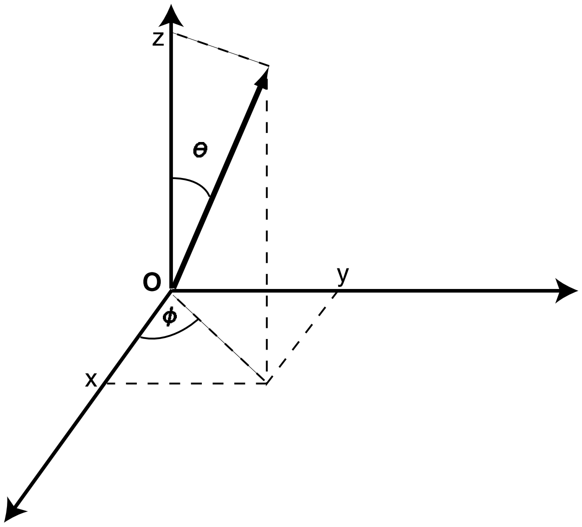

Figure 1: Spherical coordinates

§ 6 *Spherical coordinates.* Angular momentum is an extremely useful quantity for analyzing the motion of a particle in a "central field". This means a potential energy $V(r)$ that depends only on the length of the vector $\vec{r}$ and not on its orientation. A well-known example is the hydrogen atom, when we consider the nucleus to be fixed at the origin of the coordinate system; the electron interacts with it through a Coulomb force, which depends *only* on the electron-nucleus distance. The force acting on the electron is the same at any point on a sphere whose center is on the nucleus. We say that the system has spherical symmetry. For such a system, it is convenient to use spherical coordinates. The "coordinates" in this system are r, θ, ϕ (see Figure 1), and

$$x = r\sin\theta\cos\phi \tag{16}$$

$$y = r\sin\theta\sin\phi \tag{17}$$

$$z = r\cos\theta \tag{18}$$

with r, θ, ϕ in the range

$$0 \le r \le \infty, \quad 0 \le \theta \le \pi, \quad 0 \le \phi \le 2\pi \tag{19}$$

We can invert these equations to get

$$r = \sqrt{x^2+y^2+z^2} \tag{20}$$

$$\cos\theta = \frac{z}{\sqrt{x^2+y^2+z^2}} \tag{21}$$

$$\tan\phi = \frac{y}{x} \tag{22}$$

We convert Eqs. 10–12 for $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ to spherical coordinates to obtain

$$\hat{L}_x = \mathrm{i}\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right) \tag{23}$$

$$\hat{L}_y = \mathrm{i}\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right) \tag{24}$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi} \tag{25}$$

These expressions can be found by straightforward algebra. For example, by using Eqs. 16–18 for x, y, and z, $\psi(x,y,z)$ is transformed into

$$\psi(r\sin\theta\cos\phi, r\sin\theta\sin\phi, r\cos\theta) \equiv \psi(r,\theta,\phi)$$

Also, using the chain rule,

$$\frac{\partial}{\partial x}\psi(x,y,z) = \frac{\partial\psi(r,\theta,\phi)}{\partial r}\,\frac{\partial r}{\partial x} + \frac{\partial\psi(r,\theta,\phi)}{\partial\theta}\,\frac{\partial\theta}{\partial x} + \frac{\partial\psi(r,\theta,\phi)}{\partial\phi}\,\frac{\partial\phi}{\partial x}$$

$\partial r/\partial x$, $\partial\theta/\partial x$, and $\partial\phi/\partial x$ are calculated from Eqs. 20–22. We are very grateful to our predecessors who have done the required algebra and arrived at Eqs. 23–25. The last, tedious calculation is that of converting the Laplace operator to spherical coordinates. Luckily this is available in many books.[2]

The kinetic energy $-(\hbar^2/2\mu)\nabla^2$ becomes

$$\begin{aligned}\hat{K}\psi(r,\theta,\phi) &= -\frac{\hbar^2}{2\mu}\nabla^2\psi(r,\theta,\phi) \\ &= -\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\phi^2}\right]\end{aligned} \tag{26}$$

If we calculate $\hat{L}^2$ using Eqs. 23–25, we get

$$\hat{L}^2 = -\hbar^2\left[\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)\right] \tag{27}$$

Comparing Eqs. 26 and 27 gives

$$\hat{K}\psi(r,\theta,\phi) = -\frac{\hbar^2}{2\mu r^2}\,\frac{\partial}{\partial r}r^2\,\frac{\partial\psi(r,\theta,\phi)}{\partial r} + \frac{\hat{L}^2}{2\mu r^2}\psi(r,\theta,\phi) \tag{28}$$

As in classical mechanics, the kinetic energy has a radial part and an angular part. The angular part, $\hat{L}^2/(2\mu r^2)$, is the rotational energy of the particle.

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[2] For example, P. M. Moore and H. Feshbach, *Methods of Theoretical Physics, Volume 1*, McGraw-Hill, New York, @year, edition

§ 7 *The eigenfunctions of $\hat{L}^2$.* The eigenfunctions of $\hat{L}^2$ in spherical coordinates are given by

$$\hat{L}^2\,\psi(r,\theta,\phi) = \hbar^2\ell(\ell+1)\,\psi(r,\theta,\phi) \tag{29}$$

Since $\hat{L}^2$ depends only on angles, we can write

$$\psi(r,\theta,\phi) = f(r)Y(\theta,\phi) \tag{30}$$

where $f(r)$ is a function of radius r, which cannot be determined from Eq. 29. Normalization requires

$$\int \mathrm{d}x\ \mathrm{d}y\ \mathrm{d}z\,\psi(x,y,z)^*\,\psi(x,y,z) = 1 \tag{31}$$

Converting to spherical coordinates gives

$$\int_0^\infty r^2\,\mathrm{d}r \int_0^\pi \sin\theta\ \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, f(r)^*\, f(r)\, Y(\theta,\phi)^*\, Y(\theta,\phi) = 1 \tag{32}$$

If we separately normalize the radial function to

$$\int_0^\infty r^2\,\mathrm{d}r\, f(r)^*\, f(r) = 1 \tag{33}$$

then Eq. 32 gives (use Eq. 33)

$$\int_0^\pi \sin\theta\ \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\phi\, Y(\theta,\phi)^*\, Y(\theta,\phi) = 1 \tag{34}$$

To find the eigenfunctions of $\hat{L}^2$ (we already know that the eigenvalues are $\hbar\ell(\ell+1)$ with $\ell \geq 0$), we must solve

$$\hat{L}^2 Y(\theta,\phi) = \hbar\ell(\ell+1)Y(\theta,\phi) \tag{35}$$

where $\hat{L}^2$ is given by Eq. 27 and the normalization by Eq. 34. Fortunately, the solution was known to mathematicians before quantum mechanics was developed. The solutions are called the spherical harmonics and take the form

$$Y_\ell^m(\theta,\phi) = \frac{(-1)^{\ell+m}}{2^\ell \ell!}\sqrt{\frac{2\ell+1}{4\pi}\frac{(\ell-m)!}{(\ell+m)!}}e^{im\phi}(\sin\theta)^m \frac{d^{\ell+m}}{d(\cos\theta)^{\ell+m}}\left(1-\cos^2\theta\right)^\ell \tag{36}$$

A few examples are

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{2\sqrt{\pi}}\\
Y_1^{-1}(\theta,\phi) &= \frac{1}{2}\,e^{-i\phi}\sqrt{\frac{3}{2\pi}}\,\sin\theta\\
Y_1^0(\theta,\phi) &= \frac{1}{2}\sqrt{\frac{3}{\pi}}\,\cos\theta\\
Y_1^1(\theta,\phi) &= -\frac{1}{2}\,e^{i\phi}\sqrt{\frac{3}{2\pi}}\,\sin\theta\\
Y_2^{-2}(\theta,\phi) &= \frac{1}{4}\,e^{-2i\phi}\sqrt{\frac{15}{2\pi}}\,\sin^2\theta\\
Y_2^{-1}(\theta,\phi) &= \frac{1}{2}\,e^{-i\phi}\sqrt{\frac{15}{2\pi}}\,\cos\theta\,\sin 2\theta
\end{aligned}$$

More examples are given in the Appendix.

Since $\hat{L}^2$ and $\hat{L}_z$ commute, the functions $Y_\ell^m(\theta,\phi)$ are chosen to be eigenfunctions of both operators. This means that

$$\hat{L}_z Y_\ell^m(\theta,\phi) = \hbar m\, Y_\ell^m(\theta,\phi), \quad m = -\ell, -\ell+1, \ldots, \ell-1, \ell \tag{37}$$

The eigenstates of $\hat{L}^2$ are degenerate: for each value of ℓ, there are $2\ell+1$ states that correspond to different projection of $\hat{\vec{L}}$ on the OZ axis.

You are aware, of course, that if $Y_\ell^m(\theta,\phi)$ is an normalized eigenfunction of $\hat{L}^2$ and $\hat{L}_z$, then, for any real number α, $\mathrm{e}^{+\mathrm{i}\alpha}Y_\ell^m(\theta,\phi)$ is also a normalized eigenfunction. It is unfortunate that various books use different such phase factors. As long as you do not mix formulae from different sources, which might use different phase factors, you do not have to worry about them.

Spherical harmonics have many interesting properties and I give some of them in the Appendix. I will also give more details about the functions $Y_\ell^m(\theta, \phi)$ when I discuss the hydrogen atom.

Appendix 15.1. Examples of Spherical Harmonics

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{2\sqrt{\pi}} \\
Y_1^{-1}(\theta,\phi) &= \frac{1}{2}\, e^{-i\phi} \sqrt{\frac{3}{2\pi}}\, \sin\theta \\
Y_1^{0}(\theta,\phi) &= \frac{1}{2} \sqrt{\frac{3}{\pi}}\, \cos\theta \\
Y_1^{1}(\theta,\phi) &= -\frac{1}{2}\, e^{i\phi} \sqrt{\frac{3}{2\pi}}\, \sin\theta \\
Y_2^{-2}(\theta,\phi) &= \frac{1}{4}\, e^{-2i\phi} \sqrt{\frac{15}{2\pi}}\, \sin^2\theta \\
Y_2^{-1}(\theta,\phi) &= \frac{1}{2}\, e^{-i\phi} \sqrt{\frac{15}{2\pi}}\, \cos\theta\, \sin 2\theta \\
Y_2^{0}(\theta,\phi) &= \frac{1}{4} \sqrt{\frac{5}{\pi}}\, (-1 + 3\cos^2\theta) \\
Y_2^{1}(\theta,\phi) &= -\frac{1}{2}\, e^{i\phi} \sqrt{\frac{15}{2\pi}}\, \cos\theta\, \sin\theta \\
Y_2^{2}(\theta,\phi) &= \frac{1}{4}\, e^{2i\phi} \sqrt{\frac{15}{2\pi}}\, \sin^2\theta \\
Y_3^{-3}(\theta,\phi) &= \frac{1}{8}\, e^{-3i\phi} \sqrt{\frac{35}{\pi}}\, \sin^3\theta \\
Y_3^{-2}(\theta,\phi) &= \frac{1}{4}\, e^{-2i\phi} \sqrt{\frac{105}{2\pi}}\, \cos\theta\, \sin^2\theta
\end{aligned}$$

$$\begin{aligned}
Y_3^{-1}(\theta,\phi) &= \frac{1}{8}\,e^{-i\phi}\sqrt{\frac{21}{\pi}}\,(-1+5\cos^2\theta)\sin\theta \\
Y_3^{0}(\theta,\phi) &= \frac{1}{4}\sqrt{\frac{7}{\pi}}\,(-3\cos\theta+5\cos^3\theta) \\
Y_3^{1}(\theta,\phi) &= -\frac{1}{8}\,e^{i\phi}\sqrt{\frac{21}{\pi}}\,(-1+5\cos^2\theta)\sin\theta \\
Y_3^{2}(\theta,\phi) &= \frac{1}{4}\,e^{2i\phi}\sqrt{\frac{105}{2\pi}}\,\cos\theta\,\sin^2\theta \\
Y_3^{3}(\theta,\phi) &= -\frac{1}{8}\,e^{3i\phi}\sqrt{\frac{35}{\pi}}\,\sin^3\theta \\
Y_4^{-4}(\theta,\phi) &= \frac{3}{16}\,e^{-4i\phi}\sqrt{\frac{35}{2\pi}}\,\sin^4\theta \\
Y_4^{-3}(\theta,\phi) &= \frac{3}{8}\,e^{-3i\phi}\sqrt{\frac{35}{\pi}}\,\cos\theta\,\sin^3\theta \\
Y_4^{-2}(\theta,\phi) &= \frac{3}{8}\,e^{-2i\phi}\sqrt{\frac{5}{2\pi}}\,(-1+7\cos^2\theta)\sin^2\theta \\
Y_4^{-1}(\theta,\phi) &= \frac{3}{8}\,e^{-i\phi}\sqrt{\frac{5}{\pi}}\,(-3+7\cos^2\theta)\cos\theta\,\sin\theta \\
Y_4^{0}(\theta,\phi) &= \frac{3}{16\sqrt{\pi}}\,(3-30\cos^2\theta+35\cos^4\theta) \\
Y_4^{1}(\theta,\phi) &= -\frac{3}{8}\,e^{-i\phi}\sqrt{\frac{5}{\pi}}\,(-3+7\cos^2\theta)\cos\theta\,\sin\theta \\
Y_4^{2}(\theta,\phi) &= \frac{3}{8}\,e^{2i\phi}\sqrt{\frac{5}{2\pi}}\,(-1+7\cos^2\theta)\sin^2\theta \\
Y_4^{3}(\theta,\phi) &= -\frac{3}{8}\,e^{3i\phi}\sqrt{\frac{35}{\pi}}\,\cos\theta\,\sin^3\theta \\
Y_4^{4}(\theta,\phi) &= \frac{3}{16}\,e^{4i\phi}\sqrt{\frac{35}{2\pi}}\,\sin^4\theta
\end{aligned}$$