Three-Dimensional Rotation Matrices

1. 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). 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 $\det R = -1$. A real orthogonal $n \times n$ matrix with $\det R = 1$ is called a *special* orthogonal matrix and provides a matrix representation of a n-dimensional *proper* rotation[1] (i.e. no mirrors required!).

The most general three-dimensional rotation 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. This is called an *active* transformation. In these notes, we shall explore the general form for the matrix representation of a three-dimensional (proper) rotations, and examine some of its properties.

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 real 2×2 special orthogonal matrix,[2]

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

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 real 3×3 special orthogonal matrix,

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

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

The most general three-dimensional rotation, denoted by $R(\hat{\boldsymbol{n}}, \theta)$, can be specified by an axis of rotation, $\hat{\boldsymbol{n}}$, and a rotation angle θ. 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

[1] In typical parlance, a rotation refers to a proper rotation.

[2] As noted in Section 1, the term *special* refers to the property that the determinant of the matrix is equal to 1.

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 $\hat{\boldsymbol{n}}$. 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 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

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

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 $R(\hat{\boldsymbol{z}},\theta)$. Thus, there exists a real 3×3 special orthogonal matrix P such that[3]

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

and $R(\hat{\boldsymbol{z}},\theta)$ is given by eq. (1). The existence of the matrix P in eq. (8) [even without knowing its explicit form] 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.[4]

[3]Eq. (8) is a special case of a more general result given by eq. (72), which is proved in Appendix B.
[4]An explicit form for the matrix P is obtained in eq. (80) in Appendix B.

To determine the rotation angle θ, we note that the properties of the trace imply that $\mathrm{Tr}(PRP^{-1}) = \mathrm{Tr}(P^{-1}PR) = \mathrm{Tr}\,R$. 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, $0 \leq \theta \leq \pi$, which implies that $\sin\theta \geq 0$. 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 A. 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,

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

which simplifies to:

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

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

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

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

In this section, the matrix elements of $R(\hat{\boldsymbol{n}}, \theta)$ will be denoted by R_{ij}. Since $R(\hat{\boldsymbol{n}}, \theta)$ describes a 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:

$$n_1^2 + n_2^2 + n_3^2 = 1\,. \tag{12}$$

Using the techniques of tensor algebra, we can derive the formula for R_{ij} in the following way. We can regard R_{ij} as the components of a second-rank Cartesian tensor.[5] 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 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 form of the formula for R_{ij} must be:

$$R_{ij} = a\delta_{ij} + bn_in_j + c\epsilon_{ijk}n_k\,, \tag{13}$$

where there is an implicit sum over the index k in the third term of eq. (13).[6] 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 non-trivial scalar quantity in this problem. 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. (13) 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.[7]

[5]This statement is justified in Appendix C of these notes.

[6]We follow the Einstein summation convention in these notes. That is, there is an implicit sum over any pair of repeated indices in the present and all subsequent formulae.

[7]Under inversion of the coordinate system, $\theta \to -\theta$ and $\hat{\boldsymbol{n}} \to -\hat{\boldsymbol{n}}$. Since $0 \leq \theta \leq \pi$, one 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, any scalar function of θ is a true scalar and $\hat{\boldsymbol{n}}$ is a pseudovector. It follows that the product $c\hat{\boldsymbol{n}}$ is a pseudovector as asserted in the text above.

The quantities a, b and c can be determined as follows. First, we rewrite eq. (10) in terms of components,

$$R_{ij}n_j = n_i \,. \tag{14}$$

To determine the consequence of this equation, we insert eq. (13) into eq. (14) and make use of eq. (12). Noting that

$$\delta_{ij}n_j = n_i \,, \qquad n_j n_j = 1 \qquad \epsilon_{ijk}n_j n_k = 0 \,, \tag{15}$$

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

$$a + b = 1 \,. \tag{16}$$

Since the formula for R_{ij} given by eq. (13) must be completely general, it must hold for any special case. In particular, consider the case where $\boldsymbol{\hat{n}} = \boldsymbol{\hat{z}}$. In this case, eqs. (1) and (13) yields:

$$R(\boldsymbol{\hat{z}},\theta)_{11} = \cos\theta = a \,, \qquad R(\boldsymbol{\hat{z}},\theta)_{12} = -\sin\theta = c\,\epsilon_{123}n_3 = c \,. \tag{17}$$

Using eqs. (16) and (17) we conclude that,

$$a = \cos\theta \,, \qquad b = 1 - \cos\theta \,, \qquad c = -\sin\theta \,. \tag{18}$$

Inserting these results into eq. (13) yields the *Rodrigues formula*,

$$R_{ij}(\boldsymbol{\hat{n}},\theta) = \cos\theta\,\delta_{ij} + (1-\cos\theta)n_i n_j - \sin\theta\,\epsilon_{ijk}n_k \,, \tag{19}$$

which is called the *angle-and-axis parameterization* of the three-dimensional rotation matrix. In Appendix D, we show that $R(\boldsymbol{\hat{n}},\theta)$ can be expressed in exponential form,

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

where $\vec{\boldsymbol{\mathcal{S}}} = (\mathcal{S}_1\,,\,\mathcal{S}_2\,,\,\mathcal{S}_3)$ is a "vector" whose components are the three antisymmetric 3×3 matrices $\mathcal{S}_k$ $(k = 1,2,3)$, with matrix elements given by $(\mathcal{S}_k)_{ij} = -i\epsilon_{ijk}$.

Using eq. (19), we can write $R(\boldsymbol{\hat{n}},\theta)$ explicitly in 3×3 matrix form,

$$R(\boldsymbol{\hat{n}},\theta) = \begin{pmatrix} \cos\theta + n_1^2(1-\cos\theta) & n_1n_2(1-\cos\theta) - n_3\sin\theta & n_1n_3(1-\cos\theta) + n_2\sin\theta \\ n_1n_2(1-\cos\theta) + n_3\sin\theta & \cos\theta + n_2^2(1-\cos\theta) & n_2n_3(1-\cos\theta) - n_1\sin\theta \\ n_1n_3(1-\cos\theta) - n_2\sin\theta & n_2n_3(1-\cos\theta) + n_1\sin\theta & \cos\theta + n_3^2(1-\cos\theta) \end{pmatrix} . \tag{20}$$

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

$$R_{ij}(\boldsymbol{\hat{n}},\pi) = \begin{pmatrix} 2n_1^2 - 1 & 2n_1n_2 & 2n_1n_3 \\ 2n_1n_2 & 2n_2^2 - 1 & 2n_2n_3 \\ 2n_1n_3 & 2n_2n_3 & 2n_3^2 - 1 \end{pmatrix} = 2n_in_j - \delta_{ij} \,. \tag{21}$$

Finally, as expected, $R_{ij}(\boldsymbol{\hat{n}},0) = \delta_{ij}$, independently of the direction of $\boldsymbol{\hat{n}}$. I leave it as an exercise to the reader to verify explicitly that $R \equiv R(\boldsymbol{\hat{n}},\theta)$ given in eq. (20) satisfies the conditions $RR^{\mathsf{T}} = \mathbf{I}$ and $\det R = +1$.

In Section 5, we show that it is possible to express a general rotation matrix $R(\hat{\boldsymbol{n}},\theta)$ as a product of simpler rotations. This will provide further geometrical insights into the properties of rotations.

4. Determining the rotation axis and the rotation angle

Given a general three-dimensional rotation matrix, $R(\hat{\boldsymbol{n}},\theta)$, we can determine the angle of rotation θ and the axis of rotation $\hat{\boldsymbol{n}}$. Using eq. (20), the trace of $R(\hat{\boldsymbol{n}},\theta)$ is given by:

$$\text{Tr } R(\hat{\boldsymbol{n}},\theta) = 1 + 2\cos\theta\,, \tag{22}$$

which coincides with our previous result obtained in eq. (9). Thus eq. (22) yields,

$$\cos\theta = \tfrac{1}{2}\,(\text{Tr } R - 1) \quad \text{and} \quad \sin\theta = (1-\cos^2\theta)^{1/2} = \tfrac{1}{2}\sqrt{(3-\text{Tr } R)(1+\text{Tr } R)}\,, \tag{23}$$

where $\sin\theta \geq 0$ is a consequence of the range of the rotation angle, $0 \leq \theta \leq \pi$.

To determine $\hat{\boldsymbol{n}}$, we multiply eq. (19) by ϵ_{ijm} and sum over i and j. Noting that

$$\epsilon_{ijm}\delta_{ij} = \epsilon_{ijm}n_i n_j = 0\,, \qquad \epsilon_{ijk}\epsilon_{ijm} = 2\delta_{km}\,, \tag{24}$$

it follows that

$$2n_m \sin\theta = -R_{ij}\epsilon_{ijm}\,. \tag{25}$$

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 we must seek another method to determine $\hat{\boldsymbol{n}}$. If $\sin\theta \neq 0$, then one can divide both sides of eq. (25) by $\sin\theta$. Using eq. (23), we obtain:

$$n_m = -\frac{R_{ij}\epsilon_{ijm}}{2\sin\theta} = \frac{-R_{ij}\epsilon_{ijm}}{\sqrt{(3-\text{ Tr}\,R)(1+\text{Tr}\,R)}}\,, \qquad \sin\theta \neq 0\,. \tag{26}$$

More explicitly,

$$\hat{\boldsymbol{n}} = \frac{1}{\sqrt{(3-\text{Tr}\,R)(1+\text{Tr}\,R)}}\biggl(R_{32}-R_{23}\,,\, R_{13}-R_{31}\,,\, R_{21}-R_{12}\biggr)\,, \qquad \text{Tr}\,R \neq -1\,,\,3\,. \tag{27}$$

If we multiply eq. (25) by n_m and sum over m, then

$$\sin\theta = -\tfrac{1}{2}\epsilon_{ijm}R_{ij}n_m\,, \tag{28}$$

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

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

$$\begin{aligned} S_{jk} &\equiv R_{jk} + R_{kj} + (1-\text{Tr}\,R)\delta_{jk} \\ &= 2(1-\cos\theta)n_j n_k = (3-\text{Tr}\,R)n_j n_k\,, \end{aligned} \tag{29}$$

after using eq. (19) for R_{jk}. Hence,

$$n_j n_k = \frac{S_{jk}}{3 - \operatorname{Tr} R}\,, \qquad \operatorname{Tr} R \neq 3\,. \tag{30}$$

To determine $\hat{\boldsymbol{n}}$ up to an overall sign, we simply set $j = k$ (no sum) in eq. (30), which fixes the value of

$$n_j^2 = \frac{S_{jj}}{3 - \operatorname{Tr} R}\,, \qquad \operatorname{Tr} R \neq 3\,, \quad (\text{no sum over } j)\,. \tag{31}$$

If $\sin\theta \neq 0$, the overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (26). Note that eq. (29) implies that $\operatorname{Tr} S = 3 - \operatorname{Tr} R$. Summing over j in eq. (31) then yields

$$\hat{\boldsymbol{n}} \boldsymbol{\cdot} \hat{\boldsymbol{n}} = \frac{\operatorname{Tr} S}{3 - \operatorname{Tr} R} = 1\,,$$

as required for a unit vector.

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. (26). In this case, eq. (22) determines whether $\cos\theta = +1$ or $\cos\theta = -1$. For $\cos\theta = -1$, eq. (29) yields $n_j n_k = \frac{1}{4} S_{jk}$, which determines $\hat{\boldsymbol{n}}$ up to an overall sign. Equivalently, one can use eq. (20) to derive

$$\hat{\boldsymbol{n}} = \left(\epsilon_1\sqrt{\tfrac{1}{2}(1 + R_{11})}\,,\, \epsilon_2\sqrt{\tfrac{1}{2}(1 + R_{22})}\,,\, \epsilon_3\sqrt{\tfrac{1}{2}(1 + R_{33})}\right)\,, \qquad \text{if } \operatorname{Tr} R = -1\,, \tag{32}$$

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

$$\epsilon_i\epsilon_j = \frac{R_{ij}}{\sqrt{(1 + R_{ii})(1 + R_{jj})}}\,, \qquad \text{for fixed } i \neq j\,,\ R_{ii} \neq -1\,,\ R_{jj} \neq -1\,. \tag{33}$$

The ambiguity in the overall sign of $\hat{\boldsymbol{n}}$ is immaterial, in light of eq. (6). Finally, in the case of $\cos\theta = +1$ (which corresponds to $\operatorname{Tr} R = 3$), $R(\hat{\boldsymbol{n}}, 0) = \mathbf{I}$ is the 3×3 identity matrix, which is independent of the direction of $\hat{\boldsymbol{n}}$.

To summarize, eqs. (23), (27) and (30) provide a simple algorithm for determining the unit vector $\hat{\boldsymbol{n}}$ and the rotation angle θ for any rotation matrix $R(\hat{\boldsymbol{n}}, \theta) \neq \mathbf{I}$.

5. Euler angle representation of $\boldsymbol{R(\hat{n}, \theta)}$

An arbitrary rotation matrix can can be written as:

$$R(\hat{\boldsymbol{n}}, \theta) = R(\hat{\boldsymbol{z}}, \alpha) R(\hat{\boldsymbol{y}}, \beta) R(\hat{\boldsymbol{z}}, \gamma)\,, \tag{34}$$

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 $\hat{\boldsymbol{n}}$,

$$\hat{\boldsymbol{n}} = (\sin\theta_n \cos\phi_n\,,\, \sin\theta_n \sin\phi_n\,,\, \cos\theta_n)\,. \tag{35}$$

Multiplying out the three matrices on the right-hand side of eq. (34), we obtain the Euler angle parameterization of the three-dimensional rotation matrix,

$$R(\hat{\boldsymbol{n}},\theta)=\begin{pmatrix}\cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & \cos\alpha\sin\beta\\ \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma+\cos\alpha\cos\gamma & \sin\alpha\sin\beta\\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta\end{pmatrix}. \tag{36}$$

One can now make use of the results of Section 4 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. (23). Simple algebra yields:

$$\cos\theta=\cos^2(\beta/2)\cos(\gamma+\alpha)-\sin^2(\beta/2)\,, \tag{37}$$

where I have used $\cos^2(\beta/2)=\frac{1}{2}(1+\cos\beta)$ 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. (23) and the text preceding this equation]. One can also rewrite eq. (37) in a slightly more convenient form,

$$\cos\theta=-1+2\cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)\,. \tag{38}$$

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. Second, if $\theta=\pi$ then $\cos\theta=-1$ and $\hat{\boldsymbol{n}}$ is determined up to an overall sign (which is not physical). Eq. (38) then implies that $\cos^2(\beta/2)\cos^2\frac{1}{2}(\gamma+\alpha)=0$, 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. (32) and (33) 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

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

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 $\cos^2\frac{1}{2}(\gamma+\alpha)=\frac{1}{2}\,[1+\cos(\gamma+\alpha)]=0$. Thus, eqs. (32) and (33) 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

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

Finally, we consider the generic case where $\sin\theta \neq 0$. Using eqs. (27) and (36),

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

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

$$\begin{aligned}
&\left[(R_{32}-R_{23})^2 + (R_{13}-R_{31})^2 + (R_{12}-R_{21})^2\right]^{1/2}\\
&\qquad = 4\left|\cos\tfrac{1}{2}(\gamma+\alpha)\cos(\beta/2)\right|\sqrt{\sin^2(\beta/2)+\cos^2(\beta/2)\sin^2\tfrac{1}{2}(\gamma+\alpha)}\,. \qquad (39)
\end{aligned}$$

Hence,[8]

$$\begin{aligned}
\hat{\boldsymbol{n}} = &\frac{\epsilon}{\sqrt{\sin^2(\beta/2)+\cos^2(\beta/2)\sin^2\frac{1}{2}(\gamma+\alpha)}}\\
&\times\biggl(\sin(\beta/2)\sin\tfrac{1}{2}(\gamma-\alpha)\,,\ \sin(\beta/2)\cos\tfrac{1}{2}(\gamma-\alpha)\,,\ \cos(\beta/2)\sin\tfrac{1}{2}(\gamma+\alpha)\biggr)\,,
\end{aligned} \tag{40}$$

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

$$\epsilon \equiv \mathrm{sgn}\bigl\{\cos\tfrac{1}{2}(\gamma+\alpha)\cos(\beta/2)\bigr\}\,,\qquad \sin\theta \neq 0\,. \tag{41}$$

Remarkably, eq. (40) 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. (41) 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. (38) to obtain:

$$\begin{aligned}
\sin(\theta/2) &= \sqrt{\sin^2(\beta/2)+\cos^2(\beta/2)\cos^2\tfrac{1}{2}\,(\gamma+\alpha)}\,,\\
\cos(\theta/2) &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}(\gamma+\alpha)\,,
\end{aligned} \tag{42}$$

where we have used $\cos^2(\theta/2) = \frac{1}{2}(1+\cos\theta)$ and $\sin^2(\theta/2) = \frac{1}{2}(1-\cos\theta)$. 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. (41) is required in eq. (42) 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:

$$q = \Bigl(\cos(\theta/2)\,,\,\hat{\boldsymbol{n}}\sin(\theta/2)\Bigr)\,, \tag{43}$$

[8]One can can also determine $\hat{\boldsymbol{n}}$ up to an overall sign starting from eq. (36) 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. (27).

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

$$q_0 = \epsilon\cos(\beta/2)\cos\tfrac{1}{2}\left(\gamma+\alpha\right) , \qquad\qquad q_1 = \epsilon\sin(\beta/2)\sin\tfrac{1}{2}\left(\gamma-\alpha\right) ,$$
$$q_2 = \epsilon\sin(\beta/2)\cos\tfrac{1}{2}\left(\gamma-\alpha\right) , \qquad\qquad q_3 = \epsilon\cos(\beta/2)\sin\tfrac{1}{2}\left(\gamma+\alpha\right) . \tag{44}$$

Since $0 \leq \theta \leq \pi$, it follows that $q_0 \geq 0$.[9] Quaternions are especially valuable for representing rotations in computer graphics software.

If one expresses $\hat{\boldsymbol{n}}$ in terms of a polar angle θ_n and azimuthal angle ϕ_n as in eq. (35), then one can also write down expressions for θ_n and ϕ_n in terms of the Euler angles α, β and γ. Comparing eqs. (35) and (40), it follows that:

$$\tan\theta_n = \frac{(n_1^2+n_2^2)^{1/2}}{n_3} = \frac{\epsilon\tan(\beta/2)}{\sin\frac{1}{2}\left(\gamma+\alpha\right)} , \tag{45}$$

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. (41). Similarly,

$$\cos\phi_n = \frac{n_1}{(n_1^2+n_2^2)} = \epsilon\sin\tfrac{1}{2}\left(\gamma-\alpha\right) = \epsilon\cos\tfrac{1}{2}(\pi-\gamma+\alpha) , \tag{46}$$

$$\sin\phi_n = \frac{n_2}{(n_1^2+n_2^2)} = \epsilon\cos\tfrac{1}{2}\left(\gamma-\alpha\right) = \epsilon\sin\tfrac{1}{2}(\pi-\gamma+\alpha) , \tag{47}$$

or equivalently

$$\phi_n = \tfrac{1}{2}(\epsilon\pi-\gamma+\alpha) \bmod 2\pi . \tag{48}$$

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. (38) as:

$$\cos^2(\theta/2) = \cos^2(\beta/2)\cos^2\tfrac{1}{2}\left(\gamma+\alpha\right) . \tag{49}$$

Then, using eqs. (45) and (49), it follows that:

$$\sin(\beta/2) = \sin\theta_n\sin(\theta/2) . \tag{50}$$

Plugging this result back into eqs. (45) and (49) yields

$$\epsilon\sin\tfrac{1}{2}\left(\gamma+\alpha\right) = \frac{\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}} , \tag{51}$$

$$\epsilon\cos\tfrac{1}{2}\left(\gamma+\alpha\right) = \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}} . \tag{52}$$

[9]In comparing with other treatments in the mathematics literature, one should be careful to note that the convention of $\sin\theta \geq 0$ (which implies that $q_0 \geq 0$) is not universally adopted. Often, the quaternion q in eq. (43) will be re-defined as ϵq in order to remove the factors of ϵ from eq. (44), in which case $\epsilon q_0 \geq 0$.

Note that if $\beta = \pi$ then eq. (50) 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. (41)].

We shall also make use of eqs. (46) and (47),

$$\epsilon \sin \tfrac{1}{2}(\gamma - \alpha) = \cos\phi_n \,, \tag{53}$$

$$\epsilon \cos \tfrac{1}{2}(\gamma - \alpha) = \sin\phi_n \,, \tag{54}$$

Finally, we employ eqs. (52) and (53) 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

$$\epsilon = \operatorname{sgn}\left\{\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1 - \sin^2\theta_n \sin^2(\theta/2)}}\right\}\,, \tag{55}$$

If either $\gamma = 0$ or $\alpha = 0$, then the argument of sgn in eq. (55) will vanish. In this case, $\sin\frac{1}{2}(\gamma + \alpha) \geq 0$, and we may use eq. (51) 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. (41).[10] 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. (52)].

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. (20) and (36), equal to each other, where $\hat{\boldsymbol{n}}$ is given by eq. (35). For example,

$$R_{33} = \cos\beta = \cos\theta + \cos^2\theta_n(1 - \cos\theta)\,. \tag{56}$$

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

$$\sin\beta = 2\sin(\theta/2)\sin\theta_n\sqrt{1 - \sin^2\theta_n \sin^2(\theta/2)}\,, \tag{57}$$

which also can be derived from eq. (50). Next, we note that if $\sin\beta \neq 0$, then

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

[10] 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 (35)].

Using eq. (20) yields (for $\sin\beta\neq 0$):

$$\sin\alpha=\frac{\cos\theta_n\sin\phi_n\sin(\theta/2)-\cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\tag{58}$$

$$\cos\alpha=\frac{\cos\theta_n\cos\phi_n\sin(\theta/2)+\sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\tag{59}$$

$$\sin\gamma=\frac{\cos\theta_n\sin\phi_n\sin(\theta/2)+\cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\tag{60}$$

$$\cos\gamma=\frac{-\cos\theta_n\cos\phi_n\sin(\theta/2)+\sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,.\tag{61}$$

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. (56) 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 $\cos\beta=1$ and $\gamma+\alpha=\theta \mod \pi$, with $\gamma-\alpha$ indeterminate. If $\beta=\pi$ then eq. (56) yields $\theta_n=\pi/2$ and $\theta=\pi$, in which case $\cos\beta=-1$ and $\gamma-\alpha=\pi-2\phi \mod 2\pi$, with $\gamma+\alpha$ indeterminate.

One can use eqs. (58)–(61) to rederive eqs. (51)–(54). 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[11]

$$\begin{aligned}\cos\tfrac{1}{2}(\gamma\pm\alpha)&=\cos(\gamma/2)\cos(\alpha/2)\mp\sin(\gamma/2)\sin(\alpha/2)\\&=\frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)\cos(\alpha/2)\mp\sin^2(\gamma/2)\sin^2(\alpha/2)}{\sin(\gamma/2)\sin(\alpha/2)}\\&=\frac{\sin\gamma\sin\alpha\mp(1-\cos\gamma)(1-\cos\alpha)}{2(1-\cos\gamma)^{1/2}(1-\cos\alpha)^{1/2}}\,.\end{aligned}\tag{62}$$

and

$$\begin{aligned}\sin\tfrac{1}{2}(\gamma\pm\alpha)&=\sin(\gamma/2)\cos(\alpha/2)\pm\cos(\gamma/2)\sin(\alpha/2)\\&=\frac{\sin(\gamma/2)\sin(\alpha/2)\cos(\alpha/2)}{\sin(\alpha/2)}\pm\frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)}{\sin(\gamma/2)}\\&=\frac{\sin(\gamma/2)\sin\alpha}{2\sin(\alpha/2)}\pm\frac{\sin\gamma\sin(\alpha/2)}{2\sin(\gamma/2)}\\&=\tfrac{1}{2}\sin\alpha\sqrt{\frac{1-\cos\gamma}{1-\cos\alpha}}\pm\tfrac{1}{2}\sin\gamma\sqrt{\frac{1-\cos\alpha}{1-\cos\gamma}}\\&=\frac{\sin\alpha(1-\cos\gamma)\pm\sin\gamma(1-\cos\alpha)}{2(1-\cos\alpha)^{1/2}(1-\cos\gamma)^{1/2}}\,.\end{aligned}\tag{63}$$

[11]Since $\sin(\alpha/2)$ and $\sin(\gamma/2)$ are positive, one can set $\sin(\alpha/2)=\left\{\frac{1}{2}[1-\cos(\alpha/2)]\right\}^{1/2}$ and $\sin(\gamma/2)=\left\{\frac{1}{2}[1-\cos(\gamma/2)]\right\}^{1/2}$ by taking the *positive* square root in both cases, without ambiguity.

We now use eqs. (58)–(61) to evaluate the above expressions. To evaluate the denominators of eqs. (62) and (63), 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,

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

where $\epsilon=\pm 1$ is the sign defined by eq. (55). Likewise we can employ eqs. (58)–(61) 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. (62) and (63), it immediately follows that

$$
\cos\tfrac{1}{2}(\gamma+\alpha)=\frac{\epsilon\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\qquad \cos\tfrac{1}{2}(\gamma-\alpha)=\epsilon\sin\phi_n\,,\tag{64}
$$

$$
\sin\tfrac{1}{2}(\gamma+\alpha)=\frac{\epsilon\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\qquad \sin\tfrac{1}{2}(\gamma-\alpha)=\epsilon\cos\phi_n\,,\tag{65}
$$

where ϵ is given by eq. (55). We have derived eqs. (64) and (65) assuming that $\alpha\neq 0$, $\gamma\neq 0$ and $\sin\beta\neq 0$. Since $\cos(\beta/2)$ is then strictly positive, eq. (41) 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. (51)–(54).

If $\alpha=0$ and/or $\gamma=0$, then the derivation of eqs. (62) and (63) is not valid. Nevertheless, eqs. (64) and (65) are still true if $\sin\beta\neq 0$, as noted below eq. (55), 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. (61), 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. (52), $\gamma + \alpha$ is indeterminate in the exceptional case of $\beta = \pi$ (i.e., $\theta = \pi$ and $\theta_n = \pi/2$).

EXAMPLE: Suppose $\alpha = \gamma = 150°$ and $\beta = 90°$. Then $\cos\frac{1}{2}(\gamma + \alpha) = -\frac{1}{2}\sqrt{3}$, which implies that $\epsilon = -1$. Eqs. (38) and (40) then yield:

$$\cos\theta = -\tfrac{1}{4}\,, \qquad\qquad \hat{\boldsymbol{n}} = -\frac{1}{\sqrt{5}}\,(0\,,\,2\,,\,1)\,. \tag{66}$$

The polar and azimuthal angles of $\hat{\boldsymbol{n}}$ [cf. eq. (35)] are then given by $\phi_n = -90° \pmod{2\pi}$ and $\tan\theta_n = -2$. The latter can also be deduced from eqs. (45) and (48).

Likewise, given eq. (66), one obtains $\cos\beta = 0$ (i.e. $\beta = 90°$) from eq. (56), $\epsilon = -1$ from eq. (55), $\gamma = \alpha$ from eqs. (53) and (54), and $\gamma = \alpha = 150°$ from eqs. (51) and (52). One can verify these results explicitly by inserting the values of the corresponding parameters into eqs. (20) and (36) and checking that the two matrix forms for $R(\hat{\boldsymbol{n}}, \theta)$ coincide.

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

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

$$\det\,(A - \lambda\mathbf{I}) = 0\,. \tag{67}$$

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

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

Hence multiplying these two equations together yields

$$\overline{\lambda}\,\lambda\,\overline{\boldsymbol{v}}^{\mathsf{T}}\boldsymbol{v} = \overline{\boldsymbol{v}}^{\mathsf{T}} A^{\mathsf{T}} A\boldsymbol{v} = \overline{\boldsymbol{v}}^{\mathsf{T}}\boldsymbol{v}\,, \tag{68}$$

since an orthogonal matrix satisfies $A^{\mathsf{T}}A = \mathbf{I}$. Since eigenvectors must be nonzero, it follows that $\overline{\boldsymbol{v}}^{\mathsf{T}}\boldsymbol{v} \neq 0$. Hence, eq. (68) 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[13]

$$\det A\,\det(\mathbf{I} - A) = (-1)^n \det(\mathbf{I} - A)\,, \tag{69}$$

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

[13] Here, we make use of the well known properties of the determinant, namely $\det(AB) = \det A \det B$ and $\det(A^{\mathsf{T}}) = \det A$.

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. (69) yields[14]

$$\det(\mathbf{I} - A) = 0\,, \qquad \text{for any proper odd-dimensional orthogonal matrix } A. \tag{70}$$

Comparing with eq. (67), we conclude that $\lambda = 1$ is an eigenvalue of A.[15] 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 $0 \leq \theta \leq \pi$.[16]

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

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

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

$$\det A \det(\mathbf{I} + A) = \det(\mathbf{I} + A)\,, \tag{71}$$

For any improper orthogonal matrix, we have $\det A = -1$. Hence, eq. (71) yields

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

Comparing with eq. (67), 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 16).

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

In this appendix, we derive the following relation between the matrix representations of two rotations by an angle θ with respect to two different rotation axes,

$$R(\hat{\boldsymbol{n}}, \theta) = PR(\hat{\boldsymbol{n}}', \theta)P^{-1}\,, \qquad \text{where } \hat{\boldsymbol{n}} = P\hat{\boldsymbol{n}}'\,. \tag{72}$$

To prove eq. (72), we first compute the angle of the rotation $PR(\hat{\boldsymbol{n}}', \theta)P^{-1}$ using eq. (23). Since $\mathrm{Tr}[PR(\hat{\boldsymbol{n}}', \theta)P^{-1}] = \mathrm{Tr}\, R(\hat{\boldsymbol{n}}', \theta)$ using the cyclicity of the trace, it follows that the angles of rotation corresponding to $PR(\hat{\boldsymbol{n}}', \theta)P^{-1}$ 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. (25),

$$2n_m \sin\theta = -(PR'P^{-1})_{ij}\epsilon_{ijm}\,, \tag{73}$$

[14] Eq. (70) is also valid for any improper even-dimensional orthogonal matrix A since in this case $\det A = -1$ and $(-1)^n = 1$.

[15] 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 $\alpha = 0$.

[16] 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.

where $R' \equiv R(\hat{\boldsymbol{n}}', \theta)$. Since P is a rotation matrix, we have $P^{-1} = P^{\mathsf{T}}$, or equivalently $(P^{-1})_{\ell j} = P_{j\ell}$. Hence, we can rewrite eq. (73) as:

$$2n_m \sin\theta = -P_{ik} R'_{k\ell} P_{j\ell} \epsilon_{ijm}\,. \tag{74}$$

Multiplying both sides of eq. (74) by P_{mn} and using the definition of the determinant of a 3×3 matrix,

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

it then follows that:

$$2P_{mn} n_m \sin\theta = -R'_{k\ell} \epsilon_{k\ell n}\,. \tag{75}$$

after noting that $\det P = 1$ (since P is a *proper* rotation matrix). Finally, we again use eq. (25) which yields

$$2n'_n \sin\theta = -R'_{k\ell} \epsilon_{k\ell n}\,. \tag{76}$$

Assuming that $\sin\theta \neq 0$, we can subtract eqs. (75) and (76) and divide out by $2\sin\theta$. Using $(P^{\mathsf{T}})_{nm} = P_{mn}$, the end result is:

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

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

$$\hat{\boldsymbol{n}} = P\hat{\boldsymbol{n}}'\,. \tag{77}$$

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 $PR(\hat{\boldsymbol{n}}', \theta)P^{-1}$ up to an overall sign. Since $R(\hat{\boldsymbol{n}}', \theta)\hat{\boldsymbol{n}}' = \hat{\boldsymbol{n}}'$, the following eigenvalue equation is obtained:

$$PR(\hat{\boldsymbol{n}}', \theta)P^{-1}(P\hat{\boldsymbol{n}}') = PR(\hat{\boldsymbol{n}}', \theta)\hat{\boldsymbol{n}}' = P\hat{\boldsymbol{n}}'\,. \tag{78}$$

That is, $P\hat{\boldsymbol{n}}'$ is an eigenvector of $PR(\hat{\boldsymbol{n}}', \theta)P^{-1}$ with eigenvalue $+1$. It then follows that $P\hat{\boldsymbol{n}}'$ is the normalized eigenvector of $PR(\hat{\boldsymbol{n}}', \theta)P^{-1}$ up to an overall undetermined sign. For $\sin\theta \neq 0$, the overall sign is fixed and is positive by eq. (77). 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. (72) 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.

Note that for $\hat{\boldsymbol{n}}' = \hat{\boldsymbol{z}}$, eq. (72) reduces to eq. (8) as a special case. We can determine an explicit form for P by constructing the rotation such that $\hat{\boldsymbol{n}} = P\hat{\boldsymbol{z}}$. We define the angles θ_n and ϕ_n to be the polar and azimuthal angles of the unit vector $\hat{\boldsymbol{n}}$[cf. eq. (35)]. Then, the matrix P can be expressed as the product of two simple rotation matrices,

$$P = R(\hat{\boldsymbol{z}}, \phi_n) R(\hat{\boldsymbol{y}}, \theta_n)\,. \tag{79}$$

This is easily checked by noting that $R(\hat{\boldsymbol{y}}, \theta_n)\hat{\boldsymbol{z}}$ is a unit vector with polar angle θ_n that lies in the x–z plane. Multiplying the resulting vector by $R(\hat{\boldsymbol{z}}, \phi_n)$ then produces a unit vector with polar angle θ_n and azimuthal angle ϕ_n as required. Multiplying out the two rotation matrices in eq. (79) yields,

$$P = \begin{pmatrix} \dfrac{n_3 n_1}{\sqrt{n_1^2+n_2^2}} & \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & n_1 \\ \dfrac{n_3 n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & n_2 \\ -\sqrt{n_1^2+n_2^2} & 0 & n_3 \end{pmatrix} . \tag{80}$$

Since P is an orthogonal matrix, it follows that $P^{-1} = P^{\mathsf{T}}$. It is now straightforward to plug the result of eq. (80) into eq. (8) and recover the Rodrigues formula for $R(\hat{\boldsymbol{n}}, \theta)$ given in eq. (20).

Appendix C: Matrix elements of a matrix correspond to the components of a second-rank Cartesian tensor

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, the two sets of basis vectors are related by

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

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 related by a similarity transformation,

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

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 exponential representation of $R(\hat{\boldsymbol{n}}, \boldsymbol{\theta})$

Consider the matrix representation $R(\hat{\boldsymbol{n}}, \theta)$ of a counterclockwise rotation by an angle θ about a fixed axis that lies along the unit vector $\hat{\boldsymbol{n}}$. This matrix can be expressed in exponential form,

$$R(\hat{\boldsymbol{n}}, \theta) = \exp(-i\theta\hat{\boldsymbol{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}}\,)\,, \tag{81}$$

where $\vec{\boldsymbol{\mathcal{S}}} = (\mathcal{S}_1\,,\,\mathcal{S}_2\,,\,\mathcal{S}_3)$ is a "vector" whose components are the three antisymmetric 3×3 matrices $\mathcal{S}_k$, whose ij matrix elements are given by

$$(\mathcal{S}_k)_{ij} = -i\epsilon_{ijk}\,.$$

Thus, the matrix elements of the matrix that appears in the argument of the exponential in eq. (81) are given by

$$(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})_{ij} \equiv -i\epsilon_{ijk}n_k\,, \tag{82}$$

where the implicit sum over k is assumed. To prove this result, we perform an explicit computation of eq. (81) and show that the end result is eq. (19), which we rewrite as follows:

$$R_{ij}(\boldsymbol{\hat{n}},\theta) = n_i n_j + (\delta_{ij} - n_i n_j)\cos\theta - \epsilon_{ijk}n_k\sin\theta\,. \tag{83}$$

The exponential in eq. (81) is defined via its power series,

$$R(\boldsymbol{\hat{n}},\theta) = e^{-i\theta\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}}} = \sum_{k=0}^{\infty}\frac{1}{k!}(-i\theta\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^k\,. \tag{84}$$

Using eq. (82),

$$(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^2_{ij} = -\epsilon_{i\ell k}n_k\epsilon_{\ell jm}n_m = (\delta_{ij}\delta_{km} - \delta_{im}\delta_{jk})n_k n_m = \delta_{ij} - n_i n_j\,,$$

after employing the well-known ϵ-tensor identity and noting that $\delta_{km}n_k n_m = 1$ for the unit vector $\boldsymbol{\hat{n}}$. Next, we compute:

$$(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^3_{ij} = -i(\delta_{i\ell} - n_i n_\ell)\epsilon_{\ell jk}n_k = -i\epsilon_{ijk}n_k = (\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})_{ij}\,.$$

Thus, for any positive integer k,

$$(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^{2k-1} = \boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}}\,, \qquad\qquad (\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^{2k} = (\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^2\,.$$

Inserting these results in eq. (84), we obtain:

$$\begin{aligned}
R_{ij}(\boldsymbol{\hat{n}},\theta) &= \delta_{ij} - (\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})_{ij}\sum_{k=0}^{\infty}\frac{1}{(2k+1)!}(i\theta)^{2k+1} + (\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^2_{ij}\sum_{k=1}^{\infty}\frac{1}{(2k)!}(i\theta)^{2k} \\
&= \delta_{ij} - i(\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})_{ij}\sin\theta + (\boldsymbol{\hat{n}}\boldsymbol{\cdot}\vec{\boldsymbol{\mathcal{S}}})^2_{ij}(\cos\theta - 1) \\
&= \delta_{ij} - \epsilon_{ijk}n_k\sin\theta + (\delta_{ij} - n_i n_j)(\cos\theta - 1) \\
&= n_i n_j + (\delta_{ij} - n_i n_j)\cos\theta - \epsilon_{ijk}n_k\sin\theta\,,
\end{aligned}$$

which reproduces eq. (83) as advertised.

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