The Spherical Basis

1. Introducing the spherical basis

Given a real vector $\vec{\boldsymbol{v}} \in \mathbb{R}^3$, one typically writes: $\vec{\boldsymbol{v}} = (v_x, v_y, v_z)$, where v_x, v_y, and v_z are real numbers corresponding to the components of $\vec{\boldsymbol{x}}$ with respect to the standard Cartesian basis,

$$\hat{\boldsymbol{x}} = (1,0,0)\,, \qquad \hat{\boldsymbol{y}} = (0,1,0)\,, \qquad \hat{\boldsymbol{z}} = (0,0,1)\,. \tag{1}$$

That is,

$$\vec{\boldsymbol{v}} = v_x\hat{\boldsymbol{x}} + v_y\hat{\boldsymbol{y}} + v_z\hat{\boldsymbol{z}} = \sum_{i=1}^{3} v_i\hat{\boldsymbol{e}}_i\,, \tag{2}$$

in a notation where the $v_i \in \mathbb{R}$ $(i = 1, 2, 3)$ correspond to the x, y, and z components of $\vec{\boldsymbol{v}}$, and the basis unit vectors are denoted by $\hat{\boldsymbol{e}}_i = \{\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}\}$.

However, other basis choices are also useful. In these notes, I shall introduce the spherical basis,

$$\hat{\boldsymbol{e}}_1 = -\frac{1}{\sqrt{2}}\big(\hat{\boldsymbol{x}} + i\hat{\boldsymbol{y}}\big)\,, \qquad \hat{\boldsymbol{e}}_0 = \hat{\boldsymbol{z}}\,, \qquad \hat{\boldsymbol{e}}_{-1} = \frac{1}{\sqrt{2}}\big(\hat{\boldsymbol{x}} - i\hat{\boldsymbol{y}}\big)\,. \tag{3}$$

The spherical basis vectors satisfy:

$$\hat{\boldsymbol{e}}^*_m = (-1)^m\,\hat{\boldsymbol{e}}_{-m}\,, \tag{4}$$

$$(-1)^m\,\hat{\boldsymbol{e}}_{-m}\boldsymbol{\cdot}\hat{\boldsymbol{e}}_{m'} = \hat{\boldsymbol{e}}^*_m\boldsymbol{\cdot}\hat{\boldsymbol{e}}_{m'} = \delta_{mm'}\,, \qquad \text{for } m,\, m' \in \{-1,0,1\}, \tag{5}$$

where * indicates complex conjugation. With respect to the spherical basis, the components of $\vec{\boldsymbol{v}}$ are denoted by $v_m \equiv \vec{\boldsymbol{v}}\boldsymbol{\cdot}\hat{\boldsymbol{e}}_m$, with $m \in \{-1,0,1\}$. More explicitly,

$$v_1 = -\frac{1}{\sqrt{2}}\big(v_x + iv_y\big)\,, \qquad v_0 = v_z\,, \qquad v_{-1} = \frac{1}{\sqrt{2}}\big(v_x - iv_y\big)\,. \tag{6}$$

Eq. (6) implies that for a real vector $\vec{\boldsymbol{v}}$ (i.e., a vector with v_x, v_y, $v_z \in \mathbb{R}$),

$$v^*_m = (-1)^m\,v_{-m}\,, \qquad \text{for } m = -1,0,1. \tag{7}$$

It is important not confuse $v_{m=1}$ with v_x, which was defined in eq. (2) even though in the latter context, v_x is often called v_1.

The expansion of $\vec{\boldsymbol{v}}$ with respect to the spherical basis is then given by

$$\vec{\boldsymbol{v}} = \sum_m (-1)^m v_{-m}\hat{\boldsymbol{e}}_m = \sum_m (-1)^m v_m\hat{\boldsymbol{e}}_{-m}\,, \tag{8}$$

where the symbol $\sum_m$ will always mean the sum over $m = -1,0,1$. The two ways of writing $\vec{\boldsymbol{v}}$ in eq. (8) correspond simply to relabeling $m \to -m$ in the summation. One can check that inserting the expressions of eqs. (3) and (6) into eq. (8) reproduces eq. (2).

To motivate eq. (6), consider the spherical harmonics $Y_{1m}(\theta, \phi)$, for $m = -1, 0, 1$,

$$Y_{1,\pm 1}(\hat{\boldsymbol{n}}) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{\pm i\phi} = \mp\sqrt{\frac{3}{8\pi}}\frac{x \pm iy}{r}\,, \qquad Y_{10}(\hat{\boldsymbol{n}}) = \sqrt{\frac{3}{4\pi}}\cos\theta = \sqrt{\frac{3}{4\pi}}\frac{z}{r}\,, \quad (9)$$

where we have made use of the definition of spherical coordinates where

$$\vec{\boldsymbol{x}} = (x, y, z) = r(\sin\theta\cos\phi\,,\, \sin\theta\sin\phi\,,\, \cos\theta) = r\,\hat{\boldsymbol{n}}\,, \quad (10)$$

with $r \equiv |\vec{\boldsymbol{x}}|$ and the unit vector $\hat{\boldsymbol{n}}$ specifies the angles θ and ϕ (such that $0 \leq \theta \leq \pi$ and $0 \leq \phi < 2\pi$). Then, it follows that the spherical components of the vector $\vec{\boldsymbol{x}}$ are given by

$$x_m = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1m}(\hat{\boldsymbol{n}})\,, \qquad \text{for } m = -1, 0, 1. \quad (11)$$

More generally, $Y_{\ell m}(\hat{\boldsymbol{n}})$ is an example of a spherical tensor of rank ℓ, whose $2\ell + 1$ components correspond to $m = -\ell, -\ell + 1, \ldots, \ell - 1, \ell$. For more details on the distinction between Cartesian tensors and spherical tensors, see the Appendix to these notes.

The dot product of two real vectors in terms of the rectangular (Cartesian) coordinates of the two vectors is given by

$$\vec{\boldsymbol{v}} \boldsymbol{\cdot} \vec{\boldsymbol{w}} = \sum_{i=1}^{3} v_i w_i\,. \quad (12)$$

In terms of the spherical components, the dot product is given by

$$\vec{\boldsymbol{v}} \boldsymbol{\cdot} \vec{\boldsymbol{w}} = \sum_m (-1)^m v_m w_{-m} = \sum_m (-1)^m v_{-m} w_m\,. \quad (13)$$

It is easy to check that after employing eq. (6) for the v_m and the analogous formula for the w_m, one reproduces eq. (12).

We can also define the components of the gradient operator in a spherical basis:

$$\nabla_1 = -\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\,, \qquad \nabla_0 = \frac{\partial}{\partial z}\,, \qquad \nabla_{-1} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\,. \quad (14)$$

One can check that this definition is consistent by observing that

$$\begin{aligned}\vec{\boldsymbol{\nabla}} \boldsymbol{\cdot} \vec{\boldsymbol{v}} = \sum_m (-1)^m \nabla_m v_{-m} &= \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)(v_x - iv_y) + \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)(v_x + iv_y) + \frac{\partial v_z}{\partial z} \\ &= \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}\,, \end{aligned} \quad (15)$$

as expected.

One might wonder how a relation such as eq. (11) extends to the spherical harmonics with higher values of ℓ. As an example, consider the spherical harmonics with $\ell = 2$,

$$Y_{2,\pm 2}(\hat{\boldsymbol{n}}) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{\pm i\phi} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\frac{(x \pm iy)^2}{r^2}\,, \quad (16)$$

$$Y_{2,\pm 1}(\hat{\boldsymbol{n}}) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi} = \mp\sqrt{\frac{15}{8\pi}}\frac{z(x \pm iy)}{r^2}\,, \quad (17)$$

$$Y_{20}(\hat{\boldsymbol{n}}) = \frac{1}{2}\sqrt{\frac{5}{4\pi}}(3\cos^2\theta - 1) = \frac{1}{2}\sqrt{\frac{5}{4\pi}}\,\frac{2z^2 - x^2 - y^2}{r^2}\,. \quad (18)$$

In terms of the spherical components of $\vec{\boldsymbol{x}}$,

$$r^2 Y_{2,\pm 2}(\hat{\boldsymbol{n}}) = \sqrt{\frac{15}{8\pi}} x_{\pm 1}^2 \,, \tag{19}$$

$$r^2 Y_{2,\pm 1}(\hat{\boldsymbol{n}}) = \sqrt{\frac{15}{4\pi}} x_{\pm 1} x_0 \,, \tag{20}$$

$$r^2 Y_{20}(\hat{\boldsymbol{n}}) = \sqrt{\frac{5}{4\pi}} \big(x_0^2 + x_1 x_{-1} \big) \,. \tag{21}$$

Eqs. (19)–(21) can be summarized by the following formula:

$$r^2 Y_{2m}(\hat{\boldsymbol{n}}) = \sqrt{\frac{15}{8\pi}} \sum_{\substack{m'=-1 \\ |m-m'|\leq 1}}^{1} \langle 1\,, m'\,;\, 1\,, m-m' \,|\, 2\,, m \rangle x_{m'} x_{m-m'} \,, \tag{22}$$

where $\langle 1\,, m'\,;\, 1\,, m-m' \,|\, 2\,, m \rangle$ are Clebsch-Gordan coefficients, whose values are given by:

$$\begin{aligned}
&\langle 1, 1; 1, 1 \mid 2, 2 \rangle = 1 \,, \\
&\langle 1, 1; 1, 0 \mid 2, 1 \rangle = \langle 1, 0; 1, 1 \mid 2, 1 \rangle = \frac{1}{\sqrt{2}} \,, \\
&\langle 1, 1; 1, -1 \mid 2, 0 \rangle = \langle 1, -1; 1, 1 \mid 2, 0 \rangle = \frac{1}{\sqrt{6}} \,, \\
&\langle 1, 0; 1, 0 \mid 2, 0 \rangle = \sqrt{\frac{2}{3}} \,, \\
&\langle 1, -1; 1, 0 \mid 2, -1 \rangle = \langle 1, 0; 1, -1 \mid 2, -1 \rangle = \frac{1}{\sqrt{2}} \,, \\
&\langle 1, -1; 1, -1 \mid 2, -2 \rangle = 1 \,.
\end{aligned} \tag{23}$$

For the record, an explicit formula for the Clebsch-Gordan coefficients above is given by:

$$\langle 1\,, m'\,;\, 1\,, m-m' \,|\, 2\,, m \rangle = \sqrt{\frac{(2+m)!(2-m)!}{6(1+m')!(1-m')!(1+m-m')!(1-m+m')!}} \,. \tag{24}$$

One can also invert eq. (22) to obtain:[1]

$$x_{m_1} x_{m_2} = \tfrac{1}{3}(-1)^{m_1} r^2 \, \delta_{m_2,-m_1} + \sqrt{\frac{8\pi}{15}}\, r^2 \sum_{\substack{m=-2 \\ m_1+m_2=m}}^{2} \langle 1\,, m_1\,;\, 1\,, m_2 \,|\, 2\,, m \rangle Y_{2m}(\hat{\boldsymbol{n}}) \,, \tag{25}$$

Indeed, the Clebsch-Gordan coefficients appearing in eq. (25) vanish unless $m_1 + m_2 = m$.

[1] Eq. (25) can be understood from a group theoretical perspective as implying that the symmetric tensor product of two three dimensional representations of the rotation group decomposes into two irreducible representations: one representation of dimension five corresponding to the $\ell = 2$ spherical tensor of rank two and another representation of dimension one corresponding to an $\ell = 0$ scalar (i.e, a rank zero spherical tensor). See the Appendix for a brief discussion of spherical tensors in the context of irreducible representations of the rotation group.

2. Explicit evaluation of $\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(\boldsymbol{r^\ell Y^*_{\ell m}(\hat{n})}\big)$ for $\boldsymbol{\ell=1,2}$

As a pedagogical exercise, we now evaluate $\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(\boldsymbol{r^\ell Y^*_{\ell m}(\hat{n})}\big)$ when $\ell=1$ and 2, where $\vec{\boldsymbol{v}}$ is an arbitrary vector. The results of this exercise will be useful in Section 3, when we examine the electric and magnetic dipole vectors and the electric and magnetic quadrupole tensors.

First, in the case of $\ell=1$, we make use of eq. (11) to obtain

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(rY^*_{1m}(\hat{\boldsymbol{n}})\big)=\sqrt{\frac{3}{4\pi}}\sum_{m'}(-1)^{m'}v_{-m'}\nabla_{m'}x^*_m\,. \tag{26}$$

Using eqs. (6) and (14), one can easily show that

$$\nabla_{m'}\,x^*_m=\delta_{mm'}\,. \tag{27}$$

Hence, it follows that

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(rY^*_{1m}(\hat{\boldsymbol{n}})\big)=(-1)^m\sqrt{\frac{3}{4\pi}}\,v_{-m}\,. \tag{28}$$

Second, in the case of $\ell=2$, we make use of eq. (22) to obtain

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(r^2Y^*_{2m}(\hat{\boldsymbol{n}})\big)=\sqrt{\frac{15}{8\pi}}\sum_{m''}\sum_{\substack{m'=-1\\|m-m'|\leq 1}}^{1}(-1)^{m''}\langle 1\,,m'\,;\,1\,,m-m'\,|\,2\,,m\rangle v_{-m''}\nabla_{m''}\big[x^*_{m'}x^*_{m-m'}\big]\,. \tag{29}$$

After using eq. (27) and the Leibniz product rule,

$$\nabla_{m''}\big[x^*_{m'}x^*_{m-m'}\big]=x^*_{m'}\delta_{m-m',m''}+x^*_{m-m'}\delta_{m'm''}\,. \tag{30}$$

Using $\langle 1\,,m_1\,;\,1\,,m_2\,|\,2\,,m\rangle=\langle 1\,,m_2\,;\,1\,,m_1\,|\,2\,,m\rangle$, it follows that

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(r^2Y^*_{2m}(\hat{\boldsymbol{n}})\big)=\sqrt{\frac{15}{2\pi}}\sum_{\substack{m''=-1\\|m-m''|\leq 1}}^{1}(-1)^{m''}\langle 1\,,m''\,;\,1\,,m-m''\,|\,2\,,m\rangle v_{-m''}x^*_{m-m''}\,. \tag{31}$$

In particular, using the Clebsch-Gordan coefficients given in eq. (23),

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(r^2Y^*_{2,\pm 2}(\hat{\boldsymbol{n}})\big)=-\sqrt{\frac{15}{2\pi}}v_{\mp 1}x^*_{\pm 1}\,, \tag{32}$$

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(r^2Y^*_{2,\pm 1}(\hat{\boldsymbol{n}})\big)=\sqrt{\frac{15}{4\pi}}\big[v_0x^*_{\pm 1}-v_{\mp 1}x^*_0\big]\,, \tag{33}$$

$$\vec{\boldsymbol{v}}\cdot\vec{\boldsymbol{\nabla}}\big(r^2Y^*_{20}(\hat{\boldsymbol{n}})\big)=\sqrt{\frac{5}{4\pi}}\big[2v_0x^*_0-v_1x^*_1-v_{-1}x^*_{-1}\big]\,. \tag{34}$$

In all the cases above, one is free to use eq. (7) to set $x^*_m=(-1)^m\,x_{-m}$.

3. Application to the electromagnetic dipole and quadrupole moments

In the derivation of the multipole expansion in electrodynamics, one introduces the electric multipole and magnetic multipole spherical tensors in gaussian units [cf. eqs. (9.170) and (9.172) of Jackson, where the latter is given in SI units],[2]

$$Q_{\ell m} = \int d^3x\, r^\ell\, Y^*_{\ell m}(\hat{\boldsymbol{n}})\rho(\vec{\boldsymbol{x}})\,, \tag{35}$$

$$M_{\ell m} = \frac{1}{c(\ell+1)}\int d^3x\, \bigl(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)\boldsymbol{\cdot}\vec{\boldsymbol{\nabla}}\bigl(r^\ell\, Y^*_{\ell m}(\hat{\boldsymbol{n}})\bigr)\,. \tag{36}$$

First, we consider the electric dipole moment, which corresponds to $\ell = 1$ in eq. (35). Then, in light of eqs. (6) and (11),

$$Q_{1m} = \sqrt{\frac{3}{4\pi}}\int d^3x\, x^*_m\,\rho(\vec{\boldsymbol{x}}) = (-1)^m\sqrt{\frac{3}{4\pi}}\int d^3x\, x_{-m}\,\rho(\vec{\boldsymbol{x}}) = \sqrt{\frac{3}{4\pi}}(-1)^m p_{-m}\,, \tag{37}$$

where

$$\vec{\boldsymbol{p}} = \int d^3x\, \vec{\boldsymbol{x}}\,\rho(\vec{\boldsymbol{x}})\,, \tag{38}$$

and p_m is the corresponding component of the electric dipole moment vector with respect to the spherical basis. It then follows from eq. (6) that

$$Q_{11} = -\sqrt{\frac{3}{8\pi}}\bigl(p_x - ip_y\bigr)\,, \qquad Q_{10} = \sqrt{\frac{3}{4\pi}}\,p_z\,, \qquad Q_{1,-1} = \sqrt{\frac{3}{8\pi}}\bigl(p_x + ip_y\bigr)\,, \tag{39}$$

in agreement with eq. (4.5) of Jackson.

Next, we consider the magnetic dipole moment, which corresponds to $\ell = 1$ in eq. (36). Using eq. (28),

$$M_{1m} = (-1)^m\sqrt{\frac{3}{4\pi}}\int d^3x\, \bigl(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_m = \sqrt{\frac{3}{4\pi}}\,(-1)^m m_{-m}\,, \tag{40}$$

where

$$\vec{\boldsymbol{m}} = \frac{1}{2c}\int d^3x\, \vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\,, \tag{41}$$

and m_m is the corresponding component of the magnetic dipole moment vector with respect to the spherical basis. It then follows from eq. (6) that

$$M_{11} = -\sqrt{\frac{3}{8\pi}}\bigl(m_x - im_y\bigr)\,, \qquad M_{10} = \sqrt{\frac{3}{4\pi}}\,m_z\,, \qquad M_{1,-1} = \sqrt{\frac{3}{8\pi}}\bigl(m_x + im_y\bigr)\,. \tag{42}$$

As expected, one can obtain eq. (42) from eq. (39) by replacing $\vec{\boldsymbol{p}}\to\vec{\boldsymbol{m}}$.

[2]The formula for $M_{\ell m}$ given in eq. (36) can be obtained from eq. (9.172) of Jackson by an integration by parts.

Second, we consider the electric quadrupole moment, which corresponds to $\ell = 2$ in eq. (35). Then, in light of the complex conjugate of eqs. (19)–(21),

$$Q_{2,\pm 2} = \sqrt{\frac{15}{8\pi}} \int d^3x\, x_{\mp 1}^2\, \rho(\vec{\boldsymbol{x}})\,, \tag{43}$$

$$Q_{2,\pm 1} = -\sqrt{\frac{15}{4\pi}} \int d^3x\, x_{\mp 1} x_0\, \rho(\vec{\boldsymbol{x}})\,, \tag{44}$$

$$Q_{2,0} = \sqrt{\frac{5}{4\pi}} \int d^3x\, \bigl[x_0^2 + x_1 x_{-1}\bigr]\rho(\vec{\boldsymbol{x}})\,. \tag{45}$$

Using eq. (6), and noting that the Cartesian electric quadrupole tensor, which is symmetric and traceless, is given by [cf. Jackson eq. (4.9)]:

$$Q_{ij} = \int d^3x\, \bigl(3x_i x_i - \delta_{ij}|\vec{\boldsymbol{x}}|^2\bigr)\rho(\vec{\boldsymbol{x}})\,, \qquad \text{for } i,j \in \{x,y,z\}\,, \tag{46}$$

we obtain

$$Q_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \int d^3x\, \bigl(x^2 - y^2 \mp 2ixy\bigr)\, \rho(\vec{\boldsymbol{x}}) = \frac{1}{6}\sqrt{\frac{15}{8\pi}}\bigl[Q_{xx} - Q_{yy} \mp 2iQ_{xy}\bigr]\,, \tag{47}$$

$$Q_{2,\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \int d^3x\, z(x \mp iy)\, \rho(\vec{\boldsymbol{x}}) = \mp\frac{1}{3}\sqrt{\frac{15}{8\pi}}\bigl(Q_{xz} \mp iQ_{yz}\bigr)\,, \tag{48}$$

$$Q_{2,0} = \sqrt{\frac{5}{16\pi}} \int d^3x\, \bigl[2z^2 - x^2 - y^2\bigr]\rho(\vec{\boldsymbol{x}}) = \sqrt{\frac{5}{16\pi}}\, Q_{zz}\,, \tag{49}$$

in agreement with eq. (4.6) of Jackson.

Next, we consider the magnetic quadrupole moment, which corresponds to $\ell = 2$ in eq. (36). Then, in light of the complex conjugate of eqs. (32)–(34),

$$M_{2,\pm 2} = \frac{1}{3c}\sqrt{\frac{15}{2\pi}} \int d^3x\, \bigl(\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_{\mp 1} x_{\mp 1}\,, \tag{50}$$

$$M_{2,\pm 1} = -\frac{1}{3c}\sqrt{\frac{15}{4\pi}} \int d^3x\, \Bigl[\bigl(\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_0 x_{\mp 1} + \bigl(\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_{\mp 1} x_0\Bigr]\,, \tag{51}$$

$$M_{20} = \frac{1}{3c}\sqrt{\frac{5}{4\pi}} \int d^3x\, \Bigl[2\bigl(\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_0 x_0 + \bigl(\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_1 x_1 + \bigl(\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr)_{-1} x_{-1}\Bigr]\,. \tag{52}$$

Using eq. (6), and noting that the Cartesian magnetic quadrupole tensor, which is symmetric and traceless, is given by[3]

$$M_{ij} = \frac{1}{c}\int d^3x\, \Bigl\{x'_i\bigl[\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr]_j + x'_j\bigl[\vec{\boldsymbol{x}} \times \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})\bigr]_i\Bigr\}\,, \qquad \text{for } i,j \in \{x,y,z\}\,, \tag{53}$$

[3] I have seen the magnetic quadrupole tensor defined by some authors with an overall factor of 1/2 as compared to eq. (53). If you adopt this convention, then you lose the symmetry between Q_{ij} and M_{ij}. Other authors choose to define both the electric quadrupole tensor [eq. (46)] and magnetic quadrupole tensor [eq. (53)] by multiplying the corresponding definitions by an overall factor of 1/3. Such a choice does not upset the symmetry between expressions containing Q_{ij} and M_{ij}.

we obtain

$$M_{2,\pm 2} = \frac{1}{3c}\sqrt{\frac{15}{8\pi}}\int d^3x\left\{x(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_x - y(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_y \mp i\big[x(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_y + y(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_x\big]\right\}$$

$$= \frac{1}{6}\sqrt{\frac{15}{8\pi}}\Big(M_{xx} - M_{yy} \mp 2iM_{xy}\Big)\,, \tag{54}$$

$$M_{2,\pm 1} = \mp\frac{1}{3c}\sqrt{\frac{15}{8\pi}}\int d^3x\left\{x(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_z + z(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_x \mp iy(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_z \mp iz(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_y\right\}$$

$$= \mp\frac{1}{3}\sqrt{\frac{15}{8\pi}}\Big(M_{xz} \mp iM_{yz}\Big)\,, \tag{55}$$

$$M_{20} = \frac{1}{3c}\sqrt{\frac{5}{4\pi}}\int d^3x\left\{2z(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_z - x(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_x - y(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_y\right\}$$

$$= \frac{1}{6}\sqrt{\frac{5}{4\pi}}\Big(2M_{zz} - M_{xx} - M_{yy}\Big) = \sqrt{\frac{5}{16\pi}}\,M_{zz}\,, \tag{56}$$

after making use of the traceless condition, $M_{xx} + M_{yy} + M_{zz} = 0$. Eq. (56) can also be derived by employing the identity:

$$2z(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_z - x(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_x - y(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_y = 2z(xJ_y - yJ_x) - y(zJ_x - xJ_z) - x(yJ_z - zJ_y)$$

$$= 3z(xJ_y - yJ_x) = 3z(\vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}})_z\,. \tag{57}$$

As expected, one can obtain eqs. (54)–(57) from eqs. (47)–(49) by replacing $Q_{ij} \to M_{ij}$. Moreover, this computation verifies that the normalization of M_{ij} in the definition of the magnetic quadrupole tensor given by eq. (53) is consistent with the normalization of Q_{ij} exhibited in eq. (46) [see footnote 3].

4. Extension to complex vectors and tensors

If $\vec{\boldsymbol{v}} \in \mathbb{C}^3$ is a complex vector (in which case the Cartesian coordinates v_x, v_y, $v_z \in \mathbb{C}$), then eq. (6) can still be used to define the spherical components of a complex vector $\vec{\boldsymbol{v}} \in \mathbb{C}^3$. Indeed, all equations in Section 1 remain valid with one exception. Namely, one cannot use eq. (7) to relate v_{-m} and v_m^*, as these are now independent quantities. The formulae derived in Section 2 also remain valid if $\vec{\boldsymbol{v}}$ is a complex vector, since we have been careful not to apply eq. (7) to the vector $\vec{\boldsymbol{v}}$ in deriving eq. (28) and eqs. (32)–(34).

In applications involving harmonically varying charge and current densities, where $\rho(\vec{\boldsymbol{x}}, t) = \rho(\vec{\boldsymbol{x}})e^{-i\omega t}$ and $\vec{\boldsymbol{J}}(\vec{\boldsymbol{x}}, t) = \vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})e^{-i\omega t}$ (where $\omega > 0$), the quantities $\rho(\vec{\boldsymbol{x}})$ and $\vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})$ are complex. It then follows that $\vec{\boldsymbol{p}}$ and $\vec{\boldsymbol{m}}$ [defined in eqs. (38) and (41)] are complex vectors, and Q_{ij} and M_{ij} [defined in eqs. (46) and (53)] are complex second rank Cartesian tensors. Moreover, in Section 3, we employed the results of Section 2 to the complex vector $\vec{\boldsymbol{v}} = \vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}}$. Note that we were again careful not to apply eq. (7) to $\vec{\boldsymbol{v}} = \vec{\boldsymbol{x}}\times\vec{\boldsymbol{J}}$ in obtaining the results of Section 3, which remain valid in the case of complex $\rho(\vec{\boldsymbol{x}})$ and $\vec{\boldsymbol{J}}(\vec{\boldsymbol{x}})$.

However, one must be careful in identifying the *physical* electric and magnetic multipole moments. For example, the physical time-dependent multipole moment $q_{\ell m}(t)$ is given by [cf. eq. (4.3) of Jackson]:

$$q_{\ell m}(t) = \int Y^*_{\ell m}(\hat{\boldsymbol{n}})\, r^\ell\, \rho_R(\vec{\boldsymbol{x}}, t)\, d^3x\,, \tag{58}$$

where $\rho_R(\vec{\boldsymbol{x}}, t)$ is the physical (real) time-dependent charge density. The subscript R is employed here to emphasize that $\rho_R(\vec{\boldsymbol{x}}, t)$ is a real quantity. In contrast, $q_{\ell m}(t)$ is not a real quantity if $m \neq 0$, since

$$q^*_{\ell m}(t) = (-1)^m q_{\ell,-m}(t)\,, \tag{59}$$

which follows from the corresponding property of the spherical harmonics,

$$Y^*_{\ell m}(\hat{\boldsymbol{n}}) = (-1)^m Y_{\ell,-m}(\hat{\boldsymbol{n}})\,. \tag{60}$$

Consider the case where $\rho(\vec{\boldsymbol{x}}, t) = \rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}$, and the physical charge distribution is given by $\operatorname{Re}\rho(\vec{\boldsymbol{x}}, t)$. We then define the corresponding multipole moments,[4]

$$Q_{\ell m}(t) = \int Y^*_{\ell m}(\hat{\boldsymbol{n}})\, r^\ell\, \rho(\vec{\boldsymbol{x}}, t)\, d^3x = Q_{\ell m}\, e^{-i\omega t}\,, \tag{61}$$

where

$$Q_{\ell m} \equiv \int Y^*_{\ell m}(\hat{\boldsymbol{n}})\, r^\ell\, \rho(\vec{\boldsymbol{x}})\, d^3x\,. \tag{62}$$

However, the *physical* time-dependent multipole moment is $q_{\ell m}(t)$, which is not the same as $\operatorname{Re}[Q_{\ell m}\, e^{-i\omega t}]$. Indeed, $q_{\ell m}(t)$ is complex when $m \neq 0$, whereas $\operatorname{Re}[Q_{\ell m}\, e^{-i\omega t}]$ is real.

The central issue here is the relation between $q_{\ell m}(t)$ and $Q_{\ell m}$. The real physical time-dependent charge distribution for a given harmonic frequency is given by

$$\rho_R(\vec{\boldsymbol{x}}, t) = \operatorname{Re}\left[\rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}\right]\,. \tag{63}$$

Inserting this result into eq. (58) yields

$$q_{\ell m}(t) = \int Y^*_{\ell m}(\hat{\boldsymbol{n}})\, r^\ell\, \operatorname{Re}\left[\rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}\right]\, d^3x\,. \tag{64}$$

Using eqs. (60) and (64), it follows that[5]

$$\begin{aligned} q_{\ell m}(t) + q^*_{\ell m}(t) &= \int \left[Y^*_{\ell m}(\hat{\boldsymbol{n}}) + (-1)^m Y^*_{\ell,-m}(\hat{\boldsymbol{n}})\right] r^\ell\, \operatorname{Re}\left[\rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}\right]\, d^3x \\ &= \operatorname{Re}\int \left[Y^*_{\ell m}(\hat{\boldsymbol{n}}) + (-1)^m Y^*_{\ell,-m}(\hat{\boldsymbol{n}})\right] r^\ell\, \rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}\, d^3x \\ &= \operatorname{Re}\left[Q_{\ell m}(t) + (-1)^m Q_{\ell,-m}(t)\right]\,, \end{aligned} \tag{65}$$

[4]Note that because $\rho(\vec{\boldsymbol{x}}, t)$ and $\rho(\vec{\boldsymbol{x}})$ are generally complex, neither $Q_{\ell m}(t)$ nor $Q_{\ell m}$ satisfies a condition analogous to eq. (59).

[5]Note that for any complex number z and real number c, we have $c\operatorname{Re} z = \operatorname{Re}(cz)$.

and

$$i[q_{\ell m}(t) - q^*_{\ell m}(t)] = \int i\left[Y^*_{\ell m}(\hat{\boldsymbol{n}}) - (-1)^m Y^*_{\ell,-m}(\hat{\boldsymbol{n}})\right] r^\ell \,\mathrm{Re}\left[\rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}\right]\, d^3x$$

$$= \mathrm{Re}\int i\left[Y^*_{\ell m}(\hat{\boldsymbol{n}}) - (-1)^m Y^*_{\ell,-m}(\hat{\boldsymbol{n}})\right] r^\ell \rho(\vec{\boldsymbol{x}})\, e^{-i\omega t}\, d^3x$$

$$= \mathrm{Re}\Big\{ i\left[Q_{\ell m}(t) - (-1)^m Q_{\ell,-m}(t)\right]\Big\} = -\,\mathrm{Im}\left[Q_{\ell m}(t) - (-1)^m Q_{\ell,-m}(t)\right] . \quad (66)$$

In the last step above, we noted that for any complex number z, we have $\mathrm{Re}(iz) = -\,\mathrm{Im}\, z$. Thus,

$$q_{\ell m}(t) - q^*_{\ell m}(t) = i\,\mathrm{Im}\left[Q_{\ell m}(t) - (-1)^m Q_{\ell,-m}(t)\right] . \quad (67)$$

Combining eqs. (65) and (67) yields

$$q_{\ell m}(t) = \tfrac{1}{2}\left[Q_{\ell m}(t) + (-1)^m Q^*_{\ell,-m}(t)\right] . \quad (68)$$

Using eq. (61), we can rewrite the above result as

$$q_{\ell m}(t) = \tfrac{1}{2}\left[Q_{\ell m}\, e^{-i\omega t} + (-1)^m Q^*_{\ell,-m}\, e^{i\omega t}\right] . \quad (69)$$

Eq. (69) shows us how to obtain the physical electric multipole moments for a given harmonic frequency from the $Q_{\ell m}$. Note that $q_{\ell m}(t)$ given by eq. (69) automatically satisfies eq. (59). The analogous result for the physical magnetic multipole moments also applies.

Appendix: The distinction between Cartesian tensors and spherical tensors

Consider the distinction between Cartesian tensors and spherical tensors. Under an active transformation corresponding to a three-dimensional counterclockwise rotation by an angle θ about an axis pointing along the unit vector $\hat{\boldsymbol{n}}$, the Cartesian components of a vector $\vec{\boldsymbol{v}}$ transform as

$$v_i \to v'_i = R_{ij} v_j\,, \quad (70)$$

with an implicit sum over the repeated index j,[6] where $i, j \in \{1, 2, 3\} = \{x, y, z\}$, and the matrix elements of the rotation matrix R are given by Rodrigues' rotation formula,

$$R_{ij}(\hat{\boldsymbol{n}}, \theta) = \cos\theta\, \delta_{ij} + (1 - \cos\theta) n_i n_j - \sin\theta\, \epsilon_{ijk} n_k\,. \quad (71)$$

Likewise, a second rank Cartesian tensor transforms as

$$T_{ij} \to T'_{ij} = R_{ik} R_{j\ell} T_{k\ell}\,. \quad (72)$$

In this case, T_{ij} is said to transform reducibly under rotations. This means that for any second rank Cartesian tensor, one can decompose it into smaller objects, each of which

[6] In these notes, we typically employ the Einstein summation convention where a pair of repeated indices are implicitly summed over.

transforms separately under rotations. In the case of T_{ij}, one can always write:

$$T_{ij} = S_{ij} + A_{ij} + c\delta_{ij}\,, \tag{73}$$

where S_{ij} is a traceless symmetric tensor [i.e., $\delta_{ij}S_{ij} = 0$] and A_{ij} is an antisymmetric tensor. A little algebra shows that:

$$S_{ij} = \tfrac{1}{2}\big(T_{ij}+T_{ji}\big)-\tfrac{1}{3}\delta_{ij}\,\mathrm{Tr}\,T\,, \qquad A_{ij} = \tfrac{1}{2}\big(T_{ij}-T_{ji}\big)\,, \qquad c = \tfrac{1}{3}\,\mathrm{Tr}\,T = \tfrac{1}{3}\delta_{ij}T_{ij}\,. \tag{74}$$

If one now defines $a_k \equiv \epsilon_{ijk}A_{jk}$, then one can verify that under a rotation,

$$S_{ij} \to S'_{ij} = R_{ik}R_{j\ell}S_{k\ell}\,, \qquad a_i \to a'_i = R_{ij}a_j\,, \qquad c \to c' = c\,. \tag{75}$$

That is S_{ij}, which has five independent components, transforms under rotations like a second rank tensor, a_k, which has three independent components, transforms like a vector, and $c\,\delta_{ij}$ transforms as a scalar (since δ_{ij} is an *invariant* tensor under rotations [i.e., $\delta_{ij} \to \delta'_{ij} = \delta_{ij}$] as a consequence of the fact that R is an orthogonal matrix). One cannot decompose T_{ij} further, which means that each of the pieces S_{ij}, a_k and c, transforms *irreducibly* under rotations.

An example of a spherical tensor of rank ℓ is the spherical harmonic $Y_{\ell m}(\boldsymbol{\hat{n}})$. The components of this rank ℓ spherical tensor are indicated by $m = -\ell, \ell+1, \ldots, \ell-1, \ell$. That is, a spherical tensor of rank ℓ has $2\ell+1$ components. Consider a generic spherical tensor of rank ℓ, denoted by $Q_{\ell m}$. One can show that all spherical tensors transform irreducibly under a rotation. Specifically, $Q_{\ell m}$ cannot be further decomposed in a way similar to that of eq. (73). For example, Q_{00} is a scalar under rotations, whereas Q_{1m} is a vector under rotations with three components ($m = -1, 0, 1$). The relation between these components and the rectangular (Cartesian) components of a vector are precisely those given in eq. (6). The $\ell = 2$ spherical tensor Q_{2m} has 5 independent components, and it also transforms irreducibly under rotations. Indeed, in light of eqs. (47)–(49), the Q_{2m} ($m = -2, -1, 0, 1, 2$) can be re-expressed in terms of the five independent components of the traceless symmetric second rank tensor Q_{ij} [c.f. eq. (46)], which like S_{ij} in eq. (75) transforms irreducibly under rotations.

Although we will not need it in these notes, one can write down the transformation law for a rank ℓ spherical tensor $Q_{\ell m}$ under an active rotation $R(\boldsymbol{\hat{n}}, \theta)$. It is given by[7]

$$Q_{\ell m} \to Q'_{\ell m} = \sum_{m'} Q_{\ell m'}\mathcal{D}^{(\ell)\,*}_{mm'}(\boldsymbol{\hat{n}}, \theta)\,, \tag{76}$$

where the unitary matrix $\mathcal{D}^{(\ell)}(\boldsymbol{\hat{n}}, \theta)$ is called the Wigner $\mathcal{D}$-matrix.

The presence of the complex conjugation $(*)$ in eq. (76) can be understood as follows. The correct way to sum over two spherical basis labels is by summing m against $-m$, with an extra factor of $(-1)^m$ inserted, as indicated by eq. (13). Consequently, the correct form for the transformation of a spherical tensor of rank ℓ under an active rotation $R(\boldsymbol{\hat{n}}, \theta)$ is

$$(-1)^m Q_{\ell,-m} \to (-1)^m Q'_{\ell,-m} = \sum_{m'} (-1)^{m'} Q_{\ell,-m'}\mathcal{D}^{(\ell)}_{mm'}(\boldsymbol{\hat{n}}, \theta)\,. \tag{77}$$

[7]Here, we follow the conventions advocated by Kurt Gottfried and Tung-Mow Yan, *Quantum Mechanics: Fundamentals*, Second Edition (Springer-Verlag, New York, NY, USA, 2003) in Section 7.6.

That is,

$$Q'_{\ell,-m} = \sum_{m'} (-1)^{m'-m} Q_{\ell,-m'} \mathcal{D}^{(\ell)}_{mm'}(\hat{\boldsymbol{n}}, \theta) \,. \tag{78}$$

Relabeling by $m \to -m$ and $m' \to -m'$, it follows that

$$Q'_{\ell m} = \sum_{m'} (-1)^{m-m'} Q_{\ell m} \mathcal{D}^{(\ell)}_{-m,-m'}(\hat{\boldsymbol{n}}, \theta) \,. \tag{79}$$

Finally, using eq. (98), one can derive the following identity,

$$\mathcal{D}^{(\ell)*}_{mm'}(\hat{\boldsymbol{n}}, \theta) = \mathcal{D}^{(\ell)}_{m'm}(\hat{\boldsymbol{n}}, -\theta) = (-1)^{m-m'} \mathcal{D}^{(\ell)}_{-m,-m'}(\hat{\boldsymbol{n}}, \theta) \,. \tag{80}$$

Hence, we end up with

$$Q'_{\ell m} = \sum_{m'} Q_{\ell m'} \mathcal{D}^{(\ell)\,*}_{mm'}(\hat{\boldsymbol{n}}, \theta) \,, \tag{81}$$

as quoted in eq. (76).

It is instructive to write out eq. (76) explicitly for the case of $\ell = 1$. The explicit form for $\mathcal{D}^{(1)}(\hat{\boldsymbol{n}}, \theta)$ [derived in the Bonus Material below] is:

$$\mathcal{D}^{(1)}(\hat{\boldsymbol{n}}, \theta) = \begin{pmatrix} 1 - \frac{1}{2}(1+\hat{n}_3^2)(1-c_\theta) - i\hat{n}_3 s_\theta & -\frac{1}{\sqrt{2}}(\hat{n}_1 - i\hat{n}_2)\big[\hat{n}_3(1-c_\theta) + is_\theta\big] & -\frac{1}{2}(\hat{n}_1 - i\hat{n}_2)^2(1-c_\theta) \\ -\frac{1}{\sqrt{2}}(\hat{n}_1 + i\hat{n}_2)\big[\hat{n}_3(1-c_\theta) + is_\theta\big] & 1 - (1-\hat{n}_3^2)(1-c_\theta) & \frac{1}{\sqrt{2}}(\hat{n}_1 - i\hat{n}_2)\big[\hat{n}_3(1-c_\theta) - is_\theta\big] \\ -\frac{1}{2}(\hat{n}_1 + i\hat{n}_2)^2(1-c_\theta) & \frac{1}{\sqrt{2}}(\hat{n}_1 + i\hat{n}_2)\big[\hat{n}_3(1-c_\theta) - is_\theta\big] & 1 - \frac{1}{2}(1+\hat{n}_3^2)(1-c_\theta) + i\hat{n}_3 s_\theta \end{pmatrix}, \tag{82}$$

where $s_\theta \equiv \sin\theta$ and $c_\theta \equiv \cos\theta$. Note that $\hat{n}_1^2 + \hat{n}_2{}^2 + \hat{n}_3^2 = 1$. We can apply eq. (76) to $Y_{1m}(\vec{\boldsymbol{n}})$, which is a rank-one spherical vector. In particular, under an active rotation, $\hat{\boldsymbol{n}} \to \hat{\boldsymbol{n}}\,' = R\hat{\boldsymbol{n}}$, where the matrix elements of R are given in eq. (71), it follows that[8]

$$Y_{1m}(R\hat{\boldsymbol{n}}) = \sum_{m'} \mathcal{D}^{(1)*}_{mm'}(R) Y_{1m'}(\hat{\boldsymbol{n}}) \,. \tag{83}$$

Indeed, after relating $Y_{1m'}(\hat{\boldsymbol{n}})$ to x_m via eq. (11), and relating x_m to the Cartesian coordinates of $\vec{\boldsymbol{x}}$ via eq. (6), one can verify explicitly using eqs. (71) and (82) that eq. (83) is equivalent to the equation $\hat{\boldsymbol{n}}\,' = R\hat{\boldsymbol{n}}$.

In particular, under an active rotation R, the Cartesian components of a vector transform as $v_i \to R_{ij} v_j$, where R_{ij} is given by eq. (71), whereas the spherical components of a vector transform as $v_m \to \mathcal{D}^{(1)*}_{mm'}(R) v_{m'}$. In light of eq. (6), we have

$$\begin{pmatrix} v_1 \\ v_0 \\ v_{-1} \end{pmatrix} = M \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \qquad \text{where } M = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix}. \tag{84}$$

Note that M is unitary, i.e., $M^{-1} = M^\dagger$. Then, under a rotation R,

$$\begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = M^\dagger \begin{pmatrix} v_1 \\ v_0 \\ v_{-1} \end{pmatrix} \longrightarrow M^\dagger \mathcal{D}^{(1)*} \begin{pmatrix} v_1 \\ v_0 \\ v_{-1} \end{pmatrix} = M^\dagger \mathcal{D}^{(1)*} M \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \tag{85}$$

[8] Another derivation of eq. (83) can be found on p. 312 of Kurt Gottfried and Tung-Mow Yan, *Quantum Mechanics: Fundamentals*, Second Edition (Springer-Verlag, New York, NY, USA, 2003).

after applying eq. (84) in the last step above. Therefore, we can conclude that the rotation matrix R is given by

$$R = M^\dagger \mathcal{D}^{(1)*} M = \begin{pmatrix} c_\theta + \hat{n}_1^2(1-c_\theta) & \hat{n}_1\hat{n}_2(1-c_\theta) - \hat{n}_3 s_\theta & \hat{n}_1\hat{n}_3(1-c_\theta) + \hat{n}_2 s_\theta \\ \hat{n}_1\hat{n}_2(1-c_\theta) + \hat{n}_3 s_\theta & c_\theta + \hat{n}_2^2(1-c_\theta) & \hat{n}_2\hat{n}_3(1-c_\theta) - \hat{n}_1 s_\theta \\ \hat{n}_1\hat{n}_3(1-c_\theta) - \hat{n}_2 s_\theta & \hat{n}_2\hat{n}_3(1-c_\theta) + \hat{n}_1 s_\theta & c_\theta + \hat{n}_3^2(1-c_\theta) \end{pmatrix}, \tag{86}$$

which coincides with eq. (71) [after employing a Mathematica calculation to perform the matrix multiplications using eqs. (82) and (84)]. Equivalently, one could have used eq. (86) to deduce the form of $\mathcal{D}^{(1)}(\hat{\boldsymbol{n}}, \theta)$,

$$\mathcal{D}^{(1)}(\hat{\boldsymbol{n}}, \theta) = \big[M R(\hat{\boldsymbol{n}}, \theta) M^\dagger\big]^*, \tag{87}$$

in terms of the rotation matrix given by eq. (71).

<u>*BONUS MATERIAL:*</u> The Wigner $\mathcal{D}^{(\ell)}$ matrix

In order to define the Wigner $\mathcal{D}^{(\ell)}$ matrix, we will first examine finite-dimensional matrix representations of the operator,[9] $\vec{\boldsymbol{L}} \equiv -i\vec{\boldsymbol{x}} \times \vec{\boldsymbol{\nabla}}$. Since the spherical harmonics $Y_{\ell m}(\hat{\boldsymbol{n}})$ are a complete set of eigenstates defined on the sphere, we can form, for a fixed value of ℓ, three $(2\ell+1) \times (2\ell+1)$ matrices by defining their matrix elements as follows

$$\vec{\boldsymbol{L}}^{(\ell)}_{mm'} = \int Y^*_{\ell m}(\hat{\boldsymbol{n}}) \vec{\boldsymbol{L}}\, Y_{\ell m'}(\hat{\boldsymbol{n}})\, d\Omega\,, \quad \text{where } m, m' \in \{-\ell, -\ell+1, \ldots, \ell-1, \ell\}. \tag{88}$$

For example, using $L_z\, Y_{\ell m}(\hat{\boldsymbol{n}}) = m Y_{\ell m}(\hat{\boldsymbol{n}})$ and the orthogonality properties of the spherical harmonics,

$$\int Y^*_{\ell' m'}(\hat{\boldsymbol{n}})\, Y_{\ell m}(\hat{\boldsymbol{n}})\, d\Omega = \delta_{\ell\ell'}\delta_{mm'}\,, \tag{89}$$

it follows that the z-component of $\vec{\boldsymbol{L}}^{(\ell)}_{mm'}$ is a diagonal $(2\ell+1) \times (2\ell+1)$ matrix with matrix elements

$$\big(L^{(\ell)}_{mm'}\big)_z = m\delta_{mm'}\,. \tag{90}$$

To evaluate the x and y components of $\vec{\boldsymbol{L}}^{(\ell)}_{mm'}$, we write $L_\pm \equiv L_x \pm i L_y$, which implies that

$$L_x = \tfrac{1}{2}(L_+ + L_-)\,, \qquad L_y = -\tfrac{1}{2}i(L_+ - L_-)\,. \tag{91}$$

Then, after making use of

$$L_+ Y_{\ell m}(\hat{\boldsymbol{n}}) = \sqrt{(\ell-m)(\ell+m+1)}\, Y_{\ell, m+1}(\hat{\boldsymbol{n}})\,, \tag{92}$$

$$L_- Y_{\ell m}(\hat{\boldsymbol{n}}) = \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell, m-1}(\hat{\boldsymbol{n}})\,, \tag{93}$$

we obtain

$$L_x Y_{\ell m}(\hat{\boldsymbol{n}}) = \tfrac{1}{2}\big[\sqrt{(\ell-m)(\ell+m+1)}\, Y_{\ell, m+1}(\hat{\boldsymbol{n}}) + \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell, m-1}(\hat{\boldsymbol{n}})\big], \tag{94}$$

$$L_y Y_{\ell m}(\hat{\boldsymbol{n}}) = -\tfrac{1}{2}i\big[\sqrt{(\ell-m)(\ell+m+1)}\, Y_{\ell, m+1}(\hat{\boldsymbol{n}}) - \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell, m-1}(\hat{\boldsymbol{n}})\big]. \tag{95}$$

[9] For detailed properties of $\vec{\boldsymbol{L}}$, see the class handout entitled: *Properties of the differential operator* $\vec{\boldsymbol{L}}$.

Using the above results in eq. (88),

$$(L^{(\ell)}_{mm'})_x = \tfrac{1}{2}\big[\sqrt{(\ell-m)(\ell+m+1)}\,\delta_{m',m+1} + \sqrt{(\ell+m)(\ell-m+1)}\,\delta_{m,m-1}\big], \tag{96}$$

$$(L^{(\ell)}_{mm'})_y = -\tfrac{1}{2}i\big[\sqrt{(\ell-m)(\ell+m+1)}\,\delta_{m',m+1} - \sqrt{(\ell+m)(\ell-m+1)}\,\delta_{m,m-1}\big], \tag{97}$$

The Wigner $\mathcal{D}^{(\ell)}$-matrix is a $(2\ell+1)\times(2\ell+1)$ matrix that is defined as

$$\mathcal{D}^{(\ell)}(\boldsymbol{\hat{n}},\theta) \equiv \exp\big[-i\theta\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(\ell)}\big]\,. \tag{98}$$

Let us evaluate explicitly the case of $\ell = 1$. Then, eqs. (90), (96) and (97) yield

$$L^{(1)}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0\end{pmatrix}\,,\qquad L^{(1)}_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0\end{pmatrix}\,,\qquad L^{(1)}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1\end{pmatrix}\,, \tag{99}$$

and

$$\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)} = \begin{pmatrix} \hat{n}_3 & \frac{\hat{n}_1 - i\hat{n}_2}{\sqrt{2}} & 0 \\ \frac{\hat{n}_1 + i\hat{n}_2}{\sqrt{2}} & 0 & \frac{\hat{n}_1 - i\hat{n}_2}{\sqrt{2}} \\ 0 & \frac{\hat{n}_1 + i\hat{n}_2}{\sqrt{2}} & -\hat{n}_3 \end{pmatrix}\,. \tag{100}$$

It follows that

$$(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)})^2 = \begin{pmatrix} \frac{1}{2}(1+\hat{n}_3^2) & \frac{\hat{n}_3(\hat{n}_1 - i\hat{n}_2)}{\sqrt{2}} & \frac{1}{2}(\hat{n}_1 - i\hat{n}_2)^2 \\ \frac{\hat{n}_3(\hat{n}_1 + i\hat{n}_2)}{\sqrt{2}} & 1-\hat{n}_3^2 & -\frac{\hat{n}_3(\hat{n}_1 - i\hat{n}_2)}{\sqrt{2}} \\ \frac{1}{2}(\hat{n}_1 + i\hat{n}_2)^2 & -\frac{\hat{n}_3(\hat{n}_1 + i\hat{n}_2)}{\sqrt{2}} & \frac{1}{2}(1+\hat{n}_3^2) \end{pmatrix}\,, \tag{101}$$

$$(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)})^3 = \boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\,. \tag{102}$$

Hence,

$$\begin{aligned}\exp\big[-i\theta\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\big] &= \mathbb{1} - i\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\left[\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots\right] + \big(-i\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\big)^2\left[\theta^2 - \frac{\theta^4}{4!} + \frac{\theta^6}{6!} - \cdots\right] \\ &= \mathbb{1} - i\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\sin\theta - \big(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\big)^2(1-\cos\theta)\,,\end{aligned} \tag{103}$$

where $\mathbb{1}$ is the 3×3 identity matrix. That is,

$$\mathcal{D}^{(1}(\boldsymbol{\hat{n}},\theta) = \mathbb{1} - i\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\sin\theta - \big(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\big)^2(1-\cos\theta)\,, \tag{104}$$

which coincides with the result quoted in eq. (82).

The $\mathcal{D}^{(\ell)}$-matrices beyond $\ell = 1$ can be obtained from eq. (98), although their explicit forms are rather complicated. Further details can be found in the references below. It is noteworthy that, excluding the reference to Jackson, all the references cited below are books that focus on the properties of angular momentum in quantum mechanics. However, nothing in these notes depends on quantum mechanics. The mathematics underlying the material in these notes are closely associated with the properties of the rotation group SO(3) and its matrix representations.

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