Three-Dimensional Rotations as Products of Simpler Rotations

1. The most general 3×3 rotation matrix

In a class handout entitled, *Three-Dimensional Proper and Improper Rotation Matrices*, I derived the following general form for a 3×3 matrix representation of a proper rotation by an angle θ in a counterclockwise direction about a fixed rotation axis parallel to the unit vector $\hat{\boldsymbol{n}} = (n_1, n_2, n_3)$,

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

which is called the *angle-and-axis parameterization* of a three-dimensional rotation. In deriving eq. (1), we showed in the class handout cited above that

$$R(\hat{\boldsymbol{n}}, \theta) = P R(\boldsymbol{k}, \theta) P^{-1}\,, \tag{2}$$

where P is given by

$$P = \begin{pmatrix} \dfrac{n_3 n_1}{\sqrt{n_1^2+n_2^2}} & \dfrac{-n_2}{\sqrt{n_1^2+n_2^2}} & n_1 \\[2ex] \dfrac{n_3 n_2}{\sqrt{n_1^2+n_2^2}} & \dfrac{n_1}{\sqrt{n_1^2+n_2^2}} & n_2 \\[2ex] -\sqrt{n_1^2+n_2^2} & 0 & n_3 \end{pmatrix}. \tag{3}$$

The general rotation matrix $R(\hat{\boldsymbol{n}}, \theta)$ given in eq. (1) satisfies the following two relations:

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

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

which implies that any proper three-dimensional rotation can be described by a counterclockwise rotation by θ about an arbitrary axis $\hat{\boldsymbol{n}}$, where $0 \leq \theta \leq \pi$. The angle θ can be obtained from the trace of $R(\hat{\boldsymbol{n}}, \theta)$,

$$\cos\theta = \tfrac{1}{2}\left(\mathrm{Tr}\ R - 1\right) \quad \text{and} \quad \sin\theta = (1-\cos^2\theta)^{1/2} = \tfrac{1}{2}\sqrt{(3-\mathrm{Tr}\ R)(1+\mathrm{Tr}\ R)}\,. \tag{6}$$

In this convention for the range of the angle θ, the overall sign of $\hat{\boldsymbol{n}}$ is meaningful for $0 < \theta < \pi$. In this case, we showed in the class handout cited above that

$$\hat{\boldsymbol{n}} = \frac{1}{\sqrt{(3 - \text{Tr } R)(1 + \text{Tr } R)}} \Big(R_{32} - R_{23} \,,\, R_{13} - R_{31} \,,\, R_{21} - R_{12} \Big) \,, \qquad \text{Tr } R \neq -1 \,,\, 3 \,. \tag{7}$$

In the case of $\theta = \pi$ (which corresponds to $\text{Tr}\, R = -1$), eq. (5) implies that

$$R(\hat{\boldsymbol{n}}, \pi) = R(-\hat{\boldsymbol{n}}, \pi) \,, \tag{8}$$

which means that $R(\hat{\boldsymbol{n}}, \pi)$ and $R(-\hat{\boldsymbol{n}}, \pi)$ represent the *same* rotation. In this case, one can use eq. (1) to derive

$$\hat{\boldsymbol{n}} = \left(\epsilon_1 \sqrt{\tfrac{1}{2}(1 + R_{11})} \,,\, \epsilon_2 \sqrt{\tfrac{1}{2}(1 + R_{22})} \,,\, \epsilon_3 \sqrt{\tfrac{1}{2}(1 + R_{33})} \right) \,, \qquad \text{if Tr}\, R = -1 \,, \tag{9}$$

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

$$\epsilon_i \epsilon_j = \frac{R_{ij}}{\sqrt{(1 + R_{ii})(1 + R_{jj})}} \,, \qquad \text{for fixed } i \neq j \,,\, R_{ii} \neq -1 \,,\, R_{jj} \neq -1 \,. \tag{10}$$

The ambiguity of the overall sign of $\hat{\boldsymbol{n}}$ is not significant in light of eq. (8). Finally, in the case of $\theta = 0$ (which corresponds to $\text{Tr}\, R = 3$), $R(\hat{\boldsymbol{n}}, 0) = \mathbf{I}$ is the 3×3 identity matrix, which is independent of the direction of $\hat{\boldsymbol{n}}$.

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

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

$$\hat{\boldsymbol{n}} = (\sin\theta_n \cos\phi_n \,,\, \sin\theta_n \sin\phi_n \,,\, \cos\theta_n) \,, \tag{11}$$

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. (3) as:

$$P = R(\boldsymbol{k}, \phi_n) R(\boldsymbol{j}, \theta_n) = \begin{pmatrix} \cos\theta_n \cos\phi_n & -\sin\phi_n & \sin\theta \cos\phi_n \\ \cos\theta_n \sin\phi_n & \cos\phi_n & \sin\theta \sin\phi_n \\ -\sin\theta_n & 0 & \cos\theta_n \end{pmatrix} \,. \tag{12}$$

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. (1) then yields:

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

$$= R(\boldsymbol{k},\phi_n)R(\boldsymbol{j},\theta_n)R(\boldsymbol{k},-\phi_n) = PR(\boldsymbol{k},-\phi_n)\,, \tag{13}$$

after using eq. (12) in the final step. Eqs. (4) and (13) then imply that

$$P = R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\phi_n)\,, \tag{14}$$

One can now use eqs. (4), (2) and (14) to obtain:

$$R(\hat{\boldsymbol{n}},\theta) = PR(\boldsymbol{k},\theta)P^{-1} = R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\phi_n)R(\boldsymbol{k},\theta)R(\boldsymbol{k},-\phi_n)R(\hat{\boldsymbol{\varphi}},-\theta_n)\,. \tag{15}$$

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. (15) yields:

$$\boxed{R(\hat{\boldsymbol{n}},\theta) = R(\hat{\boldsymbol{\varphi}},\theta_n)R(\boldsymbol{k},\theta)R(\hat{\boldsymbol{\varphi}},-\theta_n)} \tag{16}$$

The geometrical interpretation of eq. (16) 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 $\hat{\boldsymbol{n}}$.[1]

One can derive one more interesting relation by combining the results of eqs. (12), (14) and (16):

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

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*. Details of the Euler angle representation of $R(\hat{\boldsymbol{n}},\theta)$ will be presented in Section 3.

[1] Using eq. (13), one can easily verify that $R(\hat{\boldsymbol{\varphi}},-\theta_n)\hat{\boldsymbol{n}} = \boldsymbol{k}$ and $R(\hat{\boldsymbol{\varphi}},\theta_n)\boldsymbol{k} = \hat{\boldsymbol{n}}$.

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

An arbitrary rotation matrix can can be written as:

$$R(\hat{\boldsymbol{n}},\theta)=R(\boldsymbol{k},\alpha)R(\boldsymbol{j},\beta)R(\boldsymbol{k},\gamma)\,, \tag{17}$$

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. (11)]. These relations can be obtained by multiplying out the three matrices on the right-hand side of eq. (17) to obtain

$$R(\hat{\boldsymbol{n}},\theta)=\begin{pmatrix}\cos\alpha\cos\beta\cos\gamma-\sin\alpha\sin\gamma & -\cos\alpha\cos\beta\sin\gamma-\sin\alpha\cos\gamma & \cos\alpha\sin\beta\\ \sin\alpha\cos\beta\cos\gamma+\cos\alpha\sin\gamma & -\sin\alpha\cos\beta\sin\gamma+\cos\alpha\cos\gamma & \sin\alpha\sin\beta\\ -\sin\beta\cos\gamma & \sin\beta\sin\gamma & \cos\beta\end{pmatrix}. \tag{18}$$

One can now make use of the results of Section 1 to obtain θ and $\hat{\boldsymbol{n}}$ in terms of the Euler angles α, β and γ. For example, $\cos\theta$ is obtained from eq. (6). Simple algebra yields:

$$\boxed{\cos\theta=\cos^2(\beta/2)\cos(\gamma+\alpha)-\sin^2(\beta/2)} \tag{19}$$

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. (6) and the text preceding this equation]. One can also rewrite eq. (19) in a slightly more convenient form,

$$\cos\theta=-1+2\cos^2(\beta/2)\cos^2\tfrac{1}{2}(\gamma+\alpha)\,. \tag{20}$$

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. (20) 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. (9) and (10) 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

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

since $\cos^2\tfrac{1}{2}(\gamma+\alpha)=\tfrac{1}{2}\left[1+\cos(\gamma+\alpha)\right]=0$. Thus, eqs. (9) and (10) yield

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

where

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

Finally, we consider the generic case where $\sin\theta\neq 0$. Using eqs. (7) and (18),

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

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

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

Hence,[2]

$$\begin{aligned}\hat{\boldsymbol{n}}=&\frac{\epsilon}{\sqrt{\sin^2(\beta/2)+\cos^2(\beta/2)\sin^2\tfrac{1}{2}(\gamma+\alpha)}}\\ &\times\Bigl(\sin(\beta/2)\sin\tfrac{1}{2}(\gamma-\alpha)\,,\,\sin(\beta/2)\cos\tfrac{1}{2}(\gamma-\alpha)\,,\,\cos(\beta/2)\sin\tfrac{1}{2}(\gamma+\alpha)\Bigr)\,,\end{aligned}\tag{22}$$

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

$$\epsilon\equiv\operatorname{sgn}\bigl\{\cos\tfrac{1}{2}(\gamma+\alpha)\cos(\beta/2)\bigr\}\,,\qquad\sin\theta\neq 0\,.\tag{23}$$

Remarkably, eq. (22) reduces to the correct results obtained above in the two subcases corresponding to $\theta=\pi$, where $\cos(\beta/2)=0$ and/or $\cos\tfrac{1}{2}(\gamma+\alpha)=0$, respectively. Note that in the latter two subcases, ϵ as defined in eq. (23) is indeterminate. This is consistent

[2] One can can also determine $\hat{\boldsymbol{n}}$ up to an overall sign starting from eq. (18) 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. (7).

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. (20) to obtain:

$$\begin{aligned} \sin(\theta/2) &= \sqrt{\sin^2(\beta/2) + \cos^2(\beta/2)\cos^2\tfrac{1}{2}\left(\gamma+\alpha\right)}\,, \\ \cos(\theta/2) &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}(\gamma+\alpha)\,, \end{aligned} \tag{24}$$

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. (23) is required in eq. (24) 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:

$$q = \biggl(\cos(\theta/2)\,,\,\hat{\boldsymbol{n}}\sin(\theta/2)\biggr)\,, \tag{25}$$

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

$$\begin{aligned} q_0 &= \epsilon\cos(\beta/2)\cos\tfrac{1}{2}\left(\gamma+\alpha\right)\,, \qquad & q_1 &= \epsilon\sin(\beta/2)\sin\tfrac{1}{2}\left(\gamma-\alpha\right)\,, \\ q_2 &= \epsilon\sin(\beta/2)\cos\tfrac{1}{2}\left(\gamma-\alpha\right)\,, \qquad & q_3 &= \epsilon\cos(\beta/2)\sin\tfrac{1}{2}\left(\gamma+\alpha\right)\,. \end{aligned} \tag{26}$$

In the convention of $0 \leq \theta \leq \pi$, we have $q_0 \geq 0$.[3] 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. (11), 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. (11) and (22), it follows that:

$$\boxed{\tan\theta_n = \frac{(n_1^2+n_2^2)^{1/2}}{n_3} = \frac{\epsilon\tan(\beta/2)}{\sin\frac{1}{2}\left(\gamma+\alpha\right)}} \tag{27}$$

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. (23). Similarly,

$$\cos\phi_n = \frac{n_1}{(n_1^2+n_2^2)} = \epsilon\sin\tfrac{1}{2}\left(\gamma-\alpha\right) = \epsilon\cos\tfrac{1}{2}(\pi-\gamma+\alpha)\,, \tag{28}$$

$$\sin\phi_n = \frac{n_2}{(n_1^2+n_2^2)} = \epsilon\cos\tfrac{1}{2}\left(\gamma-\alpha\right) = \epsilon\sin\tfrac{1}{2}(\pi-\gamma+\alpha)\,, \tag{29}$$

or equivalently

$$\boxed{\phi_n = \tfrac{1}{2}(\epsilon\pi-\gamma+\alpha) \bmod 2\pi} \tag{30}$$

[3] 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. (25) will be re-defined as ϵq in order to remove the factors of ϵ from eq. (26), in which case $\epsilon q_0 \geq 0$.

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. (20) as:

$$\cos^2(\theta/2) = \cos^2(\beta/2)\cos^2 \tfrac{1}{2}(\gamma+\alpha)\,. \tag{31}$$

Then, using eqs. (27) and (31), it follows that:

$$\sin(\beta/2) = \sin\theta_n \sin(\theta/2)\,. \tag{32}$$

Plugging this result back into eqs. (27) and (31) yields

$$\epsilon \sin \tfrac{1}{2}(\gamma+\alpha) = \frac{\cos\theta_n \sin(\theta/2)}{\sqrt{1-\sin^2\theta_n \sin^2(\theta/2)}}\,, \tag{33}$$

$$\epsilon \cos \tfrac{1}{2}(\gamma+\alpha) = \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n \sin^2(\theta/2)}}\,. \tag{34}$$

Note that if $\beta = \pi$ then eq. (32) 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. (23)].

We shall also make use of eqs. (28) and (29),

$$\epsilon \sin \tfrac{1}{2}(\gamma-\alpha) = \cos\phi_n\,, \tag{35}$$

$$\epsilon \cos \tfrac{1}{2}(\gamma-\alpha) = \sin\phi_n\,, \tag{36}$$

Finally, we employ eqs. (34) and (35) 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

$$\epsilon = \operatorname{sgn}\left\{\sin\phi_n - \frac{\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n \sin^2(\theta/2)}}\right\}\,, \tag{37}$$

If either $\gamma = 0$ or $\alpha = 0$, then the argument of sgn in eq. (37) will vanish. In this case, $\sin\frac{1}{2}(\gamma+\alpha) \geq 0$, and we may use eq. (33) 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. (23).[4] 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. (34)].

[4]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. (8) and (11)].

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. (1) and (18), equal to each other, where $\hat{\boldsymbol{n}}$ is given by eq. (11). For example,

$$R_{33}=\cos\beta=\cos\theta+\cos^2\theta_n(1-\cos\theta)\,. \tag{38}$$

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

$$\sin\beta=2\sin(\theta/2)\sin\theta_n\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}\,, \tag{39}$$

which also can be derived from eq. (32). 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. (1) yields (for $\sin\beta\neq 0$):

$$\sin\alpha=\frac{\cos\theta_n\sin\phi_n\sin(\theta/2)-\cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{40}$$

$$\cos\alpha=\frac{\cos\theta_n\cos\phi_n\sin(\theta/2)+\sin\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{41}$$

$$\sin\gamma=\frac{\cos\theta_n\sin\phi_n\sin(\theta/2)+\cos\phi_n\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,, \tag{42}$$

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

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. (38) 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. (38) 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. (40)–(43) to rederive eqs. (33)–(36). 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[5]

$$\begin{aligned}\cos\tfrac{1}{2}(\gamma\pm\alpha)&=\cos(\gamma/2)\cos(\alpha/2)\mp\sin(\gamma/2)\sin(\alpha/2)\\ &=\frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)\cos(\alpha/2)\mp\sin^2(\gamma/2)\sin^2(\alpha/2)}{\sin(\gamma/2)\sin(\alpha/2)}\\ &=\frac{\sin\gamma\sin\alpha\mp(1-\cos\gamma)(1-\cos\alpha)}{2(1-\cos\gamma)^{1/2}(1-\cos\alpha)^{1/2}}\,.\end{aligned} \tag{44}$$

[5]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.

and

$$\begin{aligned}
\sin \tfrac{1}{2}(\gamma \pm \alpha) &= \sin(\gamma/2)\cos(\alpha/2) \pm \cos(\gamma/2)\sin(\alpha/2) \\
&= \frac{\sin(\gamma/2)\sin(\alpha/2)\cos(\alpha/2)}{\sin(\alpha/2)} \pm \frac{\sin(\gamma/2)\cos(\gamma/2)\sin(\alpha/2)}{\sin(\gamma/2)} \\
&= \frac{\sin(\gamma/2)\sin\alpha}{2\sin(\alpha/2)} \pm \frac{\sin\gamma\sin(\alpha/2)}{2\sin(\gamma/2)} \\
&= \tfrac{1}{2}\sin\alpha\sqrt{\frac{1-\cos\gamma}{1-\cos\alpha}} \pm \tfrac{1}{2}\sin\gamma\sqrt{\frac{1-\cos\alpha}{1-\cos\gamma}} \\
&= \frac{\sin\alpha(1-\cos\gamma) \pm \sin\gamma(1-\cos\alpha)}{2(1-\cos\alpha)^{1/2}(1-\cos\gamma)^{1/2}}\,. \qquad (45)
\end{aligned}$$

We now use eqs. (40)–(43) to evaluate the above expressions. To evaluate the denominators of eqs. (44) and (45), 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. (37). Likewise we can employ eqs. (40)–(43) 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. (44) and (45), it immediately follows that

$$\cos\tfrac{1}{2}(\gamma+\alpha)=\frac{\epsilon\cos(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\qquad\qquad \cos\tfrac{1}{2}(\gamma-\alpha)=\epsilon\sin\phi_n\,,\tag{46}$$

$$\sin\tfrac{1}{2}(\gamma+\alpha)=\frac{\epsilon\cos\theta_n\sin(\theta/2)}{\sqrt{1-\sin^2\theta_n\sin^2(\theta/2)}}\,,\qquad\qquad \sin\tfrac{1}{2}(\gamma-\alpha)=\epsilon\cos\phi_n\,,\tag{47}$$

where ϵ is given by eq. (37). We have derived eqs. (46) and (47) assuming that $\alpha\neq 0$, $\gamma\neq 0$ and $\sin\beta\neq 0$. Since $\cos(\beta/2)$ is then strictly positive, eq. (23) 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. (33)–(36).

If $\alpha=0$ and/or $\gamma=0$, then the derivation of eqs. (44) and (45) is not valid. Nevertheless, eqs. (46) and (47) are still true if $\sin\beta\neq 0$, as noted below eq. (37), with $\epsilon=\mathrm{sgn}(\cos\theta_n)$ for $\theta_n\neq\pi/2$ and $\epsilon=+1$ for $\theta_n=\phi_n=\pi/2$. If $\beta=0$, then as noted below eq. (43), 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. (34), $\gamma+\alpha$ is indeterminate in the exceptional case of $\beta=\pi$ (i.e., $\theta=\pi$ and $\theta_n=\pi/2$).

<u>*EXAMPLE*</u>: Suppose $\alpha=\gamma=150^\circ$ and $\beta=90^\circ$. Then $\cos\frac{1}{2}(\gamma+\alpha)=-\frac{1}{2}\sqrt{3}$, which implies that $\epsilon=-1$. Eqs. (20) and (22) then yield:

$$\cos\theta=-\tfrac{1}{4}\,,\qquad\qquad \hat{\boldsymbol{n}}=-\frac{1}{\sqrt{5}}\,(0\,,\,2\,,\,1)\,.\tag{48}$$

The polar and azimuthal angles of $\hat{\boldsymbol{n}}$ [cf. eq. (11)] are then given by $\phi_n=-90^\circ \pmod{2\pi}$ and $\tan\theta_n=-2$. The latter can also be deduced from eqs. (27) and (30).

Likewise, given eq. (48), one obtains $\cos\beta=0$ (i.e. $\beta=90^\circ$) from eq. (38), $\epsilon=-1$ from eq. (37), $\gamma=\alpha$ from eqs. (35) and (36), and $\gamma=\alpha=150^\circ$ from eqs. (33) and (34). One can verify these results explicitly by inserting the values of the corresponding parameters into eqs. (1) and (18) and checking that the two matrix forms for $R(\hat{\boldsymbol{n}},\theta)$ coincide.

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