Clebsch-Gordon coefficients and the tensor spherical harmonics

Consider a system with orbital angular momentum $\vec{\boldsymbol{L}}$ and spin angular momentum $\vec{\boldsymbol{S}}$. The total angular momentum of the system is denoted by $\vec{\boldsymbol{J}} = \vec{\boldsymbol{L}} + \vec{\boldsymbol{S}}$. Clebsch Gordon coefficients allow us to express the total angular momentum basis $|j\,m\,;\,\ell\,s\rangle$ in terms of the direct product basis, $|\ell\,m_\ell\,;\,s\,m_s\rangle \equiv |\ell\,m_\ell\rangle \otimes |s\,m_s\rangle$,

$$|j\,m\,;\,\ell\,s\rangle = \sum_{m_\ell=-\ell}^{\ell}\ \sum_{m_s=-s}^{s} \langle \ell\,m_\ell\,;\,s\,m_s\,|\,j\,m\,;\,\ell\,s\rangle |\ell\,m_\ell\,;\,s\,m_s\rangle\,. \tag{1}$$

The Clebsch-Gordon coefficient is often denoted by

$$\langle \ell\,m_\ell\,;\,s\,m_s\,|\,j\,m\rangle \equiv \langle \ell\,m_\ell\,;\,s\,m_s\,|\,j\,m\,;\,\ell\,s\rangle\,,$$

since including $\ell\,s$ in $|j\,m\,;\,\ell\,s\rangle$ above is redundant information. In Appendix A, we discuss the Clebsch-Gordon series and its applications.

One important property of the Clebsch-Gordon coefficients is

$$\langle \ell\,m_\ell\,;\,s\,m_s\,|\,j\,m\rangle = \delta_{m\,,\,m_\ell+m_s}\langle \ell\,m_\ell\,;\,s\ m_s\,|\,j\ m_\ell+m_s\rangle\,, \tag{2}$$

which implies that if $m \neq m_\ell + m_s$ then the corresponding Clebsch-Gordon coefficient must vanish. This is simply a consequence of $J_z = L_z + S_z$. Likewise, $|\ell - s| \leq j \leq \ell + s$ (where $2j$, ℓ and $2s$ are non-negative integers), otherwise the corresponding Clebsch-Gordon coefficients vanish.

Recall that in the coordinate representation, the angular moment operator is a differential operator given by

$$\vec{\boldsymbol{L}} = -i\hbar\,\vec{\boldsymbol{x}} \times \vec{\boldsymbol{\nabla}}\,.$$

The spherical harmonics, $Y_{\ell m_\ell}(\theta,\phi)$ are simultaneous eigenstates of $\vec{\boldsymbol{L}}^2$ and L_z,

$$\vec{\boldsymbol{L}}^2\, Y_{\ell m_\ell}(\theta,\phi) = \hbar^2\ell(\ell+1)\, Y_{\ell m_\ell}(\theta,\phi)\,, \qquad L_z\, Y_{\ell m_\ell}(\theta,\phi) = \hbar m_\ell\, Y_{\ell m_\ell}(\theta,\phi)\,.$$

We can generalize these results to systems with non-zero spin. First, we define $\chi_{s\,m_s}$ to be the simultaneous eigenstates of $\vec{\boldsymbol{S}}^2$ and S_z ,

$$\vec{\boldsymbol{S}}^2\chi_{s\,m_s} = \hbar^2 s(s+1)\chi_{s\,m_s}\,, \qquad S_z\chi_{s\,m_s} = \hbar m_s\chi_{s\,m_s}\,.$$

The direct product basis in the coordinate representation is given by $Y_{\ell m_\ell}(\theta,\phi)\chi_{s\,m_s}$.

In the coordinate representation, the total angular momentum basis consists of simultaneous eigenstates of $\vec{\boldsymbol{J}}^2$, J_z , $\vec{\boldsymbol{L}}^2$, $\vec{\boldsymbol{S}}^2$. These are the *tensor spherical harmonics*, which satisfy,

$$\begin{aligned}
&\vec{\boldsymbol{J}}^2\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi) = \hbar^2 j(j+1)\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi)\,, \qquad && J_z\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi) = \hbar m\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi)\,, \\
&\vec{\boldsymbol{L}}^2\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi) = \hbar^2 \ell(\ell+1)\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi)\,, \qquad && \vec{\boldsymbol{S}}^2\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi) = \hbar^2 s(s+1)\, \mathcal{Y}^{\ell s}_{jm}(\theta,\phi)\,.
\end{aligned}$$

As a consequence of eq. (1), the tensor spherical harmonics are defined by

$$\mathcal{Y}^{\ell s}_{jm}(\theta,\phi) = \sum_{m_\ell=-\ell}^{\ell} \sum_{m_s=-s}^{s} \langle \ell\, m_\ell\,;\, s\, m_s\,|\, j\, m\rangle Y_{\ell m_\ell}(\theta,\phi)\chi_{s\, m_s}$$

$$= \sum_{m_s=-s}^{s} \langle \ell\,,\, m-m_s\,;\, s\, m_s\,|\, j\, m\rangle Y_{\ell\,,\, m-m_s}(\theta,\phi)\chi_{s\, m_s}\,, \tag{3}$$

where the second line follows from the first line above since the Clebsch-Gordon coefficient above vanishes unless $m = m_\ell + m_s$.

The general expressions for the Clebsch-Gordon coefficients in terms of j, m_ℓ, ℓ, s and m_s are very complicated to write down. Nevertheless, the explicit expressions in the simplest cases of $s = 1/2$ and $s = 1$ are manageable. Thus, we shall exhibit these two special cases below.

For spin $s = 1/2$, the possible values of j are $j = \ell + \frac{1}{2}$ and $\ell - \frac{1}{2}$, for $\ell = 1, 2, 3, \ldots$. If $\ell = 0$ then only $j = \frac{1}{2}$ is possible (and the last row of Table 1 should be omitted). The corresponding table of Clebsch-Gordon coefficients is exhibited in Table 1.

Table 1: the Clebsch-Gordon coefficients, $\langle \ell\, m - m_s\,;\, \frac{1}{2}\, m_s\,|\, jm\rangle$.

j	$m_s = \frac{1}{2}$	$m_s = -\frac{1}{2}$
$\ell + \frac{1}{2}$	$\left(\dfrac{\ell + m + \frac{1}{2}}{2\ell+1}\right)^{1/2}$	$\left(\dfrac{\ell - m + \frac{1}{2}}{2\ell+1}\right)^{1/2}$
$\ell - \frac{1}{2}$	$-\left(\dfrac{\ell - m + \frac{1}{2}}{2\ell+1}\right)^{1/2}$	$\left(\dfrac{\ell + m + \frac{1}{2}}{2\ell+1}\right)^{1/2}$

Comparing with eq. (3), the entries in Table 1 are equivalent to the following result:

$$\left| j = \ell \pm \tfrac{1}{2}\, m \right\rangle = \frac{1}{\sqrt{2\ell+1}} \left[\pm\sqrt{\ell + \tfrac{1}{2} \pm m}\, \left| \ell\, m - \tfrac{1}{2}\,;\, \tfrac{1}{2}\, \tfrac{1}{2} \right\rangle + \sqrt{\ell + \tfrac{1}{2} \mp m}\, \left| \ell\, m + \tfrac{1}{2}\,;\, \tfrac{1}{2}\, -\tfrac{1}{2} \right\rangle \right].$$

We can represent $|\frac{1}{2}\,\frac{1}{2}\rangle = \binom{1}{0}$ and $|\frac{1}{2}\, -\frac{1}{2}\rangle = \binom{0}{1}$. Then in the coordinate representation, the *spin spherical harmonics* are given by

$$\mathcal{Y}^{\ell\,\frac{1}{2}}_{j=\ell\pm\frac{1}{2}\,,\,m}(\theta,\phi) \equiv \langle \theta\,\phi\,|\, j = \ell \pm \tfrac{1}{2}\,,\, m\rangle = \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} \pm\sqrt{\ell \pm m + \frac{1}{2}}\; Y_{\ell,m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\ell \mp m + \frac{1}{2}}\; Y_{\ell,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}. \tag{4}$$

If $\ell = 0$, there is only one spin spherical harmonic,

$$\mathcal{Y}^{0\,\frac{1}{2}}_{j=\frac{1}{2}\,,\,m}(\theta,\phi) \equiv \langle \theta\,\phi\,|\, j = \tfrac{1}{2}\,,\, m\rangle = \frac{1}{\sqrt{2\ell+1}} \begin{pmatrix} \sqrt{\frac{1}{2} + m}\; Y_{0,m-\frac{1}{2}}(\theta,\phi) \\ \sqrt{\frac{1}{2} - m}\; Y_{0,m+\frac{1}{2}}(\theta,\phi) \end{pmatrix}. \tag{5}$$

Note that when $m=\frac{1}{2}$ the lower component of eq. (5) vanishes and when $m=-\frac{1}{2}$ the upper component of eq. (5) vanishes. In both cases, the non-vanishing component is proportional to $Y_{00}(\theta,\phi)=1/\sqrt{4\pi}$.

For spin $s=1$, the possible values of j are $j=\ell+1\,,\,\ell\,,\,\ell-1$ for $\ell=1,2,3,\ldots$. If $\ell=0$ then only $j=1$ is possible (and the last two rows exhibited in Table 2 should be omitted). The corresponding table of Clebsch-Gordon coefficients is exhibited in Table 2.

Table 2: the Clebsch-Gordon coefficients, $\langle \ell\, m-m_s\,;\,1\,m_s\,|\,jm\rangle$.

j	$m_s=1$	$m_s=0$	$m_s=-1$
$\ell+1$	$\left[\dfrac{(\ell+m)(\ell+m+1)}{(2\ell+1)(2\ell+2)}\right]^{1/2}$	$\left[\dfrac{(\ell-m+1)(\ell+m+1)}{(\ell+1)(2\ell+1)}\right]^{1/2}$	$\left[\dfrac{(\ell-m)(\ell-m+1)}{(2\ell+1)(2\ell+2)}\right]^{1/2}$
ℓ	$-\left[\dfrac{(\ell-m+1)(\ell+m)}{2\ell(\ell+1)}\right]^{1/2}$	$\dfrac{m}{\sqrt{\ell(\ell+1)}}$	$\left[\dfrac{(\ell-m)(\ell+m+1)}{2\ell(\ell+1)}\right]^{1/2}$
$\ell-1$	$\left[\dfrac{(\ell-m)(\ell-m+1)}{2\ell(2\ell+1)}\right]^{1/2}$	$-\left[\dfrac{(\ell-m)(\ell+m)}{\ell(2\ell+1)}\right]^{1/2}$	$\left[\dfrac{(\ell+m)(\ell+m+1)}{2\ell(2\ell+1)}\right]^{1/2}$

Using a spherical basis, we can represent $|1\,1\rangle=\left(\begin{smallmatrix}1\\0\\0\end{smallmatrix}\right)$, $|1\,0\rangle=\left(\begin{smallmatrix}0\\1\\0\end{smallmatrix}\right)$ and $|1\,-1\rangle=\left(\begin{smallmatrix}0\\0\\1\end{smallmatrix}\right)$. With respect to this basis, we can explicitly write out the three *vector spherical harmonics*, $\mathcal{Y}^{\ell\,1}_{j=\ell\pm1\,,\,m}(\theta,\phi)$ and $\mathcal{Y}^{\ell\,1}_{j=\ell\,,\,m}(\theta,\phi)$. For example, if $\ell\neq 0$ then,

$$\mathcal{Y}^{\ell\,1}_{j=\ell\,,\,m}(\theta,\phi)=\begin{pmatrix} -\left[\dfrac{(\ell-m+1)(\ell+m)}{2\ell(\ell+1)}\right]^{1/2} Y_{\ell,m-1}(\theta,\phi) \\ \dfrac{m}{\sqrt{\ell(\ell+1)}}\,Y_{\ell m}(\theta,\phi) \\ \left[\dfrac{(\ell+m+1)(\ell-m)}{2\ell(\ell+1)}\right]^{1/2} Y_{\ell,m-1}(\theta,\phi)\end{pmatrix}.$$

The other two vector spherical harmonics can be written out in a similar fashion. If $\ell=0$ then $\mathcal{Y}^{\ell\,1}_{j=\ell+1\,,\,m}(\theta,\phi)$ is the only surviving vector spherical harmonic.

It is instructive to work in a Cartesian basis, where the χ_{1,m_s} are eigenvectors of $\mathcal{S}_3$, and the spin-1 spin matrices are given by $\hbar\vec{\boldsymbol{\mathcal{S}}}$, where $(\mathcal{S}_k)_{ij}=-i\epsilon_{ijk}$. In particular,

$$\mathcal{S}_3=\begin{pmatrix}0 & -i & 0\\ i & 0 & 0\\ 0 & 0 & 0\end{pmatrix}.$$

and $\mathcal{S}_3\chi_{1,m_s}=m_s\chi_{1,m_s}$. This yields the orthonormal eigenvectors,

$$\chi_{1,\pm1}=\frac{1}{\sqrt{2}}\begin{pmatrix}\mp1\\ -i\\ 0\end{pmatrix}, \qquad \chi_{1,0}=\begin{pmatrix}0\\0\\1\end{pmatrix}. \tag{6}$$

where the arbitrary overall phase factors are conventionally chosen to be unity. As an example, in the Cartesian basis,

$$\mathcal{Y}^{\ell 1}_{j=\ell\,,\,m}(\theta,\phi)=\frac{1}{2\sqrt{\ell(\ell+1)}}\begin{pmatrix}[(\ell-m+1)(\ell+m)]^{1/2}\,Y_{\ell,m-1}(\theta,\phi)+[(\ell+m+1)(\ell-m)]^{1/2}\,Y_{\ell,m+1}(\theta,\phi)\\ i\,[(\ell-m+1)(\ell+m)]^{1/2}\,Y_{\ell,m-1}(\theta,\phi)-i\,[(\ell+m+1)(\ell-m)]^{1/2}\,Y_{\ell,m+1}(\theta,\phi)\\ 2mY_{\ell m}(\theta,\phi)\end{pmatrix}. \tag{7}$$

This is a vector with respect to the basis $\{\hat{\boldsymbol{x}}\,,\,\hat{\boldsymbol{y}}\,,\,\hat{\boldsymbol{z}}\}$. It is convenient to rewrite eq. (7) in terms of the basis $\{\hat{\boldsymbol{r}}\,,\,\hat{\boldsymbol{\theta}}\,,\,\hat{\boldsymbol{\phi}}\}$ using

$$\begin{aligned}\hat{\boldsymbol{x}}&=\hat{\boldsymbol{r}}\sin\theta\cos\phi+\hat{\boldsymbol{\theta}}\cos\theta\cos\phi-\hat{\boldsymbol{\phi}}\sin\phi\,,\\ \hat{\boldsymbol{y}}&=\hat{\boldsymbol{r}}\sin\theta\sin\phi+\hat{\boldsymbol{\theta}}\cos\theta\sin\phi+\hat{\boldsymbol{\phi}}\cos\phi\,,\\ \hat{\boldsymbol{z}}&=\hat{\boldsymbol{r}}\cos\theta-\hat{\boldsymbol{\theta}}\sin\theta\,.\end{aligned}$$

We can then greatly simplify the resulting expression for $\mathcal{Y}^{\ell 1}_{j=\ell\,,\,m}(\theta,\phi)$ by employing the recursion relation,

$$\begin{aligned}-2m\cos\theta\,Y_{\ell m}(\theta,\phi)=\sin\theta\Big\{&[(\ell+m+1)(\ell-m)]^{1/2}\,e^{-i\phi}\,Y_{\ell,m+1}(\theta,\phi)\\ &+[(\ell-m+1)(\ell+m)]^{1/2}\,e^{i\phi}\,Y_{\ell,m-1}(\theta,\phi)\Big\}\,,\end{aligned}$$

and the following two differential relations,

$$\begin{aligned}\frac{\partial}{\partial\phi}\,Y_{\ell m}(\theta,\phi)&=imY_{\ell m}(\theta,\phi)\,,\\ \frac{\partial}{\partial\theta}\,Y_{\ell m}(\theta,\phi)&=\tfrac{1}{2}\,[(\ell+m+1)(\ell-m)]^{1/2}\,e^{-i\phi}\,Y_{\ell,m+1}(\theta,\phi)\\ &\qquad-\tfrac{1}{2}\,[(\ell-m+1)(\ell+m)]^{1/2}\,e^{i\phi}\,Y_{\ell,m-1}(\theta,\phi)\,.\end{aligned}$$

Following a straightforward but tedious computation, the end result is:

$$\mathcal{Y}^{\ell 1}_{j=\ell\,,\,m}(\theta,\phi)=\frac{i}{\sqrt{\ell(\ell+1)}}\left[\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\,\frac{\partial}{\partial\phi}\,Y_{\ell m}(\theta,\phi)-\hat{\boldsymbol{\phi}}\,\frac{\partial}{\partial\theta}\,Y_{\ell m}(\theta,\phi)\right].$$

At this point, one should recognize the differential operator $\vec{\boldsymbol{L}}$ expressed in the $\{\hat{\boldsymbol{r}}\,,\,\hat{\boldsymbol{\theta}}\,,\,\hat{\boldsymbol{\phi}}\}$ basis,

$$\vec{\boldsymbol{L}}=-i\hbar\,\vec{\boldsymbol{x}}\times\vec{\boldsymbol{\nabla}}=i\hbar\left[\frac{\hat{\boldsymbol{\theta}}}{\sin\theta}\,\frac{\partial}{\partial\phi}-\hat{\boldsymbol{\phi}}\,\frac{\partial}{\partial\theta}\right].$$

Hence, we end up with

$$\mathcal{Y}^{\ell 1}_{j=\ell\,,\,m}(\theta,\phi)=\frac{1}{\sqrt{\hbar^2\ell(\ell+1)}}\,\vec{\boldsymbol{L}}\,Y_{\ell m}(\theta,\phi)\,,\qquad\text{for }\ell\neq 0\,. \tag{8}$$

This is the vector spherical harmonic,

$$\vec{\boldsymbol{X}}_{\ell m}(\theta,\phi) = \frac{-i}{\sqrt{\ell(\ell+1)}}\,\vec{\boldsymbol{x}}\times\vec{\boldsymbol{\nabla}}\,Y_{\ell m}(\theta,\phi)\,,$$

employed by J.D. Jackson, *Classical Electrodynamics*, 3rd Edition (John Wiley & Sons, Inc., New York, 1999).

Using the same methods, one can derive the following expressions for the other two vector spherical harmonics,

$$\mathcal{Y}^{\ell\,1}_{j=\ell-1\,,\,m}(\theta,\phi) = \frac{-1}{\sqrt{(j+1)(2j+1)}}\left[(j+1)\hat{\boldsymbol{n}} - r\vec{\boldsymbol{\nabla}}\right]Y_{jm}(\theta,\phi)\,, \qquad \text{for } \ell\neq 0\,, \tag{9}$$

$$\mathcal{Y}^{\ell\,1}_{j=\ell+1\,,\,m}(\theta,\phi) = \frac{1}{\sqrt{j(2j+1)}}\left[j\hat{\boldsymbol{n}} + r\vec{\boldsymbol{\nabla}}\right]Y_{jm}(\theta,\phi)\,, \tag{10}$$

where $\vec{\boldsymbol{x}} = r\vec{\boldsymbol{n}}$ and $\hat{\boldsymbol{n}}\equiv\hat{\boldsymbol{r}}$. That is, the three independent normalized vector spherical harmonics can be chosen as:[1]

$$\left\{\frac{-ir}{\sqrt{j(j+1)}}\,\hat{\boldsymbol{n}}\times\vec{\boldsymbol{\nabla}}\,Y_{jm}(\theta,\phi)\,,\quad \frac{r}{\sqrt{j(j+1)}}\vec{\boldsymbol{\nabla}}\,Y_{jm}(\theta,\phi)\,,\quad \hat{\boldsymbol{n}}\,Y_{jm}(\theta,\phi)\right\}. \tag{11}$$

Note that $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\,Y_{jm}(\theta,\phi) = \partial Y_{jm}(\theta,\phi)/\partial r = 0$. Hence, it follows that the first two vector spherical harmonics of eq. (11) are transverse (i.e., perpendicular to $\hat{\boldsymbol{n}}$), whereas the third vector spherical harmonic in eq. (11) is longitudinal (i.e., parallel to $\hat{\boldsymbol{n}}$). This is convenient for the multipole expansion of the transverse electric and magnetic radiation fields, where only the first two vector spherical harmonics of eq. (11) appear. However, $r\vec{\boldsymbol{\nabla}}\,Y_{jm}(\theta,\phi)$ and $\hat{\boldsymbol{n}}\,Y_{jm}(\theta,\phi)$ are not eigenstates of $\vec{\boldsymbol{L}}^2$ since they consist of linear combinations of states with $\ell = j\pm 1$ [which can be explicitly derived by inverting eqs. (9) and (10)].

The algebraic steps involved in establishing eqs. (8)–(10) are straightforward but tedious. A more streamlined approach to the derivation of these results is given in Appendix B.

Appendix A: The Clebsch-Gordon series and some applications

The Clebsch-Gordon coefficients form a unitary matrix. It is standard practice to employ a phase convention in defining the Clebsch-Gordon coefficients (called the *Condon-Shortly phase convention*) such that all the Clebsch-Gordon coefficients are real. In particular,

$$\langle j_1\,m_1\,;\,j_2\,m_2\,|\,jm\rangle = \langle jm\,|\,j_1\,m_1\,;\,j_2\,m_2\rangle\,.$$

[1]It is often convenient to rewrite $r\,\vec{\boldsymbol{\nabla}}\;Y_{jm}(\theta,\phi) = -r[\hat{\boldsymbol{n}}(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}) - \vec{\boldsymbol{\nabla}}]Y_{jm}(\theta,\phi) = -r\,\hat{\boldsymbol{n}}\times(\hat{\boldsymbol{n}}\times\vec{\boldsymbol{\nabla}})Y_{jm}(\theta,\phi)$, since $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\,Y_{jm}(\theta,\phi) = \partial Y_{jm}(\theta,\phi)/\partial r = 0$ as noted above. This alternative form is often used for the second vector spherical harmonic of eq. (11).

In this convention, the Clebsch-Gordon coefficients form an orthogonal matrix and therefore satisfy orthogonality relations,

$$\sum_{j,m} \langle j_1\, m_1\,;\, j_2\, m_2\,|\, j\, m\rangle\langle j_1\, m_1'\,;\, j_2\, m_2'\,|\, j\, m\rangle = \delta_{m_1,m_1'}\delta_{m_2,m_2'}\,, \tag{12}$$

$$\sum_{m_1,m_2} \langle j_1\, m_1\,;\, j_2\, m_2\,|\, j\, m\rangle\langle j_1\, m_1\,;\, j_2\, m_2\,|\, j'\, m'\rangle = \delta_{j\,j'}\delta_{m,m'}\Delta(j_1 j_2 j)\,, \tag{13}$$

where j_1, j_2 and j are non-negative integers or half-integers and

$$\Delta(j_1 j_2 j) = \begin{cases} 1\,, & \text{if } |j_1 - j_2| \leq j \leq j_1 + j_2\,, \\ 0\,, & \text{otherwise.} \end{cases} \tag{14}$$

Consider a system whose total angular momentum is $\vec{\boldsymbol{J}} = \vec{\boldsymbol{J}}_1 + \vec{\boldsymbol{J}}_2$. Clebsch-Gordon coefficients provide the connection between the total angular momentum basis $|j\, m\,;\, j_1\, j_2\rangle$ and the direct product basis, $|j_1\, m_1\,;\, j_2\, m_1\rangle \equiv |j_1\, m_1\rangle \otimes |j_2\, m_2\rangle$,

$$|j\, m\rangle = \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} \langle j_1\, m_1\,;\, j_2\, m_2\,|\, j\, m\rangle |j_1\, m_1\,;\, j_2\, m_2\rangle\,. \tag{15}$$

The unitary operator that (actively) rotates states by an angle θ about an axis $\hat{\boldsymbol{n}}$ is

$$U[R(\hat{\boldsymbol{n}},\theta)] = \exp\left(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{J}}/\hbar\right)\,.$$

Applying $U[R(\hat{\boldsymbol{n}},\theta)]$ to the state $|j\, m\rangle$ does not change the value of j since $\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{J}}$ commutes with $\vec{\boldsymbol{J}}^2$. Then, inserting a complete set of states, one obtains

$$U[R(\hat{\boldsymbol{n}},\theta)]|j\, m'\rangle = \sum_m |j\, m\rangle\langle j\, m|\exp(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{J}}/\hbar)|j\, m'\rangle = \sum_m D^{(j)}_{mm'}(R)|j\, m\rangle\,,$$

$$\langle j\, m'|U[R(\hat{\boldsymbol{n}},\theta)] = \sum_m \langle j\, m|\exp(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{J}}/\hbar)|j\, m'\rangle\langle j\, m| = \sum_m \langle j\, m|\, D^{(j)}_{mm'}(R)\,,$$

which defines the $(2j+1)\times(2j+1)$ unitary matrix $D^{(j)}(R)$ that represents the rotation R.

Consider the matrix element $\langle j_1\, m_1\,;\, j_2\, m_2|U[R(\hat{\boldsymbol{n}},\theta)]|j\, m\rangle$. We can compute this in two different ways by letting the operator $U[R(\hat{\boldsymbol{n}},\theta)]$ act either to the right or to the left.

$$\langle j_1\, m_1\,;\, j_2\, m_2|U[R(\hat{\boldsymbol{n}},\theta)]|j\, m'\rangle = \sum_q D^{(j)}_{qm'}(R)\langle j_1\, m_1\,;\, j_2\, m_2\,|\, j\, q\rangle\,,$$

$$\langle j_1\, m_1\,;\, j_2\, m_2|U[R(\hat{\boldsymbol{n}},\theta)]|j\, m'\rangle = \sum_{m_1',m_2'} \langle j_1\, m_1'\,;\, j_2\, m_2'\,|\, j\, m'\rangle\, D^{(j_1)}_{m_1 m_1'}(R)\, D^{(j_2)}_{m_2 m_2'}(R)\,.$$

Equating these two expressions yields

$$\sum_q D^{(j)}_{qm'}(R)\langle j_1\, m_1\,;\, j_2\, m_2\,|\, j\, q\rangle = \sum_{m_1',m_2'} \langle j_1\, m_1'\,;\, j_2\, m_2'\,|\, j\, m'\rangle\, D^{(j_1)}_{m_1\, m_1'}(R)\, D^{(j_2)}_{m_2\, m_2'}(R)\,.$$

Multiplying this result by $\langle j_1\, q_1\, ;\, j_2\, q_2\,|\, j\, m'\rangle$ and summing over j and m' using the orthogonality relation given in eq. (12), we end up with

$$D^{(j_1)}_{m_1\, q_1}(R)\, D^{(j_2)}_{m_2\, q_2}(R) = \sum_{q,j,m'} \langle j_1\, m_1\, ;\, j_2\, m_2\,|\, j\, q\rangle \langle j_1\, q_1\, ;\, j_2\, q_2\,|\, j\, m'\rangle D^{(j)}_{qm'}(R)\,,$$

which is called the *Clebsch-Gordon series*. The sum over q and m' can be performed immediately since the Clebsch-Gordon coefficients above vanish unless $q = m_1 + m_2$ and $m' = q_1 + q_2$, respectively. After relabeling, we are left with

$$D^{(j_1)}_{m_1\, m_1'}(R)\, D^{(j_2)}_{m_2\, m_2'}(R) = \sum_j \langle j_1\, m_1\, ;\, j_2\, m_2\,|\, j\, ,\, m_1{+}m_2\rangle\, \langle j_1\, m_1'\, ;\, j_2\, m_2'\,|\, j\, ,\, m_1'{+}m_2'\rangle\, D^{(j)}_{m_1+m_2,m_1'+m_2'}(R)\,. \tag{16}$$

For non-negative integer ℓ, one can prove that

$$D^{(\ell)}_{m\,0}(\alpha,\beta,\gamma) = \sqrt{\frac{4\pi}{2\ell+1}}\, Y^*_{\ell m}(\beta,\alpha)\,, \tag{17}$$

where $(\alpha,\,\beta,\,\gamma)$ are the Euler angles that specify the rotation R. Thus, setting $q_1 = q_2 = 0$ and taking integer values $j_1 = \ell_1$ and $j_2 = \ell_2$ in eq. (16), it follows that

$$Y_{\ell_1\, m_1}(\hat{\boldsymbol{n}})\, Y_{\ell_2\, m_2}(\hat{\boldsymbol{n}}) = \sum_{\ell,m} \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell+1)}} \langle \ell_1\, m_1\, ;\, \ell_2\, m_2\,|\, \ell\, m\rangle \langle \ell_1\, 0\, ;\, \ell_2\, 0\,|\, \ell\, 0\rangle\, Y_{\ell m}(\hat{\boldsymbol{n}})\,. \tag{18}$$

To establish eq. (17), recall that the Euler angle representation of the rotation R, described in the handout, *Three-Dimensional Rotation Matrices*, is given by

$$R(\hat{\boldsymbol{n}},\theta) = R(\hat{\boldsymbol{z}},\alpha)R(\hat{\boldsymbol{y}},\beta)R(\hat{\boldsymbol{z}},\gamma)\,. \tag{19}$$

Likewise,[2]

$$D^{(j)}_{mm'}(R) \equiv D^{(j)}_{mm'}(\alpha,\beta,\gamma) = \langle j\, m|\, e^{-i\alpha J_z/\hbar}\, e^{-i\beta J_y/\hbar}\, e^{-i\gamma J_z/\hbar}\, |jm'\rangle = e^{-i(\alpha m+\gamma m')}\, d^{(j)}_{mm'}(\beta)\,, \tag{20}$$

where $d^{(j)}(\beta) \equiv \langle j\, m|\, e^{-i\beta J_y/\hbar}\, |jm'\rangle$.

A relation between the $D^{(j)}_{mm'}(R)$ and the spherical harmonics can be determined as follows. First, note that $U[R(\hat{\boldsymbol{n}},\theta)]|\vec{\boldsymbol{x}}\rangle = |R\vec{\boldsymbol{x}}\rangle$, where $(R\vec{\boldsymbol{x}})_i \equiv R_{ij}x_j$ (with an implicit sum over the repeated index j). Since $U[R_1]U[R_2] = U[R_1R_2]$ it follows that $U^\dagger[R] = U^{-1}[R] = U[R^{-1}]$. Hence, $U^\dagger[R(\hat{\boldsymbol{n}},\theta)]|\vec{\boldsymbol{x}}\rangle = |R^{-1}\vec{\boldsymbol{x}}\rangle$ and the corresponding adjoint is $\langle\vec{\boldsymbol{x}}|U[R(\hat{\boldsymbol{n}},\theta)] = \langle R^{-1}\vec{\boldsymbol{x}}|$. Thus, we

[2] In order to avoid minus sign errors in extracting the phase factors, consider the following computation. If U is a unitary operator, then $UU^\dagger = U^\dagger U = \mathbf{I}$, or equivalently $U^\dagger = U^{-1}$. Consider the eigenvalue problem $U\vec{\boldsymbol{v}} = \lambda\vec{\boldsymbol{v}}$. Then it is straightforward to prove that $|\lambda| = 1$, or equivalently $\lambda^{-1} = \lambda^*$. Thus, using Dirac bracket notation, we have $U|v\rangle = \lambda|v\rangle$, and

$$\langle v|U = \langle U^\dagger v| = \langle U^{-1}v| = \langle\lambda^{-1}v| = \langle\lambda^* v| = \lambda\langle v|\,.$$

The key observation is that a constant inside the bra is complex-conjugated when moved outside the bra.

can evaluate $\langle\vec{\boldsymbol{x}}|U[R(\hat{\boldsymbol{n}},\theta)]|\ell\, m\rangle$ in two different ways by letting the operator $U[R(\hat{\boldsymbol{n}},\theta)]$ act either to the left or to the right.

$$\langle\vec{\boldsymbol{x}}|U[R(\hat{\boldsymbol{n}},\theta)]|\ell\, m\rangle = \langle R^{-1}\vec{\boldsymbol{x}}\,|\,\ell\, m\rangle = Y_{\ell m}(R^{-1}\hat{\boldsymbol{n}})\,,$$

$$\langle\vec{\boldsymbol{x}}|U[R(\hat{\boldsymbol{n}},\theta)]|\ell\, m\rangle = \sum_{m'}\langle\vec{\boldsymbol{x}}\,|\,\ell\, m'\rangle\,\langle\ell\, m'|U[R(\hat{\boldsymbol{n}},\theta)]|\ell\, m\rangle = \sum_{m'} D^{(\ell)}_{m'm}(R)\,Y_{\ell m'}(\hat{\boldsymbol{n}})\,,$$

where $\hat{\boldsymbol{n}} \equiv \vec{\boldsymbol{x}}/r$. Equating these two expressions yields

$$Y_{\ell m}(R^{-1}\hat{\boldsymbol{n}}) = \sum_{m'} D^{(\ell)}_{m'm}(R)\,Y_{\ell m'}(\hat{\boldsymbol{n}})\,. \tag{21}$$

Replacing R with R^{-1} and using $D^{(\ell)}_{m'm}(R^{-1}) = D^{(\ell)\,\dagger}_{m'm}(R) = D^{(\ell)\,*}_{mm'}(R)$, it follows that eq. (21) is equivalent to

$$Y_{\ell m}(R\hat{\boldsymbol{n}}) = \sum_{m'} D^{(\ell)\,*}_{mm'}(R)\,Y_{\ell m'}(\hat{\boldsymbol{n}})\,. \tag{22}$$

If we parameterize the rotation R with Euler angles $(\phi,\,\theta,\,\gamma)$ as in eq. (19), then we can write $\hat{\boldsymbol{n}} = R(\phi,\theta,\gamma)\hat{\boldsymbol{z}}$. Note that $\hat{\boldsymbol{n}}$ is a unit vector with polar angle θ and azimuthal angle ϕ. In particular, the angle γ has no effect since $R(\hat{\boldsymbol{z}},\gamma)\hat{\boldsymbol{z}} = \hat{\boldsymbol{z}}$ independently of the angle γ. Thus, replacing $\hat{\boldsymbol{n}}$ with $\hat{\boldsymbol{z}}$ in eq. (22), it follows that

$$Y_{\ell m}(\hat{\boldsymbol{n}}) = \sum_{m'} D^{(\ell)\,*}_{mm'}(R)\,Y_{\ell m'}(\hat{\boldsymbol{z}})\,.$$

Finally, using the fact that

$$Y_{\ell m'}(\hat{\boldsymbol{z}}) = \sqrt{\frac{2\ell+1}{4\pi}}\,\delta_{m,0}$$

it follows that

$$D^{(\ell)}_{m\,0}(\phi,\theta,\gamma) = \sqrt{\frac{4\pi}{2\ell+1}}\,Y^*_{\ell m}(\theta,\phi)\,,$$

which confirms eq. (17) quoted above.

Next, we note the orthogonality relations satisfied by the D-matrices,[3]

$$\int dR\, D^{(j)\,*}_{m_1\, m_2}(R)\, D^{(j')}_{m_1'\, m_2'}(R) = \frac{8\pi^2}{2j+1}\,\delta_{jj'}\,\delta_{m_1\, m_1'}\,\delta_{m_2\, m_2'}\,, \tag{23}$$

where

$$\int dR \equiv \int_0^{2\pi} d\alpha \int_0^{2\pi} d\gamma \int_0^{\pi} \sin\beta\, d\beta\,. \tag{24}$$

By setting $m_2 = m_2' = 0$ and taking $j = \ell$ and $j' = \ell'$ to be integers, one can check that in light of eq. (17), the spherical harmonics satisfy the expected orthogonality relation,

$$\int d\Omega\, Y_{\ell m}(\theta,\phi)\, Y^*_{\ell' m'}(\theta,\phi) = \delta_{\ell\ell'}\,\delta_{mm'}\,. \tag{25}$$

[3]The orthogonality relations can be derived by integrating eq. (16) over the Euler angles [cf. eq. (24)]. The resulting integral is straightforward and after some manipulations one simply needs a closed form expression for the Clebsch-Gordon coefficient $\langle j\,,\,-m\,;\,j\,m\,|\,00\rangle = (-1)^{j+m}/\sqrt{2j+1}$. For further details, see e.g. Ref. [8].

We can use eqs. (16) and (23) to derive an important integral:

$$\begin{aligned}\int dR\, D^{(j_1)}_{m_1 m_1'}(R)\, D^{(j_2)}_{m_2 m_2'}(R)\, D^{(j_3)\,*}_{m_3 m_3'}(R) &= \int dR \sum_j \langle j_1\, m_1\, ;\, j_2\, m_2 \,|\, j\, m\rangle \,\langle j_1\, m_1'\, ;\, j_2\, m_2' \,|\, j\, m'\rangle \\ &\qquad\qquad \times D^{(j)}_{m_1+m_2, m_1'+m_2'}(R)\, D^{(j_3)\,*}_{m_3 m_3'}(R) \\ &= \frac{8\pi^2}{2j_3+1} \langle j_1\, m_1\, ;\, j_2\, m_2 \,|\, j_3\, m_3\rangle \,\langle j_1\, m_1'\, ;\, j_2\, m_2' \,|\, j_3\, m_3'\rangle \,.\end{aligned} \tag{26}$$

Note that the integral above vanishes unless $m_3 = m_1 + m_2$, $m_3' = m_1' + m_2'$ and $\Delta(j_1 j_2 j_3) = 1$ due to the properties of the Clebsch-Gordon coefficients [cf. eq. (14)].

If we take $j_1 = \ell_1$, $j_2 = \ell_2$ and $j_3 = \ell_3$ to be integers and set $m_1' = m_2' = m_3' = 0$, then in light of eq. (17), we obtain

$$\int d\Omega\, Y_{\ell_1 m_1}(\theta,\phi)\, Y_{\ell_2 m_2}(\theta,\phi)\, Y^*_{\ell_3 m_3}(\theta,\phi) = \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell_3+1)}}\, \langle \ell_1\, m_1\, ;\, \ell_2\, m_2 \,|\, \ell_3\, m_3\rangle \,\langle \ell_1\, 0\, ;\, \ell_2\, 0 \,|\, \ell_3\, 0\rangle \,. \tag{27}$$

Finally, using $Y_{\ell 0}(\hat{\boldsymbol{n}}) = \left[(2\ell+1)/(4\pi)\right]^{1/2} P_\ell(\cos\theta)$, it follows that

$$\int_{-1}^{1} P_{\ell_1}(x) P_{\ell_2}(x) P_{\ell_3}(x)\, dx = \frac{2}{2\ell_3+1}\, \langle \ell_1\, 0\, ;\, \ell_2\, 0 \,|\, \ell_3\, 0\rangle^2 \,. \tag{28}$$

For completeness, we note the remarkable formula given in Ref. [5],

$$\frac{1}{2\ell_3+1}\, \langle \ell_1\, 0\, ;\, \ell_2\, 0 \,|\, \ell_3\, 0\rangle^2 = \left(\frac{g!}{(g-\ell_1)!(g-\ell_2)!(g-\ell_3)!}\right)^2 \frac{(2g-2\ell_1)!(2g-2\ell_2)!(2g-2\ell_3)!}{(2g+1)!}\,,$$

where [cf. eq. (14)]:

$$2g \equiv \ell_1 + \ell_2 + \ell_3 \text{ is an even integer and } \Delta(\ell_1 \ell_2 \ell_3) = 1\,.$$

If $\ell_1 + \ell_2 + \ell_3$ is an odd integer and/or $\Delta(\ell_1 \ell_2 \ell_3) = 0$ then $\langle \ell_1\, 0\, ;\, \ell_2\, 0 \,|\, \ell_3\, 0\rangle = 0$. As a result, the right hand side of eq. (28) is symmetric under the interchange of the ℓ_i as expected.

Appendix B: The vector spherical harmonics revisited

Since $Y_{\ell m}(\hat{\boldsymbol{n}})$ is a spherical tensor of rank-ℓ, and $\hat{\boldsymbol{n}} \equiv \vec{\boldsymbol{x}}/r$, $\vec{\boldsymbol{L}} \equiv -i\hbar\vec{\boldsymbol{x}} \times \vec{\boldsymbol{\nabla}}$ and $r\vec{\boldsymbol{\nabla}}$ are vector operators, it is not surprising that the vector spherical harmonics are linear combinations of the quantities given in eq. (11). It is instructive to derive this result directly. For convenience, we denote the vector spherical harmonics in this appendix by

$$\vec{\boldsymbol{Y}}_{j\ell m}(\hat{\boldsymbol{n}}) \equiv \mathcal{Y}^{\ell\,1}_{j\,m}(\theta,\phi)\,, \quad \text{for } j = \ell+1\,,\ \ell\,,\ \ell-1\,, \tag{29}$$

where $\hat{\boldsymbol{n}}$ is a unit vector with polar angle θ and azimuthal angle ϕ.

First, we recall that [cf. eq. (12.5.20) of Shankar]:

$$L_{\pm}|\ell\, m\rangle = \hbar\left[(\ell \mp m)(\ell \pm m+1)\right]^{1/2}|j\, m\pm 1\rangle\,, \qquad L_z|\ell\, m\rangle = \hbar m|\ell\, m\rangle\,, \tag{30}$$

where $L_{\pm} \equiv L_x \pm iL_y$. The spherical components of $\vec{\boldsymbol{L}}$ are L_q ($q = +1, 0, -1$) where

$$L_{\pm 1} \equiv \pm\frac{L_{\pm}}{\sqrt{2}} = \frac{1}{\sqrt{2}}\left(L_x \pm iL_y\right)\,, \qquad L_0 \equiv L_z\,.$$

Using the Clebsch-Gordon coefficients given in Table 2, it follows that

$$L_q|\ell\, m\rangle = \hbar(-1)^q\sqrt{\ell(\ell+1)}\,\langle \ell\,,\, m+q\,;\, 1\,,\, -q\,|\,\ell\, m\rangle\,|\ell\,,\, m+q\rangle\,. \tag{31}$$

In the coordinate representation, eq. (31) is equivalent to

$$L_q\, Y_{\ell m}(\hat{\boldsymbol{n}}) = \hbar(-1)^q\sqrt{\ell(\ell+1)}\,\langle \ell\,,\, m+q\,;\, 1\,,\, -q\,|\,\ell\, m\rangle\, Y_{\ell\,,\,m+q}(\hat{\boldsymbol{n}})\,. \tag{32}$$

It is convenient to introduce a set of spherical basis vectors,

$$\hat{\boldsymbol{e}}_{\pm 1} \equiv \mp\frac{1}{\sqrt{2}}\left(\hat{\boldsymbol{x}} \pm i\hat{\boldsymbol{y}}\right)\,, \qquad \hat{\boldsymbol{e}}_0 \equiv \hat{\boldsymbol{z}}\,. \tag{33}$$

It is not surprising that $\hat{\boldsymbol{e}}_q = \chi_{1,q}$ [cf. eq. (6)]. One can check that

$$\vec{\boldsymbol{L}} = L_x\hat{\boldsymbol{x}} + L_y\hat{\boldsymbol{y}} + L_z\hat{\boldsymbol{z}} = \sum_q (-1)^q L_q \hat{\boldsymbol{e}}_{-q}\,, \tag{34}$$

where the sum over q runs over $q = -1, 0, +1$.[4] Hence, eqs. (32) and (34) yield

$$\vec{\boldsymbol{L}}Y_{\ell m}(\hat{\boldsymbol{n}}) = \hbar\sqrt{\ell(\ell+1)}\,\sum_q \hat{\boldsymbol{e}}_{-q}\langle \ell\,,\, m+q\,;\, 1\,,\, -q\,|\,\ell\, m\rangle\, Y_{\ell\,,\,m+q}(\hat{\boldsymbol{n}})\,.$$

Since the sum is taken over $q = -1, 0, 1$, we are free to relabel $q \to -q$. Writing $\hat{\boldsymbol{e}}_q = \chi_{1,q}$, we end up with

$$\vec{\boldsymbol{L}}Y_{\ell m}(\hat{\boldsymbol{n}}) = \hbar\sqrt{\ell(\ell+1)}\,\sum_q \langle \ell\,,\, m-q\,;\, 1\,,\, q\,|\,\ell\, m\rangle\, Y_{\ell\,,\,m-q}(\hat{\boldsymbol{n}})\chi_{1\,q}\,.$$

Comparing with eq. (3) for $s = 1$, it follows that [in the notation of eq. (29)]:

$$\boxed{\vec{\boldsymbol{L}}Y_{\ell m}(\hat{\boldsymbol{n}}) = \hbar\sqrt{\ell(\ell+1)}\,\vec{\boldsymbol{Y}}_{\ell\ell m}(\hat{\boldsymbol{n}})} \tag{35}$$

in agreement with eq. (8).

Next, we examine $\hat{\boldsymbol{n}}Y_{\ell m}(\hat{\boldsymbol{n}})$. It is convenient to expand $\hat{\boldsymbol{n}} \equiv \vec{\boldsymbol{x}}/r$ in a spherical basis. Using eq. (33), the following expression is an identity,

$$\hat{\boldsymbol{n}} = \hat{\boldsymbol{x}}\sin\theta\cos\phi + \hat{\boldsymbol{y}}\sin\theta\sin\phi + \hat{\boldsymbol{z}}\cos\theta = \sqrt{\frac{4\pi}{3}}\sum_q (-1)^q\, Y_{1q}(\hat{\boldsymbol{n}})\,\hat{\boldsymbol{e}}_{-q}\,. \tag{36}$$

[4]Henceforth, if left unspecified, sums over q will run over $q = -1, 0, +1$.

Hence,

$$\hat{\boldsymbol{n}} Y_{\ell m}(\hat{\boldsymbol{n}}) = \sqrt{\frac{4\pi}{3}} \sum_q (-1)^q \, Y_{1q}(\hat{\boldsymbol{n}}) Y_{\ell m}(\hat{\boldsymbol{n}}) \, \hat{\boldsymbol{e}}_{-q} \,. \tag{37}$$

Using eq. (18) [after using eq. (2) to reduce the double sum down to a single sum],

$$Y_{1q}(\hat{\boldsymbol{n}}) Y_{\ell m}(\hat{\boldsymbol{n}}) = \sqrt{\frac{3(2\ell+1)}{4\pi}} \sum_{\ell'} \frac{1}{\sqrt{2\ell'+1}} \langle \ell\, m\, ;\, 1\, q \,|\, \ell'\, ,\, m+q \rangle \langle \ell\, 0\, ;\, 1\, 0 \,|\, \ell'\, 0 \rangle \, Y_{\ell'\, , m+q}(\hat{\boldsymbol{n}}) \,. \tag{38}$$

Only two terms, corresponding to $\ell' = \ell \pm 1$, can contribute to the sum over ℓ' since [cf. Table 2]:

$$\langle \ell\, 0\, ;\, 1\, 0 \,|\, \ell'\, 0 \rangle = \begin{cases} \left(\dfrac{\ell+1}{2\ell+1}\right)^{1/2} , & \text{for } \ell' = \ell+1\,, \\[2ex] 0\,, & \text{for } \ell' \neq \ell \pm 1\,, \\[2ex] -\left(\dfrac{\ell}{2\ell+1}\right)^{1/2} , & \text{for } \ell' = \ell - 1\,. \end{cases} \tag{39}$$

Inserting eq. (38) on the right hand side of eq. (37) and employing eq. (39) then yields

$$\begin{aligned} \hat{\boldsymbol{n}} Y_{\ell m}(\hat{\boldsymbol{n}}) = \sum_q (-1)^q \, \hat{\boldsymbol{e}}_{-q} \biggl\{ & \left(\frac{\ell+1}{2\ell+3}\right)^{1/2} \langle \ell\, m\, ;\, 1\, q \,|\, \ell+1\, ,\, m+q \rangle \, Y_{\ell+1\, , m+q}(\hat{\boldsymbol{n}}) \\ & - \left(\frac{\ell}{2\ell-1}\right)^{1/2} \langle \ell\, m\, ;\, 1\, q \,|\, \ell+1\, ,\, m+q \rangle \, Y_{\ell-1\, , m+q}(\hat{\boldsymbol{n}}) \biggr\} . \end{aligned} \tag{40}$$

It is convenient to rewrite eq. (40) with the help of the following two relations, which can be obtained from Table 2,

$$\langle \ell\, m\, ;\, 1\, q \,|\, \ell+1\, ,\, m+q \rangle = -(-1)^q \left(\frac{2\ell+3}{2\ell+1}\right)^{1/2} \langle \ell+1\, ,\, m+q\, ;\, 1\, ,\, -q \,|\, \ell\, m \rangle \,, \tag{41}$$

$$\langle \ell\, m\, ;\, 1\, q \,|\, \ell-1\, ,\, m+q \rangle = -(-1)^q \left(\frac{2\ell-1}{2\ell+1}\right)^{1/2} \langle \ell-1\, ,\, m+q\, ;\, 1\, ,\, -q \,|\, \ell\, m \rangle \,. \tag{42}$$

The end result is:

$$\begin{aligned} \hat{\boldsymbol{n}} Y_{\ell m}(\hat{\boldsymbol{n}}) = -\sum_q \hat{\boldsymbol{e}}_{-q} \biggl\{ & \left(\frac{\ell+1}{2\ell+1}\right)^{1/2} \langle \ell+1\, ,\, m+q\, ;\, 1\, ,\, -q \,|\, \ell\, m \rangle \, Y_{\ell+1\, , m+q}(\hat{\boldsymbol{n}}) \\ & - \left(\frac{\ell}{2\ell+1}\right)^{1/2} \langle \ell-1\, ,\, m+q\, ;\, 1\, ,\, -q \,|\, \ell\, m \rangle \, Y_{\ell-1\, , m+q}(\hat{\boldsymbol{n}}) \biggr\} . \end{aligned} \tag{43}$$

Using eq. (3) with $s = 1$ and $\chi_{1\,q} = \hat{\boldsymbol{e}}_q$ and employing the notation of eq. (29), it follows that

$$\vec{\boldsymbol{Y}}_{\ell\, , \ell\pm 1\, , m}(\hat{\boldsymbol{n}}) = \sum_q \hat{\boldsymbol{e}}_{-q} \, \langle \ell \pm 1\, ,\, m+q\, ;\, 1\, ,\, -q \,|\, \ell\, m \rangle \, Y_{\ell\pm 1\, , m+q}(\hat{\boldsymbol{n}}) \,, \tag{44}$$

after relabeling the summation index by $q \to -q$. Hence, eq. (43) yields

$$\boxed{\hat{\boldsymbol{n}} Y_{\ell m}(\hat{\boldsymbol{n}}) = -\left(\frac{\ell+1}{2\ell+1}\right)^{1/2} \vec{\boldsymbol{Y}}_{\ell\,,\,\ell+1\,,\,m}(\hat{\boldsymbol{n}}) + \left(\frac{\ell}{2\ell+1}\right)^{1/2} \vec{\boldsymbol{Y}}_{\ell\,,\,\ell-1\,,\,m}(\hat{\boldsymbol{n}})} \tag{45}$$

Finally, we examine $r\vec{\boldsymbol{\nabla}} Y_{\ell m}(\hat{\boldsymbol{n}})$. First, we introduce the gradient operator in a spherical basis, $\nabla_q = (\nabla_{+1}\,,\ \nabla_0\,,\ \nabla_{-1})$, where

$$\nabla_{+1} = \mp\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x} \pm i\frac{\partial}{\partial y}\right) = \mp\frac{e^{\pm i\phi}}{\sqrt{2}}\left[\sin\theta\frac{\partial}{\partial r} + \frac{\cos\theta}{r}\frac{\partial}{\partial\theta} \pm \frac{i}{r\sin\theta}\frac{\partial}{\partial\phi}\right], \tag{46}$$

$$\nabla_0 = \frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}. \tag{47}$$

We can introduce a formal operator ∇_q on the Hilbert space by defining the coordinate space representation,

$$\langle\vec{\boldsymbol{x}}|\nabla_q|\ell\, m\rangle = \nabla_q Y_{\ell m}(\hat{\boldsymbol{n}})\,.$$

Note that ∇_q is a vector operator. We shall employ the Wigner-Eckart theorem, which states that

$$\langle\ell'\, m'|\nabla_q|\ell\, m\rangle = \langle\ell\, m\,;\, 1\, q\,|\,\ell'\, m'\rangle\,\langle\ell'\|\nabla\|\ell\rangle\,, \tag{48}$$

where the reduced matrix element $\langle\ell\|\nabla\|\ell'\rangle$ is independent of q, m and m'. To evaluate the reduced matrix element, we consider the case of $q = m = m' = 0$. Then,

$$\langle\ell'\, 0|\nabla_0|\ell\, 0\rangle = \langle\ell\, 0\,;\, 1\, 0\,|\,\ell'\, 0\rangle\,\langle\ell'\|\nabla\|\ell\rangle\,.$$

Thus,

$$\langle\ell'\|\nabla\|\ell\rangle = \frac{\langle\ell'\, 0|\nabla_0|\ell\, 0\rangle}{\langle\ell\, 0\,;\, 1\, 0\,|\,\ell'\, 0\rangle}\,.$$

Inserting this result into eq. (48) yields

$$\langle\ell'\, m'|\nabla_q|\ell\, m\rangle = \frac{\langle\ell\, m\,;\, 1\, q\,|\,\ell'\, m'\rangle}{\langle\ell\, 0\,;\, 1\, 0\,|\,\ell'\, 0\rangle}\,\langle\ell'\, 0|\nabla_0|\ell\, 0\rangle\,. \tag{49}$$

We can evaluate $\langle\ell'\, 0|\nabla_0|\ell\, 0\rangle$ explicitly in the coordinate representation using eq. (47),

$$\langle\ell'\, 0|\nabla_0|\ell\, 0\rangle = -\frac{1}{r}\int d\Omega\, Y^*_{\ell'\,0}(\hat{\boldsymbol{n}})\sin\theta\,\frac{\partial}{\partial\theta}\,Y_{\ell 0}(\hat{\boldsymbol{n}})\,.$$

Using $Y_{\ell 0}(\hat{\boldsymbol{n}}) = [(2\ell+1)/(4\pi)]^{1/2}\,P_\ell(\cos\theta)$, and substituting $x \equiv \cos\theta$,

$$\langle\ell'\, 0|\nabla_0|\ell\, 0\rangle = \frac{\sqrt{(2\ell+1)(2\ell'+1)}}{2r}\int_{-1}^{1}(1-x^2)P_{\ell'}(x)P'_\ell(x)\, dx\,, \tag{50}$$

where $P'_\ell(x) = dP_\ell(x)/dx$. To evaluate eq. (50), we employ the recurrence relation,

$$(1-x^2)P'_\ell(x) = \ell P_{\ell-1}(x) - \ell x P_\ell(x)\,,$$

and the orthogonality relation of the Legendre polynomials,

$$\int_{-1}^{1} P_\ell(x) P_{\ell'}(x)\, dx = \frac{2}{2\ell+1}\,\delta_{\ell\ell'}\,.$$

It follows that

$$\langle \ell'\, 0|\nabla_0|\ell\, 0\rangle = \frac{\sqrt{(2\ell+1)(2\ell'+1)}}{2r}\left\{\frac{2\ell}{2\ell-1}\,\delta_{\ell',\ell-1} - \ell\int_{-1}^{1} xP_\ell(x)P_{\ell'}(x)\,dx\right\}. \tag{51}$$

To evaluate the remaining integral, we use $x = P_1(x)$ and the result of eq. (28) to write:

$$\int_{-1}^{1} xP_\ell(x)P_{\ell'}(x)\,dx = \int_{-1}^{1} P_1(x)P_\ell(x)P_{\ell'}(x)\,dx = \frac{2}{2\ell'+1}\langle 1\,0\,;\,\ell\,0\,|\,\ell'\,0\rangle^2\,.$$

Using eq. (39), the above integral is equal to

$$\int_{-1}^{1} xP_\ell(x)P_{\ell'}(x)\,dx = \frac{2(\ell+1)}{(2\ell+1)(2\ell+3)}\,\delta_{\ell',\ell+1} + \frac{2\ell}{(2\ell-1)(2\ell+1)}\,\delta_{\ell',\ell-1}\,.$$

Inserting this result back into eq. (51) yields

$$\begin{aligned}\langle \ell'\, 0|\nabla_0|\ell\, 0\rangle &= \frac{\sqrt{(2\ell+1)(2\ell'+1)}}{2r}\left\{\frac{2\ell(\ell+1)}{(2\ell-1)(2\ell+1)}\,\delta_{\ell',\ell-1} - \frac{2\ell(\ell+1)}{(2\ell+1)(2\ell+3)}\,\delta_{\ell',\ell+1}\right\} \\ &= \frac{\ell(\ell+1)}{r\sqrt{2\ell+1}}\left[\frac{1}{\sqrt{2\ell-1}}\,\delta_{\ell',\ell-1} - \frac{1}{\sqrt{2\ell+3}}\,\delta_{\ell',\ell+1}\right].\end{aligned}$$

Using eq. (49), it follows that:

$$\begin{aligned}\langle \ell'\, m'|\nabla_q|\ell\, m\rangle &= \frac{\langle \ell\, m\,;\,1\,q\,|\,\ell'\,m'\rangle}{\langle \ell\, 0\,;\,1\,0\,|\,\ell'\,0\rangle}\,\frac{\ell(\ell+1)}{r\sqrt{2\ell+1}}\left[\frac{1}{\sqrt{2\ell-1}}\,\delta_{\ell',\ell-1} - \frac{1}{\sqrt{2\ell+3}}\,\delta_{\ell',\ell+1}\right] \\ &= -\frac{1}{r}\langle \ell\, m\,;\,1\,q\,|\,\ell'\,m'\rangle\left[(\ell+1)\sqrt{\frac{\ell}{2\ell-1}}\,\delta_{\ell',\ell-1} + \ell\sqrt{\frac{\ell+1}{2\ell+3}}\,\delta_{\ell',\ell+1}\right],\end{aligned} \tag{52}$$

after using eq. (39) to evaluate $\langle \ell\, 0\,;\,1\,0\,|\,\ell'\,0\rangle$.

We are now ready to evaluate $r\vec{\boldsymbol{\nabla}}Y_{\ell m}(\hat{\boldsymbol{n}})$. First, we insert a complete set of states to obtain

$$\begin{aligned}\nabla_q|\ell\, m\rangle &= \sum_{\ell',m'}|\ell'\,m'\rangle\langle \ell'\,m'|\nabla_q|\ell\,m\rangle \\ &= -\frac{1}{r}\sum_{\ell',m'}|\ell'\,m'\rangle\left\{\langle \ell\, m\,;\,1\,q\,|\,\ell'\,m'\rangle\left[(\ell+1)\sqrt{\frac{\ell}{2\ell-1}}\,\delta_{\ell',\ell-1} + \ell\sqrt{\frac{\ell+1}{2\ell+3}}\,\delta_{\ell',\ell+1}\right]\right\}.\end{aligned} \tag{53}$$

Note that in the sum over m', only the terms corresponding to $m' = m + q$ survive, due to the presence of the Clebsch-Gordon coefficient $\langle \ell\, m\,;\, 1\, q\,|\,\ell'\, m'\rangle$. Likewise, in the sum over ℓ', only the terms corresponding to $\ell' = \ell \pm 1$ survive. In the coordinate representation, eq. (53) is equivalent to

$$\nabla_q Y_{\ell m}(\hat{\boldsymbol{n}}) = -\frac{1}{r}\sum_{\ell'} Y_{\ell',m+q}(\hat{\boldsymbol{n}})\left\{\langle \ell\, m\,;\, 1\, q\,|\,\ell'\,,\, m{+}q\rangle \left[(\ell+1)\sqrt{\frac{\ell}{2\ell-1}}\,\delta_{\ell',\ell-1} + \ell\,\sqrt{\frac{\ell+1}{2\ell+3}}\,\delta_{\ell',\ell+1}\right]\right\}.$$

In analogy with eq. (34), we have

$$\vec{\boldsymbol{\nabla}} = \sum_q (-1)^q\, \hat{\boldsymbol{e}}_{-q}\nabla_q\,.$$

Hence, it follows that

$$-r\vec{\boldsymbol{\nabla}}Y_{\ell m}(\hat{\boldsymbol{n}}) = \sum_q (-1)^q\, \hat{\boldsymbol{e}}_{-q}\left\{(\ell+1)\sqrt{\frac{\ell}{2\ell-1}}\,\langle \ell\, m\,;\, 1\, q\,|\,\ell-1\,,\, m+q\rangle Y_{\ell-1,m+q}(\hat{\boldsymbol{n}})\right.$$
$$\left. +\ell\,\sqrt{\frac{\ell+1}{2\ell+3}}\,\langle \ell\, m\,;\, 1\, q\,|\,\ell+1\,,\, m+q\rangle Y_{\ell+1,m+q}(\hat{\boldsymbol{n}})\right\}.$$

It is convenient to employ eqs. (41) and (42) and rewrite the above result as

$$r\vec{\boldsymbol{\nabla}}Y_{\ell m}(\hat{\boldsymbol{n}}) = \sum_q \hat{\boldsymbol{e}}_{-q}\left\{(\ell+1)\sqrt{\frac{\ell}{2\ell+1}}\,\langle \ell-1\,,\, m+q\,;\, 1\,,\, -q\,|\,\ell\, m\rangle Y_{\ell-1,m+q}(\hat{\boldsymbol{n}})\right.$$
$$\left. +\ell\,\sqrt{\frac{\ell+1}{2\ell+1}}\,\langle \ell+1\,,\, m+q\,;\, 1\,,\, -q\,|\,\ell\, m\rangle Y_{\ell+1,m+q}(\hat{\boldsymbol{n}})\right\}.$$

Finally, using eq. (44), we end up with

$$\boxed{r\vec{\boldsymbol{\nabla}}Y_{\ell m}(\hat{\boldsymbol{n}}) = (\ell+1)\sqrt{\frac{\ell}{2\ell+1}}\,\vec{\boldsymbol{Y}}_{\ell,\ell-1,m}(\hat{\boldsymbol{n}}) + \ell\,\sqrt{\frac{\ell+1}{2\ell+1}}\,\vec{\boldsymbol{Y}}_{\ell,\ell+1,m}(\hat{\boldsymbol{n}})} \tag{54}$$

which is known in the literature as the *gradient formula.*

We can now use eqs. (45) and (54) to solve for $\vec{\boldsymbol{Y}}_{\ell,\ell+1,m}(\hat{\boldsymbol{n}})$ and $\vec{\boldsymbol{Y}}_{\ell,\ell-1,m}(\hat{\boldsymbol{n}})$ in terms of $\hat{\boldsymbol{n}}Y_{\ell m}(\hat{\boldsymbol{n}})$ and $r\vec{\boldsymbol{\nabla}}Y_{\ell m}(\hat{\boldsymbol{n}})$. Since these are linear equations, they are easily inverted, and we find

$$\vec{\boldsymbol{Y}}_{\ell,\ell+1,m}(\hat{\boldsymbol{n}}) = \frac{1}{\sqrt{(\ell+1)(2\ell+1)}}\left[-(\ell+1)\hat{\boldsymbol{n}} + r\vec{\boldsymbol{\nabla}}\right]Y_{\ell m}(\hat{\boldsymbol{n}})\,, \qquad \text{for } \ell = 0, 1, 2, 3, \ldots,$$

$$\vec{\boldsymbol{Y}}_{\ell,\ell-1,m}(\hat{\boldsymbol{n}}) = \frac{1}{\sqrt{\ell(2\ell+1)}}\left[\ell\hat{\boldsymbol{n}} + r\vec{\boldsymbol{\nabla}}\right]Y_{\ell m}(\hat{\boldsymbol{n}})\,, \qquad \text{for } \ell = 1, 2, 3, \ldots,$$

which are equivalent to the results of eqs. (9) and (10) previously obtained. In addition, we also have eq. (35), which we can rewrite as

$$\vec{\boldsymbol{Y}}_{\ell,\ell,m} = \frac{-ir}{\sqrt{\ell(\ell+1)}}\,\hat{\boldsymbol{n}} \times \vec{\boldsymbol{\nabla}} Y_{\ell m}(\hat{\boldsymbol{n}})\,, \qquad \text{for } \ell = 1, 2, 3, \ldots, .$$

Thus, we have identified the three linearly independent vector spherical harmonics in terms of differential vector operators acting on $Y_{\ell m}(\hat{\boldsymbol{n}})$. For the special case of $\ell = 0$, only one vector spherical harmonic, $\vec{\boldsymbol{Y}}_{010}(\hat{\boldsymbol{n}}) = (-\hat{\boldsymbol{n}} + r\vec{\boldsymbol{\nabla}})Y_{\ell m}(\hat{\boldsymbol{n}})$, survives.

In books, one often encounters the vector spherical harmonic defined by $\hat{\boldsymbol{n}} \times \vec{\boldsymbol{L}}\, Y_{\ell m}(\hat{\boldsymbol{n}})$. However, this is not independent of the vector spherical harmonics obtained above, since

$$\hat{\boldsymbol{n}} \times \vec{\boldsymbol{L}}\, Y_{\ell m}(\hat{\boldsymbol{n}}) = -i\hbar r\, \hat{\boldsymbol{n}} \times (\hat{\boldsymbol{n}} \times \vec{\boldsymbol{\nabla}}) Y_{\ell m}(\hat{\boldsymbol{n}}) = -i\hbar r \left[\hat{\boldsymbol{n}}\frac{\partial}{\partial r} - \vec{\boldsymbol{\nabla}}\right] Y_{\ell m}(\hat{\boldsymbol{n}}) = i\hbar r\, \vec{\boldsymbol{\nabla}} Y_{\ell m}(\hat{\boldsymbol{n}})\,.$$

An alternative method for deriving the gradient formula [obtained in eq. (54)] is to evaluate $\hat{\boldsymbol{n}} \times \vec{\boldsymbol{L}}\, Y_{\ell m}(\hat{\boldsymbol{n}})$ using the same technique employed in the computation of $\hat{\boldsymbol{n}} Y_{\ell m}(\hat{\boldsymbol{n}})$ given in this Appendix. However, this calculation is much more involved and involves a product of four Clebsch-Gordon coefficients. A certain sum involving a product of three Clebsch-Gordon coefficients needs to be performed in closed form. This summation can be done (e.g., see Ref. [9] for the gory details), but the computation is much more involved than the simple analysis presented in this Appendix based on the Wigner-Eckart theorem.

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