Properties of Proper and Improper Rotation Matrices

1. Proper and improper rotation matrices

A real orthogonal matrix R is a matrix whose elements are real numbers and satisfies $R^{-1} = R^{\mathsf{T}}$ (or equivalently, $RR^{\mathsf{T}} = \mathbf{I}$, where $\mathbf{I}$ is the $n \times n$ identity matrix). The set of all such matrices provides the n-dimensional defining representation of the Lie group $\mathrm{O}(n)$. Taking the determinant of the equation $RR^{\mathsf{T}} = \mathbf{I}$ and using the fact that $\det(R^{\mathsf{T}}) = \det R$, it follows that $(\det R)^2 = 1$, which implies that either $\det R = 1$ or $\det R = -1$. The real orthogonal $n \times n$ matrices with $\det R = 1$ are called *special* real orthogonal matrices and provide the n-dimensional defining matrix representation of the group of *proper* n-dimensional rotations, denoted by $\mathrm{SO}(n)$. Note that $\mathrm{SO}(n)$ is a normal subgroup of $\mathrm{O}(n)$ since $g\,\mathrm{SO}(n)g^{-1}$ is a real orthogonal matrix with unit determinant for any $g \in \mathrm{O}(n)$ and hence is an element of $\mathrm{SO}(n)$.

We shall henceforth focus on the case of $n = 3$. The most general 3×3 special orthogonal matrix represents a counterclockwise rotation by an angle θ about a fixed axis that lies along the unit vector $\hat{\boldsymbol{n}}$. The rotation matrix operates on vectors to produce rotated vectors, while the coordinate axes are held fixed.[1] In typical parlance, a rotation refers to a proper rotation. Thus, in the following sections of these notes we will often omit the adjective *proper* when referring to a proper rotation. The 3×3 real orthogonal matrix with $\det R = -1$ provides a matrix representation of a three-dimensional *improper* rotation. To perform an improper rotation requires mirrors. That is, the most general improper rotation matrix is a product of a proper rotation by an angle θ about some axis $\hat{\boldsymbol{n}}$ and a mirror reflection through a plane that passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$.

In these notes, I shall present a detailed treatment of the matrix representations of three-dimensional proper and improper rotations. By determining the most general form for a three-dimensional proper and improper rotation matrix, we can then examine any 3×3 orthogonal matrix and determine the rotation and/or reflection it produces as an operator acting on vectors. If the matrix represents a proper rotation, then the axis of rotation and angle of rotation can be determined. If the matrix represents an improper rotation, then the reflection plane and the rotation, if any, about the normal to that plane can be determined. For additional material on these topics, I highly recommend Refs. 1–3 listed at the end of these notes.

2. Properties of the 3 × 3 rotation matrix

A rotation in the x–y plane by an angle θ measured counterclockwise from the positive x-axis is represented by the 2×2 real orthogonal matrix with determinant

[1]This is called an *active* transformation.

equal to 1 given by

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} .$$

If we consider this rotation as occurring in three-dimensional space, then it can be described as a counterclockwise rotation by an angle θ about the z-axis. The matrix representation of this three-dimensional rotation is given by the 3×3 real orthogonal matrix with determinant equal to 1 given by

$$R(\hat{\boldsymbol{z}}, \theta) \equiv \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} , \tag{1}$$

where the axis of rotation and the angle of rotation are specified as arguments of R.

The most general three-dimensional proper rotation, denoted by $R(\hat{\boldsymbol{n}}, \theta)$, can be specified by an axis of rotation, $\hat{\boldsymbol{n}}$, and a rotation angle θ.[2] Conventionally, a positive rotation angle corresponds to a counterclockwise rotation. The direction of the axis is determined by the right hand rule. Namely, curl the fingers of your right hand around the axis of rotation, where your fingers point in the θ direction. Then, your thumb points perpendicular to the plane of rotation in the direction of $\hat{\boldsymbol{n}}$. $R(\hat{\boldsymbol{n}}, \theta)$ is called the *angle-and-axis parameterization* of a general three-dimensional proper rotation.

In general, rotation matrices do not commute under multiplication. However, if both rotations are taken with respect to the *same* fixed axis, then

$$R(\hat{\boldsymbol{n}}, \theta_1) R(\hat{\boldsymbol{n}}, \theta_2) = R(\hat{\boldsymbol{n}}, \theta_1 + \theta_2) . \tag{2}$$

Simple geometric considerations will convince you that the following relations are also satisfied:

$$R(\hat{\boldsymbol{n}}, \theta + 2\pi k) = R(\hat{\boldsymbol{n}}, \theta) , \qquad k = 0, \pm 1 \pm 2 \ldots , \tag{3}$$

$$[R(\hat{\boldsymbol{n}}, \theta)]^{-1} = R(\hat{\boldsymbol{n}}, -\theta) = R(-\hat{\boldsymbol{n}}, \theta) . \tag{4}$$

Combining these two results, it follows that

$$R(\hat{\boldsymbol{n}}, 2\pi - \theta) = R(-\hat{\boldsymbol{n}}, \theta) , \tag{5}$$

which implies that any three-dimensional rotation can be described by a counterclockwise rotation by an angle θ about an arbitrary axis $\hat{\boldsymbol{n}}$, where $0 \leq \theta \leq \pi$. However, if we substitute $\theta = \pi$ in eq. (5), we conclude that

$$R(\hat{\boldsymbol{n}}, \pi) = R(-\hat{\boldsymbol{n}}, \pi) , \tag{6}$$

[2]There is an alternative convention for the range of possible angles θ and rotation axes $\hat{\boldsymbol{n}}$. We say that $\hat{\boldsymbol{n}} = (n_1, n_2, n_3) > 0$ if the first nonzero component of $\hat{\boldsymbol{n}}$ is positive. That is $n_3 > 0$ if $n_1 = n_2 = 0$, $n_2 > 0$ if $n_1 = 0$, and $n_1 > 0$ otherwise. Then, all possible rotation matrices $R(\hat{\boldsymbol{n}}, \theta)$ correspond to $\hat{\boldsymbol{n}} > 0$ and $0 \leq \theta < 2\pi$. However, we will not employ this convention in these notes.

which means that for the special case of $\theta = \pi$, $R(\hat{\boldsymbol{n}}, \pi)$ and $R(-\hat{\boldsymbol{n}}, \pi)$ represent the *same* rotation. In particular, note that

$$[R(\hat{\boldsymbol{n}}, \pi)]^2 = \mathbf{I}\,. \tag{7}$$

Indeed for any choice of $\hat{\boldsymbol{n}}$, the $R(\hat{\boldsymbol{n}}, \pi)$ are the only non-trivial rotation matrices whose square is equal to the identity operator. Finally, if $\theta = 0$ then $R(\hat{\boldsymbol{n}}, 0) = \mathbf{I}$ is the identity operator (sometimes called the trivial rotation), independently of the direction of $\hat{\boldsymbol{n}}$.

To learn more about the properties of a general three-dimensional rotation, consider the matrix representation $R(\hat{\boldsymbol{n}}, \theta)$ with respect to the standard basis $\mathcal{B}_s = \{\hat{\boldsymbol{x}}\,,\, \hat{\boldsymbol{y}}\,,\, \hat{\boldsymbol{z}}\}$. We can define a new coordinate system in which the unit vector $\hat{\boldsymbol{n}}$ points in the direction of the new z-axis; the corresponding new basis will be denoted by $\mathcal{B}'$. The matrix representation of the rotation with respect to $\mathcal{B}'$ is then given by $R(\hat{\boldsymbol{z}}, \theta)$. Consequently, there exists an invertible matrix P such that[3]

$$R(\hat{\boldsymbol{n}}, \theta) = P R(\hat{\boldsymbol{z}}, \theta) P^{-1}\,, \tag{8}$$

where $\hat{\boldsymbol{n}} = P\hat{\boldsymbol{z}}$ and $R(\hat{\boldsymbol{z}}, \theta)$ is given by eq. (1). An explicit form for P is obtained in Appendix A. However, the mere existence of the matrix P in eq. (8) is sufficient to provide a simple algorithm for determining the rotation axis $\hat{\boldsymbol{n}}$ (up to an overall sign) and the rotation angle θ that characterize a general three-dimensional rotation matrix.

To determine the rotation angle θ, we note that the properties of the trace imply that $\mathrm{Tr}(PRP^{-1}) = \mathrm{Tr}(P^{-1}PR) = \mathrm{Tr}\,R$, since one can cyclically permute the matrices within the trace without modifying its value. Hence, it immediately follows from eq. (8) that

$$\mathrm{Tr}\; R(\hat{\boldsymbol{n}}, \theta) = \mathrm{Tr}\; R(\hat{\boldsymbol{z}}, \theta) = 2\cos\theta + 1\,, \tag{9}$$

after taking the trace of eq. (1). By convention, $0 \le \theta \le \pi$, which implies that $\sin\theta \ge 0$. Hence, the rotation angle is uniquely determined by eq. (9) To identify $\hat{\boldsymbol{n}}$, we observe that any vector that is parallel to the axis of rotation is unaffected by the rotation itself. This last statement can be expressed as an eigenvalue equation,

$$R(\hat{\boldsymbol{n}}, \theta)\hat{\boldsymbol{n}} = \hat{\boldsymbol{n}}\,. \tag{10}$$

Thus, $\hat{\boldsymbol{n}}$ is an eigenvector of $R(\hat{\boldsymbol{n}}, \theta)$ corresponding to the eigenvalue 1. In particular, the eigenvalue 1 is unique for any $\theta \neq 0$, in which case $\hat{\boldsymbol{n}}$ can be determined up to an overall sign by computing the eigenvalues and the normalized eigenvectors of $R(\hat{\boldsymbol{n}}, \theta)$. A simple proof of this result is given in Appendix B. Here, we shall establish this assertion by noting that the eigenvalues of any matrix are invariant with respect to a similarity transformation. Using eq. (8), it follows that the eigenvalues of $R(\hat{\boldsymbol{n}}, \theta)$ are identical to the eigenvalues of $R(\hat{\boldsymbol{z}}, \theta)$. The latter can be obtained from the characteristic equation,

$$(1 - \lambda)\left[(\cos\theta - \lambda)^2 + \sin^2\theta\right] = 0\,,$$

[3]Eq. (8) is a special case of a more general result, $R(\hat{\boldsymbol{n}}, \theta) = PR(\hat{\boldsymbol{n}}', \theta)P^{-1}$, where $\hat{\boldsymbol{n}} = P\hat{\boldsymbol{n}}'$. The derivation of this result, which makes use of eqs. (57) and (59) of Section 7, is presented in Appendix D.

which simplifies to:

$$(1-\lambda)(\lambda^2 - 2\lambda\cos\theta + 1) = 0\,,$$

after using $\sin^2\theta + \cos^2\theta = 1$. Solving the quadratic equation, $\lambda^2 - 2\lambda\cos\theta + 1 = 0$, yields:

$$\lambda = \cos\theta \pm \sqrt{\cos^2\theta - 1} = \cos\theta \pm i\sqrt{1-\cos^2\theta} = \cos\theta \pm i\sin\theta = e^{\pm i\theta}\,. \qquad (11)$$

It follows that the three eigenvalues of $R(\hat{\boldsymbol{z}},\theta)$ are given by,

$$\lambda_1 = 1\,, \quad \lambda_2 = e^{i\theta}\,, \quad \lambda_3 = e^{-i\theta}\,, \qquad \text{for } \; 0 \leq \theta \leq \pi\,.$$

There are three distinct cases:

Case 1:	$\theta = 0$	$\lambda_1 = \lambda_2 = \lambda_3 = 1\,,$	$R(\hat{\boldsymbol{n}},0) = \mathbf{I}\,,$
Case 2:	$\theta = \pi$	$\lambda_1 = 1\,,\, \lambda_2 = \lambda_3 = -1\,,$	$R(\hat{\boldsymbol{n}},\pi)\,,$
Case 3:	$0 < \theta < \pi$	$\lambda_1 = 1, \lambda_2 = e^{i\theta}\,,\, \lambda_3 = e^{-i\theta}\,,$	$R(\hat{\boldsymbol{n}},\theta)\,,$

where the corresponding rotation matrix is indicated for each of the three cases. Indeed, for $\theta \neq 0$ the eigenvalue 1 is unique. Moreover, the other two eigenvalues are complex conjugates of each other, whose real part is equal to $\cos\theta$, which uniquely fixes the rotation angle in the convention where $0 \leq \theta \leq \pi$. Case 1 corresponds to the identity (i.e. no rotation) and Case 2 corresponds to a 180° rotation about the axis $\hat{\boldsymbol{n}}$. In Case 2, the interpretation of the the doubly degenerate eigenvalue -1 is clear. Namely, the corresponding two linearly independent eigenvectors span the plane that passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$. In particular, the two doubly degenerate eigenvectors (along with any linear combination $\vec{\boldsymbol{v}}$ of these eigenvectors that lies in the plane perpendicular to $\hat{\boldsymbol{n}}$) are inverted by the 180° rotation and hence must satisfy $R(\hat{\boldsymbol{n}},\pi)\vec{\boldsymbol{v}} = -\vec{\boldsymbol{v}}$.

Since $\hat{\boldsymbol{n}}$ is a real vector of unit length, it is determined only up to an overall sign by eq. (10) when its corresponding eigenvalue 1 is unique. This sign ambiguity is immaterial in Case 2 in light of eq. (6). The sign ambiguity in Case 3 cannot be resolved without further analysis. To make further progress, in Section 3 we shall obtain the general expression for the three dimensional rotation matrix $R(\hat{\boldsymbol{n}},\theta)$.

3. An explicit formula for the matrix elements of a general 3×3 rotation matrix

The matrix elements of $R(\hat{\boldsymbol{n}},\theta)$ will be denoted by R_{ij}. Since $R(\hat{\boldsymbol{n}},\theta)$ describes a counterclockwise rotation by an angle θ about an axis $\hat{\boldsymbol{n}}$, the formula for R_{ij} that we seek will depend on θ and on the coordinates of $\hat{\boldsymbol{n}} = (n_1\,,\, n_2\,,\, n_3)$ with respect to a fixed Cartesian coordinate system. Note that since $\hat{\boldsymbol{n}}$ is a unit vector, it follows that:

$$n_1^2 + n_2^2 + n_3^2 = 1\,. \qquad (12)$$

An explicit formula for R_{ij} is obtained by noting that a general element of SO(3) in the angle-and-axis parameterization is given by $R_{ij}(\hat{\boldsymbol{n}},\theta) = \exp(-i\theta\hat{\boldsymbol{n}}\cdot\vec{\boldsymbol{J}})_{ij}$, with $(\hat{\boldsymbol{n}}\cdot\vec{\boldsymbol{J}})_{ij} \equiv -i\epsilon_{ijk}n_k$ [where there is an implicit sum over the index k due to the Einstein summation convention]. The explicit evaluation of the exponential can be carried out by employing the Taylor series definition of the matrix exponential [cf. problem 7(b) of Problem Set 2] and yields:

$$R_{ij}(\hat{\boldsymbol{n}},\theta) = n_i n_j + (\delta_{ij} - n_i n_j)\cos\theta - \epsilon_{ijk}n_k\sin\theta\,. \tag{13}$$

Eq. (13) can also be derived using the techniques of tensor algebra in a clever way as follows. Employing the arguments given in Appendix C, one can regard R_{ij} as the components of a second-rank tensor. Likewise, the n_i are components of a vector (equivalently, a first-rank tensor). Two other important quantities for the analysis are the *invariant* tensors δ_{ij} (the Kronecker delta) and ϵ_{ijk} (the Levi-Civita tensor). If we invoke the covariance of Cartesian tensor equations, then one must be able to express R_{ij} in terms of a second-rank tensor composed of n_i, δ_{ij} and ϵ_{ijk}, as there are no other tensors in the problem that could provide a source of indices. Thus, the explicit formula for R_{ij} must be of the following form:

$$R_{ij} = a\delta_{ij} + bn_i n_j + c\epsilon_{ijk}n_k\,. \tag{14}$$

The numbers a, b and c are real scalar quantities. As such, a, b and c are functions of θ, since the rotation angle is the only relevant scalar quantity in this problem.[4] If we also allow for transformations between right-handed and left-handed orthonormal coordinate systems, then R_{ij} and δ_{ij} are true second-rank tensors and ϵ_{ijk} is a third-rank pseudotensor. Thus, to ensure that eq. (14) is covariant with respect to transformations between two bases that are related by either a proper or an improper rotation, we conclude that a and b are true scalars, and the product $c\hat{\boldsymbol{n}}$ is a pseudovector.[5]

We now propose to deduce conditions that are satisfied by a, b and c. The first condition is given by eq. (10), which in terms of components is

$$R_{ij}n_j = n_i\,. \tag{15}$$

To determine the consequence of this equation, we insert eq. (14) into eq. (15) and make use of eq. (12). Noting that

$$\delta_{ij}n_j = n_i\,, \qquad n_j n_j = 1 \qquad \epsilon_{ijk}n_j n_k = 0\,, \tag{16}$$

[4]One can also construct a scalar by taking the dot product of $\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}}$, but this quantity is equal to 1 [cf. eq. (12)], since $\hat{\boldsymbol{n}}$ is a unit vector.

[5]Under inversion of the coordinate system, $\theta \to -\theta$ and $\hat{\boldsymbol{n}} \to -\hat{\boldsymbol{n}}$. However, since $0 \leq \theta \leq \pi$ (by convention), we must then use eq. (4) to flip the signs of both θ and $\hat{\boldsymbol{n}}$ to represent the rotation $R(\hat{\boldsymbol{n}},\theta)$ in the new coordinate system. Hence, the signs of θ and $\hat{\boldsymbol{n}}$ effectively *do not change* under the inversion of the coordinate system. That is, θ is a true scalar and $\hat{\boldsymbol{n}}$ is a pseudovector, in which case c is also a true scalar. In a different convention where $-\pi \leq \theta \leq \pi$ (which we do not adopt in these notes), θ is a pseudoscalar and $\hat{\boldsymbol{n}}$ is a true vector, in which case c is also a pseudoscalar. Independent of these conventions, the product $c\hat{\boldsymbol{n}}$ is a pseudovector as asserted in the text above.

it follows immediately that $n_i(a+b) = n_i$. Hence,

$$a + b = 1\,. \tag{17}$$

Since the formula for R_{ij} given by eq. (14) must be completely general, it must hold for any special case. In particular, consider the case where $\hat{\boldsymbol{n}} = \hat{\boldsymbol{z}}$. In this case, eqs. (1) and (14) yields:

$$R(\hat{\boldsymbol{z}},\theta)_{11} = \cos\theta = a\,, \qquad\qquad R(\hat{\boldsymbol{z}},\theta)_{12} = -\sin\theta = c\,\epsilon_{123}n_3 = c\,. \tag{18}$$

Using eqs. (17) and (18) we conclude that,

$$a = \cos\theta\,, \qquad\quad b = 1-\cos\theta\,, \qquad\quad c = -\sin\theta\,. \tag{19}$$

Inserting these results into eq. (14) yields the *Rodriguez formula*:

$$\boxed{R_{ij}(\hat{\boldsymbol{n}},\theta) = \cos\theta\,\delta_{ij} + (1-\cos\theta)n_i n_j - \sin\theta\,\epsilon_{ijk}n_k} \tag{20}$$

which reproduces the result of eq. (13). We can write $R(\hat{\boldsymbol{n}},\theta)$ explicitly in 3×3 matrix form,

$$R(\hat{\boldsymbol{n}},\theta) = \begin{pmatrix} \cos\theta + n_1^2(1-\cos\theta) & n_1n_2(1-\cos\theta) - n_3\sin\theta & n_1n_3(1-\cos\theta)+n_2\sin\theta \\ n_1n_2(1-\cos\theta)+n_3\sin\theta & \cos\theta+n_2^2(1-\cos\theta) & n_2n_3(1-\cos\theta)-n_1\sin\theta \\ n_1n_3(1-\cos\theta)-n_2\sin\theta & n_2n_3(1-\cos\theta)+n_1\sin\theta & \cos\theta+n_3^2(1-\cos\theta) \end{pmatrix}. \tag{21}$$

One can easily check that eqs. (3) and (4) are satisfied. In particular, as indicated by eq. (5), the rotations $R(\hat{\boldsymbol{n}},\pi)$ and $R(-\hat{\boldsymbol{n}},\pi)$ represent the same rotation,

$$R_{ij}(\hat{\boldsymbol{n}},\pi) = \begin{pmatrix} 2n_1^2-1 & 2n_1n_2 & 2n_1n_3 \\ 2n_1n_2 & 2n_2^2-1 & 2n_2n_3 \\ 2n_1n_3 & 2n_2n_3 & 2n_3^2-1 \end{pmatrix} = 2n_in_j - \delta_{ij}\,. \tag{22}$$

Finally, as expected, $R_{ij}(\hat{\boldsymbol{n}},0) = \delta_{ij}$, independently of the direction of $\hat{\boldsymbol{n}}$. I leave it as an exercise to the reader to verify explicitly that $R = R(\hat{\boldsymbol{n}},\theta)$ given in eq. (21) satisfies the conditions $RR^{\mathsf{T}} = \mathbf{I}$ and $\det R = +1$.

The two rotation matrices $R(\hat{\boldsymbol{n}},\theta)$ and $R(\hat{\boldsymbol{n}}',\theta)$ are related in an interesting way that generalizes the result of eq. (8). Details can be found in Appendix D.

4. $\boldsymbol{R(\hat{n},\theta)}$ expressed as a product of simpler rotation matrices

In this section, we shall demonstrate that it is possible to express a general three-dimensional rotation matrix $R(\hat{\boldsymbol{n}},\theta)$ as a product of simpler rotations. This will provide further geometrical insights into the properties of rotations. First, it will be convenient to express the unit vector $\hat{\boldsymbol{n}}$ in spherical coordinates,

$$\hat{\boldsymbol{n}} = (\sin\theta_n\cos\phi_n\,,\ \sin\theta_n\sin\phi_n\,,\ \cos\theta_n)\,, \tag{23}$$

where θ_n is the polar angle and ϕ_n is the azimuthal angle that describe the direction of the unit vector $\hat{\boldsymbol{n}}$. Noting that

$$R(\hat{\boldsymbol{z}},\phi_n)=\begin{pmatrix}\cos\phi_n & -\sin\phi_n & 0\\ \sin\phi_n & \cos\phi_n & 0\\ 0 & 0 & 1\end{pmatrix}\,,\qquad R(\hat{\boldsymbol{y}},\theta_n)=\begin{pmatrix}\cos\theta_n & 0 & \sin\theta_n\\ 0 & 1 & 0\\ -\sin\theta_n & 0 & \cos\theta_n\end{pmatrix}\,,$$

one can identify the matrix P given in eq. (71) as:

$$P=R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{y}},\theta_n)=\begin{pmatrix}\cos\theta_n\cos\phi_n & -\sin\phi_n & \sin\theta\cos\phi_n\\ \cos\theta_n\sin\phi_n & \cos\phi_n & \sin\theta\sin\phi_n\\ -\sin\theta_n & 0 & \cos\theta_n\end{pmatrix}\,. \tag{24}$$

We now introduce a unit vector in the azimuthal direction,

$$\hat{\boldsymbol{\varphi}}=(-\sin\phi_n\,,\,\cos\phi_n\,,\,0)\,.$$

Inserting $n_1=-\sin\phi_n$ and $n_2=\cos\phi_n$ into eq. (21) then yields:

$$R(\hat{\boldsymbol{\varphi}},\theta_n)=\begin{pmatrix}\cos\theta_n+\sin^2\!\phi_n(1-\cos\theta_n) & -\sin\phi_n\cos\phi_n(1-\cos\theta_n) & \sin\theta_n\cos\phi_n\\ -\sin\phi_n\cos\phi_n(1-\cos\theta_n) & \cos\theta_n+\cos^2\!\phi_n(1-\cos\theta_n) & \sin\theta_n\sin\phi_n\\ -\sin\theta_n\cos\phi_n & -\sin\theta_n\sin\phi_n & \cos\theta_n\end{pmatrix}$$

$$=R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{y}},\theta_n)R(\hat{\boldsymbol{z}},-\phi_n)=PR(\hat{\boldsymbol{z}},-\phi_n)\,, \tag{25}$$

after using eq. (24) in the final step. Eqs. (4) and (25) then imply that

$$P=R(\hat{\boldsymbol{\varphi}},\theta_n)R(\hat{\boldsymbol{z}},\phi_n)\,, \tag{26}$$

One can now use eqs. (4), (8) and (26) to obtain:

$$R(\hat{\boldsymbol{n}},\theta)=PR(\hat{\boldsymbol{z}},\theta)P^{-1}=R(\hat{\boldsymbol{\varphi}},\theta_n)R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{z}},\theta)R(\hat{\boldsymbol{z}},-\phi_n)R(\hat{\boldsymbol{\varphi}},-\theta_n)\,. \tag{27}$$

Since rotations about a fixed axis commute, it follows that

$$R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{z}},\theta)R(\hat{\boldsymbol{z}},-\phi_n)=R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{z}},-\phi_n)R(\hat{\boldsymbol{z}},\theta)=R(\hat{\boldsymbol{z}},\theta)\,,$$

after using eq. (2). Hence, eq. (27) yields:

$$R(\hat{\boldsymbol{n}},\theta)=R(\hat{\boldsymbol{\varphi}},\theta_n)R(\hat{\boldsymbol{z}},\theta)R(\hat{\boldsymbol{\varphi}},-\theta_n)\,. \tag{28}$$

To appreciate the geometrical interpretation of eq. (28), consider $R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{v}}$ for any vector $\vec{\boldsymbol{v}}$. This is equivalent to $R(\hat{\boldsymbol{\varphi}},\theta_n)R(\hat{\boldsymbol{z}},\theta)R(\hat{\boldsymbol{\varphi}},-\theta_n)\vec{\boldsymbol{v}}$. The effect of $R(\hat{\boldsymbol{\varphi}},-\theta_n)$ is to rotate the axis of rotation $\hat{\boldsymbol{n}}$ to $\hat{\boldsymbol{z}}$ (which lies along the z-axis). Then, $R(\hat{\boldsymbol{z}},\theta)$ performs the rotation by θ about the z-axis. Finally, $R(\hat{\boldsymbol{\varphi}},\theta_n)$ rotates $\hat{\boldsymbol{z}}$ back to the original rotation axis $\hat{\boldsymbol{n}}$.[6]

[6]Using eq. (25), one can easily verify that $R(\hat{\boldsymbol{\varphi}},-\theta_n)\hat{\boldsymbol{n}}=\hat{\boldsymbol{z}}$ and $R(\hat{\boldsymbol{\varphi}},\theta_n)\hat{\boldsymbol{z}}=\hat{\boldsymbol{n}}$.

By combining the results of eqs. (25) and (28), one obtains:

$$\begin{aligned} R(\hat{\boldsymbol{n}},\theta) &= R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{y}},\theta_n)R(\hat{\boldsymbol{z}},-\phi_n)R(\hat{\boldsymbol{z}},\theta)R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{y}},-\theta_n)R(\hat{\boldsymbol{z}},-\phi_n) \\ &= R(\hat{\boldsymbol{z}},\phi_n)R(\hat{\boldsymbol{y}},\theta_n)R(\hat{\boldsymbol{z}},\theta)R(\hat{\boldsymbol{y}},-\theta_n)R(\hat{\boldsymbol{z}},-\phi_n)\,. \end{aligned} \tag{29}$$

That is, a rotation by an angle θ about a fixed axis $\hat{\boldsymbol{n}}$ (whose direction is described by polar and azimuthal angles θ_n and ϕ_n) is equivalent to a sequence of rotations about a fixed z and a fixed y-axis. In fact, one can do somewhat better. One can prove that an arbitrary rotation can be written as:

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

where α, β and γ are called the *Euler angles*. Details of the Euler angle representation of $R(\hat{\boldsymbol{n}},\theta)$ are presented in Appendix E.

5. Properties of the 3 × 3 improper rotation matrix

An improper rotation matrix is a real orthogonal matrix, $\overline{R}$, such that $\det\overline{R} = -1$. That is, $\overline{R} \in \mathrm{O}(n)$ but $\overline{R} \notin \mathrm{SO}(n)$. Specializing to the case of $n = 3$, the most general three-dimensional improper rotation, denoted by $\overline{R}(\hat{\boldsymbol{n}},\theta)$, consists of a product of a proper rotation matrix, $R(\hat{\boldsymbol{n}},\theta)$, and a mirror reflection through a plane normal to the unit vector $\hat{\boldsymbol{n}}$, which shall be denoted by $\overline{R}(\hat{\boldsymbol{n}})$. In particular, the reflection plane passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$. In equations,

$$\overline{R}(\hat{\boldsymbol{n}},\theta) \equiv R(\hat{\boldsymbol{n}},\theta)\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}},\theta)\,. \tag{30}$$

The improper rotation defined in eq. (30) does not depend on the order in which the proper rotation and reflection are applied. The matrix $\overline{R}(\hat{\boldsymbol{n}})$ is called a *reflection matrix*, since it is a representation of a mirror reflection through a fixed plane. In particular,

$$\overline{R}(\hat{\boldsymbol{n}}) = \overline{R}(-\hat{\boldsymbol{n}}) = \overline{R}(\hat{\boldsymbol{n}},0)\,, \tag{31}$$

after using $R(\hat{\boldsymbol{n}},0) = \mathbf{I}$. Thus, the overall sign of $\hat{\boldsymbol{n}}$ for a reflection matrix has no physical meaning. Note that all reflection matrices are orthogonal matrices with $\det\overline{R}(\hat{\boldsymbol{n}}) = -1$, with the property that:

$$[\overline{R}(\hat{\boldsymbol{n}})]^2 = \mathbf{I}\,. \tag{32}$$

In general, the product of a two proper and/or improper rotation matrices is not commutative. However, if $\hat{\boldsymbol{n}}$ is the same for both matrices, then eq. (2) implies that:[7]

$$R(\hat{\boldsymbol{n}},\theta_1)\overline{R}(\hat{\boldsymbol{n}},\theta_2) = \overline{R}(\hat{\boldsymbol{n}},\theta_1)R(\hat{\boldsymbol{n}},\theta_2) = \overline{R}(\hat{\boldsymbol{n}},\theta_1+\theta_2)\,, \tag{33}$$

$$\overline{R}(\hat{\boldsymbol{n}},\theta_1)\overline{R}(\hat{\boldsymbol{n}},\theta_2) = \overline{R}(\hat{\boldsymbol{n}},\theta_1)\overline{R}(\hat{\boldsymbol{n}},\theta_2) = R(\hat{\boldsymbol{n}},\theta_1+\theta_2)\,, \tag{34}$$

after making use of eqs. (30) and (32).

[7]Since $\det[R(\hat{\boldsymbol{n}},\theta_1)\overline{R}(\hat{\boldsymbol{n}},\theta_2)] = \det R(\hat{\boldsymbol{n}},\theta_1)\det\overline{R}(\hat{\boldsymbol{n}},\theta_2) = -1$, it follows that $R(\hat{\boldsymbol{n}},\theta_1)\overline{R}(\hat{\boldsymbol{n}},\theta_2)$ must be an improper rotation matrix. Likewise, $\overline{R}(\hat{\boldsymbol{n}},\theta_1)\overline{R}(\hat{\boldsymbol{n}},\theta_2)$ must be a proper rotation matrix. Eqs. (33) and (34) are consistent with these expectations.

The properties of the improper rotation matrices mirror those of the proper rotation matrices given in eqs. (3)–(7). Indeed the properties of the latter combined with eqs. (31) and (32) yield:

$$\overline{R}(\hat{\boldsymbol{n}},\theta+2\pi k)=\overline{R}(\hat{\boldsymbol{n}},\theta)\,,\qquad k=0,\pm 1\,\pm 2\,\ldots\,, \tag{35}$$

$$[\overline{R}(\hat{\boldsymbol{n}},\theta)]^{-1}=\overline{R}(\hat{\boldsymbol{n}},-\theta)=\overline{R}(-\hat{\boldsymbol{n}},\theta)\,. \tag{36}$$

Combining these two results, it follows that

$$\overline{R}(\hat{\boldsymbol{n}},2\pi-\theta)=\overline{R}(-\hat{\boldsymbol{n}},\theta)\,. \tag{37}$$

We shall adopt the convention (employed in Section 2) in which the angle θ is defined to lie in the interval $0\leq\theta\leq\pi$. In this convention, the overall sign of $\hat{\boldsymbol{n}}$ is meaningful when $0<\theta<\pi$.

The matrix $\overline{R}(\hat{\boldsymbol{n}},\pi)$ is special. Geometric considerations will convince you that

$$\overline{R}(\hat{\boldsymbol{n}},\pi)=R(\hat{\boldsymbol{n}},\pi)\overline{R}(\hat{\boldsymbol{n}})=\overline{R}(\hat{\boldsymbol{n}})R(\hat{\boldsymbol{n}},\pi)=-\mathbf{I}\,. \tag{38}$$

That is, $\overline{R}(\hat{\boldsymbol{n}},\pi)$ represents an *inversion*, which is a linear operator that transforms all vectors $\vec{\boldsymbol{x}}\to-\vec{\boldsymbol{x}}$. In particular, $\overline{R}(\hat{\boldsymbol{n}},\pi)$ is *independent* of the unit vector $\hat{\boldsymbol{n}}$. Eq. (38) is equivalent to the statement that an inversion is equivalent to a mirror reflection through a plane that passes through the origin and is perpendicular to an arbitrary unit vector $\hat{\boldsymbol{n}}$, followed by a proper rotation of 180° around the axis $\hat{\boldsymbol{n}}$. Sometimes, $\overline{R}(\hat{\boldsymbol{n}},\pi)$ is called a point reflection through the origin (to distinguish it from a reflection through a plane). Just like a reflection matrix, the inversion matrix satisfies

$$[\overline{R}(\hat{\boldsymbol{n}},\pi)]^2=\mathbf{I}\,. \tag{39}$$

In general, any improper 3×3 rotation matrix $\overline{R}$ with the property that $\overline{R}^2=\mathbf{I}$ is a representation of either an inversion or a reflection through a plane that passes through the origin.

Given any proper 3×3 rotation matrix $R(\hat{\boldsymbol{n}},\theta)$, the matrix $-R(\hat{\boldsymbol{n}},\theta)$ has determinant equal to -1 and therefore represents some improper rotation, which can be determined as follows:

$$-R(\hat{\boldsymbol{n}},\theta)=R(\hat{\boldsymbol{n}},\theta)\overline{R}(\hat{\boldsymbol{n}},\pi)=\overline{R}(\hat{\boldsymbol{n}},\theta+\pi)=\overline{R}(-\hat{\boldsymbol{n}},\pi-\theta)\,, \tag{40}$$

after employing eqs. (38), (33) and (37). Two noteworthy consequences of eq. (40) are:

$$\overline{R}(\hat{\boldsymbol{n}},\tfrac{1}{2}\pi)=-R(-\hat{\boldsymbol{n}},\tfrac{1}{2}\pi)\,, \tag{41}$$

$$\overline{R}(\hat{\boldsymbol{n}})=\overline{R}(\hat{\boldsymbol{n}},0)=-R(\hat{\boldsymbol{n}},\pi)\,, \tag{42}$$

after using eq. (6) in the second equation above.

To learn more about the properties of a general three-dimensional improper rotation, consider the matrix representation $\overline{R}(\hat{\boldsymbol{n}},\theta)$ with respect to the standard basis $\mathcal{B}_s=\{\hat{\boldsymbol{x}}\,,\,\hat{\boldsymbol{y}}\,,\,\hat{\boldsymbol{z}}\}$. We can define a new coordinate system in which the unit normal to the reflection plane $\hat{\boldsymbol{n}}$ points in the direction of the new z-axis; the corresponding new basis will be denoted by $\mathcal{B}'$. The matrix representation of the improper rotation with respect to $\mathcal{B}'$ is then given by

$$\overline{R}(\hat{\boldsymbol{z}},\theta) = R(\hat{\boldsymbol{z}},\theta)\overline{R}(\hat{\boldsymbol{z}}) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & -1 \end{pmatrix} .$$

Similar to the case of eq. (8), there exists an invertible matrix P (which has been explicitly obtained in Appendix A) such that

$$\overline{R}(\hat{\boldsymbol{n}},\theta) = P\overline{R}(\hat{\boldsymbol{z}},\theta)P^{-1} . \tag{43}$$

The rest of the analysis mirrors the discussion of Section 2. It immediately follows that

$$\text{Tr } \overline{R}(\hat{\boldsymbol{n}},\theta) = \text{Tr } \overline{R}(\hat{\boldsymbol{z}},\theta) = 2\cos\theta - 1 , \tag{44}$$

after taking the trace of eq. (43). By convention, $0 \leq \theta \leq \pi$, which implies that $\sin\theta \geq 0$. Hence, the rotation angle is uniquely determined by eq. (44) To identify $\hat{\boldsymbol{n}}$ (up to an overall sign), we observe that any vector that is parallel to $\hat{\boldsymbol{n}}$ (which points along the normal to the reflection plane) is inverted. This last statement can be expressed as an eigenvalue equation,

$$\overline{R}(\hat{\boldsymbol{n}},\theta)\hat{\boldsymbol{n}} = -\hat{\boldsymbol{n}} . \tag{45}$$

Thus, $\hat{\boldsymbol{n}}$ is an eigenvector of $\overline{R}(\hat{\boldsymbol{n}},\theta)$ corresponding to the eigenvalue -1. In particular, the eigenvalue -1 is unique for any $\theta \neq \pi$, in which case $\hat{\boldsymbol{n}}$ can be determined up to an overall sign by computing the eigenvalues and the normalized eigenvectors of $\overline{R}(\hat{\boldsymbol{n}},\theta)$. A simple proof of this result is given in Appendix B. Here, we shall establish this assertion by noting that the eigenvalues of any matrix are invariant with respect to a similarity transformation. Using eq. (43), it follows that the eigenvalues of $\overline{R}(\hat{\boldsymbol{n}},\theta)$ are identical to the eigenvalues of $\overline{R}(\hat{\boldsymbol{z}},\theta)$. The latter can be obtained from the characteristic equation,

$$-(1+\lambda)\left[(\cos\theta - \lambda)^2 + \sin^2\theta\right] = 0 ,$$

which simplifies to:

$$(1+\lambda)(\lambda^2 - 2\lambda\cos\theta + 1) = 0 .$$

The solution to the quadratic equation, $\lambda^2 - 2\lambda\cos\theta + 1 = 0$, was given in eq. (11). It follows that the three eigenvalues of $\overline{R}(\hat{\boldsymbol{z}},\theta)$ are given by,

$$\lambda_1 = -1 , \quad \lambda_2 = e^{i\theta} , \quad \lambda_3 = e^{-i\theta} , \qquad \text{for } \ 0 \leq \theta \leq \pi .$$

There are three distinct cases:

$$
\begin{array}{llll}
\textit{Case 1:} & \theta = 0 & \lambda_1 = \lambda_2 = \lambda_3 = -1\,, & \overline{R}(\boldsymbol{\hat{n}}, \pi) = -\mathbf{I}\,, \\
\textit{Case 2:} & \theta = \pi & \lambda_1 = -1\,,\, \lambda_2 = \lambda_3 = 1\,, & \overline{R}(\boldsymbol{\hat{n}}, 0) \equiv \overline{R}(\boldsymbol{\hat{n}})\,, \\
\textit{Case 3:} & 0 < \theta < \pi & \lambda_1 = -1, \lambda_2 = e^{i\theta}\,,\, \lambda_3 = e^{-i\theta}\,, & \overline{R}(\boldsymbol{\hat{n}}, \theta)\,,
\end{array}
$$

where the corresponding improper rotation matrix is indicated for each of the three cases. Indeed, for $\theta \neq \pi$, the eigenvalue -1 is unique. Moreover, the other two eigenvalues are complex conjugates of each other, whose real part is equal to $\cos\theta$, which uniquely fixes the rotation angle in the convention where $0 \leq \theta \leq \pi$. Case 1 corresponds to inversion and Case 2 corresponds to a mirror reflection through a plane that passes through the origin and is perpendicular to $\boldsymbol{\hat{n}}$. In Case 2, the doubly degenerate eigenvalue $+1$ is a consequence of the two linearly independent eigenvectors that span the reflection plane. In particular, any linear combination $\vec{\boldsymbol{v}}$ of these eigenvectors that lies in the reflection plane is unaffected by the reflection and thus satisfies $\overline{R}(\boldsymbol{\hat{n}})\vec{\boldsymbol{v}} = \vec{\boldsymbol{v}}$. In contrast, the improper rotation matrices of Case 3 do not possess an eigenvalue of $+1$, since the vectors that lie in the reflection plane transform non-trivially under the proper rotation $R(\boldsymbol{\hat{n}}, \theta)$.

Since $\boldsymbol{\hat{n}}$ is a real vector of unit length, it is determined only up to an overall sign by eq. (45) when its corresponding eigenvalue -1 is unique. This sign ambiguity is immaterial in Case 2 in light of eq. (31). The sign ambiguity in Case 3 cannot be resolved without further analysis. To make further progress, in Section 6 we shall obtain the general expression for the three dimensional improper rotation matrix $\overline{R}(\boldsymbol{\hat{n}}, \theta)$.

6. An explicit formula for the matrix elements of a general 3×3 improper rotation matrix

In this section, the matrix elements of $\overline{R}(\boldsymbol{\hat{n}}, \theta)$ will be denoted by $\overline{R}_{ij}$. The derivation of an explicit form for $\overline{R}(\boldsymbol{\hat{n}}, \theta)$ follows closely the derivation of $R(\boldsymbol{\hat{n}}, \theta)$ given in Section 3. In particular, one can also express $\overline{R}_{ij}$ in terms of a second-rank tensor composed of n_i, δ_{ij} and ϵ_{ijk}, since there are no other tensors in the problem that could provide a source of indices. Thus, the form of the formula for $\overline{R}_{ij}$ must be:

$$
\overline{R}_{ij} = a\delta_{ij} + bn_in_j + c\epsilon_{ijk}n_k\,, \tag{46}
$$

where the coefficients of a, b and c need not be the same as those that appear in eq. (14).

In this case, a, b and c can be determined as follows. The first condition is given by eq. (45), which in terms of components is

$$
\overline{R}_{ij}n_j = -n_i\,. \tag{47}
$$

To determine the consequence of this equation, we insert eq. (46) into eq. (47) and make use of eq. (12). using eq. (16), it follows immediately that $n_i(a+b) = -n_i$. Hence,

$$
a + b = -1\,. \tag{48}
$$

Since the formula for $\overline{R}_{ij}$ given by eq. (46) must be completely general, it must hold for any special case. In particular, consider the case where $\hat{\boldsymbol{n}} = \hat{\boldsymbol{z}}$. In this case, eqs. (32) and (46) yields:

$$\overline{R}(\hat{\boldsymbol{z}}, \theta)_{11} = \cos\theta = a\,, \qquad\qquad \overline{R}(\hat{\boldsymbol{z}}, \theta)_{12} = -\sin\theta = c\,\epsilon_{123} n_3 = c\,. \tag{49}$$

Using eqs. (48) and (49) we conclude that,

$$a = \cos\theta\,, \qquad\qquad b = -1 - \cos\theta\,, \qquad\qquad c = -\sin\theta\,. \tag{50}$$

Inserting these results into eq. (46) yields the analog of the Rodriguez formula for improper rotation matrices:

$$\boxed{\overline{R}_{ij}(\hat{\boldsymbol{n}}, \theta) = \cos\theta\,\delta_{ij} - (1+\cos\theta) n_i n_j - \sin\theta\,\epsilon_{ijk} n_k} \tag{51}$$

We can write $\overline{R}(\hat{\boldsymbol{n}}, \theta)$ explicitly in 3×3 matrix form,

$$\overline{R}(\hat{\boldsymbol{n}}, \theta) = \begin{pmatrix} \cos\theta - n_1^2(1+\cos\theta) & -n_1 n_2(1+\cos\theta) - n_3\sin\theta & -n_1 n_3(1+\cos\theta) + n_2\sin\theta \\ -n_1 n_2(1+\cos\theta) + n_3\sin\theta & \cos\theta - n_2^2(1+\cos\theta) & -n_2 n_3(1+\cos\theta) - n_1\sin\theta \\ -n_1 n_3(1+\cos\theta) - n_2\sin\theta & -n_2 n_3(1+\cos\theta) + n_1\sin\theta & \cos\theta - n_3^2(1+\cos\theta) \end{pmatrix}. \tag{52}$$

One can easily check that eqs. (35) and (36) are satisfied. In particular, as indicated by eq. (31), the improper rotations $\overline{R}(\hat{\boldsymbol{n}}, 0)$ and $\overline{R}(-\hat{\boldsymbol{n}}, 0)$ represent the same reflection matrix,[8]

$$\overline{R}_{ij}(\hat{\boldsymbol{n}}, 0) \equiv \overline{R}_{ij}(\hat{\boldsymbol{n}}) = \begin{pmatrix} 1-2n_1^2 & -2n_1 n_2 & -2n_1 n_3 \\ -2n_1 n_2 & 1-2n_2^2 & -2n_2 n_3 \\ -2n_1 n_3 & 2 - n_2 n_3 & 1-2n_3^2 \end{pmatrix} = \delta_{ij} - 2n_i n_j\,. \tag{53}$$

Finally, as expected, $\overline{R}_{ij}(\hat{\boldsymbol{n}}, \pi) = -\delta_{ij}$, independently of the direction of $\hat{\boldsymbol{n}}$. I leave it as an exercise to the reader to verify explicitly that $\overline{R} = \overline{R}(\hat{\boldsymbol{n}}, \theta)$ given in eq. (52) satisfies the conditions $\overline{R}\,\overline{R}^{\mathsf{T}} = \mathbf{I}$ and $\det \overline{R} = -1$.

7. Determining the parameters $\hat{\boldsymbol{n}}$ and $\boldsymbol{\theta}$ of a general 3×3 orthogonal matrix.

The results obtained in eqs. (20) and (51) can be expressed as a single equation. Consider a general 3×3 orthogonal matrix R, corresponding to *either* a proper or improper rotation. Then its matrix elements are given by:

$$R_{ij}(\hat{\boldsymbol{n}}, \theta) = \cos\theta\,\delta_{ij} + (\varepsilon - \cos\theta) n_i n_j - \sin\theta\,\epsilon_{ijk} n_k\,, \tag{54}$$

where

$$\varepsilon \equiv \det R(\hat{\boldsymbol{n}}, \theta)\,. \tag{55}$$

[8]Indeed, eqs. (22) and (53) are consistent with eq. (42) as expected.

That is, $\varepsilon = 1$ for a proper rotation and $\varepsilon = -1$ for an improper rotation. Using eq. (54), one can derive expressions for the unit vector $\hat{\boldsymbol{n}}$ and the angle θ in terms of the matrix elements of R. With some tensor algebra manipulations involving the Levi-Civita tensor, we can quickly obtain the desired results.

First, we compute the trace of $R(\hat{\boldsymbol{n}}, \theta)$. In particular, using eq. (54) it follows that:[9]

$$\text{Tr } R(\hat{\boldsymbol{n}}, \theta) \equiv R_{ii} = \varepsilon + 2\cos\theta\,. \tag{56}$$

In deriving this result, we used the fact that $\delta_{ii} = \text{Tr }\mathbf{I} = 3$ (since the indices run over $i = 1, 2, 3$ in three-dimensional space) and $\epsilon_{iik} = 0$ (the latter is a consequence of the fact that the Levi-Civita tensor is totally antisymmetric under the interchange of any two indices). By convention, $0 \leq \theta \leq \pi$, which implies that $\sin\theta \geq 0$. Thus,

$$\cos\theta = \tfrac{1}{2}(\text{Tr}\,R - \varepsilon) \quad \text{and} \quad \sin\theta = (1-\cos^2\theta)^{1/2} = \tfrac{1}{2}\sqrt{(3-\varepsilon\,\text{Tr}\,R)(1+\varepsilon\,\text{Tr}\,R)}\,, \tag{57}$$

where $\cos\theta$ is determined from eq. (56) and we have used $\varepsilon^2 = 1$. All that remains is to determine the unit vector $\hat{\boldsymbol{n}}$.

Let us multiply eq. (20) by ϵ_{ijm} and sum over i and j. Noting that

$$\epsilon_{ijm}\delta_{ij} = \epsilon_{ijm}n_i n_j = 0\,, \qquad \epsilon_{ijk}\epsilon_{ijm} = 2\delta_{km}\,, \tag{58}$$

it follows that

$$2n_m \sin\theta = -R_{ij}\epsilon_{ijm}\,. \tag{59}$$

If R is a symmetric matrix (i.e. $R_{ij} = R_{ji}$), then $R_{ij}\epsilon_{ijm} = 0$ automatically since ϵ_{ijk} is antisymmetric under the interchange of the indices i and j. In this case $\sin\theta = 0$, and eq. (59) cannot be used to determine $\hat{\boldsymbol{n}}$. If $\sin\theta \neq 0$, then one can divide both sides of eq. (59) by $\sin\theta$. Using eq. (57), we obtain:

$$n_m = -\frac{R_{ij}\epsilon_{ijm}}{2\sin\theta} = \frac{-R_{ij}\epsilon_{ijm}}{\sqrt{(3-\varepsilon\,\text{Tr}\,R)(1+\varepsilon\,\text{Tr}\,R)}}\,, \qquad \sin\theta \neq 0\,. \tag{60}$$

More explicitly,

$$\hat{\boldsymbol{n}} = \frac{1}{\sqrt{(3-\varepsilon\,\text{Tr}\,R)(1+\varepsilon\,\text{Tr}\,R)}}\bigg(R_{32}-R_{23}\,,\, R_{13}-R_{31}\,,\, R_{21}-R_{12}\bigg)\,, \qquad \varepsilon\,\text{Tr}R \neq -1\,,\,3\,. \tag{61}$$

In Appendix F, we verify that $\hat{\boldsymbol{n}}$ as given by eq. (60) is a vector of unit length [as required by eq. (12)]. The overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (60) due to our convention in which $\sin\theta \geq 0$. If we multiply eq. (59) by n_m and sum over m, then

$$\sin\theta = -\tfrac{1}{2}\epsilon_{ijm}R_{ij}n_m\,, \tag{62}$$

after using $n_m n_m = 1$. This provides an additional check on the determination of the rotation angle.

[9]The quantities $R_{ii} \equiv \text{Tr}\,R$ and $\delta_{ii} \equiv \text{Tr}\,\mathbf{I} = 3$ each involve an implicit sum over i (following the Einstein summation convention), and thus define the trace of R and $\mathbf{I}$, respectively.

If $\sin\theta = 0$, then there are two possible cases to consider depending on the sign of $\cos\theta$. In the case of $\cos\theta = -\varepsilon$ (which corresponds to $\varepsilon\,\mathrm{Tr}\,R = -1$), one can use eq. (54) to derive

$$\hat{\boldsymbol{n}} = \left(\epsilon_1\sqrt{\tfrac{1}{2}(1+\varepsilon R_{11})}\,,\,\epsilon_2\sqrt{\tfrac{1}{2}(1+\varepsilon R_{22})}\,,\,\epsilon_3\sqrt{\tfrac{1}{2}(1+\varepsilon R_{33})}\right)\,, \qquad \text{if } \varepsilon\,\mathrm{Tr}\,R = -1\,, \tag{63}$$

where the individual signs $\epsilon_i = \pm 1$ are determined up to an overall sign via

$$\epsilon_i\epsilon_j = \frac{\varepsilon R_{ij}}{\sqrt{(1+\varepsilon R_{ii})(1+\varepsilon R_{jj})}}\,, \qquad \text{for fixed } i \neq j\,,\ \varepsilon R_{ii} \neq -1\,,\ \varepsilon R_{jj} \neq -1\,. \tag{64}$$

The ambiguity of the overall sign of $\hat{\boldsymbol{n}}$ is not significant in light of eqs. (6) and (31). Finally, in the case of $\cos\theta = \varepsilon$ (which corresponds to $\varepsilon\,\mathrm{Tr}\,R = 3$), we have $R = \varepsilon\mathbf{I}$ independently of the direction of $\hat{\boldsymbol{n}}$.

Alternatively, we can define a matrix S whose matrix elements are given by:

$$\begin{aligned} S_{jk} &\equiv R_{jk} + R_{kj} + (\varepsilon - \mathrm{Tr}\,R)\delta_{jk} \qquad (65)\\ &= 2(\varepsilon - \cos\theta)n_j n_k = (3\varepsilon - \mathrm{Tr}\,R)n_j n_k\,, \end{aligned}$$

after using eq. (54) for R_{jk}. Hence,[10]

$$n_j n_k = \frac{S_{jk}}{3\varepsilon - \mathrm{Tr}\,R}\,, \qquad \mathrm{Tr}\,R \neq 3\varepsilon\,. \tag{66}$$

To determine $\hat{\boldsymbol{n}}$ up to an overall sign, we simply set $j = k$ (no sum) in eq. (66), which fixes the value of n_j^2. If $\sin\theta \neq 0$, the overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (59).

As noted above, if R is a symmetric matrix (i.e. $R_{ij} = R_{ji}$), then $\sin\theta = 0$ and $\hat{\boldsymbol{n}}$ cannot be determined from eq. (60). In this case, eq. (56) determines whether $\cos\theta = +1$ or $\cos\theta = -1$. If $\cos\theta = \varepsilon$, then $R_{ij} = \varepsilon\delta_{ij}$, in which case $S = \mathbf{0}$ and the axis $\hat{\boldsymbol{n}}$ is undefined. For $\cos\theta = -\varepsilon$, one can determine $\hat{\boldsymbol{n}}$ up to an overall sign using eq. (66). As previously remarked, in this latter case the overall sign of $\hat{\boldsymbol{n}}$ is not meaningful.

To summarize, eqs. (57), (61) and (66) provide a simple algorithm for determining the unit vector $\hat{\boldsymbol{n}}$ and the rotation angle θ for any proper or improper rotation matrix $R(\hat{\boldsymbol{n}},\theta) \neq \varepsilon\mathbf{I}$.

8. Determining the reflection plane corresponding to an improper rotation

As noted in Section 5, the most general three-dimensional improper rotation, denoted by $\overline{R}(\hat{\boldsymbol{n}},\theta)$, consists of a product of a proper rotation matrix, $R(\hat{\boldsymbol{n}},\theta)$, and a mirror reflection through a plane normal to the unit vector $\hat{\boldsymbol{n}}$, which we denote by

[10]Eq. (65) yields $\mathrm{Tr}\,S = 3\varepsilon - \mathrm{Tr}\,R$. One can then use eq. (66) to verify once again that $\hat{\boldsymbol{n}}$ is a unit vector.

$\overline{R}(\hat{\boldsymbol{n}})$[cf. eq. (30)]. In particular, the reflection plane passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$. In this section, we shall derive an equation for the reflection plane, which passes through the origin and is perpendicular to $\hat{\boldsymbol{n}}$.

Consider a plane that passes through the point (x_0, y_0, z_0) that is perpendicular to the unit vector $\hat{\boldsymbol{n}} = n_1\hat{\boldsymbol{x}} + n_2\hat{\boldsymbol{y}} + n_2\hat{\boldsymbol{z}} = (n_1, n_2, n_3)$. Then it is straightforward to show that the equation of the plane is given by:

$$n_1(x - x_0) + n_2(y - y_0) + n_3(z - z_0) = 0\,. \tag{67}$$

It is then a simple matter to apply this result to the reflection plane, which is perpendicular to $\hat{\boldsymbol{n}}$ and passes through the origin, i.e. the point $(x_0, y_0, z_0) = (0, 0, 0)$. Then, eq. (67) immediately yields the equation of the reflection plane,

$$n_1 x + n_2 y + n_3 z = 0\,. \tag{68}$$

Note that the equation for the reflection plane does not depend on the overall sign of $\hat{\boldsymbol{n}}$ [cf. eq. (31)]. This makes sense, as both $\hat{\boldsymbol{n}}$ and $-\hat{\boldsymbol{n}}$ are perpendicular to the reflection plane.

The equation for the reflection plane can also be derived directly as follows. If $\theta \neq \pi$,[11] then the reflection plane corresponding to the improper rotation $\overline{R}(\hat{\boldsymbol{n}}, \theta)$ is perpendicular to $\hat{\boldsymbol{n}}$, independently of the value of θ. Thus without loss of generality, one can take $\theta = 0$ and consider $\overline{R}(\hat{\boldsymbol{n}}) \equiv \overline{R}(\hat{\boldsymbol{n}}, 0)$, which represents a mirror reflection through the reflection plane. Any vector $\vec{\boldsymbol{v}} = (x, y, z)$ that lies in the reflection plane is an eigenvector of $\overline{R}(\hat{\boldsymbol{n}})$ with eigenvalue $+1$, as indicated at the end of Section 5. Thus, the equation of the reflection plane is $\overline{R}(\hat{\boldsymbol{n}})\vec{\boldsymbol{v}} = \vec{\boldsymbol{v}}$, which is explicitly given by [cf. eq. (53)]:

$$\begin{pmatrix} 1 - 2n_1^2 & -2n_1 n_2 & -2n_1 n_3 \\ -2n_1 n_2 & 1 - 2n_2^2 & -2n_2 n_3 \\ -2n_1 n_3 & 2 - n_2 n_3 & 1 - 2n_3^2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{69}$$

The matrix equation, eq. (69), is equivalent to:

$$\begin{pmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ n_1 n_2 & n_2^2 & n_2 n_3 \\ n_1 n_3 & n_2 n_3 & n_3^2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0\,. \tag{70}$$

Applying two elementary row operations, the matrix equation, eq. (70), can be transformed into reduced row echelon form,

$$\begin{pmatrix} n_1^2 & n_1 n_2 & n_1 n_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = 0\,.$$

The solution to this equation is all x, y and z that satisfy eq. (68), which corresponds to the equation of the reflection plane.

[11]In the case of $\theta = \pi$, the unit normal to the reflection plane $\hat{\boldsymbol{n}}$ is undefined so we exclude this case from further consideration.

Appendix A: An explicit computation of the matrix $\boldsymbol{P}$ defined in eq. (8)

The matrix $R(\hat{\boldsymbol{n}},\theta)$ is specified with respect to the standard basis $\mathcal{B}_s = \{\hat{\boldsymbol{x}}\,,\,\hat{\boldsymbol{y}}\,,\,\hat{\boldsymbol{z}}\}$. One can always rotate to a new orthonormal basis, $\mathcal{B}' = \{\hat{\boldsymbol{x}}'\,,\,\hat{\boldsymbol{y}}'\,,\,\hat{\boldsymbol{z}}'\}$, in which new positive z-axis points in the direction of $\hat{\boldsymbol{n}}$. That is,

$$\hat{\boldsymbol{z}}' = \hat{\boldsymbol{n}} \equiv (n_1, n_2, n_3)\,, \qquad \text{where}\ \ n_1^2+n_2^2+n_3^2 = 1\,.$$

The new positive y-axis can be chosen to lie along

$$\hat{\boldsymbol{y}}' = \left(\frac{-n_2}{\sqrt{n_1^2+n_2^2}}\,,\,\frac{n_1}{\sqrt{n_1^2+n_2^2}}\,,\,0\right)\,,$$

since by construction, $\hat{\boldsymbol{y}}'$ is a unit vector orthogonal to $\hat{\boldsymbol{z}}'$. We complete the new right-handed coordinate system by choosing:

$$\hat{\boldsymbol{x}}' = \hat{\boldsymbol{y}}'\times\hat{\boldsymbol{z}}' = \begin{vmatrix} \hat{\boldsymbol{x}} & \hat{\boldsymbol{y}} & \hat{\boldsymbol{z}} \\ \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & 0 \\ n_1 & n_2 & n_3 \end{vmatrix} = \left(\frac{n_3 n_1}{\sqrt{n_1^2+n_2^2}}\,,\,\frac{n_3 n_2}{\sqrt{n_1^2+n_2^2}}\,,\,-\sqrt{n_1^2+n_2^2}\right)\,.$$

One can now determine the matrix P whose matrix elements are defined by

$$\boldsymbol{b}'_j = \sum_{i=1}^{n} P_{ij}\hat{\boldsymbol{e}}_i\,,$$

where the $\hat{\boldsymbol{e}}_i$ are the basis vectors of $\mathcal{B}_s$ and the $\boldsymbol{b}'_j$ are the basis vectors of $\mathcal{B}'$. The columns of P are the coefficients of the expansion of the new basis vectors in terms of the old basis vectors. Thus,

$$P = \begin{pmatrix} \dfrac{n_3 n_1}{\sqrt{n_1^2+n_2^2}} & \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & n_1 \\ \dfrac{n_3 n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & n_2 \\ -\sqrt{n_1^2+n_2^2} & 0 & n_3 \end{pmatrix}\,. \qquad (71)$$

Note that the columns of P are orthonormal and $\det P = 1$. That is, P is an SO(3) matrix. Using eq. (10) of the class handout cited above, we recover eq. (8). It is straightforward to check that $\hat{\boldsymbol{n}} = P\hat{\boldsymbol{z}}$, which is not surprising since the matrix P was constructed so that the vector $\hat{\boldsymbol{n}}$, which is represented by $\hat{\boldsymbol{n}} = (n_1\,,\,n_2\,,\,n_3)$ with respect to the standard basis $\mathcal{B}_s$ would have coordinates $(0\,,\,0\,,\,1)$ with respect to the basis $\mathcal{B}'$.

Appendix B: The eigenvalues of a 3 × 3 orthogonal matrix[12]

Given any matrix A, the eigenvalues are the solutions to the characteristic equation,

$$\det\,(A-\lambda\mathbf{I})=0\,. \tag{72}$$

Suppose that A is an $n\times n$ real orthogonal matrix. The eigenvalue equation for A and its complex conjugate transpose are given by:

$$A\boldsymbol{v}=\lambda\boldsymbol{v}\,,\qquad \boldsymbol{v}^\dagger A^{\mathsf{T}}=\lambda^*\,\boldsymbol{v}^\dagger\,.$$

Hence multiplying these two equations together yields

$$\lambda^*\,\lambda\,\boldsymbol{v}^\dagger\boldsymbol{v}=\boldsymbol{v}^\dagger A^{\mathsf{T}}A\boldsymbol{v}=\boldsymbol{v}^\dagger\boldsymbol{v}\,, \tag{73}$$

since an orthogonal matrix satisfies $A^{\mathsf{T}}A=\mathbf{I}$. Since eigenvectors must be nonzero, it follows that $\boldsymbol{v}^\dagger\boldsymbol{v}\neq 0$. Hence, eq. (73) yields $|\lambda|=1$. Thus, the eigenvalues of a real orthogonal matrix must be complex numbers of unit modulus. That is, $\lambda=e^{i\alpha}$ for some α in the interval $0\leq\alpha<2\pi$.

Consider the following product of matrices, where A satisfies $A^{\mathsf{T}}A=\mathbf{I}$,

$$A^{\mathsf{T}}(\mathbf{I}-A)=A^{\mathsf{T}}-\mathbf{I}=-(\mathbf{I}-A)^{\mathsf{T}}\,.$$

Taking the determinant of both sides of this equation, it follows that

$$\det A\,\det(\mathbf{I}-A)=(-1)^n\det(\mathbf{I}-A)\,, \tag{74}$$

since for the $n\times n$ identity matrix, $\det(-\mathbf{I})=(-1)^n$. For a proper odd-dimensional orthogonal matrix, we have $\det A=1$ and $(-1)^n=-1$. Hence, eq. (74) yields[13]

$$\det(\mathbf{I}-A)=0\,,\qquad \text{for any proper odd-dimensional orthogonal matrix } A. \tag{75}$$

Comparing with eq. (72), we conclude that $\lambda=1$ is an eigenvalue of A.[14] Since $\det A$ is the product of its three eigenvalues and each eigenvalue is a complex number of unit modulus, it follows that the eigenvalues of any proper 3×3 orthogonal matrix must be 1, $e^{i\theta}$ and $e^{-i\theta}$ for some value of θ that lies in the interval $0\leq\theta\leq\pi$.[15]

Next, we consider the following product of matrices, where A satisfies $A^{\mathsf{T}}A=\mathbf{I}$,

$$A^{\mathsf{T}}(\mathbf{I}+A)=A^{\mathsf{T}}+\mathbf{I}=(\mathbf{I}+A)^{\mathsf{T}}\,.$$

[12] A nice reference to the results of this Appendix can be found in L. Mirsky, *An Introduction to Linear Algebra* (Dover Publications, Inc., New York, 1982).

[13] Eq. (75) is also valid for any improper even-dimensional orthogonal matrix A since in this case $\det A=-1$ and $(-1)^n=1$.

[14] Of course, this is consistent with the result that the eigenvalues of a real orthogonal matrix are of the form $e^{i\alpha}$ for $0\leq\alpha<2\pi$, since the eigenvalue 1 corresponds to $\alpha=0$.

[15] There is no loss of generality in restricting the interval of the angle to satisfy $0\leq\theta\leq\pi$. In particular, under $\theta\to 2\pi-\theta$, the two eigenvalues $e^{i\theta}$ and $e^{-i\theta}$ are simply interchanged.

Taking the determinant of both sides of this equation, it follows that

$$\det A \det(\mathbf{I} + A) = \det(\mathbf{I} + A)\,, \tag{76}$$

For any improper orthogonal matrix, we have $\det A = -1$. Hence, eq. (76) yields

$$\det(\mathbf{I} + A) = 0\,, \qquad \text{for any improper orthogonal matrix } A.$$

Comparing with eq. (72), we conclude that $\lambda = -1$ is an eigenvalue of A. Since $\det A$ is the product of its three eigenvalues and each eigenvalue is a complex number of unit modulus, it follows that the eigenvalues of any improper 3×3 orthogonal matrix must be -1, $e^{i\theta}$ and $e^{-i\theta}$ for some value of θ that lies in the interval $0 \leq \theta \leq \pi$ (cf. footnote 15).

Appendix C: Matrix elements of matrices correspond to the components of second rank tensors

Consider the matrix elements of a linear operator with respect to two different orthonormal bases, $\mathcal{B} = \{\hat{\boldsymbol{e}}_1\,,\,\hat{\boldsymbol{e}}_2\,,\,\hat{\boldsymbol{e}}_3\}$ and $\mathcal{B}' = \{\hat{\boldsymbol{e}}'_1\,,\,\hat{\boldsymbol{e}}'_2\,,\,\hat{\boldsymbol{e}}'_3\}$. Then, using the Einstein summation convention,

$$\hat{\boldsymbol{e}}'_j = P_{ij}\hat{\boldsymbol{e}}_i\,,$$

where P is an orthogonal matrix. Given any linear operator A with matrix elements a_{ij} with respect to the basis $\mathcal{B}$, the matrix elements a'_{ij} with respect to the basis $\mathcal{B}'$ are given by

$$a'_{k\ell} = (P^{-1})_{ki}a_{ij}P_{j\ell} = P_{ik}a_{ij}P_{j\ell}\,,$$

where we have used the fact that $P^{-1} = P^{\mathsf{T}}$ in the second step above. Finally, identifying $P = R^{-1}$, where R is also an orthogonal matrix, it follows that

$$a'_{k\ell} = R_{ki}R_{\ell j}a_{ij}\,,$$

which we recognize as the transformation law for the components of a second rank Cartesian tensor.

Appendix D: The relation between $R(\hat{\boldsymbol{n}}, \theta)$ and $R(\hat{\boldsymbol{n}}', \theta)$

Eq. (8) is a special case of a more general result,

$$R(\hat{\boldsymbol{n}}, \theta) = \mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}\,, \qquad \text{where } \hat{\boldsymbol{n}} = \mathcal{R}\hat{\boldsymbol{n}}'\,. \tag{77}$$

That is, $\mathcal{R}$ is the rotation matrix that rotates the unit vector $\hat{\boldsymbol{n}}'$ into the unit vector $\hat{\boldsymbol{n}}$.[16] The group theoretical interpretation of this result is that elements of SO(3) corresponding to a rotation by a fixed angle θ about an arbitrary axis are members of the same

[16] An explicit form for the matrix $\mathcal{R}$ can be obtained using the methods of Appendix A.

conjugacy class. In particular, the independent (disjoint) conjugacy classes of SO(3) are in one to one correspondence with the possible choices of θ (where $0 \leq \theta \leq \pi$).

Eq. (77) is a consequence of a well known result of the theory of Lie groups and Lie algebras. I will discuss this result at the end of this Appendix. First, I will provide a direct proof of eq. (77). First, we shall compute the angle of the rotation $\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}$ using eq. (57) with $\varepsilon = 1$. Since $\mathrm{Tr}[\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}] = \mathrm{Tr}\, R(\hat{\boldsymbol{n}}', \theta)$ using the cyclicity of the trace, it follows that the angles of rotation corresponding to $\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}$ and $R(\hat{\boldsymbol{n}}', \theta)$ coincide and are both equal to θ. To compute the corresponding axis of rotation $\hat{\boldsymbol{n}}$, we employ eq. (59),

$$2n_m \sin\theta = -(\mathcal{R}\, R'\, \mathcal{R}^{-1})_{ij}\epsilon_{ijm}\,, \tag{78}$$

where $R' \equiv R(\hat{\boldsymbol{n}}', \theta)$. Since $\mathcal{R}^{-1} = \mathcal{R}^{\mathsf{T}}$, or equivalently $(\mathcal{R}^{-1})_{\ell j} = \mathcal{R}_{j\ell}$, one can rewrite eq. (78) as:

$$2n_m \sin\theta = -\mathcal{R}_{ik}\, R'_{k\ell}\, \mathcal{R}_{j\ell}\, \epsilon_{ijm}\,, \tag{79}$$

Multiplying both sides of eq. (79) by $\mathcal{R}_{mn}$ and using the definition of the determinant of a 3×3 matrix,

$$\mathcal{R}_{ik}\mathcal{R}_{j\ell}\mathcal{R}_{mn}\epsilon_{ijm} = (\det P)\epsilon_{k\ell n}\,,$$

it then follows that:

$$2\mathcal{R}_{mn}n_m \sin\theta = -R'_{k\ell}\epsilon_{k\ell n}\,, \tag{80}$$

after noting that $\det \mathcal{R} = 1$. Finally, we again use eq. (59) which yields

$$2n'_n \sin\theta = -R'_{k\ell}\epsilon_{k\ell n}\,. \tag{81}$$

Assuming that $\sin\theta \neq 0$, we can subtract eqs. (80) and (81) and divide out by $2\sin\theta$. Using $(\mathcal{R}^{\mathsf{T}})_{nm} = \mathcal{R}_{mn}$, the end result is:

$$\hat{\boldsymbol{n}}' - \mathcal{R}^{\mathsf{T}}\hat{\boldsymbol{n}} = 0\,.$$

Since $\mathcal{R}\,\mathcal{R}^{\mathsf{T}} = \mathcal{R}^{\mathsf{T}}\,\mathcal{R} = \mathbf{I}$, we conclude that

$$\hat{\boldsymbol{n}} = \mathcal{R}\hat{\boldsymbol{n}}'\,. \tag{82}$$

The case of $\sin\theta = 0$ must be treated separately. Using eq. (10), one can determine the axis of rotation $\hat{\boldsymbol{n}}$ of the rotation matrix $\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}$ up to an overall sign. Since $R(\hat{\boldsymbol{n}}', \theta)\hat{\boldsymbol{n}}' = \hat{\boldsymbol{n}}'$, the following eigenvalue equation is obtained:

$$\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}(\mathcal{R}\hat{\boldsymbol{n}}') = \mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\hat{\boldsymbol{n}}' = \mathcal{R}\hat{\boldsymbol{n}}'\,. \tag{83}$$

That is, $\mathcal{R}\hat{\boldsymbol{n}}'$ is an eigenvector of $\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}$ with eigenvalue $+1$. It then follows that $\mathcal{R}\hat{\boldsymbol{n}}'$ is the normalized eigenvector of $\mathcal{R}\, R(\hat{\boldsymbol{n}}', \theta)\mathcal{R}^{-1}$ up to an overall undetermined sign. For $\sin\theta \neq 0$, the overall sign is fixed and is positive by eq. (82). If $\sin\theta = 0$, then there are two cases to consider. If $\theta = 0$, then $R(\hat{\boldsymbol{n}}, 0) = R(\hat{\boldsymbol{n}}', 0) = \mathbf{I}$ and eq. (77) is trivially satisfied. If $\theta = \pi$, then eq. (6) implies that the unit vector parallel to the rotation axis is only defined up to an overall sign. Hence, eq. (77) is valid even in the case of $\sin\theta = 0$, and the proof is complete.

As noted above eq. (77) is a consequence of a well known result of the theory of Lie groups and Lie algebra of SO(3). The matrices R_{ij} given in eq. (20) constitutes the defining representation of SO(3). The operator $\mathrm{Ad}\,\mathcal{R}$ acts on elements of the SO(3) Lie algebra, henceforth denoted by $\mathfrak{so}(3)$, and is defined by

$$\mathrm{Ad}\,\mathcal{R}(x) = \mathcal{R}x\mathcal{R}^{-1}\,, \quad x \in \mathfrak{so}(3)\,. \tag{84}$$

The matrix elements of $\mathrm{Ad}\,\mathcal{R}$ are obtained in the usual way by considering the action of $\mathrm{Ad}\,\mathcal{R}$ on the basis vectors, namely the generators of $\mathfrak{so}(3)$,

$$\mathrm{Ad}\,\mathcal{R}(e_i) = (\mathrm{Ad}\,\mathcal{R})_{ji}e_j\,, \tag{85}$$

where there is an implicit sum over the repeated index j. The generators of $\mathfrak{so}(3)$ satisfy the commutation relations, $[e_i\,,\,e_j] = \epsilon_{ijk}e_k$.[17] We identify $(\mathrm{Ad}\,\mathcal{R})_{ji} = R_{ji}$, since the adjoint representation and the defining representation of SO(3) coincide. Thus, combining eqs. (84) and (85),

$$\mathcal{R}e_i\mathcal{R}^{-1} = R_{ji}e_j\,, \tag{86}$$

which applies to *any* matrix representation of the $\mathfrak{so}(3)$ generators, e_i.

We shall make use of eq. (86) by taking the e_i to be the matrix generators of $\mathfrak{so}(3)$ in the defining representation (which in this case is equivalent to the adjoint representation) of $\mathfrak{so}(3)$. In the notation of problem 7(b) of problem set 2, we identify $e_k = -iJ_k$, where $(J_k)_{ij} = -i\epsilon_{ijk}$. Then, multiplying both sides of eq. (86) by $\theta\hat{n}'_i$ and defining $\hat{n}_j = R_{ji}\hat{n}'_i$ [cf. eq. (82)], it follows that

$$\mathcal{R}\left(-i\theta\boldsymbol{\hat{n}'}\boldsymbol{\cdot}\vec{\boldsymbol{J}}\right)\mathcal{R}^{-1} = -i\theta\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{J}}, \tag{87}$$

after combining the three matrix generators, $\{-iJ_1\,,\,-iJ_2\,,\,-iJ_3\}$, of $\mathfrak{so}(3)$ into a vector by writing $\vec{\boldsymbol{J}} = (J_1\,,\,J_2\,,\,J_3)$. Finally, we exponentiate both sides of eq. (87), and recognize that $R(\boldsymbol{\hat{n}},\theta) = \exp(-i\theta\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{J}})$ as noted below eq. (12).[18] Hence, we end up with

$$\mathcal{R}\,R(\boldsymbol{\hat{n}'},\theta)\mathcal{R}^{-1} = R(\boldsymbol{\hat{n}},\theta)\,, \qquad \text{where } \boldsymbol{\hat{n}} = \mathcal{R}\boldsymbol{\hat{n}'}\,. \tag{88}$$

which is eq. (77).

Appendix E: Euler angle representation of $\boldsymbol{R(\hat{n},\theta)}$

The angle-and-axis parameterization, denoted by $R(\boldsymbol{\hat{n}},\theta)$, is only one of a number of ways of parameterizing the most general three-dimensional proper rotation. In this Appendix, we examine an alternative parameterization called the Euler angle representation.

[17] Here, we use the mathematician's convention in which the generators of $\mathfrak{so}(3)$ in the defining representation are antihermitian. In the physicist's convention, one replaces $e_i \to ie_i$ and employs hermitian generators.

[18] Note that for any invertible matrix S, it follows that $\exp(SAS^{-1}) = Se^AS^{-1}$. This result is easily established by using the Taylor series expansion for the exponential function.

An arbitrary three-dimensional proper rotation matrix can be written as the product of the following *three* simpler rotations,[19]

$$R(\hat{\boldsymbol{n}},\theta)=R(\hat{\boldsymbol{z}},\alpha)R(\hat{\boldsymbol{y}},\beta)R(\hat{\boldsymbol{z}},\gamma)\,, \qquad (89)$$

where α, β and γ are called the *Euler angles*. The ranges of the Euler angles are: $0\leq\alpha,\gamma<2\pi$ and $0\leq\beta\leq\pi$. We shall prove these statements "by construction." That is, we shall explicitly derive the relations between the Euler angles and the angles θ, θ_n and ϕ_n that characterize the rotation $R(\hat{\boldsymbol{n}},\theta)$ [where θ_n and ϕ_n are the polar and azimuthal angle that define the axis of rotation $\hat{\boldsymbol{n}}$ as specified in eq. (23)]. These relations can be obtained by multiplying out the three matrices on the right-hand side of eq. (89) to obtain

$$R(\hat{\boldsymbol{n}},\theta)=\begin{pmatrix}\cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & \cos\alpha\sin\beta\\ \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma+\cos\alpha\cos\gamma & \sin\alpha\sin\beta\\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta\end{pmatrix}. \qquad (90)$$

If the matrix elements of R_{ij} are known, then the Euler angles can be determined from the following relations,

$$\tan\alpha=\frac{R_{23}}{R_{13}}\,,\qquad \cos\beta=R_{33}\,,\qquad \tan\gamma=-\frac{R_{32}}{R_{31}}\,, \qquad (91)$$

where $0\leq\alpha,\gamma<2\pi$ and $0\leq\beta\leq\pi$, as noted above. Eq. (91) leaves the quadrants of the angles α and γ ambiguous, but these can be fixed from the signs of R_{23} and R_{32}, respectively, which determine the respective signs of $\sin\alpha$ and $\sin\gamma$ (in light of the fact that $0\leq\sin\beta\leq 1$).

One can now make use of the results of Section 7 (with $\varepsilon=1$) to obtain θ and $\hat{\boldsymbol{n}}$ in terms of the Euler angles α, β and γ. For example, $\cos\theta$ is obtained from eq. (57). Simple algebra yields:

$$\boxed{\cos\theta=\cos^2(\beta/2)\cos(\gamma+\alpha)-\sin^2(\beta/2)} \qquad (92)$$

after using $\cos^2(\beta/2)=\frac{1}{2}(1+\cos\beta)$ and $\sin^2(\beta/2)=\frac{1}{2}(1-\cos\beta)$. Thus, we have determined θ mod π, consistent with our convention that $0\leq\theta\leq\pi$ [cf. eq. (57) and the text preceding this equation]. One can also rewrite eq. (92) in a slightly more convenient form,

$$\cos\theta=-1+2\cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)\,. \qquad (93)$$

We examine separately the cases for which $\sin\theta=0$. First, $\cos\beta=\cos(\gamma+\alpha)=1$ implies that $\theta=0$ and $R(\hat{\boldsymbol{n}},\theta)=\mathbf{I}$. In this case, the axis of rotation, $\hat{\boldsymbol{n}}$, is undefined.

[19]There are many possible Euler angle parameterizations of a rotation matrix. See, e.g., Ref. 3 for a catalog of different possible parameterizations (note that this paper employs passive rather than active rotations, so to match the results in these notes, one must change the signs of all angles). The Euler angle parameterization employed in eq. (89) follows that standard convention adopted in most books on angular momentum in quantum mechanics.

Second, if $\theta=\pi$ then $\cos\theta=-1$ and $\hat{\boldsymbol{n}}$ is determined up to an overall sign (which is not physical). Eq. (93) then implies that $\cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)=0$, or equivalently $(1+\cos\beta)\,[1+\cos(\gamma+\alpha)]=0$, which yields two possible subcases,

$$\text{(i)}\quad \cos\beta=-1 \quad \text{and/or} \quad \text{(ii)}\quad \cos(\gamma+\alpha)=-1\,.$$

In subcase (i), if $\cos\beta=-1$, then eqs. (63) and (64) yield

$$R(\hat{\boldsymbol{n}},\pi)=\begin{pmatrix}-\cos(\gamma-\alpha) & \sin(\gamma-\alpha) & 0\\ \sin(\gamma-\alpha) & \cos(\gamma-\alpha) & 0\\ 0 & 0 & -1\end{pmatrix}\,,$$

where

$$\hat{\boldsymbol{n}}=\pm\bigl(\sin\tfrac{1}{2}(\gamma-\alpha)\,,\,\cos\tfrac{1}{2}(\gamma-\alpha)\,,\,0\bigr)\,.$$

In subcase (ii), if $\cos(\gamma+\alpha)=-1$, then

$$\begin{aligned}\cos\gamma+\cos\alpha&=2\cos\tfrac{1}{2}\,(\gamma-\alpha)\cos\tfrac{1}{2}\,(\gamma+\alpha)=0\,,\\ \sin\gamma-\sin\alpha&=2\sin\tfrac{1}{2}\,(\gamma-\alpha)\cos\tfrac{1}{2}\,(\gamma+\alpha)=0\,,\end{aligned}$$

since $\cos^2\tfrac{1}{2}(\gamma+\alpha)=\tfrac{1}{2}\,[1+\cos(\gamma+\alpha)]=0$. Thus, eqs. (63) and (64) yield

$$R(\hat{\boldsymbol{n}},\pi)=\begin{pmatrix}-\cos\beta-2\sin^2\!\alpha\sin^2(\beta/2) & \sin(2\alpha)\sin^2(\beta/2) & \cos\alpha\sin\beta\\ \sin(2\alpha)\sin^2(\beta/2) & -1+2\sin^2\!\alpha\sin^2(\beta/2) & \sin\alpha\sin\beta\\ \cos\alpha\sin\beta & \sin\alpha\sin\beta & \cos\beta\end{pmatrix}\,,$$

where

$$\hat{\boldsymbol{n}}=\pm\bigl(\sin(\beta/2)\cos\alpha\,,\,\sin(\beta/2)\sin\alpha\,,\,\cos(\beta/2)\bigr)\,.$$

Finally, we consider the generic case where $\sin\theta\neq 0$. Using eqs. (61) and (91),

$$\begin{aligned}R_{32}-R_{23}&=2\sin\beta\sin\tfrac{1}{2}(\gamma-\alpha)\cos\tfrac{1}{2}(\gamma+\alpha)\,,\\ R_{13}-R_{31}&=2\sin\beta\cos\tfrac{1}{2}(\gamma-\alpha)\cos\tfrac{1}{2}(\gamma+\alpha)\,,\\ R_{21}-R_{12}&=2\cos^2(\beta/2)\sin(\gamma+\alpha)\,.\end{aligned}$$

In normalizing the unit vector $\hat{\boldsymbol{n}}$, it is convenient to write $\sin\beta=2\sin(\beta/2)\cos(\beta/2)$ and $\sin(\gamma+\alpha)=2\sin\tfrac{1}{2}(\gamma+\alpha)\cos\tfrac{1}{2}(\gamma+\alpha)$. Then, we compute:

$$\begin{aligned}&\bigl[(R_{32}-R_{23})^2+(R_{13}-R_{31})^2+(R_{12}-R_{21})^2\bigr]^{1/2}\\ &\qquad=4\left|\cos\tfrac{1}{2}(\gamma+\alpha)\cos(\beta/2)\right|\sqrt{\sin^2(\beta/2)+\cos^2(\beta/2)\sin^2\tfrac{1}{2}(\gamma+\alpha)}\,.\end{aligned}\tag{94}$$

Hence,[20]

$$\begin{aligned}\hat{\boldsymbol{n}}=&\frac{\epsilon}{\sqrt{\sin^2(\beta/2)+\cos^2(\beta/2)\sin^2\tfrac{1}{2}(\gamma+\alpha)}}\\ &\times\Bigl(\sin(\beta/2)\sin\tfrac{1}{2}(\gamma-\alpha)\,,\,\sin(\beta/2)\cos\tfrac{1}{2}(\gamma-\alpha)\,,\,\cos(\beta/2)\sin\tfrac{1}{2}(\gamma+\alpha)\Bigr)\,,\end{aligned}\tag{95}$$

[20]One can can also determine $\hat{\boldsymbol{n}}$ up to an overall sign starting from eq. (90) by employing the relation $R(\hat{\boldsymbol{n}},\theta)\hat{\boldsymbol{n}}=\hat{\boldsymbol{n}}$. The sign of $\hat{\boldsymbol{n}}\sin\theta$ can then be determined from eq. (61).

where $\epsilon = \pm 1$ according to the following sign,

$$\epsilon \equiv \operatorname{sgn}\bigl\{\cos\tfrac{1}{2}(\gamma+\alpha)\cos(\beta/2)\bigr\}\,, \qquad \sin\theta \neq 0\,. \tag{96}$$

Remarkably, eq. (95) reduces to the correct results obtained above in the two subcases corresponding to $\theta = \pi$, where $\cos(\beta/2) = 0$ and/or $\cos\frac{1}{2}(\gamma+\alpha) = 0$, respectively. Note that in the latter two subcases, ϵ as defined in eq. (96) is indeterminate. This is consistent with the fact that the sign of $\hat{\boldsymbol{n}}$ is indeterminate when $\theta = \pi$. Finally, one can easily verify that when $\theta = 0$ [corresponding to $\cos\beta = \cos(\gamma+\alpha) = 1$], the direction of $\hat{\boldsymbol{n}}$ is indeterminate and hence arbitrary.

One can rewrite the above results as follows. First, use eq. (93) to obtain:

$$\begin{aligned} \sin(\theta/2) &= \sqrt{\sin^2(\beta/2) + \cos^2(\beta/2)\cos^2\tfrac{1}{2}\,(\gamma+\alpha)}\,, \\ \cos(\theta/2) &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}(\gamma+\alpha)\,. \end{aligned} \tag{97}$$

Since $0 \leq \theta \leq \pi$, it follows that $0 \leq \sin(\theta/2)\,,\ \cos(\theta/2) \leq 1$. Hence, the factor of ϵ defined by eq. (96) is required in eq. (97) to ensure that $\cos(\theta/2)$ is non-negative. In the mathematics literature, it is common to define the following vector consisting of four-components, $q = (q_0\,,\ q_1\,,\ q_2\,,\ q_3)$, called a *quaternion*, as follows:[21]

$$q = \Bigl(\cos(\theta/2)\,,\ \hat{\boldsymbol{n}}\sin(\theta/2)\Bigr)\,, \tag{98}$$

where the components of $\hat{\boldsymbol{n}}\sin(\theta/2)$ comprise the last three components of the quaternion q and

$$\begin{aligned} q_0 &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}\,(\gamma+\alpha)\ , \\ q_1 &= \epsilon\sin(\beta/2)\sin\tfrac{1}{2}\,(\gamma-\alpha)\ , \\ q_2 &= \epsilon\sin(\beta/2)\cos\tfrac{1}{2}\,(\gamma-\alpha)\ , \\ q_3 &= \epsilon\cos(\beta/2)\sin\tfrac{1}{2}\,(\gamma+\alpha)\ . \end{aligned} \tag{99}$$

In the convention of $0 \leq \theta \leq \pi$, we have $q_0 \geq 0$.[22] Quaternions are especially valuable for representing rotations in computer graphics software.[23]

If one expresses $\hat{\boldsymbol{n}}$ in terms of a polar angle θ_n and azimuthal angle ϕ_n as in eq. (23), then one can also write down expressions for θ_n and ϕ_n in terms of the Euler angles α,

[21] The connection between q and the quaternion division algebra $\mathbb{H}$ discussed in class is treated in some detail in Ref. 4. The relation between quaternions and the rotation group is also discussed in Ref. 5 along with applications to molecular symmetry.

[22] In comparing with other treatments in the mathematics literature, one should be careful to note that the convention of $q_0 \geq 0$ is not universally adopted. Often, the quaternion q in eq. (98) will be re-defined as ϵq in order to remove the factors of ϵ from eq. (99), in which case $\epsilon q_0 \geq 0$.

[23] See Ref. 6 for a very readable introduction to quaternions and their applications to visual representations and computer graphics.

β and γ. Comparing eqs. (23) and (95), it follows that:

$$\boxed{\tan\theta_n = \frac{(n_1^2+n_2^2)^{1/2}}{n_3} = \frac{\epsilon\tan(\beta/2)}{\sin\frac{1}{2}(\gamma+\alpha)}} \tag{100}$$

where we have noted that $(n_1^2+n_2^2)^{1/2} = \sin(\beta/2) \geq 0$, since $0 \leq \beta \leq \pi$, and the sign $\epsilon = \pm 1$ is defined by eq. (96). Similarly,

$$\cos\phi_n = \frac{n_1}{(n_1^2+n_2^2)} = \epsilon\sin\tfrac{1}{2}(\gamma-\alpha) = \epsilon\cos\tfrac{1}{2}(\pi-\gamma+\alpha)\,, \tag{101}$$

$$\sin\phi_n = \frac{n_2}{(n_1^2+n_2^2)} = \epsilon\cos\tfrac{1}{2}(\gamma-\alpha) = \epsilon\sin\tfrac{1}{2}(\pi-\gamma+\alpha)\,, \tag{102}$$

or equivalently

$$\boxed{\phi_n = \tfrac{1}{2}(\epsilon\pi-\gamma+\alpha)\ \bmod 2\pi} \tag{103}$$

Indeed, given that $0 \leq \alpha, \gamma < 2\pi$ and $0 \leq \beta \leq \pi$, we see that θ_n is determined mod π and ϕ_n is determine mod 2π as expected for a polar and azimuthal angle, respectively.

One can also solve for the Euler angles in terms of θ, θ_n and ϕ_n. First, we rewrite eq. (93) as:

$$\cos^2(\theta/2) = \cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)\ . \tag{104}$$

Then, using eqs. (100) and (104), it follows that:

$$\sin(\beta/2) = \sin\theta_n\sin(\theta/2)\,. \tag{105}$$

Plugging this result back into eqs. (100) and (104) yields

$$\epsilon\sin\tfrac{1}{2}(\gamma+\alpha) = \frac{\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{106}$$

$$\epsilon\cos\tfrac{1}{2}(\gamma+\alpha) = \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,. \tag{107}$$

Note that if $\beta = \pi$ then eq. (105) yields $\theta = \pi$ and $\theta_n = \pi/2$, in which case $\gamma+\alpha$ is indeterminate. This is consistent with the observation that ϵ is indeterminate if $\cos(\beta/2) = 0$ [cf. eq. (96)].

We shall also make use of eqs. (101) and (102), which we repeat here:

$$\epsilon\sin\tfrac{1}{2}(\gamma-\alpha) = \cos\phi_n\,, \qquad \epsilon\cos\tfrac{1}{2}(\gamma-\alpha) = \sin\phi_n\,. \tag{108}$$

Finally, we employ eq. (108) to obtain (assuming $\beta \neq \pi$):

$$\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}} = \epsilon\left[\cos\tfrac{1}{2}(\gamma-\alpha) - \cos\tfrac{1}{2}(\gamma+\alpha)\right] = 2\epsilon\sin(\gamma/2)\sin(\alpha/2)\,.$$

Since $0 \leq \frac{1}{2}\gamma, \frac{1}{2}\alpha < \pi$, it follows that $\sin(\gamma/2)\sin(\alpha/2) \geq 0$. Thus, we may conclude that if $\gamma \neq 0$, $\alpha \neq 0$ and $\beta \neq \pi$ then

$$\epsilon = \operatorname{sgn}\left\{\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right\}, \tag{109}$$

If either $\gamma = 0$ or $\alpha = 0$, then the argument of sgn in eq. (109) will vanish. In this case, $\sin\frac{1}{2}(\gamma+\alpha) \geq 0$, and we may use eq. (106) to conclude that $\epsilon = \operatorname{sgn}\{\cos\theta_n\}$, if $\theta_n \neq \pi/2$. The case of $\theta_n = \phi_n = \pi/2$ must be separately considered and corresponds simply to $\beta = \theta$ and $\alpha = \gamma = 0$, which yields $\epsilon = 1$. The sign of ϵ is indeterminate if $\sin\theta = 0$ as noted below eq. (96).[24] The latter includes the case of $\beta = \pi$, which implies that $\theta = \pi$ and $\theta_n = \pi/2$, where $\gamma + \alpha$ is indeterminate [cf. eq. (107)].

There is an alternative strategy for determining the Euler angles in terms of θ, θ_n and ϕ_n. Simply set the two matrix forms for $R(\hat{\boldsymbol{n}},\theta)$, eqs. (21) and (90), equal to each other, where $\hat{\boldsymbol{n}}$ is given by eq. (23). For example,

$$R_{33} = \cos\beta = \cos\theta + \cos^2\theta_n(1-\cos\theta)\,. \tag{110}$$

where the matrix elements of $R(\hat{\boldsymbol{n}},\theta)$ are denoted by R_{ij}. It follows that

$$\sin\beta = 2\sin(\theta/2)\sin\theta_n\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}\,, \tag{111}$$

which also can be derived from eq. (105). Next, we note that if $\sin\beta \neq 0$, then

$$\sin\alpha = \frac{R_{23}}{\sin\beta}\,, \qquad \cos\alpha = \frac{R_{13}}{\sin\beta}\,, \qquad \sin\gamma = \frac{R_{32}}{\sin\beta}\,, \qquad \cos\gamma = -\frac{R_{31}}{\sin\beta}\,.$$

Using eq. (21) yields (for $\sin\beta \neq 0$):

$$\sin\alpha = \frac{\cos\theta_n\sin\phi_n\sin(\theta/2) - \cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{112}$$

$$\cos\alpha = \frac{\cos\theta_n\cos\phi_n\sin(\theta/2) + \sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{113}$$

$$\sin\gamma = \frac{\cos\theta_n\sin\phi_n\sin(\theta/2) + \cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{114}$$

$$\cos\gamma = \frac{-\cos\theta_n\cos\phi_n\sin(\theta/2) + \sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,. \tag{115}$$

The cases for which $\sin\beta = 0$ must be considered separately. Since $0 \leq \beta \leq \pi$, $\sin\beta = 0$ implies that $\beta = 0$ or $\beta = \pi$. If $\beta = 0$ then eq. (110) yields either (i) $\theta = 0$, in which case $R(\hat{\boldsymbol{n}},\theta) = \mathbf{I}$ and $\cos\beta = \cos(\gamma+\alpha) = 1$, or (ii) $\sin\theta_n = 0$, in which case

[24] In particular, if $\theta = 0$ then θ_n and ϕ_n are not well-defined, whereas if $\theta = \pi$ then the signs of $\cos\theta_n$, $\sin\phi_n$ and $\cos\phi_n$ are not well-defined [cf. eqs. (6) and (23)].

$\cos\beta = 1$ and $\gamma + \alpha = \theta \bmod \pi$, with $\gamma - \alpha$ indeterminate. If $\beta = \pi$ then eq. (110) yields $\theta_n = \pi/2$ and $\theta = \pi$, in which case $\cos\beta = -1$ and $\gamma - \alpha = \pi - 2\phi \bmod 2\pi$, with $\gamma + \alpha$ indeterminate.

One can use eqs. (112)–(115) to rederive eqs. (106)–(108). For example, if $\gamma \neq 0$, $\alpha \neq 0$ and $\sin\beta \neq 0$, then we can employ a number of trigonometric identities to derive[25]

$$\begin{aligned}\cos\tfrac{1}{2}(\gamma \pm \alpha) &= \cos(\gamma/2)\cos(\alpha/2) \mp \sin(\gamma/2)\sin(\alpha/2) \\ &= \frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)\cos(\alpha/2) \mp \sin^2(\gamma/2)\sin^2(\alpha/2)}{\sin(\gamma/2)\sin(\alpha/2)} \\ &= \frac{\sin\gamma\sin\alpha \mp (1-\cos\gamma)(1-\cos\alpha)}{2(1-\cos\gamma)^{1/2}(1-\cos\alpha)^{1/2}}\,. \end{aligned} \tag{116}$$

and

$$\begin{aligned}\sin\tfrac{1}{2}(\gamma \pm \alpha) &= \sin(\gamma/2)\cos(\alpha/2) \pm \cos(\gamma/2)\sin(\alpha/2) \\ &= \frac{\sin(\gamma/2)\sin(\alpha/2)\cos(\alpha/2)}{\sin(\alpha/2)} \pm \frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)}{\sin(\gamma/2)} \\ &= \frac{\sin(\gamma/2)\sin\alpha}{2\sin(\alpha/2)} \pm \frac{\sin\gamma\sin(\alpha/2)}{2\sin(\gamma/2)} \\ &= \tfrac{1}{2}\sin\alpha\sqrt{\frac{1-\cos\gamma}{1-\cos\alpha}} \pm \tfrac{1}{2}\sin\gamma\sqrt{\frac{1-\cos\alpha}{1-\cos\gamma}} \\ &= \frac{\sin\alpha(1-\cos\gamma) \pm \sin\gamma(1-\cos\alpha)}{2(1-\cos\alpha)^{1/2}(1-\cos\gamma)^{1/2}}\,. \end{aligned} \tag{117}$$

We now use eqs. (112)–(115) to evaluate the above expressions. To evaluate the denominators of eqs. (116) and (117), we compute:

$$\begin{aligned}(1-\cos\gamma)(1-\cos\alpha) &= 1 - \frac{2\sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}} + \frac{\sin^2\phi_n\cos^2(\theta/2) - \cos^2\theta_n\cos^2\phi_n\sin^2(\theta/2)}{1-\sin^2\theta_n\sin^2(\theta/2)} \\ &= \sin^2\phi_n - \frac{2\sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}} + \frac{\cos^2(\theta/2)}{1-\sin^2\theta_n\sin^2(\theta/2)} \\ &= \left(\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right)^2 . \end{aligned}$$

Hence,

$$(1-\cos\gamma)^{1/2}(1-\cos\alpha)^{1/2} = \epsilon\left(\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right),$$

[25]Since $\sin(\alpha/2)$ and $\sin(\gamma/2)$ are positive, one can set $\sin(\alpha/2) = \left\{\tfrac{1}{2}[1-\cos(\alpha/2)]\right\}^{1/2}$ and $\sin(\gamma/2) = \left\{\tfrac{1}{2}[1-\cos(\gamma/2)]\right\}^{1/2}$ by taking both square roots to be *positive*, without ambiguity.

where $\epsilon = \pm 1$ is the sign defined by eq. (109). Likewise we can employ eqs. (112)–(115) to evaluate:

$$\sin\gamma\sin\alpha - (1-\cos\gamma)(1-\cos\alpha) = \frac{2\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\left[\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right],$$

$$\sin\gamma\sin\alpha + (1-\cos\gamma)(1-\cos\alpha) = 2\sin\phi_n\left[\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right],$$

$$\sin\alpha(1-\cos\gamma) + \sin\gamma(1-\cos\alpha) = \frac{2\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\left[\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right],$$

$$\sin\alpha(1-\cos\gamma) + \sin\gamma(1-\cos\alpha) = 2\cos\phi_n\left[\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\right].$$

Inserting the above results into eqs. (116) and (117), it immediately follows that

$$\cos\tfrac{1}{2}(\gamma+\alpha) = \frac{\epsilon\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \qquad \cos\tfrac{1}{2}(\gamma-\alpha) = \epsilon\sin\phi_n\,, \tag{118}$$

$$\sin\tfrac{1}{2}(\gamma+\alpha) = \frac{\epsilon\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \qquad \sin\tfrac{1}{2}(\gamma-\alpha) = \epsilon\cos\phi_n\,, \tag{119}$$

where ϵ is given by eq. (109). We have derived eqs. (118) and (119) assuming that $\alpha \neq 0$, $\gamma \neq 0$ and $\sin\beta \neq 0$. Since $\cos(\beta/2)$ is then strictly positive, eq. (96) implies that ϵ is equal to the sign of $\cos\frac{1}{2}(\gamma+\alpha)$, which is consistent with the expression for $\cos\frac{1}{2}(\gamma+\alpha)$ obtained above. Thus, we have confirmed the results of eqs. (106)–(108).

If $\alpha = 0$ and/or $\gamma = 0$, then the derivation of eqs. (116) and (117) is not valid. Nevertheless, eqs. (118) and (119) are still true if $\sin\beta \neq 0$, as noted below eq. (109), with $\epsilon = \text{sgn}(\cos\theta_n)$ for $\theta_n \neq \pi/2$ and $\epsilon = +1$ for $\theta_n = \phi_n = \pi/2$. If $\beta = 0$, then as noted below eq. (115), either $\theta = 0$ in which case $\hat{\boldsymbol{n}}$ is undefined, or $\theta \neq 0$ and $\sin\theta_n = 0$ in which case the azimuthal angle ϕ_n is undefined. Hence, $\beta = 0$ implies that $\gamma - \alpha$ is indeterminate. Finally, as indicated below eq. (107), $\gamma + \alpha$ is indeterminate in the exceptional case of $\beta = \pi$ (i.e., $\theta = \pi$ and $\theta_n = \pi/2$).

EXAMPLE: Suppose $\alpha = \gamma = 150^\circ$ and $\beta = 90^\circ$. Then $\cos\frac{1}{2}(\gamma+\alpha) = -\frac{1}{2}\sqrt{3}$, which implies that $\epsilon = -1$. Eqs. (93) and (95) then yield $\hat{\boldsymbol{n}} = -\frac{1}{\sqrt{5}}(0\,,\,2\,,\,1)$ and $\cos\theta = -\frac{1}{4}$. The polar and azimuthal angles of $\hat{\boldsymbol{n}}$ [cf. eq. (23)] are then given by $\phi_n = -90^\circ \pmod{2\pi}$ and $\tan\theta_n = -2$. The latter can also be deduced from eqs. (100) and (103).

Likewise, given $\cos\theta$ and $\hat{\boldsymbol{n}}$ computed above, one obtains $\cos\beta = 0$ (i.e. $\beta = 90^\circ$) from eq. (110), $\epsilon = -1$ from eq. (109), $\gamma = \alpha$ from eq. (108), and $\gamma = \alpha = 150^\circ$ from eqs. (106) and (107). One can verify these results explicitly by inserting the values of the corresponding parameters into eqs. (21) and (90) and checking that the two matrix forms for $R(\hat{\boldsymbol{n}}, \theta)$ coincide.

Appendix F: Verifying that $\hat{\boldsymbol{n}}$ obtained from eq. (60) is a unit vector

We first need some preliminary results. The characteristic equation of an arbitrary 3×3 matrix R is given by:

$$p(\lambda) = \det(R - \lambda \mathbf{I}) = -\left[\lambda^3 - \lambda^2 \text{Tr } R + c_2 \lambda - \det R\right] \,,$$

where[26]

$$c_2 = \tfrac{1}{2}\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] \,. \qquad (120)$$

For an orthogonal matrix, $\varepsilon \equiv \det R = \pm 1$. Hence,

$$p(\lambda) = -\lambda^3 + \lambda^2 \text{Tr } R - \tfrac{1}{2}\lambda \left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] + \varepsilon \,.$$

We now employ the Cayley-Hamilton theorem, which states that a matrix satisfies its own characteristic equation, i.e. $p(R) = 0$. That is,

$$R^3 - R^2 \,\text{Tr } R + \tfrac{1}{2} R \left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] - \varepsilon \mathbf{I} = 0 \,.$$

Multiplying the above equation by R^{-1}, and using the fact that $R^{-1} = R^{\mathsf{T}}$ for an orthogonal matrix,

$$R^2 - R \,\text{Tr } R + \tfrac{1}{2}\mathbf{I}\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] - \varepsilon R^{\mathsf{T}} = 0 \,.$$

Finally, we take the trace of the above equation and solve for $\text{Tr}(R^2)$. Using $\text{Tr } \mathbf{I} = 3$, the end result is given by:

$$\text{Tr}(R^2) = (\text{Tr } R)^2 - 2\varepsilon \,\text{Tr}\, R \,, \qquad (121)$$

which is satisfied by all 3×3 orthogonal matrices.

We now verify that $\hat{\boldsymbol{n}}$ as determined from eq. (60) is a unit vector. For convenience, we repeat eq. (60) here:

$$n_m = -\frac{R_{ij}\epsilon_{ijm}}{2\sin\theta} = \frac{-R_{ij}\epsilon_{ijm}}{\sqrt{(3 - \varepsilon\, R_{ii})(1 + \varepsilon\, R_{ii})}} \,, \qquad \sin\theta \neq 0 \,,$$

where $R_{ii} \equiv \text{Tr } R$. We evaluate $\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}} = n_m n_m$ as follows:

$$n_m n_m = \frac{R_{ij}\epsilon_{ijm} R_{k\ell}\epsilon_{k\ell m}}{(3 - \varepsilon\, R_{ii})(1 + \varepsilon\, R_{ii})} = \frac{R_{ij} R_{k\ell}(\delta_{ik}\delta_{j\ell} - \delta_{i\ell}\delta_{jk})}{(3 - \varepsilon\, R_{ii})(1 + \varepsilon\, R_{ii})} = \frac{R_{ij}R_{ij} - R_{ij}R_{ji}}{(3 - \varepsilon\, R_{ii})(1 + \varepsilon\, R_{ii})} \,, \qquad (122)$$

[26]To prove eq. (120), write $\det(R - \lambda\mathbf{I}) = (\lambda_1 - \lambda)(\lambda_2 - \lambda)(\lambda_3 - \lambda)$, where the λ_i are the roots of the characteristic equation. By diagonalizing R, it follows that $\text{Tr}\, R = \lambda_1 + \lambda_2 + \lambda_3$ and $\text{Tr}\, R^2 = \lambda_1^2 + \lambda_2^2 + \lambda_3^2$. Therefore,

$$c_2 = \lambda_1\lambda_2 + \lambda_1\lambda_3 + \lambda_2\lambda_3 = \tfrac{1}{2}\left[(\lambda_1 + \lambda_2 + \lambda_3)^2 - (\lambda_1^2 + \lambda_2^2 + \lambda_3^2)\right] = \tfrac{1}{2}\left[(\text{Tr } R)^2 - \text{Tr}(R^2)\right] \,.$$

after making use of the well-known identity,

$$\epsilon_{ijm}\epsilon_{k\ell m} = \delta_{ik}\delta_{j\ell} - \delta_{i\ell}\delta_{jk}\,. \tag{123}$$

The numerator of eq. (122) is equal to:

$$\begin{aligned} R_{ij}R_{ij} - R_{ij}R_{ji} &= \mathrm{Tr}(R^{\mathsf{T}}R) - \mathrm{Tr}(R^2) = \mathrm{Tr}\,\mathbf{I} - \mathrm{Tr}(R^2) \\ &= 3 - \mathrm{Tr}(R^2) = 3 - (\mathrm{Tr}\,R)^2 + 2\varepsilon\,\mathrm{Tr}\,R \\ &= (3 - \varepsilon\,R_{ii})(1 + \varepsilon\,R_{ii})\,, \end{aligned} \tag{124}$$

after using eq. (121) for $\mathrm{Tr}(R^2)$. Hence,

$$\hat{\boldsymbol{n}}\cdot\hat{\boldsymbol{n}} = n_m n_m = \frac{R_{ij}R_{ij} - R_{ij}R_{ji}}{(3 - \varepsilon\,R_{ii})(1 + \varepsilon\,R_{ii})} = 1\,,$$

and the proof that $\hat{\boldsymbol{n}}$ is a unit vector is complete.

References

1. W.-K. Tung, *Group Theory in Physics* (World Scientific, Singapore, 1985).

2. K.N. Srinivasa Rao, *The Rotation and Lorentz Groups and their Representations for Physicists* (Wiley Eastern Limited, New Delhi, 1988).

3. James Diebel, *Representing Attitude: Euler Angles, Unit Quaternions, and Rotation Vectors*, Matrix 58 (15-16) (2006) 1–35.

4. S.L. Altmann, *Rotations, Quaternions, and Double Groups* (Dover Publications, Inc., New York, NY, 2005).

5. Harald P. Fritzer, *Molecular Symmetry with Quaternions*, Spectrochimica Acta Part A 57 (2001) 1919–1930.

6. Andrew J. Hanson, *Visualizing Quaternions* (Morgan Kaufmann Publishers, San Francisco, CA, 2006).