

3: Angular momentum in quantum mechanics

Objectives

In this chapter we discuss the angular momentum operator – one of several related operators – analogous to classical angular momentum. The angular momentum operator plays a central role in the theory of atomic physics and other quantum problems involving rotational symmetry. In both classical and quantum mechanical systems, angular momentum (together with linear momentum and energy) is one of the three fundamental properties of motion.

Prerequisites

Chapters 1 and 2. Angular momentum and its conservation in classical mechanics. Spherical coordinates, elements of vector analysis. Laplace equation.

Eigenvalue equation in polar coordinates

The classical definition of the angular momentum vector is

$$\mathcal{L} = \mathbf{r} \times \mathbf{p} \quad (3.1)$$

which depends on the choice of the point of origin where $|\mathbf{r}|=r=0$. With the definition of the position and the momentum operators we obtain the angular momentum operator as

$$\hat{\mathbf{L}} = -i\hbar(\mathbf{r} \times \nabla) \quad (3.2)$$

The Cartesian components of $\hat{\mathbf{L}}$ are then

$$\hat{L}_x = -i\hbar(y\partial_z - z\partial_y), \quad \hat{L}_y = -i\hbar(z\partial_x - x\partial_z), \quad \hat{L}_z = -i\hbar(x\partial_y - y\partial_x) \quad (3.3)$$

One frequently needs the components of $\hat{\mathbf{L}}$ in [spherical coordinates](#). In order to obtain them we have to make use of the expression of the position vector by spherical coordinates, which are connected to the Cartesian components by

$$\mathbf{r} = x\hat{\mathbf{e}}_x + y\hat{\mathbf{e}}_y + z\hat{\mathbf{e}}_z = r \sin\theta \cos\phi \hat{\mathbf{e}}_x + r \sin\theta \sin\phi \hat{\mathbf{e}}_y + r \cos\theta \hat{\mathbf{e}}_z \quad (3.4)$$

Going over to the spherical components in (3.3), and using the chain rule:

$$\partial_x = (\partial_x r) \partial_r + (\partial_x \theta) \partial_\theta + (\partial_x \phi) \partial_\phi \quad (3.5)$$

and similarly for ∂_y and ∂_z gives the following components

$$\begin{aligned} \hat{L}_x &= i\hbar(\sin\phi \partial_\theta + \cot\theta \cos\phi \partial_\phi) \\ \hat{L}_y &= i\hbar(-\cos\phi \partial_\theta + \cot\theta \sin\phi \partial_\phi) \\ \hat{L}_z &= -i\hbar \partial_\phi \end{aligned} \quad (3.6)$$

One sees at once the reason and the advantage of using spherical coordinates: the operators in question do not depend on the radial variable r . This is of course also true for $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ which turns out to be $-\hbar^2$ times the angular part of the Laplace operator $\Delta_{\theta\phi}$.

$$\hat{L}^2 = -\hbar^2 \left(\partial_\theta^2 + \cot\theta \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi^2 \right) = -\hbar^2 \Delta_{\theta\phi} \quad (3.7)$$

We shall now find the eigenfunctions of $\Delta_{\theta\phi}$, that play a very important role in quantum mechanics, and actually in several branches of theoretical physics. They will be functions of $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$, i.e. they can be considered as complex valued functions whose domain is the unit sphere. The eigenfunctions of \hat{L}^2 will be denoted by $Y(\theta, \phi)$, and the angular eigenvalue equation is:

$$\begin{aligned} -\Delta_{\theta\phi} Y(\theta, \phi) &= \ell(\ell+1) Y(\theta, \phi) \quad \text{or} \\ \left(\partial_\theta^2 + \cot\theta \partial_\theta + \frac{1}{\sin^2\theta} \partial_\phi^2 \right) Y(\theta, \phi) &= -\ell(\ell+1) Y(\theta, \phi) \end{aligned} \quad (3.8)$$

One might wonder what is the reason for writing the eigenvalue in the form $\ell(\ell+1)$, but as it will turn out soon, there is no loss of generality in this notation.

Separation of the eigenvalue equation

We try the separation of the variables:

$$Y(\theta, \phi) = \Theta(\theta)\Phi(\phi) \quad (3.9)$$

Plugging this into (3.8) and dividing by $\Theta\Phi$, we find

$$\left\{ \frac{1}{\Theta} \left[\sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) \right] + \ell(\ell+1) \sin^2 \theta \right\} + \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = 0 \quad (3.10)$$

The first term depends only on θ while the last one is a function of only ϕ . In order to satisfy this equation for all values of θ and ϕ these terms must be separately equal to a constant with opposite signs. This constant is traditionally denoted by m^2 and $-m^2$ (note that this is not the mass) and we have two equations: one for Θ , and another for Φ . We consider the second one, and have:

$$\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2 \quad (3.11)$$

Two linearly independent solutions are

$$\Phi(\phi) = \begin{cases} e^{im\phi} \\ e^{-im\phi} \end{cases} \quad (3.12)$$

and any linear combinations of them. One can choose $e^{im\phi}$, and include the other one by allowing m to be negative. As these are functions of points in real three dimensional space, the values of $\Phi(\phi)$ and $\Phi(\phi+2\pi)$ must be the same, as these values of the argument correspond to identical points in space. Then $e^{im(\phi+2\pi)} = e^{im\phi}$, and $e^{im2\pi} = 1$ must hold. From this it follows that m must be an integer

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad m = 0, \pm 1, \pm 2 \dots \quad (3.15)$$

The integration constant $\frac{1}{\sqrt{2\pi}}$ has been chosen here so that already $\Phi(\phi)$ is normalized to unity when integrating with respect to ϕ from 0 to 2π .

The equation for Θ

$$\sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + [\ell(\ell+1) \sin^2 \theta - m^2] \Theta = 0 \quad (3.16)$$

is more complicated. With $\cos \theta = z$ the solution is

$$P_\ell^m(z) := (1-z^2)^{|m|/2} \left(\frac{d}{dz} \right)^{|m|} P_\ell(z) \quad (3.17)$$

where $P_\ell(z)$ is the ℓ -th **Legendre polynomial**, defined by the following formula, (called the **Rodrigues formula**):

$$P_\ell(z) := \frac{1}{2^\ell \ell!} \left(\frac{d}{dz} \right)^\ell (z^2 - 1)^\ell \quad (3.18)$$

The functions $P_\ell^m(z)$ are called associated Legendre functions.

Problem 3.1

Find the first three Legendre polynomials $P_0(z)$, $P_1(z)$ and $P_2(z)$.

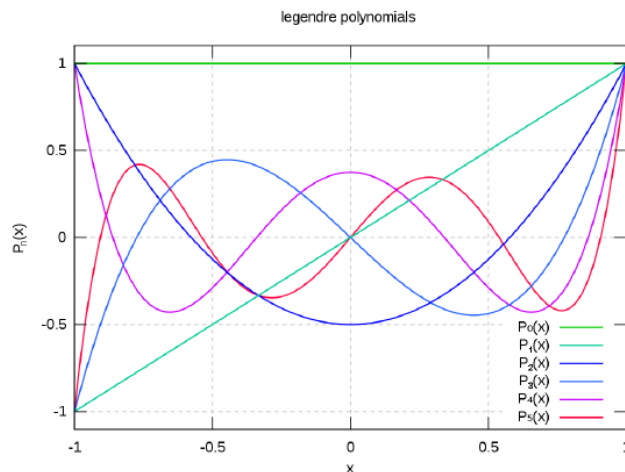


Figure 3.1: Plot of the first six Legendre polynomials.

<http://en.Wikipedia.org/wiki/File:Legendrepolynomials6.svg>

The function $P_\ell^m(z)$ is a polynomial in z only if $|m|$ is even, otherwise it contains a term $(1 - z^2)^{|m|/2}$ which is a square root. But when turning back to $\cos\theta = z$ this factor reduces to $(\sin\theta)^{|m|}$.

Problem 3.2

Find $P_2^0(\theta)$, $P_2^1(\theta)$, $P_2^2(\theta)$.

Problem 3.3

Prove that $P_\ell(z)$ are solutions of (3.16) for $m = 0$.

Problem 3.4

Prove that $P_\ell^m(z)$ are solutions of (3.16) for all ℓ and $|m|$, if $|m| \leq \ell$.

Problem 3.5

Show that $P_\ell(z)$ are either even, or odd depending on the parity of ℓ .

Notice that ℓ must be a nonnegative **integer** otherwise the definition (3.18) makes no sense, and in addition if $|\ell| > \ell$, then (3.17) yields zero. Thus for any given ℓ , there are $2\ell + 1$ allowed values of m :

$$m = -\ell, -\ell + 1, \dots, -1, 0, 1, \dots, \ell - 1, \ell, \quad \text{for } \ell = 0, 1, 2, \dots \quad (3.19)$$

Note that equation (3.16) – as all second order differential equations – must have other linearly independent solutions different from $P_\ell^m(z)$ for a given value of ℓ and m . One can show however, that these latter solutions are divergent for $\theta = 0$ and $\theta = \pi$, and therefore they are not describing physical states. The solutions

$$Y_\ell^m(\theta, \phi) = \mathcal{N}_{\ell m} P_\ell^m(\cos\theta) e^{im\phi} \quad (3.20)$$

where the absolute values of the constants $\mathcal{N}_{\ell m}$ ensure the normalization over the unit sphere, are called **spherical harmonics**. There are several different conventions for the phases of $\mathcal{N}_{\ell m}$, so one has to be careful with them.

The $Y_\ell^m(\theta)$ functions are thus the eigenfunctions of \hat{L} corresponding to the eigenvalue $\hbar^2 \ell(\ell + 1)$, and they are also eigenfunctions of $\hat{L}_z = -i\hbar \partial_\phi$, because

$$\hat{L}_z Y_\ell^m(\theta, \phi) = -i\hbar \partial_\phi Y_\ell^m(\theta, \phi) = \hbar m Y_\ell^m(\theta, \phi) \quad (3.21)$$

The quantum number ℓ is called **angular momentum quantum number**, or sometimes for a historical reason as azimuthal quantum number, while m is the **magnetic quantum number**.

Concluding the subsection let us note the following important fact. As none of the components of $\hat{\mathbf{L}}$, and thus nor \hat{L}^2 depends on the radial distance r from the origin, then any function of the form $\mathcal{R}(r)Y_\ell^m(\theta, \phi)$ will be the solution of the eigenvalue equation above, because from the point of view of the $\hat{\mathbf{L}}$ the $\mathcal{R}(r)$ function is a constant, and we can freely multiply both sides of (3.8). by $\mathcal{R}(r)$.

Orthonormality and completeness

The spherical harmonics form an infinite **system of orthonormal functions** in the sense:

$$\int_0^{2\pi} \int_0^\pi \left(Y_{\ell'}^{m'}(\theta, \phi) \right)^* Y_\ell^m(\theta, \phi) \sin \theta d\theta d\phi = \delta_{\ell\ell'} \delta_{mm'} \quad (3.22)$$

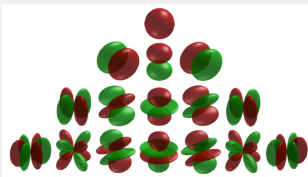
This system is also a **complete** one, which means that any complex valued function $g(\theta, \phi)$ that is square integrable on the unit sphere, i.e. $\int |g(\theta, \phi)|^2 \sin \theta d\theta d\phi < \infty$ can be expanded in terms of the $Y_\ell^m(\theta, \phi)$:

$$g(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{\ell m} Y_\ell^m(\theta, \phi) \quad (3.23)$$

where the expansion coefficients can be obtained similarly to the case of the complex Fourier expansion by

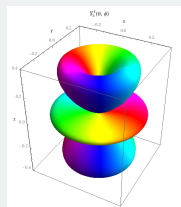
$$c_{\ell m} = \int_0^{2\pi} \int_0^\pi \left(Y_\ell^m(\theta, \phi) \right)^* g(\theta, \phi) \sin \theta d\theta d\phi \quad (3.24)$$

Further Reading



If you are interested in the topic Spherical harmonics in more details check out the Wikipedia link below:
http://en.Wikipedia.org/wiki/Spherical_harmonics

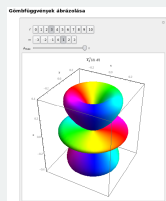
Animation



The animation shows the time dependence of the stationary state – i.e. the one containing the time dependent factor $e_{-i\epsilon t/\hbar}$ as well – given by the function $Y_1^3(\theta, \phi)$. The absolute value of the function in the direction given by θ and ϕ is equal to the distance of the point from the origin, and the argument of the complex number is obtained by the colours of the surface according to the phase code of the complex number in the chosen direction.

http://titan.physx.u-szeged.hu/~mmquantum/video/Gombfuggvény_fazis_idofejlodes.flv

Animation



The figures show the three-dimensional polar diagrams of the spherical harmonics. The state to be shown, can be chosen by setting the quantum numbers ℓ and m .

<http://titan.physx.u-szeged.hu/~mmquantum/interactive/Gombfuggvények.nbp>

Specific examples

The first few functions are the following, with one of the usual phase (sign) conventions:

$$Y_0^0(\theta, \phi) = \frac{1}{\sqrt{4\pi}} \quad (3.25)$$

$$Y_1^0(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta, \quad Y_1^1(\theta, \phi) = -\sqrt{\frac{3}{8\pi}} \sin \theta e^{i\phi}, \quad Y_1^{-1}(\theta, \phi) = \sqrt{\frac{3}{8\pi}} \sin \theta e^{-i\phi} \quad (3.26)$$

Historically the spherical harmonics with the labels $\ell = 0, 1, 2, 3, 4$ are called $s, p, d, f, g \dots$ functions respectively, the terminology is coming from spectroscopy.

If an external magnetic field $\mathbf{B} = \{0, 0, B\}$ is applied, the projection of the angular momentum onto the field direction is $\hbar m$. Since m can take only the integer values between $-\ell$ and $+\ell$, there are $2\ell + 1$ different possible projections, corresponding to the $2\ell + 1$ different functions $Y_m^\ell(\theta, \phi)$ with a given ℓ .

Very often the spherical harmonics are given by Cartesian coordinates by exploiting $\sin \theta e^{\pm i\phi} = (x \pm iy)/r$ and $\cos \theta = z/r$. Another way of using these functions is to create linear combinations of functions with opposite m -s. This is useful for instance when we illustrate the orientation of chemical bonds in molecules. We demonstrate this with the example of the p functions.

$$\begin{aligned} p_x &= \frac{x}{r} = \frac{(Y_1^{-1} - Y_1^1)}{\sqrt{2}} = \sqrt{\frac{3}{4\pi}} \sin \theta \cos \phi \\ p_y &= \frac{y}{r} = -\frac{(Y_1^{-1} + Y_1^1)}{\sqrt{2}} = \sqrt{\frac{3}{4\pi}} \sin \theta \sin \phi \\ p_z &= \frac{z}{r} = Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos \theta \end{aligned} \quad (3.27)$$

Let us also note that the $m = 0$ functions do not depend on ϕ , and they are proportional to the Legendre polynomials in $\cos \theta$.

$$Y_\ell^0(\theta) = \sqrt{\frac{2\ell+1}{4\pi}} P_\ell(\cos \theta) \quad (3.28)$$

Parity and angular momentum

The operator of parity Π is defined in the following way:

$$\Pi\psi(\mathbf{r}) = \psi(-\mathbf{r}) \quad (3.29)$$

The result of acting by the parity on a function is the mirror image of the original function with respect to the origin. Looking for the eigenvalues and eigenfunctions of Π , we note first that $\Pi^2 = 1$. Therefore the single eigenvalue of Π^2 is 1, and any function is its eigenfunction. The eigenvalues of Π itself are then ± 1 , and we have the following two possibilities:

$$\begin{aligned} \Pi\psi_+(\mathbf{r}) &= \psi_+(-\mathbf{r}) = \psi_+(\mathbf{r}) \\ \Pi\psi_-(\mathbf{r}) &= \psi_-(-\mathbf{r}) = -\psi_-(\mathbf{r}) \end{aligned} \quad (3.30)$$

In the first case the eigenfunctions $\psi_+(\mathbf{r})$ belonging to eigenvalue $+1$ are the even functions, while in the second we see that $\psi_-(\mathbf{r})$ are the odd functions belonging to the eigenvalue -1 . There are of course functions which are neither even nor odd, they do not belong to the set of eigenfunctions of Π .

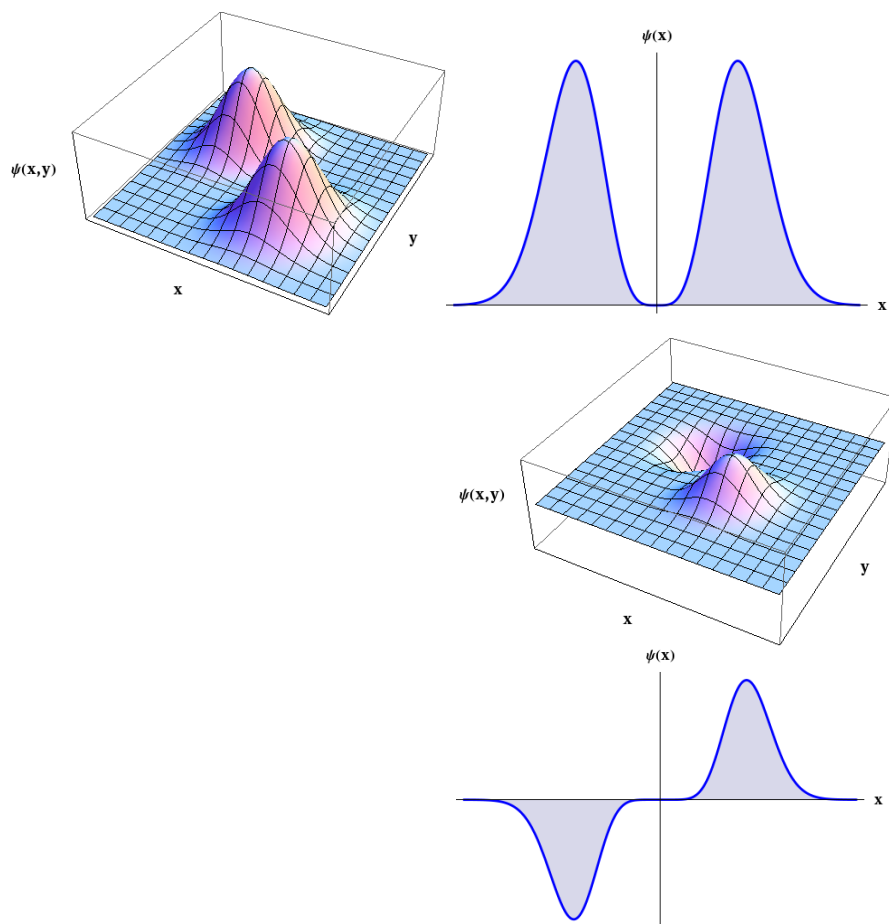


Figure 3.2: Examples of even and odd functions in one and two dimensions.

The reason why we consider parity in connection with the angular momentum is that the simultaneous eigenfunctions of \hat{L}^2 and \hat{L}_z the spherical harmonics times any function of the radial variable r are eigenfunctions of Π as well, and the corresponding eigenvalues are $(-1)^\ell$. This can be formulated as:

$$\Pi \mathcal{R}(r) Y_\ell^m(\theta, \phi) = \mathcal{R}(r) \Pi Y_\ell^m(\theta, \phi) = (-1)^\ell \mathcal{R}(r) Y_\ell^m(\theta, \phi) \quad (3.31)$$

Problem 3.6

Show that the transformation $\{x, y, z\} \longrightarrow \{-x, -y, -z\}$ is equivalent to $\theta \longrightarrow \pi - \theta$, $\phi \longrightarrow \phi + \pi$.

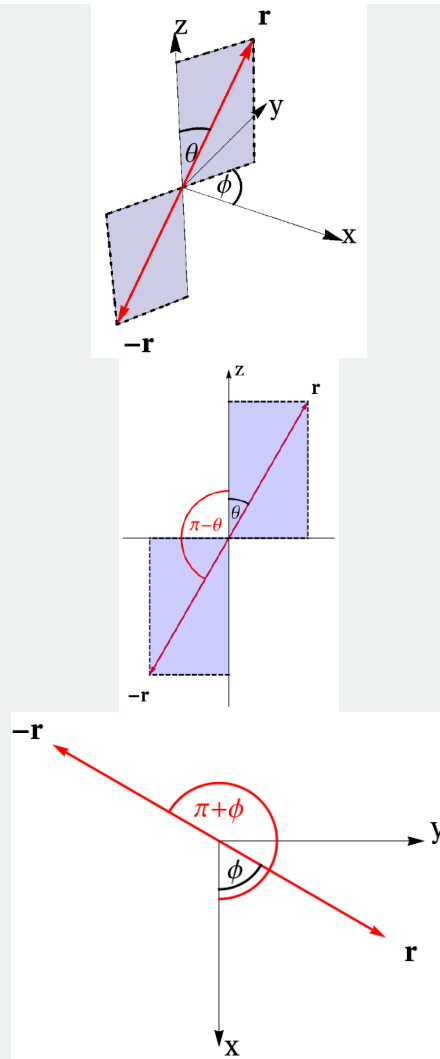


Figure 3.3: The effect of the transformation $\{x, y, z\} \rightarrow \{-x, -y, -z\}$

Problem 3.7

By using the results of the previous subsections prove the validity of Eq. (3.31).

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