The Matrix Representation of a Three-Dimensional Rotation

1. Properties of the 3 × 3 rotation matrix

An active rotation in the x–y plane by an angle θ measured counterclockwise from the positive x-axis is represented by the 2×2 special real orthogonal matrix[1]

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

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 special real orthogonal matrix [cf. eq. (7.18) on p. 129 of Boas],

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

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

The most general three-dimensional rotation,[2] denoted by $R(\boldsymbol{n},\theta)$, can be specified by an axis of rotation, $\hat{\boldsymbol{n}}$, and a rotation angle[3] 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 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 $\hat{\boldsymbol{n}}$. Simple geometrical considerations will convince you that the following relations are satisfied:

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

$$[R(\boldsymbol{n},\theta)]^{-1} = R(\boldsymbol{n},-\theta) = R(-\boldsymbol{n},\theta) . \tag{3}$$

Combining these two results, it follows that

$$R(\boldsymbol{n}, 2\pi - \theta) = R(-\boldsymbol{n},\theta) , \tag{4}$$

[1] A real orthogonal matrix R is a matrix whose elements are real numbers that satisfies $R^{-1} = R^{\mathsf{T}}$. Taking the determinant of the equation $RR^{\mathsf{T}} = \mathbf{I}$, it follows that det $R = \pm 1$. If det $R = +1$, then R represents a *proper* rotation. The adjective "special" refers to the condition of det $R = +1$.

[2] As in the two-dimensional case, the rotation matrix operates on vectors to produce rotated vectors, while the coordinate axes are held fixed. This is an *active* transformation.

[3] 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 $0 \leq \theta < 2\pi$.

which implies that any three-dimensional rotation can be described by a counter-clockwise rotation by θ about an arbitrary axis $\hat{\boldsymbol{n}}$, where $0 \leq \theta \leq \pi$. However, if we substitute $\theta = \pi$ in eq. (4), we conclude that

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

which means that for the special case of $\theta = \pi$, $R(\boldsymbol{n}, \pi)$ and $R(-\boldsymbol{n}, \pi)$ represent the *same* rotation. Finally, if $\theta = 0$, then $R(\boldsymbol{n}, 0) = \mathbf{I}$ is the identity operator, independently of the direction of $\hat{\boldsymbol{n}}$. The goal of these notes is to construct the 3×3 special real orthogonal matrix $R(\hat{\boldsymbol{n}}, \theta)$ that represents this general three-dimensional rotation

2. 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 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:

$$n_1^2 + n_2^2 + n_3^2 = 1\,. \tag{6}$$

The method employed in the solution to problem 3.11–54 on p. 161 of Boas that was given in the solutions to homework set #8 can be generalized to provide a derivation of an explicit formula for R_{ij}.

Suppose we are given a rotation matrix $R(\hat{\boldsymbol{n}}, \theta)$ and are asked to determine the axis of rotation $\hat{\boldsymbol{n}}$ and the rotation angle θ. The matrix $R(\hat{\boldsymbol{n}}, \theta)$ is specified with respect to a basis

$$\mathcal{B} = \{\boldsymbol{i}\,, \boldsymbol{j}\,, \boldsymbol{k}\}\,.$$

We shall rotate to a new orthonormal basis,

$$\mathcal{B}' = \{\boldsymbol{i}'\,, \boldsymbol{j}'\,, \boldsymbol{k}'\}\,,$$

in which $\boldsymbol{k}'$ along the new positive z-axis,

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

The new positive y axis can be chosen to lie along

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

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

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

Following the class handout entitled "*Coordinates, matrix elements and changes of basis*," we determine the matrix P whose matrix elements are defined by

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

where the $\boldsymbol{b}_i$ are the basis vectors of $\mathcal{B}$ 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,

$$P = \begin{pmatrix} \dfrac{n_3 n_1}{\sqrt{n_1^2+n_2^2}} & \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & n_1 \\[2ex] \dfrac{n_3 n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & n_2 \\[2ex] -\sqrt{n_1^2+n_2^2} & 0 & n_3 \end{pmatrix} . \tag{7}$$

The inverse P^{-1} is easily computed since the columns of P are orthonormal, which implies that P is an orthogonal matrix, i.e. $P^{-1} = P^{\mathsf{T}}$.

According to eq. (14) of the class handout, "*Coordinates, matrix elements and changes of basis*,"

$$[R]_{\mathcal{B}'} = P^{-1}\,[R]_{\mathcal{B}}\,P\,. \tag{8}$$

where $[R]_{\mathcal{B}}$ is the matrix R with respect to the standard basis, and $[R]_{\mathcal{B}'}$ is the matrix R with respect to the new basis (in which $\hat{\boldsymbol{n}}$ points along the new positive z-axis). In particular,

$$[R]_{\mathcal{B}} = R(\hat{\boldsymbol{n}},\theta)\,, \qquad\qquad [R]_{\mathcal{B}'} = R(\boldsymbol{k},\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} .$$

Hence, eq. (8) yields

$$R(\hat{\boldsymbol{n}},\theta) = PR(\boldsymbol{k},\theta)P^{-1}\,, \tag{9}$$

where P is given by eq. (7) and $P^{-1} = P^{\mathsf{T}}$. For ease of notation, we define

$$N_{12} \equiv \sqrt{n_1^2+n_2^2}\,.$$

Note that $N_{12}^2 + n_3^2 = 1$, since $\hat{\boldsymbol{n}}$ is a unit vector. Writing out the matrices in eq. (9),

$$R(\hat{\boldsymbol{n}},\theta) = \begin{pmatrix} n_3n_1/N_{12} & -n_2/N_{12} & n_1 \\ n_3n_2/N_{12} & n_1/N_{12} & n_2 \\ -N_{12} & 0 & n_3 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} n_3n_1/N_{12} & n_3n_2/N_{12} & -N_{12} \\ -n_2/N_{12} & n_1/N_{12} & 0 \\ n_1 & n_2 & n_3 \end{pmatrix}$$

$$= \begin{pmatrix} n_3n_1/N_{12} & -n_2/N_{12} & n_1 \\[2ex] n_3n_2/N_{12} & n_1/N_{12} & n_2 \\[2ex] -N_{12} & 0 & n_3 \end{pmatrix} \begin{pmatrix} \frac{n_3n_1\cos\theta+n_2\sin\theta}{N_{12}} & \frac{n_3n_2\cos\theta-n_1\sin\theta}{N_{12}} & -N_{12}\cos\theta \\[2ex] \frac{n_3n_1\sin\theta-n_2\cos\theta}{N_{12}} & \frac{n_3n_2\sin\theta+n_1\cos\theta}{N_{12}} & -N_{12}\sin\theta \\[2ex] n_1 & n_2 & n_3 \end{pmatrix} .$$

Using $N_{12}^2 = n_1^2 + n_2^2$ and $n_3^2 = 1 - N_{12}^2$, the final matrix multiplication then yields the desired result:

$$\boxed{R(\hat{\boldsymbol{n}},\theta) = \begin{pmatrix} \cos\theta + n_1^2(1-\cos\theta) & n_1 n_2(1-\cos\theta) - n_3\sin\theta & n_1 n_3(1-\cos\theta) + n_2\sin\theta \\ n_1 n_2(1-\cos\theta) + n_3\sin\theta & \cos\theta + n_2^2(1-\cos\theta) & n_2 n_3(1-\cos\theta) - n_1\sin\theta \\ n_1 n_3(1-\cos\theta) - n_2\sin\theta & n_2 n_3(1-\cos\theta) + n_1\sin\theta & \cos\theta + n_3^2(1-\cos\theta) \end{pmatrix}} \tag{10}$$

Eq. (10) is called the *Rodriguez formula* for the 3×3 rotation matrix $R(\hat{\boldsymbol{n}},\theta)$.

One can easily check that eqs. (2) and (3) are satisfied. In particular, as indicated by eq. (4), the rotations $R(\hat{\boldsymbol{n}},\pi)$ and $R(-\hat{\boldsymbol{n}},\pi)$ represent the same rotation,

$$R_{ij}(\hat{\boldsymbol{n}},\pi) = \begin{pmatrix} 2n_i^2 - 1 & 2n_1 n_2 & 2n_1 n_3 \\ 2n_1 n_2 & 2n_2^2 - 1 & 2n_2 n_3 \\ 2n_1 n_3 & 2n_2 n_3 & 2n_3^2 - 1 \end{pmatrix} = 2n_i n_j - \delta_{ij}\,, \tag{11}$$

where the Kronecker delta δ_{ij} is defined to be the matrix elements of the identity,

$$\delta_{ij} = \begin{cases} 1\,, & \text{if } i = j\,, \\ 0\,, & \text{if } i \neq j\,. \end{cases}$$

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

In Appendix A, 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.

3. Determining the rotation axis and the rotation angle

Now that we have the most general form for $R(\hat{\boldsymbol{n}},\theta)$, we ask the following question. Given $R(\hat{\boldsymbol{n}},\theta)$, can we quickly determine the direction of the rotation axis $\hat{\boldsymbol{n}}$ and the rotation angle θ? The answer is yes. First, we compute the trace of $R(\hat{\boldsymbol{n}},\theta)$. In particular, using eq. (10) it follows that:

$$\boxed{\mathrm{Tr}\ R(\hat{\boldsymbol{n}},\theta) = 1 + 2\cos\theta} \tag{12}$$

By convention, $0 \leq \theta \leq \pi$, which implies that $\sin\theta \geq 0$. Thus,

$$\boxed{\cos\theta = \tfrac{1}{2}(\mathrm{Tr}\ R - 1) \quad \text{and} \quad \sin\theta = (1-\cos^2\theta)^{1/2} = \tfrac{1}{2}\sqrt{(3 - \mathrm{Tr}\ R)(1 + \mathrm{Tr}\ R)}} \tag{13}$$

where $\cos\theta$ is determined from eq. (12). All that remains is to determine the axis of rotation $\hat{\boldsymbol{n}}$.

If $\sin\theta \neq 0$, then we can immediately use eqs. (10) and (13) to obtain

$$\hat{\boldsymbol{n}} = \frac{1}{\sqrt{(3 - \mathrm{Tr}\ R)(1 + \mathrm{Tr}\ R)}}\Big(R_{32} - R_{23}\,,\ R_{13} - R_{31}\,,\ R_{21} - R_{12}\Big)\,, \qquad \mathrm{Tr}\ R \neq -1\,,\,3\,. \tag{14}$$

The overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (3) due to our convention in which $\sin\theta \geq 0$. If $\sin\theta = 0$, then eq. (10) implies that $R_{ij} = R_{ji}$, in which case $\hat{\boldsymbol{n}}$ cannot be determined from eq. (14). In this case, eq. (12) determines whether $\cos\theta = +1$ or $\cos\theta = -1$. If $\cos\theta = +1$, then $R_{ij} = \delta_{ij}$ and the axis $\hat{\boldsymbol{n}}$ is undefined. If $\cos\theta = -1$, then eq. (11) determines the direction of $\hat{\boldsymbol{n}}$ up to an overall sign. That is,

$$\hat{\boldsymbol{n}} \text{ is undetermined if } \theta = 0\,,$$

$$\hat{\boldsymbol{n}} = \left(\epsilon_1\sqrt{\tfrac{1}{2}(1+R_{11})}\,,\,\epsilon_2\sqrt{\tfrac{1}{2}(1+R_{22})}\,,\,\epsilon_3\sqrt{\tfrac{1}{2}(1+R_{33})}\right)\,, \qquad \text{if } \theta = \pi\,, \tag{15}$$

where the individual signs $\epsilon_i = \pm 1$ are determined up to an overall sign via[4]

$$\epsilon_i\epsilon_j = \frac{R_{ij}}{\sqrt{(1+R_{ii})(1+R_{jj})}}\,, \qquad \text{for fixed } i \neq j\,,\ R_{ii} \neq -1\,,\ R_{jj} \neq -1\,. \tag{16}$$

The ambiguity of the overall sign of $\hat{\boldsymbol{n}}$ sign is not significant, since $R(\hat{\boldsymbol{n}}, \pi)$ and $R(-\hat{\boldsymbol{n}}, \pi)$ represent the same rotation [cf. eq. (5)].

One slightly inconvenient feature of the above analysis is that the case of $\theta = \pi$ (or equivalently, $\text{Tr } R = -1$) requires a separate treatment in order to determine $\hat{\boldsymbol{n}}$. Moreover, for values of θ very close to π, the numerator and denominator of eq. (14) are very small, so that a very precise numerical evaluation of both the numerator and denominator is required to accurately determine the direction of $\hat{\boldsymbol{n}}$. Thus, we briefly mention another approach for determining $\hat{\boldsymbol{n}}$ that can be employed for all possible values of R_{ii} (except for $\text{Tr } R = 3$ corresponding to the identity rotation, where $\hat{\boldsymbol{n}}$ is undefined). In this approach, we define the matrix

$$S = R + R^{\mathsf{T}} + (1 - \text{Tr } R)\mathbf{I}\,. \tag{17}$$

Then, eq. (10) yields $S_{jk} = 2(1-\cos\theta)n_j n_k = (3 - \text{Tr } R)n_j n_k$. Hence,[5]

$$\boxed{n_j n_k = \frac{S_{jk}}{3 - \text{Tr } R}\,, \qquad \text{Tr } R \neq 3} \tag{18}$$

Note that for θ close to π (which corresponds to $\text{Tr } R \simeq -1$), neither the numerator nor the denominator of eq. (18) is particularly small, and the direction of $\hat{\boldsymbol{n}}$ can be determined numerically without significant roundoff error.

To determine $\hat{\boldsymbol{n}}$ up to an overall sign, we simply set $j = k$ in eq. (18), which fixes the value of n_j^2. If $\sin\theta \neq 0$, the overall sign of $\hat{\boldsymbol{n}}$ is fixed by eq. (14). If $\sin\theta = 0$ there are two cases. For $\theta = 0$ (corresponding to the identity rotation), the rotation axis $\hat{\boldsymbol{n}}$ is undefined. For $\theta = \pi$, the ambiguity in the overall sign of $\hat{\boldsymbol{n}}$ is immaterial, in light of eq. (5).

Thus, we have achieved our goal. Eqs. (13), (14) and (15) provide a simple algorithm for determining the rotation axis $\hat{\boldsymbol{n}}$ and the rotation angle θ for any rotation matrix $R(\hat{\boldsymbol{n}}, \theta) \neq \mathbf{I}$.

[4]If $R_{ii} = -1$, where i is a fixed index, then $n_i = 0$, in which case the corresponding ϵ_i is not well-defined.

[5]Eq. (17) yields $\text{Tr}\, S = 3 - \text{Tr } R$. One can then use eq. (18) to verify that $\hat{\boldsymbol{n}}$ is a unit vector.

4. Boas, p. 161, problem 3.11–54 revisited

Show that the matrix,

$$R = \frac{1}{2}\begin{pmatrix} 1 & \sqrt{2} & -1 \\ \sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & -1 \end{pmatrix}, \tag{19}$$

is orthogonal and find the rotation it produces as an operator acting on vectors. Determine the rotation axis and the angle of rotation.

First we check that R is orthogonal.

$$R^{\mathsf{T}}R = \frac{1}{4}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 0 & -\sqrt{2} \\ -1 & \sqrt{2} & -1 \end{pmatrix}\begin{pmatrix} 1 & \sqrt{2} & -1 \\ \sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbf{I}\,.$$

Second, we compute the determinant by the expansion of the second row by cofactors:

$$\det\, R = \frac{1}{8}\begin{vmatrix} 1 & \sqrt{2} & -1 \\ \sqrt{2} & 0 & \sqrt{2} \\ 1 & -\sqrt{2} & -1 \end{vmatrix} = -\frac{1}{8}\sqrt{2}\left[\begin{vmatrix} \sqrt{2} & -1 \\ -\sqrt{2} & -1 \end{vmatrix} + \begin{vmatrix} 1 & \sqrt{2} \\ 1 & -\sqrt{2} \end{vmatrix}\right]$$

$$= -\frac{1}{8}\sqrt{2}\left[-2\sqrt{2} - 2\sqrt{2}\right] = \frac{1}{8}\sqrt{2}[4\sqrt{2}] = +1\,.$$

Since $\det\, R = +1$, we conclude that R is a proper rotation.

We can now use eqs. (13) and (14) to determine the rotation angle θ and the rotation axis $\boldsymbol{\hat{n}}$. Since $\operatorname{Tr} R = 0$, eq. (13) yields

$$\cos\theta = -\tfrac{1}{2}\,, \qquad \sin\theta = \tfrac{1}{2}\sqrt{3}\,,$$

which implies that $\theta = 120^\circ$. Next, we employ eq. (14) to obtain the axis of rotation,

$$\boldsymbol{\hat{n}} = -\frac{1}{\sqrt{3}}\left[\sqrt{2}\,\boldsymbol{i} + \boldsymbol{j}\right]\,. \tag{20}$$

In the solution to this problem given in the solutions to homework set #8, I obtained $\boldsymbol{\hat{n}} = \frac{1}{\sqrt{3}}\left[\sqrt{2}\,\boldsymbol{i} + \boldsymbol{j}\right]$ and $\theta = 240^\circ$, which corresponds to the convention defined in footnote 3 where $0 \leq \theta < 2\pi$ and $\boldsymbol{\hat{n}} > 0$. This is in contrast to eq. (20) which is based on the convention adopted in these notes where $0 \leq \theta \leq \pi$. Of course, both choices yield the same rotation matrix, in light of eq. (4).

In either convention, I am sure that you will agree that the method presented above is far simpler than the method presented in the solutions to homework set #8.

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

In this appendix, 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. First, it will be convenient to express $\hat{\boldsymbol{n}}$ in spherical coordinates,

$$\hat{\boldsymbol{n}} = (\sin\theta_n\cos\phi_n\,,\,\sin\theta_n\sin\phi_n\,,\,\cos\theta_n)\,, \tag{21}$$

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

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

one can identify the matrix P given in eq. (7) as:

$$P = R(\boldsymbol{k},\phi_n)R(\boldsymbol{j},\theta_n) = \begin{pmatrix} \cos\theta_n\cos\phi_n & -\sin\phi_n & \sin\theta\cos\phi_n \\ \cos\theta_n\sin\phi_n & \cos\phi_n & \sin\theta\sin\phi_n \\ -\sin\theta_n & 0 & \cos\theta_n \end{pmatrix}\,. \tag{22}$$

Let us introduce the 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. (10) then yields:

$$\begin{aligned} R(\hat{\boldsymbol{\varphi}},\theta_n) &= \begin{pmatrix} \cos\theta_n + \sin^2\phi_n(1-\cos\theta_n) & -\sin\phi_n\cos\phi(1-\cos\theta_n) & \sin\theta_n\cos\phi_n \\ -\sin\phi_n\cos\phi_n(1-\cos\theta_n) & \cos\theta_n + \cos^2\phi_n(1-\cos\theta_n) & \sin\theta_n\sin\phi_n \\ -\sin\theta_n\cos\phi_n & -\sin\theta_n\sin\phi_n & \cos\theta_n \end{pmatrix} \\ &= R(\boldsymbol{k},\phi_n)R(\boldsymbol{j},\theta_n)R(\boldsymbol{k},-\phi_n) = PR(\boldsymbol{k},-\phi_n)\,, \end{aligned} \tag{23}$$

after using eq. (22) in the final step. Eqs. (3) and (23) then imply that

$$P = R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\phi_n)\,, \tag{24}$$

One can now use eqs. (3), (9) and (24) to obtain:

$$R(\hat{\boldsymbol{n}},\theta) = PR(\boldsymbol{k},\theta)P^{-1} = R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\phi_n)R(\boldsymbol{k},\theta)R(\boldsymbol{k},-\phi_n)R(\hat{\boldsymbol{\varphi}},-\theta_n)\,. \tag{25}$$

Since rotations about a fixed axis commute, it follows that

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

since $R(\boldsymbol{k},\phi_n)R(\boldsymbol{k},-\phi_n) = R(\boldsymbol{k},\phi_n)[R(\boldsymbol{k},\phi_n)]^{-1} = \mathbf{I}$. Hence, eq. (25) yields:

$$\boxed{R(\hat{\boldsymbol{n}},\theta) = R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\theta)R(\hat{\boldsymbol{\varphi}},-\theta_n)} \tag{26}$$

The geometrical interpretation of eq. (26) is clear. Consider $R(\hat{\boldsymbol{n}},\theta)\vec{\boldsymbol{v}}$ for any vector $\vec{\boldsymbol{v}}$. This is equivalent to $R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\theta)R(\hat{\boldsymbol{\varphi}},-\theta_n)\vec{\boldsymbol{v}}$. The effect of $R(\hat{\boldsymbol{\varphi}},-\theta_n)$ is to rotate the axis of rotation $\hat{\boldsymbol{n}}$ to $\boldsymbol{k}$ (which lies along the z-axis). Then, $R(\boldsymbol{k},\theta)$ performs the rotation by θ about the z-axis. Finally, $R(\hat{\boldsymbol{\varphi}},\theta_n)$ rotates $\boldsymbol{k}$ back to the original rotation axis $\hat{\boldsymbol{n}}$.[6]

One can derive one more interesting relation by combining the results of eqs. (22), (24) and (26):

$$\begin{aligned} R(\hat{\boldsymbol{n}},\theta) &= R(\boldsymbol{k},\phi_n)R(\boldsymbol{j},\theta_n)R(\boldsymbol{k},-\phi_n)R(\boldsymbol{k},\theta)R(\boldsymbol{k},\phi_n)R(\boldsymbol{j},-\theta_n)R(\boldsymbol{k},-\phi_n) \\ &= R(\boldsymbol{k},\phi_n)R(\boldsymbol{j},\theta_n)R(\boldsymbol{k},\theta)R(\boldsymbol{j},-\theta_n)R(\boldsymbol{k},-\phi_n)\,. \end{aligned}$$

That is, a rotation by an angle θ about a fixed axis $\hat{\boldsymbol{n}}$ (with 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 slightly better. One can prove that an arbitrary rotation can be written as:

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

where α, β and γ are called the *Euler angles*. For those of you who are interested, details of the Euler angle representation of $\boldsymbol{R(\hat{n},\theta)}$ can be found in Appendix B.

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

An arbitrary rotation matrix can can be written as:

$$R(\hat{\boldsymbol{n}},\theta) = R(\boldsymbol{k},\alpha)R(\boldsymbol{j},\beta)R(\boldsymbol{k},\gamma)\,, \tag{27}$$

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. (21)]. These relations can be obtained by multiplying out the three matrices on the right-hand side of eq. (27) to obtain

$$R(\hat{\boldsymbol{n}},\theta) = \begin{pmatrix} \cos\alpha\cos\beta\cos\gamma - \sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma - \sin\alpha\cos\gamma & \cos\alpha\sin\beta \\ \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma + \cos\alpha\cos\gamma & \sin\alpha\sin\beta \\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta \end{pmatrix}\,. \tag{28}$$

One can now make use of the results of Section 2 to obtain θ and $\hat{\boldsymbol{n}}$ in terms of α, β and γ. For example, $\cos\theta$ is obtained from eq. (13). Simple algebra yields:

$$\boxed{\cos\theta = \cos^2(\beta/2)\cos(\gamma+\alpha) - \sin^2(\beta/2)} \tag{29}$$

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. (13)

[6]Using eq. (22), one can easily verify that $R(\hat{\boldsymbol{\varphi}},-\theta_n)\hat{\boldsymbol{n}} = \boldsymbol{k}$ and $R(\hat{\boldsymbol{\varphi}},\theta_n)\boldsymbol{k} = \hat{\boldsymbol{n}}$.

and the text preceding this equation]. One can also rewrite eq. (29) in a slightly more convenient form,

$$\cos\theta = -1 + 2\cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)\,. \tag{30}$$

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. (30) 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. (15) and (16) 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. (15) and (16) 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. (14) and (28),

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

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:

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

Hence,[7]

$$\hat{\boldsymbol{n}} = \frac{\epsilon}{\sqrt{\sin^2(\beta/2) + \cos^2(\beta/2)\sin^2\frac{1}{2}(\gamma+\alpha)}}$$
$$\times\Big(\sin(\beta/2)\sin\tfrac{1}{2}(\gamma-\alpha)\,,\ \sin(\beta/2)\cos\tfrac{1}{2}(\gamma-\alpha)\,,\ \cos(\beta/2)\sin\tfrac{1}{2}(\gamma+\alpha)\Big)\,, \tag{32}$$

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

$$\epsilon \equiv \operatorname{sgn}\big\{\cos\tfrac{1}{2}(\gamma+\alpha)\cos(\beta/2)\big\}\,, \qquad \sin\theta \neq 0\,. \tag{33}$$

Remarkably, eq. (32) 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. (33) 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. (30) to obtain:

$$\begin{aligned}
\sin(\theta/2) &= \sqrt{\sin^2(\beta/2) + \cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)}\,,\\
\cos(\theta/2) &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}(\gamma+\alpha)\,,
\end{aligned} \tag{34}$$

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. (33) is required in eq. (34) 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:

$$q = \Big(\cos(\theta/2)\,,\ \hat{\boldsymbol{n}}\sin(\theta/2)\Big)\,, \tag{35}$$

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

$$\begin{aligned}
q_0 &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}(\gamma+\alpha)\,, & q_1 &= \epsilon\sin(\beta/2)\sin\tfrac{1}{2}(\gamma-\alpha)\,,\\
q_2 &= \epsilon\sin(\beta/2)\cos\tfrac{1}{2}(\gamma-\alpha)\,, & q_3 &= \epsilon\cos(\beta/2)\sin\tfrac{1}{2}(\gamma+\alpha)\,.
\end{aligned} \tag{36}$$

In the convention of $0 \leq \theta \leq \pi$, we have $q_0 \geq 0$.[8] Quaternions are especially valuable for representing rotations in computer graphics software.

[7] One can can also determine $\hat{\boldsymbol{n}}$ up to an overall sign starting from eq. (28) 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. (14).

[8] 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. (35) will be re-defined as ϵq in order to remove the factors of ϵ from eq. (36), in which case $\epsilon q_0 \geq 0$.

If one expresses $\hat{\boldsymbol{n}}$ in terms of a polar angle θ_n and azimuthal angle ϕ_n as in eq. (21), 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. (21) and (32), it follows that:

$$\boxed{\tan\theta_n = \frac{(n_1^2+n_2^2)^{1/2}}{n_3} = \frac{\epsilon\tan(\beta/2)}{\sin\frac{1}{2}(\gamma+\alpha)}} \tag{37}$$

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. (33). Similarly,

$$\cos\phi_n = \frac{n_1}{(n_1^2+n_2^2)} = \epsilon\sin\tfrac{1}{2}(\gamma-\alpha) = \epsilon\cos\tfrac{1}{2}(\pi-\gamma+\alpha)\,, \tag{38}$$

$$\sin\phi_n = \frac{n_2}{(n_1^2+n_2^2)} = \epsilon\cos\tfrac{1}{2}(\gamma-\alpha) = \epsilon\sin\tfrac{1}{2}(\pi-\gamma+\alpha)\,, \tag{39}$$

or equivalently

$$\boxed{\phi_n = \tfrac{1}{2}(\epsilon\pi-\gamma+\alpha) \bmod 2\pi} \tag{40}$$

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. (30) as:

$$\cos^2(\theta/2) = \cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)\,. \tag{41}$$

Then, using eqs. (37) and (41), it follows that:

$$\sin(\beta/2) = \sin\theta_n\sin(\theta/2)\,. \tag{42}$$

Plugging this result back into eqs. (37) and (41) yields

$$\epsilon\sin\tfrac{1}{2}(\gamma+\alpha) = \frac{\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{43}$$

$$\epsilon\cos\tfrac{1}{2}(\gamma+\alpha) = \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,. \tag{44}$$

Note that if $\beta = \pi$ then eq. (42) 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. (33)].

We shall also make use of eqs. (38) and (39),

$$\epsilon\sin\tfrac{1}{2}(\gamma-\alpha) = \cos\phi_n\,, \tag{45}$$

$$\epsilon\cos\tfrac{1}{2}(\gamma-\alpha) = \sin\phi_n\,, \tag{46}$$

Finally, we employ eqs. (44) and (45) 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

$$\epsilon = \operatorname{sgn}\left\{\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n \sin^2(\theta/2)}}\right\}, \tag{47}$$

If either $\gamma = 0$ or $\alpha = 0$, then the argument of sgn in eq. (47) will vanish. In this case, $\sin\frac{1}{2}(\gamma+\alpha) \geq 0$, and we may use eq. (43) 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. (33).[9] 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. (44)].

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. (10) and (28), equal to each other, where $\hat{\boldsymbol{n}}$ is given by eq. (21). For example,

$$R_{33} = \cos\beta = \cos\theta + \cos^2\theta_n(1-\cos\theta). \tag{48}$$

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

$$\sin\beta = 2\sin(\theta/2)\sin\theta_n\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}\,, \tag{49}$$

which also can be derived from eq. (42). 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. (10) yields (for $\sin\beta \neq 0$):

$$\sin\alpha = \frac{\cos\theta_n\sin\phi_n\sin(\theta/2) - \cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{50}$$

$$\cos\alpha = \frac{\cos\theta_n\cos\phi_n\sin(\theta/2) + \sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{51}$$

$$\sin\gamma = \frac{\cos\theta_n\sin\phi_n\sin(\theta/2) + \cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{52}$$

$$\cos\gamma = \frac{-\cos\theta_n\cos\phi_n\sin(\theta/2) + \sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,. \tag{53}$$

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. (48) 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 $\gamma + \alpha = \theta \bmod \pi$, with $\gamma - \alpha$ indeterminate. If $\beta = \pi$ then eq. (48)

[9]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. (5) and (21)].

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. (50)–(53) to rederive eqs. (43)–(46). 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[10]

$$\begin{aligned}
\cos\tfrac{1}{2}(\gamma \pm \alpha) &= \cos(\gamma/2)\cos(\alpha/2) \mp \sin(\gamma/2)\sin(\alpha/2) \\
&= \frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)\cos(\alpha/2) \mp \sin^2(\gamma/2)\sin^2(\alpha/2)}{\sin(\gamma/2)\sin(\alpha/2)} \\
&= \frac{\sin\gamma\sin\alpha \mp (1-\cos\gamma)(1-\cos\alpha)}{2(1-\cos\gamma)^{1/2}(1-\cos\alpha)^{1/2}}\,. \qquad (54)
\end{aligned}$$

and

$$\begin{aligned}
\sin\tfrac{1}{2}(\gamma \pm \alpha) &= \sin(\gamma/2)\cos(\alpha/2) \pm \cos(\gamma/2)\sin(\alpha/2) \\
&= \frac{\sin(\gamma/2)\sin(\alpha/2)\cos(\alpha/2)}{\sin(\alpha/2)} \pm \frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)}{\sin(\gamma/2)} \\
&= \frac{\sin(\gamma/2)\sin\alpha}{2\sin(\alpha/2)} \pm \frac{\sin\gamma\sin(\alpha/2)}{2\sin(\gamma/2)} \\
&= \tfrac{1}{2}\sin\alpha\sqrt{\frac{1-\cos\gamma}{1-\cos\alpha}} \pm \tfrac{1}{2}\sin\gamma\sqrt{\frac{1-\cos\alpha}{1-\cos\gamma}} \\
&= \frac{\sin\alpha(1-\cos\gamma) \pm \sin\gamma(1-\cos\alpha)}{2(1-\cos\alpha)^{1/2}(1-\cos\gamma)^{1/2}}\,. \qquad (55)
\end{aligned}$$

We now use eqs. (50)–(53) to evaluate the above expressions. To evaluate the denominators of eqs. (54) and (55), 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,

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

[10] 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 the *positive* square root in both cases, without ambiguity.

where $\epsilon = \pm 1$ is the sign defined by eq. (47). Likewise we can employ eqs. (50)–(53) 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. (54) and (55), it immediately follows that

$$\cos\tfrac{1}{2}(\gamma+\alpha) = \frac{\epsilon\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}, \qquad \cos\tfrac{1}{2}(\gamma-\alpha) = \epsilon\sin\phi_n, \qquad (56)$$

$$\sin\tfrac{1}{2}(\gamma+\alpha) = \frac{\epsilon\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}, \qquad \sin\tfrac{1}{2}(\gamma-\alpha) = \epsilon\cos\phi_n, \qquad (57)$$

where ϵ is given by eq. (47). We have derived eqs. (56) and (57) assuming that $\alpha \neq 0$, $\gamma \neq 0$ and $\sin\beta \neq 0$. Since $\cos(\beta/2)$ is then strictly positive, eq. (33) 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. (43)–(46).

If $\alpha = 0$ and/or $\gamma = 0$, then the derivation of eqs. (54) and (55) is not valid. Nevertheless, eqs. (56) and (57) are still true if $\sin\beta \neq 0$, as noted below eq. (47), 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. (53), 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. (44), $\gamma + \alpha$ 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. (30) and (32) then yield:

$$\cos\theta = -\tfrac{1}{4}, \qquad \hat{\boldsymbol{n}} = -\frac{1}{\sqrt{5}}(0\,,\,2\,,\,1)\,. \qquad (58)$$

The polar and azimuthal angles of $\hat{\boldsymbol{n}}$ [cf. eq. (21)] are then given by $\phi_n = -90°$ (mod 2π) and $\tan\theta_n = -2$. The latter can also be deduced from eqs. (37) and (40).

Likewise, given eq. (58), one obtains $\cos\beta = 0$ (i.e. $\beta = 90°$) from eq. (48), $\epsilon = -1$ from eq. (47), $\gamma = \alpha$ from eqs. (45) and (46), and $\gamma = \alpha = 150°$ from eqs. (43) and (44). One can verify these results explicitly by inserting the values of the corresponding parameters into eqs. (10) and (28) and checking that the two matrix forms for $R(\hat{\boldsymbol{n}}, \theta)$ coincide.