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Spherical Harmonics, Orbital Angular Momentum

We are now in a position to calculate the full angular functions for the general central force problem, using the laddering techniques for the θ equation to construct the full set of angular functions $\Theta(\theta)$ via the normalized step-down operators. Because the eigenvalue $\lambda = \lambda_0 + \frac{1}{4}$ is a function of $m_{\max} \equiv l$, we will replace the index λ by the integer l. [Recall that $\lambda = \mathcal{L}(m_{\max} + 1) = (l + \frac{1}{2})^2$.] The full angular functions are the spherical harmonics

$$Y_{lm}(\theta, \phi) = \Theta_{lm}(\theta)\Phi_m(\phi) = \frac{u_{lm}(\theta)}{\sqrt{\sin\theta}} \frac{e^{im\phi}}{\sqrt{2\pi}}. \tag{1}$$

To get the standard (universally accepted) phases for the spherical harmonics, we need to multiply the normalization coefficient in the starting function u_{ll}, with $m_{\max} = l$, by the phase factor $(-1)^l$

$$u_{ll}(\theta) = (-1)^l \sqrt{\frac{(2l+1)!!}{2[2l!!]}} \sin^{l+\frac{1}{2}}(\theta). \tag{2}$$

In addition, we need to multiply the normalized step-operators $\mathcal{O}_-(m)$ and $\mathcal{O}_+(m+1)$ of eqs. (37) and (39) of Chapter 7 by a phase factor (-1). Thus,

$$Y_{l(m-1)} = -\frac{e^{-i\phi}}{\sqrt{\sin\theta}} \frac{\left[\left(\frac{d}{d\theta} + (m - \frac{1}{2})\cot\theta\right)u_{lm}(\theta)\right]}{\sqrt{(l+\frac{1}{2})^2 - (m-\frac{1}{2})^2}} \frac{e^{im\phi}}{\sqrt{2\pi}}. \tag{3}$$

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Setting $u_{lm}(\theta) = \sqrt{\sin\theta}\,\Theta_{lm}(\theta)$ in this equation, this becomes

$$Y_{l(m-1)} = \frac{e^{-i\phi}}{\sqrt{(l+m)(l-m+1)}}\left[\left(-\frac{d}{d\theta} - m\cot\theta\right)\Theta_{lm}(\theta)\right]\frac{e^{im\phi}}{\sqrt{2\pi}}. \qquad (4)$$

Finally, putting

$$me^{im\phi} = -i\frac{\partial}{\partial\phi}e^{im\phi}, \qquad (5)$$

we obtain

$$Y_{l(m-1)}(\theta,\phi) = \frac{e^{-i\phi}}{\sqrt{(l+m)(l-m+1)}}\left[-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]Y_{lm}(\theta,\phi). \qquad (6)$$

Similarly, using the normalized, standard-phase step-up operator $-\mathcal{O}_+(m+1)$,

$$Y_{l(m+1)}(\theta,\phi) = \frac{e^{+i\phi}}{\sqrt{(l-m)(l+m+1)}}\left[+\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right]Y_{lm}(\theta,\phi). \qquad (7)$$

A Angular Momentum Operators

It will now be useful to express the operators converting the Y_{lm} into $Y_{l(m\pm1)}$ in terms of dimensionless angular momentum operators, such as

$$\frac{L_z}{\hbar} = \frac{1}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \qquad (8)$$

Transforming to spherical coordinates

$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta, \qquad (9)$$

and using

$$\begin{aligned}
&\frac{\partial r}{\partial x} = \sin\theta\cos\phi, && \frac{\partial r}{\partial y} = \sin\theta\sin\phi, && \frac{\partial r}{\partial z} = \cos\theta,\\
&\frac{\partial\theta}{\partial x} = \frac{\cos\theta\cos\phi}{r}, && \frac{\partial\theta}{\partial y} = \frac{\cos\theta\sin\phi}{r}, && \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r},\\
&\frac{\partial\phi}{\partial x} = -\frac{\sin\phi}{r\sin\theta}, && \frac{\partial\phi}{\partial y} = \frac{\cos\phi}{r\sin\theta}, && \frac{\partial\phi}{\partial z} = 0,
\end{aligned} \qquad (10)$$

we get

$$\frac{L_z}{\hbar} \equiv L_0 = \frac{1}{i}\frac{\partial}{\partial\phi}, \qquad (11)$$

$$\frac{(L_x \pm iL_y)}{\hbar} \equiv L_\pm = e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right), \qquad (12)$$

and

$$\frac{(\vec{L}\cdot\vec{L})}{\hbar^2} = L_0^2 + \frac{1}{2}(L_+L_- + L_-L_+) = -\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right). \qquad (13)$$

Hence, the spherical harmonics are simultaneous eigenfunctions of the operators, $(\vec{L} \cdot \vec{L})$, and L_z, with

$$\begin{aligned} L_z Y_{lm}(\theta, \phi) &= \hbar m Y_{lm}(\theta, \phi), \\ (\vec{L} \cdot \vec{L}) Y_{lm}(\theta, \phi) &= \hbar^2 \lambda_0 Y_{lm}(\theta, \phi) = \hbar^2 l(l+1) Y_{lm}(\theta, \phi). \end{aligned} \tag{14}$$

In addition, eqs. (6) and (7) can be put into the form

$$L_- Y_{lm} = \sqrt{(l+m)(l-m+1)}\, Y_{l(m-1)}, \tag{15}$$

$$L_+ Y_{lm} = \sqrt{(l-m)(l+m+1)}\, Y_{l(m+1)}. \tag{16}$$

The $Y_{lm}(\theta, \phi)$ form an orthonormal complete set over the surface of the unit sphere. Thus, the matrix elements of the operators $L_{\pm}$ are

$$\langle Y_{l'm'}, L_- Y_{lm} \rangle = \delta_{l'l} \delta_{m'(m-1)} \sqrt{(l+m)(l-m+1)}, \tag{17}$$

$$\langle Y_{l'm'}, L_+ Y_{lm} \rangle = \delta_{l'l} \delta_{m'(m+1)} \sqrt{(l-m)(l+m+1)}, \tag{18}$$

and

$$\langle Y_{l'm'}, L_0 Y_{lm} \rangle = \delta_{l'l} \delta_{m'm} m. \tag{19}$$

These matrix elements can also be used to obtain the matrix elements of L_x and L_y.

$$\begin{aligned} \langle Y_{l'm'}, L_x Y_{lm} \rangle &= \frac{\hbar}{2} \langle Y_{l'm'}, (L_+ + L_-) Y_{lm} \rangle \\ &= \delta_{l'l} \frac{\hbar}{2} \Big(\delta_{m'(m+1)} \sqrt{(l-m)(l+m+1)} \\ &\quad + \delta_{m'(m-1)} \sqrt{(l+m)(l-m+1)} \Big). \end{aligned} \tag{20}$$

Similarly,

$$\begin{aligned} \langle Y_{l'm'}, L_y Y_{lm} \rangle &= \frac{\hbar}{2} \langle Y_{l'm'}, (-iL_+ + iL_-) Y_{lm} \rangle \\ &= \delta_{l'l} \frac{\hbar}{2} \Big(-i\delta_{m'(m+1)} \sqrt{(l-m)(l+m+1)} \\ &\quad + i\delta_{m'(m-1)} \sqrt{(l+m)(l-m+1)} \Big). \end{aligned} \tag{21}$$

The infinite-dimensional matrices for L_x, L_y, and L_z thus factor into $(2l+1)$ by $(2l+1)$ submatrices. As a simple, specific example, the submatrices for $l = 1$ are (in units of $\hbar$),

$$\mathbf{L}_x = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

$$\mathbf{L}_y = \begin{pmatrix} 0 & \frac{-i}{\sqrt{2}} & 0 \\ \frac{+i}{\sqrt{2}} & 0 & \frac{-i}{\sqrt{2}} \\ 0 & \frac{+i}{\sqrt{2}} & 0 \end{pmatrix},$$

$$\mathbf{L}_z = \begin{pmatrix} +1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

where rows and columns are labeled in the conventional order, $m = +1, 0, -1$.

Because the spherical harmonics form a complete orthonormal set, we can translate the operators $L_\pm$ into the following functional forms. For example,

$$L_+ = \sum_{l=0}^{\infty} \sum_{m=-l}^{m=+l} Y_{l(m+1)}(\theta, \phi) Y_{lm}^*(\theta, \phi) \big(\sqrt{(l-m)(l+m+1)}\big). \tag{22}$$

In our method of constructing the $(2l+1)$ spherical harmonics for a particular l, we have started with the eigenfunction with $m = m_{\max} = l$, and we have then used the normalized step-down operators, $\mathcal{O}_-(m)$, to calculate the remaining $2l$ eigenfunctions. Alternatively, we could have started with $m = m_{\min}$ and laddered with $\mathcal{O}_+(m+1)$. A third possibility would be to start with the spherical harmonics with $m = 0$ and use successive application of $L_\pm$ to calculate the spherical harmonics with $\pm m$.

$$\begin{aligned} Y_{lm} &= \frac{(L_+)^m Y_{l0}}{\sqrt{l(l-1)\cdots(l-m+1)(l+1)(l+2)\cdots(l+m)}} \\ &= \sqrt{\frac{(l-m)!}{(l+m)!}} (L_+)^m Y_{l0}, \end{aligned} \tag{23}$$

and

$$\begin{aligned} Y_{l-m} &= \frac{(L_-)^m Y_{l0}}{\sqrt{l(l-1)\cdots(l-m+1)(l+1)(l+2)\cdots(l+m)}} \\ &= \sqrt{\frac{(l-m)!}{(l+m)!}} (L_-)^m Y_{l0}. \end{aligned} \tag{24}$$

Now, because

$$(L_+)^* = -(L_-), \tag{25}$$

we see

$$Y_{l-m}(\theta, \phi) = (-1)^m Y_{lm}^*(\theta, \phi). \tag{26}$$

Thus, it is sufficient to calculate the spherical harmonics with $m \geq 0$. As a final remark, the three operators L_x, L_y, L_z are all hermitian, and hence,

$$L_+^\dagger = L_-; \qquad L_-^\dagger = L_+. \tag{27}$$