Angular momentum in spherical coordinates

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1 Introduction

Angular momentum is a deep property and in courses on quantum mechanics a lot of time is devoted to commutator relationships and spherical harmonics. However, many basic things are actually set for proof outside lectures as problems. For instance, one of the standard quantum physics textbooks [1, pp 660-663] deals with the issue this way:

"Applying the classical technique of changing variables, we obtain, from formulas (D-1) and (D-2), the following expressions (the calculations are rather time-consuming but pose no great problems):

\[ L_x = i\hbar \left( \sin \phi \frac{\partial}{\partial \theta} + \cos \phi \frac{\partial}{\tan \theta \partial \phi} \right) \]
\[ L_y = i\hbar \left( -\cos \phi \frac{\partial}{\partial \theta} + \sin \phi \frac{\partial}{\tan \theta \partial \phi} \right) \]
\[ L_z = \hbar \frac{1}{i} \frac{\partial}{\partial \phi} \]

which yield:

\[ L^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta \frac{\partial}{\partial \theta}} - \frac{1}{\sin^2 \theta \frac{\partial^2}{\partial \phi^2}} \right) \]
\[ L_\phi = \hbar e^{i\phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) \]
\[ L_\varphi = \hbar e^{-i\phi} \left( -\frac{\partial}{\partial \vartheta} + i \cot \theta \frac{\partial}{\partial \varphi} \right) \]  

The starting point for (1) are the Cartesian expressions for the angular momentum components:

\[ L_x = \frac{\hbar}{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \]
\[ L_y = \frac{\hbar}{i} \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \]
\[ L_z = \frac{\hbar}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \]  

The spherical coordinate transformation is as follows:

\[ x = r \sin \theta \cos \phi \]
\[ y = r \sin \theta \sin \phi \]
\[ z = r \cos \theta \]  

with:

\[ r \geq 0 \]
\[ 0 \leq \theta \leq \pi \]
\[ 0 \leq \phi < 2\pi \]  

2 The derivations

The fundamental formula is this:

\[ \frac{\partial \square}{\partial x_i} = \frac{\partial \square}{\partial r} \frac{\partial r}{\partial x_i} + \frac{\partial \square}{\partial \theta} \frac{\partial \theta}{\partial x_i} + \frac{\partial \square}{\partial \phi} \frac{\partial \phi}{\partial x_i} \]  

where \( \square \) is a placeholder. In principle there is nothing particularly difficult about performing the relevant calculations but it is very easy to make small mistakes.

The Cartesian coordinates are related to the spherical coordinates as follows:
\[ r = \sqrt{x^2 + y^2 + z^2} \]
\[ \cos \theta = \frac{z}{\sqrt{x^2 + y^2 + z^2}} \]  
\[ \tan \phi = \frac{y}{x} \]  
\[ \frac{\partial r}{\partial x} = \frac{1}{2}(x^2 + y^2 + z^2)^{-\frac{1}{2}} 2x = \frac{x}{r} = \sin \theta \cos \phi \]  
\[ \frac{\partial r}{\partial y} = \frac{1}{2}(x^2 + y^2 + z^2)^{-\frac{1}{2}} 2y = \frac{y}{r} = \sin \theta \sin \phi \]  
\[ \frac{\partial r}{\partial z} = \frac{z}{r} = \cos \theta \]  
\[ \frac{\partial \theta}{\partial x} = \frac{\partial}{\partial x} \left( \cos^{-1} \left( \frac{z}{\sqrt{x^2 + y^2 + z^2}} \right) \right) \]
\[ = \frac{-1}{\sqrt{1 - \frac{z^2}{x^2 + y^2 + z^2}}} \times z \times \frac{-1}{2} (x^2 + y^2 + z^2)^{-\frac{3}{2}} \times 2x \]
\[ = \frac{zx}{\sqrt{x^2 + y^2} r^3} \]
\[ = \frac{r \cos \theta}{r \sin \theta} \cos \phi \]
\[ = \frac{r^{2} \cos \theta \sin \phi}{r^{2} \sin \theta} \]
\[ = \frac{\sin \theta}{r} \]  
Note that \( \sqrt{x^2 + y^2} = \sqrt{(r \sin \theta \cos \phi)^2 + (r \sin \theta \sin \phi)^2} = \sqrt{r^2 \sin^2 \theta (\cos^2 \phi + \sin^2 \phi)} = r \sin \theta \).  
Using (13) we can go straight to:
\[ \frac{\partial \theta}{\partial y} = \frac{zy}{r^2 \sin \theta} \]
\[ = \frac{r \cos \theta \sin \theta \sin \phi}{r^2 \sin \theta} \]
\[ = \frac{\cos \theta \sin \phi}{r} \]  
(14)
\[
\frac{\partial \theta}{\partial z} = \frac{\partial}{\partial z} \left( \cos^{-1} \left( \frac{z}{\sqrt{x^2 + y^2 + z^2}} \right) \right) \\
= \frac{-1}{\sqrt{1 - \frac{z^2}{x^2 + y^2 + z^2}}} \times \left( \frac{1}{r} + z \times \frac{-1}{2} \left( \frac{x^2 + y^2 + z^2}{r^3} \right) \times 2z \right) \\
= \frac{-r}{r \sin \theta} \times \left( \frac{1}{r} - \frac{z^2}{r^3} \right) \\
= \frac{-1}{\sin \theta} \times \left( \frac{r^2 - z^2}{r^3} \right) \\
= \frac{-r^2 \sin^2 \theta}{r^3 \sin \theta} \\
= \frac{-\sin \theta}{r}
\]

\[\frac{\partial \phi}{\partial x} = \frac{\partial}{\partial x} \left( \tan^{-1} \left( \frac{y}{x} \right) \right) \\
= \frac{1}{1 + \frac{y^2}{x^2}} \times \frac{-y}{x^2} \\
= \frac{-y}{x^2 + y^2} \\
= \frac{-r \sin \theta \sin \phi}{r^2 \sin^2 \theta} \\
= -\frac{\sin \phi}{r \sin \theta}
\]

\[\frac{\partial \phi}{\partial y} = \frac{\partial}{\partial y} \left( \tan^{-1} \left( \frac{y}{x} \right) \right) \\
= \frac{1}{1 + \frac{y^2}{x^2}} \times \frac{1}{x} \\
= \frac{x}{x^2 + y^2} \\
= \frac{r \sin \theta \cos \phi}{r^2 \sin^2 \theta} \\
= \frac{\cos \phi}{r \sin \theta}
\]

\[\frac{\partial \phi}{\partial z} = 0 \quad (18)
\]
Thus the Cartesian operators have the following form using (5):

\[
\begin{align*}
\frac{\partial}{\partial x} &= \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{1}{r} \cos \phi \cos \theta \frac{\partial}{\partial \theta} - \frac{1}{r} \sin \phi \frac{\partial}{\partial \phi} \\
\frac{\partial}{\partial y} &= \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{1}{r} \sin \phi \cos \theta \frac{\partial}{\partial \theta} + \frac{1}{r} \cos \phi \frac{\partial}{\partial \phi} \\
\frac{\partial}{\partial z} &= \cos \theta \frac{\partial}{\partial r} - \frac{1}{r} \sin \theta \frac{\partial}{\partial \theta}
\end{align*}
\]

(19)

It is now only a matter of labouriously making the relevant substitutions in (2).

\[
L_x = \frac{\hbar}{i} \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)
\]

\[
= \frac{\hbar}{i} \left( r \sin \theta \sin \phi \left[ \cos \theta \frac{\partial}{\partial r} - \frac{1}{r} \sin \theta \frac{\partial}{\partial \theta} \right] - r \cos \theta \left[ \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{1}{r} \sin \phi \cos \theta \frac{\partial}{\partial \theta} + \frac{1}{r} \cos \phi \frac{\partial}{\partial \phi} \right] \right)
\]

\[
= \frac{\hbar}{i} \left( - \sin^2 \theta \sin \phi - \cos^2 \theta \sin \phi \right) \frac{\partial}{\partial \theta} - \cos \theta \frac{\partial}{\partial \phi} - \frac{\cos \phi}{\sin \theta} \frac{\partial}{\partial \phi}
\]

\[
= i \hbar \left( \sin \phi \frac{\partial}{\partial \theta} + \cos \phi \frac{\partial}{\partial \phi} \right)
\]

(20)

\[
L_y = \frac{\hbar}{i} \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)
\]

\[
= \frac{\hbar}{i} \left( r \cos \theta \left[ \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{1}{r} \cos \phi \cos \theta \frac{\partial}{\partial \theta} - \frac{1}{r} \sin \phi \frac{\partial}{\partial \phi} \right] - r \sin \theta \cos \phi \left[ \cos \theta \frac{\partial}{\partial r} - \frac{1}{r} \sin \theta \frac{\partial}{\partial \theta} \right] \right)
\]

\[
= \frac{\hbar}{i} \left( \cos \phi \cos^2 \theta + \cos \phi \sin^2 \theta \right) \frac{\partial}{\partial \theta} - \sin \phi \frac{\partial}{\partial \phi}
\]

\[
= \frac{\hbar}{i} \left( \cos \phi \frac{\partial}{\partial \theta} - \sin \phi \frac{\partial}{\partial \phi} \right)
\]

\[
= i \hbar \left( - \cos \phi \frac{\partial}{\partial \theta} + \sin \phi \frac{\partial}{\partial \phi} \right)
\]

(21)
\[ L_z = \frac{\hbar}{i} \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) = \frac{\hbar}{i} \left( r \sin \theta \cos \phi \left[ \sin \theta \sin \phi \frac{\partial}{\partial r} + \frac{1}{r} \sin \phi \cos \theta \frac{\partial}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right] - r \sin \theta \sin \phi \left[ \sin \theta \cos \phi \frac{\partial}{\partial r} + \frac{1}{r} \cos \phi \cos \theta \frac{\partial}{\partial \theta} - \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \right] \right) \quad (22) \]

\[ = \frac{\hbar}{i} \left( \cos^2 \phi + \sin^2 \phi \right) \frac{\partial}{\partial \phi} \]

The following symbols are used in what follows to cut down keystrokes:

\[
\begin{align*}
\frac{\partial}{\partial r} &= \partial_r \\
\frac{\partial}{\partial \theta} &= \partial_\theta \\
\frac{\partial}{\partial \phi} &= \partial_\phi 
\end{align*} \quad (23)
\]

Now we have that \( \mathbf{L} \) is the orbital momentum of a spinless particle [see [1], p. 660] and the operator \( \mathbf{L}^2 \) is defined to be:

\[ \mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2 \quad (24) \]

Now all we have to do is make the relevant substitutions in (24). This is straightforward, but error prone, so each component will be done separately.

6
\[ L_x^2 = -\hbar^2 \left( \sin \phi \partial_\theta + \frac{\cos \phi}{\tan \theta} \partial_\phi \right) \left( \sin \phi \partial_\theta + \frac{\cos \phi}{\tan \theta} \partial_\phi \right) \]
\[ = -\hbar^2 \left( \sin^2 \phi \partial_\theta^2 + \sin \phi \frac{\partial}{\partial \theta} \left( \cot \theta \sin \phi \partial_\phi \right) \right) \]
\[ = -\hbar^2 \left( \sin^2 \phi \partial_\theta^2 + \sin \phi \left[ \cos \phi \partial_\phi \times -\csc^2 \theta + \cot \theta \cos \phi \partial_\theta \partial_\phi \right] \right) \]
\[ + \cot \theta \cos \phi \left[ \partial_\theta \cos \phi \partial_\phi \partial_\theta + \cot^2 \theta \csc^2 \phi \partial_\phi^2 \right] \]
\[ (25) \]

\[ L_y^2 = -\hbar^2 \left( -\cos \phi \partial_\theta + \cot \theta \sin \phi \partial_\phi \right) \left( -\cos \phi \partial_\theta + \cot \theta \sin \phi \partial_\phi \right) \]
\[ = -\hbar^2 \left( \cos^2 \phi \partial_\theta^2 - \cos \phi \frac{\partial}{\partial \theta} \left( \cot \theta \sin \phi \partial_\phi \right) \right) \]
\[ = -\hbar^2 \left( \cos^2 \phi \partial_\theta^2 - \cos \phi \left[ \sin \phi \partial_\phi \times -\csc^2 \theta + \cot \theta \sin \phi \partial_\theta \partial_\phi \right] \right) \]
\[ + \cot^2 \theta \sin^2 \phi \partial_\phi^2 \]
\[ = -\hbar^2 \left( \cos^2 \phi \partial_\theta^2 + \cos \phi \sin \phi \csc^2 \phi \partial_\phi^2 - \cos \phi \cot \theta \sin \phi \partial_\theta \partial_\phi + \cot \theta \sin^2 \phi \partial_\theta \partial_\phi - \cot \theta \sin \phi \cos \phi \partial_\theta \partial_\theta \partial_\phi \right) \]
\[ + \cot^2 \theta \csc^2 \phi \partial_\phi^2 \]
\[ (26) \]

\[ L_z^2 = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \times \frac{\hbar}{i} \frac{\partial}{\partial \phi} = -\hbar^2 \partial_\phi^2 \]
\[ (27) \]

Now pairing up the terms 1-6 we have:
\[
\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2
\]

\[
= -\hbar^2 \left( \partial_\theta^2 + \cot \theta \partial_\theta + (\cot^2 \theta + 1)\partial_\phi^2 \right)
\]

\[
= -\hbar^2 \left( \partial_\theta^2 + \frac{1}{\tan \theta} \partial_\theta + \left( \frac{\cos^2 \theta + \sin^2 \theta}{\sin^2 \theta} \right) \partial_\phi^2 \right)
\]

\[
= -\hbar^2 \left( \partial_\theta^2 + \frac{1}{\tan \theta} \partial_\theta + \frac{1}{\sin^2 \theta} \partial_\phi^2 \right)
\]

Thus the textbook answer is indeed obtained.

Equations (3) and (4) are easily derived once it is known that \([1], p.647\):

\[
L_+ = L_x + i L_y
\]

and

\[
L_- = L_x - i L_y
\]

Thus:

\[
L_+ = L_x + i L_y = i h \left( \sin \phi \partial_\theta + \cot \theta \cos \phi \partial_\phi \right) - h \left( -\cos \phi \partial_\theta + \cot \theta \sin \phi \partial_\phi \right)
\]

\[
= h \left( \cos \phi \partial_\theta + i \cot \theta \cos \phi \partial_\phi + i \sin \phi \partial_\theta - \cot \theta \sin \phi \partial_\phi \right)
\]

\[
= h \left( \cos \phi + i \sin \phi \right) \left( \partial_\theta + i \cot \theta \partial_\phi \right)
\]

\[
= h e^{i\phi} \left( \partial_\theta + i \cot \theta \partial_\phi \right)
\]

Similarly:

\[
L_- = L_x + i L_y = i h \left( \sin \phi \partial_\theta + \cot \theta \cos \phi \partial_\phi \right) + h \left( -\cos \phi \partial_\theta + \cot \theta \sin \phi \partial_\phi \right)
\]

\[
= h \left( -\cos \phi \partial_\theta + i \cot \theta \cos \phi \partial_\phi + i \sin \phi \partial_\theta + \cot \theta \sin \phi \partial_\phi \right)
\]

\[
= h \left( \cos \phi - i \sin \phi \right) \left( -\partial_\theta + i \cot \theta \partial_\phi \right)
\]

\[
= h e^{-i\phi} \left( \partial_\theta + i \cot \theta \partial_\phi \right)
\]
2.1 Solving the partial differential equations

There is a substantial preliminary overhead in establishing that the eigenvalues of $L^2$ are $l(l+1)\hbar^2$ and those of $L_z$ are $m\hbar$. (see [1], pages 643-662). Using (2) we have:

$$-\hbar^2\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}\right) \psi(r, \theta, \phi) = l(l+1)\hbar^2 \psi(r, \theta, \phi)$$

\[33\]

Using (22) we have:

$$\frac{\hbar}{i} \frac{\partial}{\partial \phi} \psi(r, \theta, \phi) = m\hbar \psi(r, \theta, \phi)$$

\[34\]

Because $r$ does not appear as a differential operator in either (33) or (34) we assume an eigenfunction which depends only on the angular variables $\theta$ and $\phi$. Note that if we assumed a solution of the form $\psi(r, \theta, \phi) = Y_{l,m}(\theta, \phi) f(r)$ (see [2], p.314) the term $f(r)$ simply cancels because of the lack of derivatives in $r$ (or viewed as a constant of integration). However, once (33) and (34) have been solved for $Y_{l,m}(\theta, \phi)$ the eigenfunctions will be of the form $\psi_{l,m}(r, \theta, \phi) = Y_{l,m}(\theta, \phi) f(r)$. Denoting the common eigenfunction of $L^2$ and $L_z$ by $Y_{l,m}(\theta, \phi)$ we have that:

$$-\left(\frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2}\right) Y_{l,m}(\theta, \phi) = l(l+1)\hbar^2 Y_{l,m}(\theta, \phi)$$

\[35\]

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

\[36\]

Integration of (36) leads straightaway to:

$$Y_{l,m}(\theta, \phi) = F_{l,m}(\theta) e^{im\phi}$$

\[37\]

Noting here that $F_{l,m}(\theta)$ is like a constant given the lack of $\theta$ dependence in (36). A wave function must be continuous throughout space if the differential development of the operators is to make any sense. This is the case because differentiability implies continuity, thus if the wave function were not continuous it could not be differentiable and hence none of the above development would make any sense. So let’s take some boundary values and exploit the continuity:
\[
Y_l^m(\theta, \phi = 0) = Y_l^m(\theta, \phi = 2\pi) \tag{38}
\]

thus we have that:

\[
\begin{align*}
Y_l^m(\theta, \phi = 0) &= F_l^m(\theta) \\
Y_l^m(\theta, \phi = 2\pi) &= F_l^m(\theta) e^{2im\phi} \tag{39}
\end{align*}
\]

Thus we must have:

\[
e^{2im\phi} = 1 \tag{40}
\]

Because \(m\) is integral or half-integral (see [1], pages 647-660), (40) shows that orbital angular momentum must be integral and because \(m\) and \(l\) must be either both integral or half-integral, it follows that \(l\) must be integral too.

On the basis of general theory (see [1], pages 647-664) the \(Y_l^m(\theta, \phi)\) must satisfy:

\[
L_+ Y_l^m(\theta, \phi) = 0 \tag{41}
\]

Using (31) and (37) we have:

\[
\begin{align*}
& L_+ Y_l^m(\theta, \phi) = 0 \\
& \hbar e^{i\phi} \left( \partial_\theta + i \cot \theta \partial_\phi \right) F_l^m(\theta) e^{il\phi} = 0 \\
& \hbar e^{i\phi} \left( e^{il\phi} \frac{d}{d\theta} F_l^m(\theta) + i \cot \theta F_l^m(\theta) il e^{il\phi} \right) = 0 \tag{42} \\
& \hbar e^{i(l+1)\phi} \left( \frac{d}{d\theta} - l \cot \theta \right) F_l^m(\theta) = 0 \\
& \left( \frac{d}{d\theta} - l \cot \theta \right) F_l^m(\theta) = 0
\end{align*}
\]

To solve (42) note that:

\[
\cot \theta \, d\theta = \frac{d(\sin \theta)}{\sin \theta} \tag{43}
\]

Thus we have:
\[ \begin{align*}
    dF_l^j(\theta) &= l \cot \theta F_l^j(\theta) \, d\theta \\
    &= l F_l^j(\theta) \frac{d(\sin \theta)}{\sin \theta} \\
    \int \frac{dF_l^j(\theta)}{F_l^j(\theta)} &= l \int \frac{d(\sin \theta)}{\sin \theta} \\
    \ln F_l^j(\theta) &= l \ln(\sin \theta) + c \\
    \therefore F_l^j(\theta) &= c_l (\sin \theta)^l \\
    \text{and so } Y_l^j(\theta, \phi) &= c_l (\sin \theta)^l e^{il\phi}
\end{align*} \]

This is just touching the surface of the detailed treatment of eigenfunctions represented as spherical harmonics. Courant and Hilbert give proofs, for instance, of how one can expand a function in terms of spherical harmonics (see [2], page 513). Reference [1] covers the ground well with many detailed calculations but the authors often leave out specific justifications eg for expansions in terms of spherical harmonics.

### 3 References


### 4 History

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