Vectors and Tensors in the Spherical Basis

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Abstract

Vectors and tensors are usually introduced with respect to a Cartesian basis. However, Cartesian tensors of rank two and higher do not transform irreducibly under rotations. This motivates the introduction of the spherical basis. In these notes, the spherical basis is discussed first in the context of a vector quantity (which corresponds to a rank-one spherical tensor). For tensors of higher rank, the spherical tensors are identified as the objects that transform irreducibly under rotations. The corresponding transformation laws are derived both for the spherical components of a vector and for the components of a spherical tensor of arbitrary rank ℓ.

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,

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

We can rewrite eq. (6) in matrix form:

$$\begin{pmatrix} v_1 \\ v_0 \\ v_{-1} \end{pmatrix} = M \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix}, \qquad \text{where } M = \begin{pmatrix} -\frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix}. \tag{7}$$

Note that M is unitary, i.e., $M^{-1} = M^\dagger$.

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

$$v_m^* = (-1)^m\, v_{-m}\,, \qquad \text{for } m = -1, 0, 1. \tag{8}$$

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

$$\vec{\boldsymbol{v}} = \sum_m (-1)^m v_{-m} \hat{\boldsymbol{e}}_m = \sum_m (-1)^m v_m \hat{\boldsymbol{e}}_{-m}\,, \tag{9}$$

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. (9) correspond simply to relabeling $m \to -m$ in the summation. One can check that inserting the expressions of eqs. (3) and (6) into eq. (9) reproduces eq. (2).

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

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

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

$$\vec{\boldsymbol{x}} = (x, y, z) = r(\sin\theta\cos\phi\,,\, \sin\theta\sin\phi\,,\, \cos\theta) = r\,\hat{\boldsymbol{n}}\,, \tag{11}$$

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

$$x_m = \sqrt{\frac{4\pi}{3}}\, r\, Y_{1m}(\hat{\boldsymbol{n}})\,, \qquad \text{for } m = -1, 0, 1. \tag{12}$$

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 Section 5.

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

$$\vec{\boldsymbol{v}} \boldsymbol{\cdot} \vec{\boldsymbol{w}} = \sum_{i=1}^{3} v_i w_i\,. \tag{13}$$

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

$$\vec{\boldsymbol{v}} \boldsymbol{\cdot} \vec{\boldsymbol{w}} = \sum_m (-1)^m v_m w_{-m} = \sum_m (-1)^m v_{-m} w_m\,. \tag{14}$$

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. (13).

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

$$\nabla_1 = -\frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right), \qquad \nabla_0 = \frac{\partial}{\partial z}, \qquad \nabla_{-1} = \frac{1}{\sqrt{2}}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right). \tag{15}$$

One can check that this definition is consistent by observing that

$$\begin{aligned}\vec{\boldsymbol{\nabla}}\boldsymbol{\cdot}\vec{\boldsymbol{v}} = \sum_m (-1)^m \nabla_m v_{-m} &= \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)(v_x - iv_y) + \frac{1}{2}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)(v_x + iv_y) + \frac{\partial v_z}{\partial z} \\ &= \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}, \end{aligned} \tag{16}$$

as expected.

One might wonder how a relation such as eq. (12) extends to the spherical harmonics with higher values of ℓ. As an example, consider the spherical harmonics with $\ell = 2$,

$$Y_{2,\pm 2}(\hat{\boldsymbol{n}}) = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta e^{\pm 2i\phi} = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\frac{(x \pm iy)^2}{r^2}, \tag{17}$$

$$Y_{2,\pm 1}(\hat{\boldsymbol{n}}) = \mp\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta e^{\pm i\phi} = \mp\sqrt{\frac{15}{8\pi}}\frac{z(x \pm iy)}{r^2}, \tag{18}$$

$$Y_{20}(\hat{\boldsymbol{n}}) = \frac{1}{2}\sqrt{\frac{5}{4\pi}}(3\cos^2\theta - 1) = \frac{1}{2}\sqrt{\frac{5}{4\pi}}\,\frac{2z^2 - x^2 - y^2}{r^2}. \tag{19}$$

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

$$r^2 Y_{2,\pm 2}(\hat{\boldsymbol{n}}) = \sqrt{\frac{15}{8\pi}}x_{\pm 1}^2, \tag{20}$$

$$r^2 Y_{2,\pm 1}(\hat{\boldsymbol{n}}) = \sqrt{\frac{15}{4\pi}}x_{\pm 1}x_0, \tag{21}$$

$$r^2 Y_{20}(\hat{\boldsymbol{n}}) = \sqrt{\frac{5}{4\pi}}\left(x_0^2 + x_1 x_{-1}\right). \tag{22}$$

Eqs. (20)–(22) can be summarized by the following formula:

$$r^2 Y_{2m}(\hat{\boldsymbol{n}}) = \sqrt{\frac{15}{8\pi}} \sum_{\substack{m'=-1 \\ |m-m'|\leq 1}}^{1} \langle 1\,, m'\,;\, 1\,, m-m'\,|\,2\,, m\rangle x_{m'}x_{m-m'}, \tag{23}$$

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

$$\langle 1, 1; 1, 1 \mid 2, 2\rangle = 1, \tag{24}$$

$$\langle 1,1;1,0 \mid 2,1\rangle = \langle 1,0;1,1 \mid 2,1\rangle = \frac{1}{\sqrt{2}}\,, \tag{25}$$

$$\langle 1,1;1,-1 \mid 2,0\rangle = \langle 1,-1;1,1 \mid 2,0\rangle = \frac{1}{\sqrt{6}}\,, \tag{26}$$

$$\langle 1,0;1,0 \mid 2,0\rangle = \sqrt{\frac{2}{3}}\,, \tag{27}$$

$$\langle 1,-1;1,0 \mid 2,-1\rangle = \langle 1,0;1,-1 \mid 2,-1\rangle = \frac{1}{\sqrt{2}}\,, \tag{28}$$

$$\langle 1,-1;1,-1 \mid 2,-2\rangle = 1\,. \tag{29}$$

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

$$\langle 1\,,m'\,;\,1\,,m-m'\,|\,2\,,m\rangle = \sqrt{\frac{(2+m)!(2-m)!}{6(1+m')!(1-m')!(1+m-m')!(1-m+m')!}}\,. \tag{30}$$

One can also invert eq. (23) to obtain:[1]

$$x_{m_1}x_{m_2} = \tfrac{1}{3}(-1)^{m_1}r^2\,\delta_{m_2,-m_1} + \sqrt{\frac{8\pi}{15}}\,r^2 \sum_{\substack{m=-2\\ m_1+m_2=m}}^{2} \langle 1\,,m_1\,;\,1\,,m_2\,|\,2\,,m\rangle Y_{2m}(\hat{\boldsymbol{n}})\,, \tag{31}$$

Indeed, the Clebsch-Gordan coefficients appearing in eq. (31) vanish unless $m_1+m_2=m$.

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. (8) to relate v_{-m} and v^*_m, as these are now independent quantities.

2. Transformation law for a vector under an active rotation

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 Cartesian vector $\vec{\boldsymbol{v}}$ transform as

$$v_i \to v'_i = R_{ij}v_j\,, \tag{32}$$

with an implicit sum over the repeated index j,[2] 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,

$$R_{ij}(\hat{\boldsymbol{n}},\theta) = \cos\theta\,\delta_{ij} + (1-\cos\theta)\hat{n}_i\hat{n}_j - \sin\theta\,\epsilon_{ijk}\hat{n}_k\,. \tag{33}$$

[1] Eq. (31) 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 Section 5 for a discussion of spherical tensors in the context of irreducible representations of the rotation group.

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

Eq. (33) can be derived as follows. We begin with the generators of the SO(3) Lie algebra, which satisfy the commutation relations,

$$\big[S_i\,,\,S_j\big] = i\epsilon_{ijk}S_k\,. \tag{34}$$

The SO(3) Lie algebra generators S_i can be represented by the 3×3 real antisymmetric matrices, where the matrix elements of the matrices $\vec{\boldsymbol{S}} = (S_1, S_2, S_3)$ are given by

$$(S_i)_{jk} = -i\epsilon_{ijk}\,, \tag{35}$$

and ϵ_{ijk} is the Levi-Civita tensor. More explicitly,

$$S_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \qquad S_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}, \qquad S_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{36}$$

This three-dimensional representation is known as the adjoint representation of the SO(3) Lie algebra. One can then identify the matrix R by exponentiating the adjoint representation of the SO(3) Lie algebra. This yields the three-dimensional representation of the SO(3) Lie group, which corresponds to 3×3 orthogonal matrices of unit determinant,

$$R = \exp\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)\,, \tag{37}$$

We can compute R by way of the Taylor series of $\exp\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)$. Starting with

$$-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S} = \theta\begin{pmatrix} 0 & -\hat{n}_3 & \hat{n}_2 \\ \hat{n}_3 & 0 & -\hat{n}_1 \\ -\hat{n}_2 & \hat{n}_1 & 0 \end{pmatrix}, \tag{38}$$

it follows that

$$\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)^2 = \theta^2\begin{pmatrix} \hat{n}_1^2-1 & \hat{n}_1\hat{n}_2 & \hat{n}_1\hat{n}_3 \\ \hat{n}_1\hat{n}_2 & \hat{n}_2^2-1 & \hat{n}_2\hat{n}_3 \\ \hat{n}_1\hat{n}_2 & \hat{n}_2\hat{n}_3 & \hat{n}_3^2-1 \end{pmatrix}, \qquad \big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)^3 = -\theta^2\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)\,, \tag{39}$$

after making use of $\hat{n}_1^2+\hat{n}_2^2+\hat{n}_3^2 = 1$. Hence,

$$\begin{aligned} R = \exp\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big) &= \mathbb{1} + \frac{1}{\theta}\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)\Big[\theta - \frac{\theta^3}{3!} + \cdots\Big] + \frac{1}{\theta^2}\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\big)^2\Big[\frac{\theta^2}{2!} - \frac{\theta^4}{4!} + \cdots\Big] \\ &= \mathbb{1} + \sin\theta\begin{pmatrix} 0 & -\hat{n}_3 & \hat{n}_2 \\ \hat{n}_3 & 0 & -\hat{n}_1 \\ -\hat{n}_2 & \hat{n}_1 & 0 \end{pmatrix} + \big[1-\cos\theta\big]\begin{pmatrix} \hat{n}_1^2-1 & \hat{n}_1\hat{n}_2 & \hat{n}_1\hat{n}_3 \\ \hat{n}_1\hat{n}_2 & \hat{n}_2^2-1 & \hat{n}_2\hat{n}_3 \\ \hat{n}_1\hat{n}_2 & \hat{n}_2\hat{n}_3 & \hat{n}_3^2-1 \end{pmatrix} \\ &= \mathbb{1}\cos\theta - \sin\theta\begin{pmatrix} 0 & \hat{n}_3 & -\hat{n}_2 \\ -\hat{n}_3 & 0 & \hat{n}_1 \\ \hat{n}_2 & -\hat{n}_1 & 0 \end{pmatrix} + \big[1-\cos\theta\big]\begin{pmatrix} \hat{n}_1^2 & \hat{n}_1\hat{n}_2 & \hat{n}_1\hat{n}_3 \\ \hat{n}_1\hat{n}_2 & \hat{n}_2^2 & \hat{n}_2\hat{n}_3 \\ \hat{n}_1\hat{n}_2 & \hat{n}_2\hat{n}_3 & \hat{n}_3^2 \end{pmatrix}, \end{aligned} \tag{40}$$

where $\mathbb{1}$ is the 3×3 identity matrix. This result coincides with that of eq. (33).

It is convenient transform to a new basis in which S_3 is diagonal. The eigenvalues of S_3 are $+1$, 0, and -1. The columns of the diagonalization matrix consist of the corresponding eigenvectors of S_3, which can be chosen to be orthonormal.[3] The resulting unitary diagonalization matrix P is given by

$$P = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}, \tag{41}$$

where $P^\dagger S_3 P$, which we shall henceforth denote by $L_z^{(1)}$, is diagonal. Note that $P = M^\mathsf{T}$, where the matrix M transforms the Cartesian coordinates of a vector into its spherical coordinates [cf. eq. (6)]. This is not an accident, as we shall shortly see.

Likewise, we can work out the corresponding expressions for S_1 and S_2 in a basis where S_3 is diagonal. Denoting these quantities by $L_x^{(1)}$ and $L_y^{(1)}$, respectively, we obtain

$$L_x^{(1)} \equiv P^\dagger S_1 P = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{42}$$

$$L_y^{(1)} \equiv P^\dagger S_2 P = \frac{i}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \tag{43}$$

$$L_z^{(1)} \equiv P^\dagger S_3 P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{44}$$

One can also obtain an expression for the rotation matrix $R(\hat{\boldsymbol{n}}, \theta)$ given by eq. (37) in a basis in which S_3 is diagonal, which we denote below by $\mathcal{D}^{(1)}(\hat{\boldsymbol{n}}, \theta)$,

$$\mathcal{D}^{(1)}(\hat{\boldsymbol{n}}, \theta) = P^\dagger R P = P^\dagger \exp\bigl(-i\theta \hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{S}\bigr) P = \exp\bigl(-i\theta \hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{\boldsymbol{L}}^{(1)}\bigr). \tag{45}$$

To determine $\exp\bigl(-i\theta \hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{\boldsymbol{L}}^{(1)}\bigr)$, we first evaluate

$$\hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{\boldsymbol{L}}^{(1)} = \begin{pmatrix} \hat{n}_3 & \frac{\hat{n}_1 - i\hat{n}_2}{\sqrt{2}} & 0 \\ \frac{\hat{n}_1 + i\hat{n}_2}{\sqrt{2}} & 0 & \frac{\hat{n}_1 - i\hat{n}_2}{\sqrt{2}} \\ 0 & \frac{\hat{n}_1 + i\hat{n}_2}{\sqrt{2}} & -\hat{n}_3 \end{pmatrix}. \tag{46}$$

It follows that

$$(\hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{\boldsymbol{L}}^{(1)})^2 = \begin{pmatrix} \frac{1}{2}(1+\hat{n}_3^2) & \frac{\hat{n}_3(\hat{n}_1 - i\hat{n}_2)}{\sqrt{2}} & \frac{1}{2}(\hat{n}_1 - i\hat{n}_2)^2 \\ \frac{\hat{n}_3(\hat{n}_1 + i\hat{n}_2)}{\sqrt{2}} & 1 - \hat{n}_3^2 & -\frac{\hat{n}_3(\hat{n}_1 - i\hat{n}_2)}{\sqrt{2}} \\ \frac{1}{2}(\hat{n}_1 + i\hat{n}_2)^2 & -\frac{\hat{n}_3(\hat{n}_1 + i\hat{n}_2)}{\sqrt{2}} & \frac{1}{2}(1+\hat{n}_3^2) \end{pmatrix}, \qquad (\hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{\boldsymbol{L}}^{(1)})^3 = \hat{\boldsymbol{n}} \boldsymbol{\cdot} \vec{\boldsymbol{L}}^{(1)}. \tag{47}$$

[3]Since S_3 commutes with its hermitian conjugate, the diagonalization matrix P can be chosen to be unitary, i.e., $P^{-1} = P^\dagger$.

Hence,

$$\exp\bigl[-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\bigr] = \mathbb{1} - i\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\left[\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots\right] + \bigl(-i\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\bigr)^2\left[\theta^2 - \frac{\theta^4}{4!} + \frac{\theta^6}{6!} - \cdots\right]$$

$$= \mathbb{1} - i\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\sin\theta - \bigl(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\bigr)^2(1-\cos\theta)\,, \tag{48}$$

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

$$\mathcal{D}^{(1}(\hat{\boldsymbol{n}},\theta) = \mathbb{1} - i\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\sin\theta - \bigl(\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(1)}\bigr)^2(1-\cos\theta)\,, \tag{49}$$

More explicitly,

$$\mathcal{D}^{(1)}(\hat{\boldsymbol{n}},\theta) = P^\dagger R P = P^\dagger\exp\bigl(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{S}\bigr)P$$

$$= \begin{pmatrix} 1-\frac{1}{2}(1+\hat{n}_3^2)(1-c_\theta) - i\hat{n}_3 s_\theta & -\frac{1}{\sqrt{2}}(\hat{n}_1 - i\hat{n}_2)\bigl[\hat{n}_3(1-c_\theta)+is_\theta\bigr] & -\frac{1}{2}(\hat{n}_1-i\hat{n}_2)^2(1-c_\theta) \\ -\frac{1}{\sqrt{2}}(\hat{n}_1+i\hat{n}_2)\bigl[\hat{n}_3(1-c_\theta)+is_\theta\bigr] & 1-(1-\hat{n}_3^2)(1-c_\theta) & \frac{1}{\sqrt{2}}(\hat{n}_1-i\hat{n}_2)\bigl[\hat{n}_3(1-c_\theta)-is_\theta\bigr] \\ -\frac{1}{2}(\hat{n}_1+i\hat{n}_2)^2(1-c_\theta) & \frac{1}{\sqrt{2}}(\hat{n}_1+i\hat{n}_2)\bigl[\hat{n}_3(1-c_\theta)-is_\theta\bigr] & 1-\frac{1}{2}(1+\hat{n}_3^2)(1-c_\theta)+i\hat{n}_3 s_\theta \end{pmatrix}. \tag{50}$$

Using eq. (32), we can determine the components of $\vec{\boldsymbol{v}}$ in the basis where S_3 is diagonal. Starting from $\vec{\boldsymbol{v}}\,' = R\vec{\boldsymbol{v}}$, it follows that

$$P^\dagger\vec{\boldsymbol{v}}\,' = P^\dagger R P P^\dagger\vec{\boldsymbol{v}} = \mathcal{D}^{(1)}(\hat{\boldsymbol{n}},\theta)P^\dagger\vec{\boldsymbol{v}}\,. \tag{51}$$

Using eq. (41), it follows that

$$(P^\dagger\vec{\boldsymbol{v}})_1 = -\frac{1}{\sqrt{2}}\Bigl(v_x - iv_y\Bigr)\,,\qquad (P^\dagger\vec{\boldsymbol{v}})_0 = v_z\,,\qquad (P^\dagger\vec{\boldsymbol{v}})_- = \frac{1}{\sqrt{2}}\Bigl(v_x + iv_y\Bigr)\,, \tag{52}$$

where we have numbered the components of the vector in the basis where S_3 is diagonal by $+1$, 0, -1, respectively. Comparing this result with eq. (6), we see that for a vector $\vec{\boldsymbol{v}}$ whose Cartesian components are real,

$$v_m^* = (P^\dagger\vec{\boldsymbol{v}})_m\,. \tag{53}$$

This means that under an active rotation, the spherical components of a vector $\vec{\boldsymbol{v}}$ transform as

$$v_m' = \sum_{m'}\mathcal{D}^{(1)*}_{mm'}(\hat{\boldsymbol{n}},\theta)v_{m'}\,. \tag{54}$$

If the Cartesian components of a vector $\vec{\boldsymbol{v}}$ are complex, then it is more accurate to replace eq. (53) with[4]

$$(-1)^m v_{-m} = (P^\dagger\vec{\boldsymbol{v}})_m\,. \tag{55}$$

Using eq. (55), it follows that eq. (51) yields

$$(-1)^m v_{-m}' = \sum_{m'}(-1)^{m'}v_{-m'}\mathcal{D}^{(1)}_{mm'}(\hat{\boldsymbol{n}},\theta)\,. \tag{56}$$

[4]Of course, in the case of a vector whose Cartesian coordinates are real, we can use eq. (8) to recover eq. (53).

We can interpret eq. (56) by saying that in a basis where S_3 is diagonal, the components of a vector $\vec{\boldsymbol{v}}$ are given by its spherical components v_m. The reason why $(-1)^m v_{-m}$ appears in eq. (56) is the same reason this factor appears in eq. (14). Namely, when working in the spherical basis, 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 a sanity check, we note that under a rotation, the dot product [cf. eq. (13)]

$$\vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{w}} = \sum_m (-1)^m v_m w_{-m} \tag{57}$$

must be invariant. We can check this explicitly as follows. Using eq. (56), we can write

$$(-1)^m w'_{-m} = \sum_{m''} (-1)^{m''} w_{-m''} \mathcal{D}^{(1)}_{mm''}(\hat{\boldsymbol{n}}, \theta) \,. \tag{58}$$

Making use of eqs. (56)–(58),

$$\vec{\boldsymbol{v}}\,' \cdot \vec{\boldsymbol{w}}\,' = \sum_{m'} \sum_{m''} (-1)^{m''-m'} v_{m'} w_{-m''} \sum_m (-1)^m \mathcal{D}^{(1)}_{-m,-m'}(\hat{\boldsymbol{n}}, \theta) \mathcal{D}^{(1)}_{mm''}(\hat{\boldsymbol{n}}, \theta) \,. \tag{59}$$

We can now use the following identity:

$$(-1)^m \mathcal{D}^{(1)}_{-m,-m'}(\hat{\boldsymbol{n}}, \theta) = (-1)^{m'} \mathcal{D}^{(1)}_{m'm}(\hat{\boldsymbol{n}}, -\theta) \,. \tag{60}$$

Inserting this result back into eq. (59) and noting that

$$\sum_m \mathcal{D}^{(1)}_{m'm}(\hat{\boldsymbol{n}}, -\theta) \mathcal{D}^{(1)}_{mm''}(\hat{\boldsymbol{n}}, \theta) = \delta_{m'm''} \,, \tag{61}$$

we end up with

$$\vec{\boldsymbol{v}}\,' \cdot \vec{\boldsymbol{w}}\,' = \sum_{m'} (-1)^{m'} v_{m'} w_{-m'} = \vec{\boldsymbol{v}} \cdot \vec{\boldsymbol{w}} \,, \tag{62}$$

as expected.

Returning to eq. (56), after relabeling $m \to -m$ and $m' \to -m'$,

$$v'_m = \sum_{m'} (-1)^{m-m'} v_{m'}\, \mathcal{D}^{(1)}_{-m,-m'}(\hat{\boldsymbol{n}}, \theta) \,. \tag{63}$$

Finally, using eq. (50), one can derive the following identity,

$$\mathcal{D}^{(1)*}_{mm'}(\hat{\boldsymbol{n}}, \theta) = \mathcal{D}^{(1)}_{m'm}(\hat{\boldsymbol{n}}, -\theta) = (-1)^{m-m'} \mathcal{D}^{(1)}_{-m,-m'}(\hat{\boldsymbol{n}}, \theta) \,. \tag{64}$$

Hence, we end up with

$$v'_m = \sum_{m'} v_{m'} \mathcal{D}^{(1)\,*}_{mm'}(\hat{\boldsymbol{n}}, \theta) \,, \tag{65}$$

which reproduces eq. (54) in the more general case of a vector whose Cartesian components are complex.

Below eq. (41), we noted that $P = M^{\mathsf{T}}$, where the matrix M transforms the Cartesian coordinates of a vector into its spherical coordinates [cf. eq. (6)]. This provides a quick way to derive the transformation law for the spherical components of a vector under an active rotation:

$$\begin{pmatrix} v_1 \\ v_0 \\ v_{-1} \end{pmatrix} = M \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} \longrightarrow MR \begin{pmatrix} v_x \\ v_y \\ v_z \end{pmatrix} = MRM^\dagger \begin{pmatrix} v_1 \\ v_0 \\ v_{-1} \end{pmatrix} , \tag{66}$$

after noting that $M^{-1} = M^\dagger$. This implies that the matrix $MRM^\dagger$ transforms the spherical components of a vector under an active transformation. This is consistent with the result of eq. (65), which identifies this matrix with $\mathcal{D}^{(1)*}$. In particular,

$$\mathcal{D}^{(1)*} = MRM^\dagger = P^{\mathsf{T}} R P^* = \left[P^\dagger R P\right]^* , \tag{67}$$

where we have used the fact that R is a real matrix. Taking the complex conjugate of this equation yields

$$\mathcal{D}^{(1)} = P^\dagger R P , \tag{68}$$

in agreement with eq. (45).

3. Rank-ℓ spherical tensors

In light of eq. (12), eq. (65) is equivalent to

$$Y_{1m}(R\hat{\boldsymbol{n}}) = \sum_{m'} D^{(1)}_{mm'}(R) Y_{1m'}(\hat{\boldsymbol{n}}) . \tag{69}$$

It is instructive to extend eq. (69) to the spherical harmonics of arbitrary ℓ. In order to define $D^{(\ell)}_{mm'}$, we introduce an abstract operator $\vec{\boldsymbol{L}}$ that satisfies

$$\left[L_i \, , \, L_j\right] = i\epsilon_{ijk} L_k . \tag{70}$$

We then introduce the states $|\ell, m\rangle$, which are the simultaneous eigenstate of $\vec{\boldsymbol{L}}^{\,2}$ and L_z with corresponding eigenvalues $\ell(\ell+1)$ and m, respectively:

$$L_z \,|\ell m\rangle = m \,|\ell, m\rangle \ , \tag{71}$$

$$\vec{\boldsymbol{L}}^{\,2} \,|\ell, m\rangle = \ell(\ell+1) \,|\ell m\rangle \ . \tag{72}$$

Moreover, after defining $L_\pm \equiv L_x \pm i L_y$, one can derive the commutation relations

$$\left[L_+ \, , \, L_-\right] = 2L_z \, , \qquad \left[L_\pm \, , \, L_z\right] = \mp L_\pm \, , \tag{73}$$

and the identities

$$L_+ L_- = \vec{\boldsymbol{L}}^{\,2} - L_z(L_z - 1) \, , \tag{74}$$

$$L_- L_+ = \vec{\boldsymbol{L}}^{\,2} - L_z(L_z + 1) \, . \tag{75}$$

Using the commutation relations [eq. (73)] and the identities above, it follows that

$$L_+ \,|\ell m\rangle = \sqrt{(\ell-m)(\ell+m+1)}\;|\ell m+1\rangle\,, \tag{76}$$

$$L_- \,|\ell m\rangle = \sqrt{(\ell+m)(\ell-m+1)}\;|\ell m-1\rangle\,, \tag{77}$$

up to an overall phase which is set by convention. These two results imply that

$$L_x \,|\ell m\rangle = \tfrac{1}{2}\Big[\sqrt{(\ell-m)(\ell+m+1)}\;|\ell m+1\rangle + \sqrt{(\ell+m)(\ell-m+1)}\;|\ell m-1\rangle\Big], \tag{78}$$

$$L_y \,|\ell m\rangle = -\tfrac{1}{2}i\Big[\sqrt{(\ell-m)(\ell+m+1)}\;|\ell m+1\rangle - \sqrt{(\ell+m)(\ell-m+1)}\;|\ell m-1\rangle\Big]. \tag{79}$$

One can construct matrix representations of $\vec{\boldsymbol{L}}$ by the following method. 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

$$\vec{\boldsymbol{L}}^{(\ell)}_{mm'} = \langle \ell m|\,\vec{\boldsymbol{L}}\,|\ell m'\rangle\,. \tag{80}$$

It follows from eq. (71) that the z-component of $\vec{\boldsymbol{L}}^{(\ell)}_{mm'}$ is a diagonal $(2\ell+1)\times(2\ell+1)$ matrix with matrix elements

$$\big(L^{(\ell)}_{mm'}\big)_z = m\delta_{mm'}\,. \tag{81}$$

Likewise, we can use eqs. (78) and (79) to evaluate the x and y components of $\vec{\boldsymbol{L}}^{(\ell)}_{mm'}$,

$$\big(L^{(\ell)}_{mm'}\big)_x = \tfrac{1}{2}\Big[\sqrt{(\ell-m)(\ell+m+1)}\,\delta_{m',m+1} + \sqrt{(\ell+m)(\ell-m+1)}\,\delta_{m,m-1}\Big], \tag{82}$$

$$\big(L^{(\ell)}_{mm'}\big)_y = -\tfrac{1}{2}i\Big[\sqrt{(\ell-m)(\ell+m+1)}\,\delta_{m',m+1} - \sqrt{(\ell+m)(\ell-m+1)}\,\delta_{m,m-1}\Big], \tag{83}$$

As a check, we examine the case of $\ell = 1$. Then, eqs. (81), (82) and (83) yield

$$L^{(1)}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}, \qquad L^{(1)}_y = \frac{i}{\sqrt{2}}\begin{pmatrix} 0 & -1 & 0\\ 1 & 0 & -1\\ 0 & 1 & 0\end{pmatrix}, \qquad L^{(1)}_z = \begin{pmatrix} 1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}, \tag{84}$$

in agreement with the results obtained in eqs. (42)–(44).

The Wigner $\mathcal{D}^{(\ell)}$-matrix is a unitary $(2\ell+1)\times(2\ell+1)$ matrix whose matrix elements are defined by

$$\mathcal{D}^{(\ell)}_{m'm}(R) = \langle \ell m'|\exp\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}\,\big)\,|\ell m\rangle = \Big[\exp\big(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{L}}^{(\ell)}\big)\Big]_{m'm}\,, \tag{85}$$

where R denotes an active counterclockwise rotation by an angle θ about a fixed axis that points along the unit vector $\hat{\boldsymbol{n}}$. For $\ell = 1$, this definition coincides with that of eq. (45).

Our goal now is to extend the result of eq. (69) to $Y_{\ell m}(\hat{\boldsymbol{n}})$ for all ℓ. Here, I shall follow the derivation given in Section 7.5(a) of Kurt Gottfried and Tung-Mow Yan, *Quantum Mechanics: Fundamentals*, Second Edition (Springer-Verlag, New York, NY, USA, 2003). Under a rotation R of the basis $|\ell m\rangle$,

$$|\ell m\rangle \to |\ell m; R\rangle = D(R)\,|\ell m\rangle\,, \tag{86}$$

where $D(R) \equiv \exp\bigl(-i\theta\hat{\boldsymbol{n}}\cdot\vec{\boldsymbol{L}}\bigr)$. Therefore,

$$|\ell m; R\rangle = D(R)\,|\ell m\rangle = \sum_{\ell' m'} |\ell' m'\rangle\,\langle \ell' m'|\exp\bigl(-i\theta\hat{\boldsymbol{n}}\cdot\vec{\boldsymbol{L}}\bigr)\,|\ell m\rangle\ , \tag{87}$$

after summing over a complete set of states. In light of the properties of $\vec{\boldsymbol{L}}$ discussed above,

$$\langle \ell' m'|\exp\bigl(-i\theta\hat{\boldsymbol{n}}\cdot\vec{\boldsymbol{L}}\bigr)\,|\ell m\rangle = \delta_{\ell\ell'}\mathcal{D}^{(\ell)}_{m'm}(R)\,, \tag{88}$$

since the action of $\vec{\boldsymbol{L}}$ on $|\ell m\rangle$ does not modify the value of ℓ. Hence,

$$|\ell m; R\rangle = \sum_{m'} |\ell m'\rangle\,\mathcal{D}^{(\ell)}_{m'm}(R)\,. \tag{89}$$

In the notation employed here, one can identify the spherical harmonics by

$$Y_{\ell m}(\hat{\boldsymbol{n}}) = \langle \hat{\boldsymbol{n}}|\ell m\rangle\,. \tag{90}$$

After multiplying eq. (89) on the left by $\langle\hat{\boldsymbol{n}}|$, it is convenient to write:

$$\langle \hat{\boldsymbol{n}}|\ell m; R\rangle = \langle \hat{\boldsymbol{n}}|\,D(R)\,|\ell m\rangle = \langle R^{-1}\hat{\boldsymbol{n}}|\ell m\rangle\,. \tag{91}$$

Then, eqs. (89)–(91) yield

$$Y_{\ell m}(R^{-1}\hat{\boldsymbol{n}}) = \sum_{m'} Y_{\ell m'}(\hat{\boldsymbol{n}})D^{(\ell)}_{m'm}(R)\,. \tag{92}$$

Since $D^{(\ell)}$ is a unitary matrix, it follows that

$$D^{(\ell)}_{mm'}(R^{-1}) = D^{(\ell)*}_{m'm}(R)\,. \tag{93}$$

Inserting this result into eq. (92) yields

$$Y_{\ell m}(R^{-1}\hat{\boldsymbol{n}}) = \sum_{m'} Y_{\ell m'}(\hat{\boldsymbol{n}})D^{(\ell)*}_{mm'}(R^{-1})\,. \tag{94}$$

Since eq. (94) is true for any rotation R, we can replace R^{-1} by R to arrive at

$$Y_{\ell m}(R\hat{\boldsymbol{n}}) = \sum_{m'} D^{(\ell)*}_{mm'}(R)Y_{\ell m'}(\hat{\boldsymbol{n}})\,. \tag{95}$$

In the case of $\ell = 1$, we have succeeded in reproducing the result obtained in eq. (69).

Eq. (95) motivates the definition of a rank-ℓ spherical tensor $Q_{\ell m}$, which is defined to be a tensor that transforms under rotations according to

$$Q_{\ell m} \to Q'_{\ell m} = \sum_{m'} Q_{\ell m'}\mathcal{D}^{(\ell)\,*}_{mm'}(\hat{\boldsymbol{n}},\theta)\,. \tag{96}$$

Eq. (65) provides an example of eq. (96) in the case of $\ell = 1$. Indeed, given any vector $\vec{\boldsymbol{v}}$, which transforms under rotations according to eq. (32), the components of $\vec{\boldsymbol{v}}$ with respect to the spherical basis transform according to eq. (96) with $\ell = 1$.

4. The three-dimensional representation of SO(3) revisited

The derivation of the representation matrices $\vec{\boldsymbol{L}}^{(\ell)}_{mm'}$ in Section 3 was rather abstract. Here is a more concrete derivation. We shall examine finite-dimensional matrix representations of the operator, $\vec{\boldsymbol{L}} \equiv -i\vec{\boldsymbol{x}} \times \vec{\boldsymbol{\nabla}}$, which acts on functions defined on the sphere. This operator satisfies the commutation relations given in eq. (70). 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 its matrix elements as follows

$$\vec{\boldsymbol{L}}^{(\ell)}_{mm'} = \int Y^*_{\ell m}(\hat{\boldsymbol{n}})\vec{\boldsymbol{L}}\, Y_{\ell m'}(\hat{\boldsymbol{n}})\, d\Omega\,, \quad \text{where } m, m' \in \{-\ell, -\ell+1, \ldots, \ell-1, \ell\}. \tag{97}$$

Introducing $L_\pm \equiv L_x \pm iL_y$, the explicit forms for the operators L_z and $L_\pm$ are given by

$$L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = -i\frac{\partial}{\partial\phi}\,, \tag{98}$$

$$L_\pm \equiv L_x \pm iL_y = e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + i\cot\theta\,\frac{\partial}{\partial\phi}\right)\,. \tag{99}$$

Using eqs. (98) and (99) and the properties of the spherical harmonics,

$$L_z\, Y_{\ell m}(\hat{\boldsymbol{n}}) = mY_{\ell m}(\hat{\boldsymbol{n}})\,, \tag{100}$$

$$L_+ Y_{\ell m}(\hat{\boldsymbol{n}}) = \sqrt{(\ell-m)(\ell+m+1)}\, Y_{\ell,m+1}(\hat{\boldsymbol{n}})\,, \tag{101}$$

$$L_- Y_{\ell m}(\hat{\boldsymbol{n}}) = \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell,m-1}(\hat{\boldsymbol{n}})\,, \tag{102}$$

From the last two equations above, we can derive

$$L_x Y_{\ell m}(\hat{\boldsymbol{n}}) = \tfrac{1}{2}\left[\sqrt{(\ell-m)(\ell+m+1)}\, Y_{\ell,m+1}(\hat{\boldsymbol{n}}) + \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell,m-1}(\hat{\boldsymbol{n}})\right], \tag{103}$$

$$L_y Y_{\ell m}(\hat{\boldsymbol{n}}) = -\tfrac{1}{2}i\left[\sqrt{(\ell-m)(\ell+m+1)}\, Y_{\ell,m+1}(\hat{\boldsymbol{n}}) - \sqrt{(\ell+m)(\ell-m+1)}\, Y_{\ell,m-1}(\hat{\boldsymbol{n}})\right]. \tag{104}$$

We can now evaluate the integral in eq. (97), with the help of the orthogonality properties of the spherical harmonics,

$$\int Y^*_{\ell' m'}(\hat{\boldsymbol{n}})\, Y_{\ell m}(\hat{\boldsymbol{n}})\, d\Omega = \delta_{\ell\ell'}\delta_{mm'}\,, \tag{105}$$

it follows that

$$\left(L^{(\ell)}_{mm'}\right)_x = \tfrac{1}{2}\left[\sqrt{(\ell-m)(\ell+m+1)}\,\delta_{m',m+1} + \sqrt{(\ell+m)(\ell-m+1)}\,\delta_{m,m-1}\right], \tag{106}$$

$$\left(L^{(\ell)}_{mm'}\right)_y = -\tfrac{1}{2}i\left[\sqrt{(\ell-m)(\ell+m+1)}\,\delta_{m',m+1} - \sqrt{(\ell+m)(\ell-m+1)}\,\delta_{m,m-1}\right], \tag{107}$$

$$\left(L^{(\ell)}_{mm'}\right)_z = m\delta_{mm'}\,. \tag{108}$$

in agreement with the results of eqs. (81)–(83).

5. The distinction between Cartesian tensors and spherical tensors

Consider the distinction between Cartesian tensors and spherical tensors. As noted in Section 2, 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

$$v_i \to v_i' = R_{ij} v_j \,, \tag{109}$$

with an implicit sum over the repeated index j, where $i, j \in \{1, 2, 3\} = \{x, y, z\}$, with the R_{ij} given by Rodrigues' rotation formula [eq. (33)]. Likewise, a second rank Cartesian tensor transforms as

$$T_{ij} \to T_{ij}' = R_{ik} R_{j\ell} T_{k\ell} \,. \tag{110}$$

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

$$T_{ij} = S_{ij} + A_{ij} + c\delta_{ij} \,, \tag{111}$$

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:

$$S_{ij} = \tfrac{1}{2}\big(T_{ij} + T_{ji}\big) - \tfrac{1}{3}\delta_{ij} \,\mathrm{Tr}\, T \,, \qquad A_{ij} = \tfrac{1}{2}\big(T_{ij} - T_{ji}\big) \,, \qquad c = \tfrac{1}{3}\,\mathrm{Tr}\, T = \tfrac{1}{3}\delta_{ij} T_{ij} \,. \tag{112}$$

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

$$S_{ij} \to S_{ij}' = R_{ik} R_{j\ell} S_{k\ell} \,, \qquad a_i \to a_i' = R_{ij} a_j \,, \qquad c \to c' = c \,. \tag{113}$$

That is, the S_{ij}, which is governed by five independent components, transform under rotations like a second rank tensor (independently of the other four independent components). Likewise, the a_k, which is governed by three independent components, transform like a vector (independently of the other six independent components),. Finally, the one remaining degree of freedom, $c\,\delta_{ij}$, 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, transform *irreducibly* under rotations.

In contrast, as indicated previously in eq. (96), a spherical tensor of rank ℓ transforms according to

$$Q_{\ell m} \to Q_{\ell m}' = \sum_{m'} Q_{\ell m'} \mathcal{D}^{(\ell)\,*}_{mm'}(\hat{\boldsymbol{n}}, \theta) \,, \tag{114}$$

where the components of $Q_{\ell m}$ are labeled by $m = -\ell, \ell+1, \ldots, \ell-1, \ell$. That is, a spherical tensor of rank ℓ has $2\ell+1$ components. It is immediately apparent 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. (111). 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). Similarly, the $\ell = 2$ spherical tensor Q_{2m} possesses 5 independent components, and it also transforms irreducibly under rotations. Indeed, 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 that, like S_{ij} in eq. (113), transform irreducibly under rotations.

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