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The Second Orthogonality Conditions in the Theory of Proper and Improper Rotations. II. The Intrinsic Vector*

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The properties of the intrinsic vector associated with a real three-by-three orthogonal transformation, are derived. For proper rotations the problem of extracting the axis and angle or a rotation from its matrix representation, is considered. It is shown that the intrinsic vector allows the determination of the axis and angle as unambiguously as possible, thus remedying the ambiguous treatment of this problem in the literature. Several examples of this use of the intrinsic vector are given. Its properties for improper rotations are also discussed.

Key words: Axis and angle of rotation; coordinate inversion; coordinate reflection; improper rotations; matrices; orthogonal transformations; proper rotations; rigid rotations; rotation.

1. Introduction

It was shown in paper I [1] [1] that the intrinsic vector **V** defined in terms of the elements of the transformation matrix A by

$$V_m \equiv \epsilon_{mnr} A_{nr}. \tag{1}$$

is an eigenvector of A belonging to the eigenvalue p'/p, so that we have

$$A_{jm} V_m = \frac{p'}{p} V_j. \tag{2}$$

The symbols p and p' represent handedness factors for the initial and final coordinate systems S and S' respectively. Each factor has the value plus one if its coordinate system is right-handed, and minus one if its coordinate system is left-handed. The individual components represented by eq (1) are

$$V_1 = A_{23} - A_{32}, \tag{3a}$$

$$V_2 = A_{31} - A_{13}, \tag{3b}$$

$$V_3 = A_{12} = A_{21}. \tag{3c}$$

As pointed out in [1] any non-null vector parallel or antiparallel to **V** is a solution to eq (2). However, it is the specific vector **V** which is the object of interest in this paper. We will investigate its properties for both proper and improper rotations.

The main interest of this paper is in proper (i.e., rigid) rotations. The problem which motivates the discussion of **V** for proper rotations is that of identifying the axis and angle of a rotation directly

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[1] Figures in brackets indicate the literature references at the end of this paper.

from the matrix which represents it. The word "directly" is the key word in this statement of the problem. To be sure there are several methods for finding the axis and angle of a rotation, which are less than direct. For example, one can find the axis of rotation in the usual way by solving the eigenvalue probelm for A corresponding to the eigenvalue $+1$. It is then possible to construct vectors which are perpendicular to the axis. By observing how such vectors are transformed by A, the angle of rotation can be determined. What we are looking for, however, is a prescription which allows us to *read* the necessary information for finding the angle and the axis, directly from A. Unfortunately, the customary method which serves as the prescription is incomplete and consequently ambiguous. [2]

In section 2 we discuss the ambiguities one encounters in trying to formulate a prescription for the determination of the axis and the angle of a rotation. In section 3, it is shown how these ambiguities are overcome by the use of **V**. Section 4 gives some concrete examples of this usage. In section 5, we consider the properties of **V** for improper rotations.

2. Ambiguities in Determining the Axis and Angle of a Rotation from Its Representative Matrix

In the conventional method of finding the axis and angle of a rotation from its matrix A, the axis is found by calculating the eigenvectors of A belonging to the eigenvalue $+1$. The angle of rotation α is then found by equating the trace of A to $1+2\cos\alpha$. Each of the two steps in this procedure is a source of ambiguity in the final result. The axis is ambiguous because the homogeneous equations which determine the eigenvectors of A do not give the individual components of the eigenvectors but only their ratios to some arbitrarily chosen component. That is, the equations for the eigenvectors determine only a direction, not a sense along that direction. The result is that if the axis of rotation is specified by a unit vector $\mathbf{n}$, its sense along the direction of the axis has to be fixed by an arbitrary sign convention. Henceforth when we refer to the "axis of rotation" we will mean its chosen sense as well as its direction.

The angle determined by the conventional method is ambiguous because one cannot determine an angle from its cosine alone. Thus if α_0 is a solution of

$$\operatorname{tr} A = 1 + 2\cos\alpha \tag{4}$$

then so is $-\alpha$. The cosine determines the angle of rotation only to within an arbitrary signature. It is important to realize that the conventional method provides no correlation whatever between the choice of the arbitrary signature for the axis of rotation and that for the angle of rotation. It is this lack of correlation which makes the conventional method incomplete. The four possible choices of the two signatures correspond to a two-fold ambiguity in the orientation of the final coordinate system with respect to the initial one. It is actually this latter ambiguity which we wish to remove rather than the separate ambiguities in the signatures of the axis and angle. Those two can in fact never be removed absolutely.

In addition to the ambiguities of the conventional method just discussed there is an additional source of possible ambiguity which is present whenever one deals with rotation matrices. This is the handedness of the coordinate system which is being rotated. It is not usually thought of as a source of ambiguity since the handedness of one's coordinate system is always known. Right-handed systems are the most common ones but left-handed systems are also used occasionally. A given rotation matrix can describe the rotation of either a right-handed or a left-handed coordinate system. The possibility of ambiguity concerns the sense in which the angle of rotation is described with respect to the chosen sense of the axis of rotation.[3] The common choice is to describe the

[2] The customary method appears explicitly or implicitly in many standard works. As examples, we cite references [2] and [3].

[3] Indeed the only reason for assigning a sense to the axis of rotation is in order to be able to describe the angle of rotation by means of a handedness convention with respect to this sense. This illustrates the fact that the various ambiguities one encounters are not entirely independent of one another.

angle of rotation by means of a right-handed convention with respect to the axis. If one desires, this convention can be maintained irrespective of the handedness of the coordinate system. Alternatively one can use a convention in which the sense of description of the angle with respect to the axis is made dependent on the handedness of the coordinate system. Partially for practical convenience and partially as a matter of taste we shall adhere to the latter convention for the remainder of this paper and in the subsequent papers in this series. Specifically, we shall use the convention that the handedness of the description of the angle of rotation with respect to the axis agrees with the handedness of the coordinate system.

The choice of having the handedness of the rotation angle depend on the handedness of the coordinate system can be reinforced by considering the example of a rotation by amount α about the z axis. The matrix for this rotation is

$$R_z(\alpha) \equiv \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{5}$$

where, with the chosen convention, α would be the angle of right-handed rotation about the positive z axis in a right-handed coordinate system, and of left-handed rotation about the positive z axis

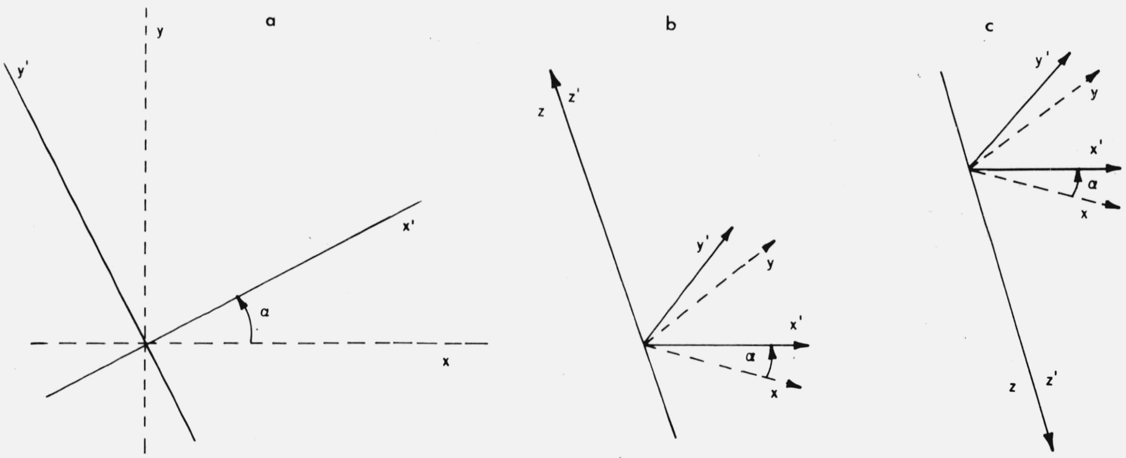

FIGURE 1. *Formation of a three-dimensional rotation from a given planar rotation.*

in a left-handed system. To see how this can come about we observe that the transformation represented by this matrix is an extension of the two dimensional transformation in the (x, y) plane which is indicated in figure 1a. In that transformation we take the angle of rotation to be positive when it is measured *from* the positive x axis *to* the positive x' axis in a rotation which initially carries the positive x' axis through the first quadrant of the (x, y) plane. Note that this convention, while arbitrary, utilizes no rule of handedness.

The two dimensional rotation of figure 1a is described by the transformation

$$x' = x\cos\alpha + y\sin\alpha, \tag{6a}$$

$$y' = -x\sin\alpha + y\cos\alpha. \tag{6b}$$

The two dimensional matrix for this rotation is

$$\begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \tag{7}$$

In order to pass from this two-dimensional rotation matrix to the three dimensional one in eq (5), we must append a z axis perpendicular to the coordinate plane in figure 1a. But there are two choices for the positive sense of this axis. These are "into the page" and "out of the page," as illustrated in figures 1b and 1c respectively. From the definition of A_{ij} (eq (5), ref. [1]),

$$A_{ij} \equiv \mathbf{b}_i' \cdot \mathbf{b}_j, \tag{8}$$

where $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, and $\mathbf{b}_1'$, $\mathbf{b}_2'$, $\mathbf{b}_3'$ are the basis vectors of S and S' respectively, we see that the resultant three dimensional rotation matrix is given by $R_z(\alpha)$ in eq (5), regardless of the choice of sense of the z axis. Now the two possible choices of sense illustrated in figures 1b and 1c correspond to coordinate systems of opposite handedness. If we now want to describe the way in which the angle of rotation is related to the positive z axis by means of a handedness convention then we see that for the right-handed choice, figure 1b, the angle α is described in the right-handed sense with respect to the z axis, while for the left-handed choice, figure 1c, the angle α is described in the left-handed sense with respect to the z axis. In each case, the handedness of the description of the rotation agrees with the handedness of the coordinate system.

What this example shows is not the inevitability of the convention we have chosen but rather that the seemingly natural way in which the three-dimensional matrix (5) was constructed from the two-dimensional transformation (6), guarantees the convention. In any event, there are subtleties connected with the handedness of a coordinate system which can lead to difficulties in interpretation unless some convention such as the one we have adopted, is clearly kept in mind. An interesting example of such a subtlety will help to clarify this.

By direct calculation one can verify that the matrix

$$\Pi_z \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \Pi_z^{-1} \tag{9}$$

effects reflections of ones coordinate system in the (x, y) plane. By further direct calculation one can verify the equation

$$R_z(\alpha)\,\Pi_z = \Pi_z R_z(\alpha), \tag{10}$$

from which one gets

$$R_z(\alpha) = \Pi_z R_z(\alpha) \Pi_z^{-1}. \tag{11}$$

This equation says that the similarity transform by a matrix which represents a reflection in the (x, y) plane, of a matrix which represents a rotation about the z axis by an angle α, is itself a matrix which represents a rotation about the z axis by an angle α. The result is a special case of the conjugacy theorem, to be discussed in paper III of this series.[4] It is not particularly subtle until one tries to follow pictorially the sequence of operations on the right side of eq (11) which leads to the left side. The sequence is illustrated in figure 2. Suppose that the initial coordinate system is right-handed (fig. 2a). Since the reflection Π_z^{-1} is applied first in the sequence, the coordinate system in which $R_z(\alpha)$ on the right side of eq (11) is carried out, is left-handed (fig. 2b). According to our convention, the angle α must then be regarded as the angle of *left-handed* rotation about the positive z axis of figure 2b. The rotation leads to the configuration in figure 2c. The final reflection restores the z axis to its initial sense and restores the initial handedness, giving the result that the entire sequence is equivalent to $R_z(\alpha)$ applied to the initial right-handed system (figure 2d). The essential point is that the handedness of the coordinate system on which $R_z(\alpha)$ on the right side of eq (11)

[4] In group theory, the right side of eq (11) would be described as the *conjugate* of a rotation about the z axis by an angle α, by a reflection in the (x, y) plane.

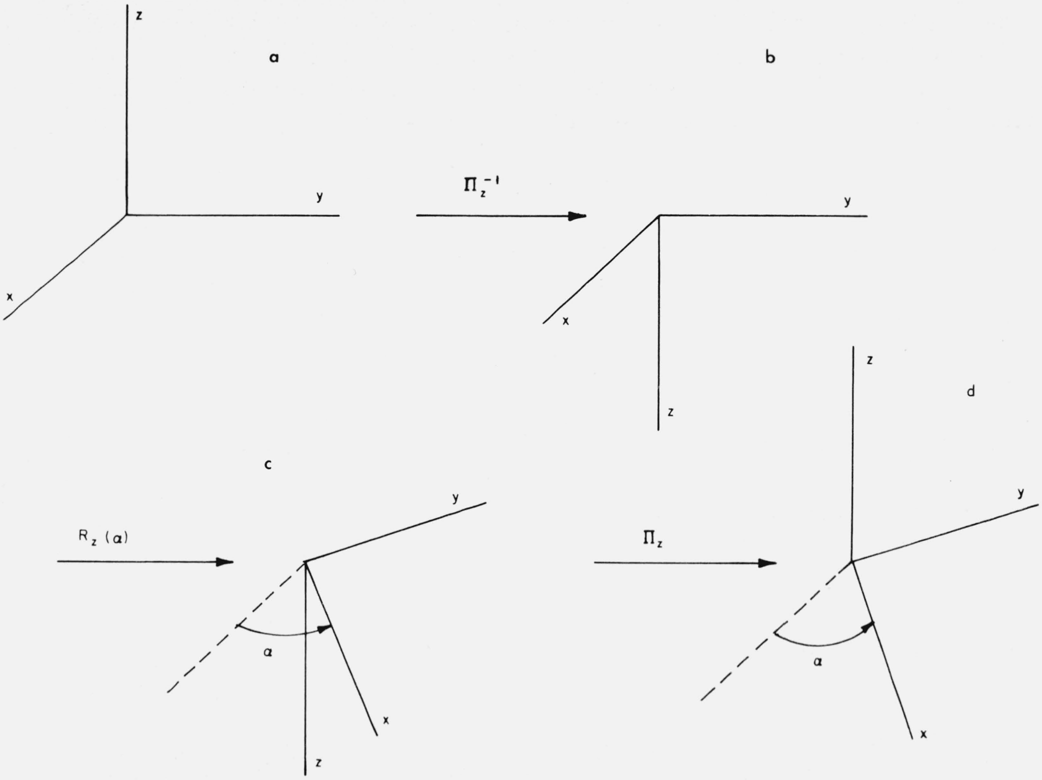

FIGURE 2. *Pictorial description of the conjugate of a general rotation about the z axis by a reflection in the x-y plane.*

operates, is opposite to that of the initial coordinate system. The interpretation of α must be changed to accommodate this change in handedness. Otherwise the orientation of the final right-handed coordinate system with respect to the initial right-handed one will be described by $R_z(-\alpha)$ rather than $R_z(\alpha)$ as called for on the left side of eq (11).

In the next section we will see how the intrinsic vector **V** overcomes the ambiguities discussed in this section.

3. The Intrinsic Vector for Rigid Rotations

We first calculate the square of the length of **V**. From eq (1) this is

$$V^2 = V_m V_m = \epsilon_{mnr}\epsilon_{mij} A_{nr} A_{ij}.$$

By using the identity (I 14a) for the product of the Levi-Civita symbols, we have[5]

$$V^2 = (\delta_{ni}\delta_{rj} - \delta_{nj}\delta_{ri}) A_{nr} A_{ij} = A_{ij} A_{ij} - A_{ji} A_{ij}. \tag{12}$$

The first term on the right side of this equation is, by either of eqs (I 7), equal to δ_{ii}, which is 3. The second term is tr (A^2), which can be expressed in terms of tr A by means of eq (I 15). Then using eq (4) for tr A, we have

$$\text{tr } (A^2) = 4 \cos^2 \alpha - 1 = 3 - 4 \sin^2 \alpha. \tag{13}$$

Inserting these results into the right side of eq (12) the result for V^2 is

$$V^2 = 4 \sin^2 \alpha. \tag{14}$$

[5] The notation eq (I n) refers to equation number n in paper I (ref. [1]). Throughout this series we will use this notation for equations in previous papers.

The length of $\mathbf{V}$ (an intrinsically nonnegative number) is seen to be twice the absolute value of $\sin\alpha$. We now observe that since $\mathbf{n}$ is either parallel or antiparallel to $\mathbf{V}$, and since $\cos\alpha$ determines $\sin\alpha$ up to an arbitrary signature, the result (14) allows us to represent the net effect of these two ambiguities as a single arbitrary signature in the equation

$$\mathbf{V} = \pm 2\mathbf{n} \sin\alpha. \tag{15}$$

This remaining ambiguity in signature can be removed by imposing the convention adopted in section 2 that the sense of description of the angle of rotation with respect to the axis agree with the handedness of the coordinate system. This is most easily done by considering the special case of rotation about the z axis since as we have seen in section 2, $R_z(\alpha)$ already has that convention built into it. We take $\mathbf{n}$ equal to $(0, 0, 1)$ since this is the positive z axis for a coordinate system of either handedness. From eqs (3) we calculate $\mathbf{V}$ for $R_z(\alpha)$ in eq (5). The result is $\mathbf{V} = (0, 0, 2\sin\alpha)$, which for this special case is equal to $2\,\mathbf{n}\sin\alpha$. Comparing this result with eq (15) we see that the positive sign is required on the right side of that equation in order to establish the desired convention. The final expression for $\mathbf{V}$ is therefore[6]

$$\mathbf{V} = 2\mathbf{n} \sin\alpha. \tag{16}$$

Equation (16) yields a value of $\sin\alpha$ which is completely unambiguous within the conventions we have adopted. The value is

$$\sin\alpha = \tfrac{1}{2}\,\mathbf{n} \cdot \mathbf{V}. \tag{17}$$

The method which emerges for finding the unambiguous orientation of the final coordinate system with respect to the initial one for a given rotation matrix, can now be summarized as follows:

(a) Compute $\cos\alpha$ from eq (4).

(b) Compute $\mathbf{V}$ from eqs (3).

(c) Compute the length of $\mathbf{V}$. If it is not zero[7] form a unit vector parallel to $\mathbf{V}$ by dividing it by its length. Arbitrarily select $\mathbf{n}$ as being either this unit vector or its negative.

(d) For the choice of $\mathbf{n}$ in step (c), compute $\sin\alpha$ from eq (17).

(e) The values of $\cos\alpha$ and $\sin\alpha$ from steps (a) and (d) uniquely determine the value of α whose sense of description with respect to $\mathbf{n}$ agrees with the handedness of the coordinate system.[8] This angle lies between 0 and 2π.

This method will be illustrated by means of several examples in the next section. For the remainder of this section we consider some general properties of $\mathbf{V}$ for rigid rotations.

We first note from eq (14) that V^2 and therefore $\mathbf{V}$ vanishes when α is 0° or 180°. From eqs (3) we see that for these angles, A is a symmetric matrix. Conversely, when A is symmetric (in addition to being orthogonal of course), eqs (3) show that $\mathbf{V}$ is identically zero. Equation (14) then shows that a symmetric A represents either the identity transformation (rigid rotation of 0°), or a rotation of 180°. When A is symmetric, the axis of rotation cannot be determined from $\mathbf{V}$ since the division in step (c) cannot be carried out. In this instance, it is necessary to solve the eigenvalue problem for A corresponding to the eigenvalue $+1$, in order to determine the direction of the axis.

Equation (17) for $\sin\alpha$ can be expressed in an interesting alternative form. Using eq (1), $\mathbf{n} \cdot \mathbf{V}$ takes the form

$$\mathbf{n} \cdot \mathbf{V} = n_i V_i = n_i \epsilon_{ijk} A_{jk} = (\epsilon_{kij} n_i)\, A_{jk}, \tag{18}$$

[6] Equation (16) should be interpreted with caution. The components of $\mathbf{V}$ do not transform as a vector under the transformation definition of a vector. The components of $\mathbf{n}$ however *do* transform as a vector. Equation (16) should not be regarded as a universal vector equation but simply as a condensed way of relating the components of $\mathbf{V}$ to those of $\mathbf{n}$ in the initial or final coordinate systems only.

[7] The case $\mathbf{V} = 0$ for rigid rotations is discussed later in this section.

[8] From now on the unqualified phrase "rotation about an axis" will imply that the sense of the rotation about the axis agrees with the handedness of the coordinate system.

where in the last step we have used the cyclic permutation property (I 10) of the Levi-Civita symbol. The object in parentheses on the right of eq (18) is the quantity N_{kj} as defined in eq (I 26), and whose matrix representation is given in eq (I 27). The quantity $\mathbf{n}\cdot\mathbf{V}$ is therefore $N_{kj}A_{jk}=\operatorname{tr}(NA)$. The sine of α is then given by

$$\sin\alpha=\tfrac{1}{2}\operatorname{tr}(NA). \tag{19}$$

Equation (19) shows that sin α, like cos α, is calculable from the trace of an appropriate matrix.

It is an interesting calculation to check the consistency between eqs (4), (19), and the exponential representation of A, eq (I 28). We imagine $\mathbf{n}$ to be fixed and α variable. Then differentiating eq (I 28) we have

$$\frac{dA}{d\alpha}=-NA. \tag{20}$$

We therefore replace the matrix NA in eq (19) by its value from eq (20). Since the operation of calculating the trace of a matrix commutes with that of differentiating the matrix with respect to a parameter, we have for sin α from eq (19)

$$\sin\alpha=-\frac{1}{2}\operatorname{tr}\frac{dA}{d\alpha}=-\frac{1}{2}\frac{d}{d\alpha}\operatorname{tr}A. \tag{21}$$

The use of eq (4) for tr A reduces eq (21) to an identity.

4. Examples of the Use of the Intrinsic Vector to Determine the Axis and Angle of a Rotation

We consider first a numerical example. The real orthogonal matrix

$$A=\frac{1}{2}\begin{pmatrix}\frac{1}{\sqrt{2}}+1 & \frac{1}{\sqrt{2}}-1 & 1\\ \frac{1}{\sqrt{2}}-1 & \frac{1}{\sqrt{2}}+1 & 1\\ -1 & -1 & \sqrt{2}\end{pmatrix}$$

has determinant unity and therefore represents a rigid rotation. Its trace is $1+\sqrt{2}$ so that from eq (4), $\cos\alpha=1/\sqrt{2}$. From eqs (3) the intrinsic vector is $\mathbf{V}=(1,-1,0)$. We choose $\mathbf{n}$ to be parallel to $\mathbf{V}$ so that $\mathbf{n}$ is $(1/\sqrt{2},-1\sqrt{2},0)$. Then from eq (17)

$$\sin\alpha=\frac{1}{2}\left(\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{2}}\right)=\frac{1}{\sqrt{2}}.$$

The angle α is therefore 45°. Its sense of description with respect to $\mathbf{n}$ is right (left)-handed in a right (left)-handed coordinate system.

As a second example we consider a rotation described by the Euler angles [4]. We assume a right-handed coordinate system. The rotation matrix expressed in terms of these angles is

$$A=\begin{pmatrix}\cos\phi\cos\psi-\cos\theta\sin\phi\sin\psi & \sin\phi\cos\psi+\cos\theta\cos\phi\sin\psi & \sin\theta\sin\psi\\ -\cos\phi\sin\psi-\cos\theta\sin\phi\cos\psi & -\sin\phi\sin\psi+\cos\theta\cos\phi\cos\psi & \sin\theta\cos\psi\\ \sin\phi\sin\theta & -\cos\phi\sin\theta & \cos\theta\end{pmatrix}$$

The trace of this equation leads to

$$\cos^2\frac{\alpha}{2}=\cos^2\frac{\theta}{2}\cos^2\frac{\phi+\psi}{2}. \tag{22}$$

In taking the square root of this equation to extract $\cos(\alpha/2)$ we choose the positive root. This has the effect of imposing the natural requirement that $\alpha=0$ when $\theta=\phi=\psi=0$. The result for $\cos(\alpha/2)$ is

$$\cos\frac{\alpha}{2}=\cos\frac{\theta}{2}\cos\frac{\phi+\psi}{2}. \tag{23}$$

The components of $\mathbf{V}$ in either the initial or final coordinate system are

$$V_1=\sin\theta\,(\cos\phi+\cos\psi), \tag{24a}$$

$$V_2=\sin\theta\,(\sin\phi-\sin\psi), \tag{24b}$$

$$V_3=(1+\cos\theta)\sin(\phi+\psi). \tag{24c}$$

The square of the length of $\mathbf{V}$ is

$$V^2=16\cos^2\frac{\theta}{2}\cos^2\frac{\phi+\psi}{2}\left[\sin^2\frac{\theta}{2}+\cos^2\frac{\theta}{2}\sin^2\frac{\phi+\psi}{2}\right] \tag{25a}$$

$$=16\cos^2\frac{\theta}{2}\cos^2\frac{\phi+\psi}{2}\left[\sin^2\frac{\phi+\psi}{2}+\sin^2\frac{\theta}{2}\cos^2\frac{\phi+\psi}{2}\right] \tag{25b}$$

From eq (23), the factor before either of the square brackets in eqs (25) will be recognized as $[4\cos(\alpha/2)]^2$.

In paper I, section 3 the point was made that $\mathbf{V}$ is a vector only in the sense of being a set of three numbers. In particular, it does not qualify as a vector under the definition based on the transformation properties of the components of a vector. Nevertheless it is possible to obtain an interesting representation of $\mathbf{V}$ by treating the components in eqs (24) as though they were the components of a true vector and then expressing this vector in the nonorthogonal basis formed by the unit vectors $\mathbf{q}$, $\mathbf{q}'$, and $(\mathbf{q}\times\mathbf{q}')/\sin\theta$. Here $\mathbf{q}$ is the axis about which the ϕ rotation is carried out and $\mathbf{q}'$ is the axis about which the ψ rotation is carried out. The representation of $\mathbf{V}$ in this basis is

$$V=(\mathbf{q}+\mathbf{q}')\sin(\phi+\psi)+(\mathbf{q}\times\mathbf{q}')[1+\cos(\phi+\psi)]. \tag{26}$$

It must be remembered however that it is legitimate to take the components of eq (26) only in either the initial or the final coordinate systems, where the components are given by eqs (24). The components of eq (26) have no significance in either of the intermediate coordinate systems in the sequence of Euler rotations.

We treat as an example now the problem of determining the equivalent single axis and single angle of rotation for a sequence of rotations of an initial coordinate system about each of two intersecting axes. The principal results of this calculation, eqs (29) and (32) are not new. However, the derivation given here is believed to be the first derivation of these results by purely matrix methods. Previous derivations have made use of the representation of rotations by means of dyadics [5], and of the methods of spherical trigonometry [6]. The latter derivation gives a very clear geometrical picture of the relation between the axes and angles of the component rotations and the equivalent single axis and angle.[9]

[9] The geometrical statement of the relation between two component rotations and the equivalent single rotation is known as the theorem of Rodrigues and Hamilton. Whittaker [7] gives one statement of the theorem. A somewhat more precise statement will be found in reference [6].

We assume a right-handed coordinate system. The first rotation is one of amount β about an axis $\mathbf{q}$. This is followed by a rotation about a second axis $\mathbf{q}'$ by an amount β'. We call θ the smaller of the two angles between $\mathbf{q}$ and $\mathbf{q}'$, and assume that its sine does not vanish. We orient the initial coordinate system in such a way that $\mathbf{q}$ is along the positive z axis, and that the colatitude and azimuth of $\mathbf{q}'$ in this system are θ and β respectively. This is illustrated in figure 3a. The

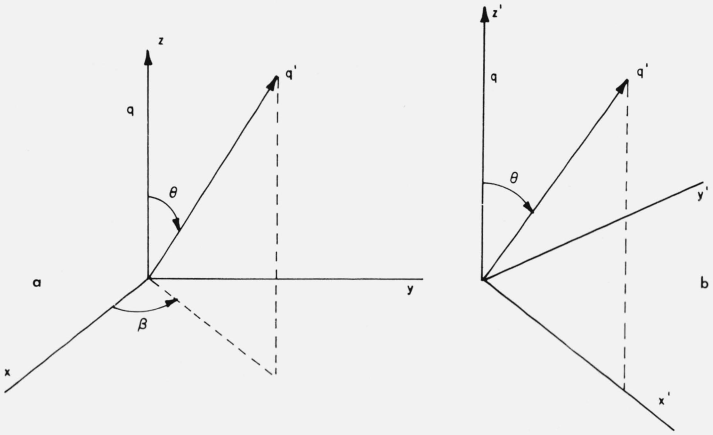

FIGURE 3. *The initial and the intermediate coordinate system for the description of consecutive finite rotations about two intersecting axes.*

first rotation of the sequence is therefore about the z axis by an angle β and brings the original x-z plane into coincidence with $\mathbf{q}'$, as illustrated in figure 3b. This rotation is described by $R_z(\beta)$. The second rotation is by an angle β' about $\mathbf{q}'$. Since $\mathbf{q}'$ is now in the x-z plane the coordinate system on which the rotation about $\mathbf{q}'$ operates is that in figure 3b. A tedious but straightforward calculation, using for example eqs (I–25) and (I–26) with $\mathbf{n}=\mathbf{q}'$, shows the matrix for this rotation to be

$$R_{\mathbf{q}'}(\beta')=\begin{pmatrix} \sin^2\theta+\cos^2\theta\cos\beta' & \cos\theta\sin\beta' & \sin\theta\cos\theta\,(1-\cos\beta') \\ -\cos\theta\sin\beta' & \cos\beta' & \sin\theta\sin\beta' \\ \sin\theta\cos\theta\,(1-\cos\beta') & -\sin\theta\sin\beta' & \cos^2\theta+\sin^2\theta\cos\beta' \end{pmatrix} \tag{27}$$

The sequence of rotations about $\mathbf{q}$ and $\mathbf{q}'$ is therefore described by the matrix

$$R_{\mathbf{n}}(\alpha)=R_{\mathbf{q}'}(\beta')R_z(\beta),$$

where $\mathbf{n}$ and α are the axis and angle of rotation for the single rotation which is equivalent to the sequence of two. By direct calculation using eqs (5) and (27) the matrix $R_{\mathbf{n}}(\alpha)$ is found to be

$$R_{\mathbf{n}}(\alpha)=$$

$$\begin{pmatrix} (\sin^2\theta+\cos^2\theta\cos\beta')\cos\beta-\cos\theta\sin\beta\sin\beta' & (\sin^2\theta+\cos^2\theta\cos\beta')\sin\beta+\cos\theta\cos\beta\sin\beta' & \sin\theta\cos\theta\,(1-\cos\beta') \\ -\cos\theta\cos\beta\sin\beta'-\sin\beta\cos\beta' & -\cos\theta\sin\beta\sin\beta'+\cos\beta\cos\beta' & \sin\theta\sin\beta' \\ \sin\theta\cos\theta\cos\beta\,(1-\cos\beta')+\sin\theta\sin\beta\sin\beta' & \sin\theta\cos\theta\sin\beta\,(1-\cos\beta')-\sin\theta\cos\beta\sin\beta' & \cos^2\theta+\sin^2\theta\cos\beta' \end{pmatrix} \tag{28}$$

The cosine of α is computed from eq (4). The previous example of a rotation described by Euler angles suggests that a simplification of the final results is achieved by working with half angles rather than angles. The trace of eq (28) then leads to

$$\cos^2 \frac{\alpha}{2} = \left(\cos \frac{\beta}{2} \cos \frac{\beta'}{2} - \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta\right)^2.$$

In taking the square root of this equation to find $\cos(\alpha/2)$ the ambiguity in sign is removed by requiring that for $\beta = \beta' = 0$, $\cos(\alpha/2) = +1$ rather than -1 so that α is zero rather than 2π. With the choice of the plus sign for the square root, we have

$$\cos \frac{\alpha}{2} = \cos \frac{\beta}{2} \cos \frac{\beta'}{2} - \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta. \tag{29}$$

The components of $\mathbf{V}$ for $R_{\mathbf{n}}(\alpha)$ in the coordinate system of figure 3a, are

$$V_1 = 4 \cos \frac{\beta}{2} \sin \frac{\beta'}{2} \sin \theta \left(\cos \frac{\beta}{2} \cos \frac{\beta'}{2} - \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta\right), \tag{30a}$$

$$V_2 = 4 \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \sin \theta \left(\cos \frac{\beta}{2} \cos \frac{\beta'}{2} - \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta\right), \tag{30b}$$

$$V_3 = 4 \left(\sin \frac{\beta}{2} \cos \frac{\beta'}{2} + \cos \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta\right)\left(\cos \frac{\beta}{2} \cos \frac{\beta'}{2} - \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta\right). \tag{30c}$$

From eq (29) we recognize the common parenthetic factor in each of the components of $\mathbf{V}$ as $\cos(\alpha/2)$. Since $\mathbf{V}$ may be written as $4\,\mathbf{n} \sin(\alpha/2) \cos(\alpha/2)$, we can cancel this common factor thereby reducing eqs (30) to the following equations for the components of $\mathbf{n}$:

$$n_1 \sin \frac{\alpha}{2} = \cos \frac{\beta}{2} \sin \frac{\beta'}{2} \sin \theta, \tag{31a}$$

$$n_2 \sin \frac{\alpha}{2} = \sin \frac{\beta}{2} \sin \frac{\beta'}{2} \sin \theta, \tag{31b}$$

$$n_3 \sin \frac{\alpha}{2} = \sin \frac{\beta}{2} \cos \frac{\beta'}{2} + \cos \frac{\beta}{2} \sin \frac{\beta'}{2} \cos \theta. \tag{31c}$$

Unlike the components of $\mathbf{V}$, those of $\mathbf{n}$ obey the transformation definition of a vector. Therefore, eqs (31) represent the components in the coordinate system of fig. 3a, of a vector equation which is valid in all coordinate systems. An instructive form of this equation is obtained by expressing it in the nonorthogonal basis consisting of the unit vectors $\mathbf{q}$, $\mathbf{q}'$, and $(\mathbf{q} \times \mathbf{q}')/\sin \theta$. Omitting the algebraic steps leading to this form, the result is

$$\mathbf{n} \sin \frac{\alpha}{2} = \mathbf{q} \sin \frac{\beta}{2} \cos \frac{\beta'}{2} + \mathbf{q}' \cos \frac{\beta}{2} \sin \frac{\beta'}{2} - (\mathbf{q} \times \mathbf{q}') \sin \frac{\beta}{2} \sin \frac{\beta'}{2}. \tag{32}$$

We observe that since α lies between 0 and 2π, $\sin(\alpha/2)$ is positive. Hence $\alpha/2$ and therefore α, are completely determined by eq (29). The axis $\mathbf{n}$ is then completely determined by eq (32) without the need to first form $\mathbf{V}$. To illustrate this procedure consider a right-handed coordinate system and the axes whose representation in this system are $\mathbf{q} = \mathbf{b}_3$, $\mathbf{q}' = \mathbf{b}_2$. The angle between these axes is 90°. We take rotation angles β and β' of 90°. The first rotation is clearly $R_z(\pi/2)$

and brings the x axis into coincidence with $\mathbf{q}'$. The second rotation is therefore $R_x(\pi/2)$. The net rotation is

$$R_{\mathbf{n}}\ (\alpha)=R_x(\pi/2)R_z(\pi/2)=\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 1\\ 0 & -1 & 0\end{pmatrix}\begin{pmatrix}0 & 1 & 0\\ -1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix}=\begin{pmatrix}0 & 1 & 0\\ 0 & 0 & 1\\ 1 & 0 & 0\end{pmatrix}. \tag{33}$$

Using eqs (3) and (4) we get from the matrix on the right that $\cos\alpha=-1/2, \mathbf{V}=(1,1,1)$. Choosing $\mathbf{n}$ parallel to $\mathbf{V}$ we find $\mathbf{n}=(1/\sqrt{3},\ 1/\sqrt{3},\ 1/\sqrt{3})$ and $\sin\alpha=\sqrt{3}/2$ so that α is 120°. The same results follow from the formalism of successive rotations without having to carry out the computation in eq (33). From eq (29) we find $\cos(\alpha/2)=1/2$. Since $\sin(\alpha/2)$ must be positive we have that $\sin(\alpha/2)=\sqrt{3}/2$.Hence $\alpha/2$ is 60° and α is 120°. From eq (32) we find that the representation of $\mathbf{n}$ in the initial coordinate system is $\mathbf{n}=(1,\ 1,\ 1)/\sqrt{3}$.

5. The Intrinsic Vector for Improper Rotations

In this section we examine the case $p'/p=-1$. We demonstrate first that A has the property of being "factorable" into a product of a pure reflection in an arbitrarily chosen plane followed or preceded by a proper rotation whose axis and angle depend on the plane of reflection. We will work out only the case where the reflection precedes the rotation. The analysis is nearly identical for the case where the reflection follows the rotation.

For an arbitrary unit vector $\boldsymbol{\sigma}$ the improper orthogonal matrix $\Pi(\boldsymbol{\sigma})$ defined by

$$\Pi_{ij}(\boldsymbol{\sigma})=\delta_{ij}-2\sigma_i\sigma_j \tag{34}$$

is the matrix for a pure reflection in a plane perpendicular to $\boldsymbol{\sigma}$. For a given improper orthogonal transformation matrix A, we define the matrix B as

$$B\equiv A\Pi(\boldsymbol{\sigma}). \tag{35}$$

The matrix B has determinant one and satisfies the first orthogonality conditions. It therefore represents a proper rotation.[10] Since $[\Pi(\boldsymbol{\sigma})]^2=1$, we can write

$$A=B\Pi(\boldsymbol{\sigma}). \tag{36}$$

This demonstrates the factorability of A into a product of a reflection in an arbitrary plane, followed by a rotation. The axis and angle of the rotation are determined from eq (35). The trace of B is given by

$$\operatorname{tr} B=\operatorname{tr} A-2\sigma_i A_{ij}\sigma_j. \tag{37}$$

The intrinsic vector $\mathbf{W}$ belonging to B is determined from eqs (1), (34), and (35). It is

$$W_i=\epsilon_{ijk}B_{jk}=V_i=2\epsilon_{ijk}(A_{jm}\sigma_m)\sigma_k. \tag{38}$$

where $\mathbf{V}$ is the intrinsic vector belonging to A.

There are interesting special cases of eqs (35)–(38). The first is the case where $\boldsymbol{\sigma}$ is chosen parallel or antiparallel to $\mathbf{V}$. In that case the last term on the right of eq (38) is proportional to $\epsilon_{ijk}V_jV_k$, which is zero. The intrinsic vector for B is therefore identical to that of A. The factorization property of A then states that A is expressible as a reflection in a plane perpendicular to the intrinsic vector of A followed by a rotation about that intrinsic vector, of a specified amount.

[10] The matrix B also satisfies the second orthogonality conditions, as is true of any product of matrices each of which obeys those conditions.

The second interesting special case is that in which A itself is a reflection in some plane. If the plane of reflection of A is perpendicular to $\boldsymbol{\sigma}$, then B in eq (36) is simply the identity matrix. Therefore, we assume that the plane of reflection of A intersects that of $\Pi(\boldsymbol{\sigma})$. We take the plane of reflection of A to be specified by the unit normal vector $\mathbf{g}$. We define the angle θ at which the plane perpendicular to $\boldsymbol{\sigma}$ and that perpendicular to $\mathbf{g}$ intersect as the smaller of the angles between $\boldsymbol{\sigma}$ and $\mathbf{g}$. This is illustrated in figure 4 which represents the normal trace of the intersecting planes in the plane of the figure.

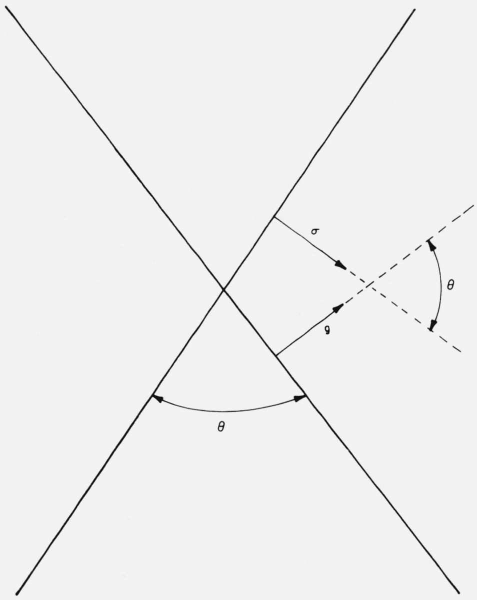

FIGURE 4. *Normal trace of a pair of intersecting planes, in the plane of the page.*

To compute the matrix B on the left side of eq (35) we observe that the application of $\Pi(\boldsymbol{\sigma})$ reflects the initial coordinate system in the plane perpendicular to $\boldsymbol{\sigma}$. This means that the appropriate A to use in eq (35) is not $\Pi(\mathbf{g})$ but rather $\Pi(\mathbf{g}')$, where the primed argument implies that the components of $\mathbf{g}$ to be used are those in the coordinate system which results from the initial one by the application of $\Pi(\boldsymbol{\sigma})$. From eq (34), these components are

$$g_i' = \Pi_{ij}(\boldsymbol{\sigma})g_j = g_i - 2(\mathbf{g}\cdot\boldsymbol{\sigma})\sigma_i.$$

Since $\mathbf{g}\cdot\boldsymbol{\sigma}$ is $\cos\theta$, we have

$$g_i' = g_i - (2\cos\theta)\sigma_i. \tag{39}$$

In terms of these components the matrix B in eq (35) is given by

$$B_{ij} = (\delta_{ik} - 2g_i'g_k')(\delta_{kj} - 2\sigma_k\sigma_j),$$

$$= \delta_{ij} + 4(g_k'\sigma_k)g_i'\sigma_j - 2\sigma_i\sigma_j - 2g_i'g_j'. \tag{40}$$

Letting α denote the angle of the rotation represented by B, eq (37) leads to

$$\cos\alpha = 2(g_k'\sigma_k)^2 - 1.$$

Using eq (39) for the g_k' in the product $g_k'\sigma_k$, we have $g_k'\sigma_k = -\cos\theta$. Therefore

$$\cos\alpha = \cos 2\theta. \tag{41}$$

The intrinsic vector W for B is computed from eq (38). Observing that $\mathbf{V}$ is identically zero for a pure reflection we have

$$W_i = -4 \cos \theta \epsilon_{ijk} g_j' \sigma_k. \tag{42}$$

The product $\epsilon_{ijk} g_j' \sigma_k$ may be computed with the help of eq (39) and is seen to be identical to $\epsilon_{ijk} g_j \sigma_k$. Therefore

$$W_i = 4\epsilon_{ikj} \sigma_k g_j \cos \theta, \tag{43}$$

where we have used the antisymmetry property of the Levi-Civita symbol. Now the *vector* product $\epsilon_{ikj}\sigma_k g_j$ is identical to the conventional right-handed *cross* product of $\boldsymbol{\sigma}$ and $\mathbf{g}$ if the initial coordinate system is right-handed. However, since ϵ has no intrinsic handedness, the vector product is identical to a *left-handed* cross product of $\boldsymbol{\sigma}$ and $\mathbf{g}$ if the initial coordinate system is left-handed.[11] We may therefore rewrite eq (43) in the form

$$\mathbf{W} = 4\mathbf{n} \sin \theta \cos \theta = 2\mathbf{n} \sin (2\theta), \tag{44}$$

where $\mathbf{n}$ has the sense of the right-(left-)handed cross product of $\boldsymbol{\sigma}$ and $\mathbf{g}$ when the initial coordinate system is right-(left-)handed. If we now define the axis of rotation of B to be always identical to $\mathbf{n}$, then we may write

$$\mathbf{W} = 2\mathbf{n} \sin \alpha. \tag{45}$$

Comparing eqs (44) and (45) we have

$$\sin \alpha = \sin 2\theta \tag{46}$$

From eqs (41) and (46) we can set

$$\alpha = 2\theta. \tag{47}$$

We have therefore proven by matrix methods, with the help of the intrinsic vector, the classical property that a sequence of reflections in each of two intersecting planes is equivalent to a rotation about an axis along the line of intersection of the planes by an angle which is twice that between the planes. This method of representing a rotation by a sequence of reflections can be used to construct a less cumbersome (but less direct) derivation of eqs (29) and (32) for a sequence of rotations about intersecting axes. Since one of the planes of reflection in the pair of reflections equivalent to a given rotation, is arbitrary, one simply has to choose the plane of the *second* reflection for the *first* rotation in the sequence to be identical to the plane of the *first* reflection for the *second* rotation of the sequence. Thus the sequence of two rotations is shown to be equivalent to a sequence of two reflections. Equations (29) and (32) then follow from a calculation which is much less laborious than the one presented in section 4.

The third special case of eqs (35)–(38) which is of interest is the case where A is a coordinate inversion with respect to the origin,

$$A_{ij} = -\delta_{ij}.$$

From eq (37) we compute tr $B = -1$ for this case so that the angle of rotation of B is 180°. No additional information is furnished by eq (38), which gives $\mathbf{W} = 0$. The characteristic direction of B for this case must be found by solving for the real eigenvectors of B belonging to the eigenvalue $+1$. From eqs (34) and (35) we see that

$$B_{ij} = 2\sigma_i \sigma_j - \delta_{ij}.$$

One readily finds that the characteristic direction of B is the direction of $\boldsymbol{\sigma}$. Thus we have the well-known result that a coordinate inversion is equivalent to a reflection in an arbitrary plane followed by a rotation of 180° about the normal to that plane.[12]

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[11] This distinction between the vector product and the cross product is almost universally ignored in the literature. As a result, the transformation properties of the cross product are usually confused with those of the vector product. In particular, the cross product of two polar vectors is usually held up as the prototype of an axial vector whereas in fact the cross product is a polar vector. It is the vector product which is an axial vector. These points will be amplified in a forthcoming paper.

[12] In addition to its factorability as a product of a reflection and a rotation, A can also be factored into a product of a rotation preceded or followed by a coordinate inversion.

When we discussed rigid rotations we saw that the vanishing of **V** implied that A was either the identity matrix or a matrix representing a rotation of 180°. For improper rotations a vanishing **V** means that A represents either an inversion with respect to the origin or a reflection in some plane. To see this we observe that when **V** vanishes, A is both symmetric and orthogonal and hence its eigenvalues are each plus one or minus one. Since the product of the eigenvalues must be minus one we get two distinct situations, one with two-fold degeneracy and one with three-fold degeneracy. In the two-fold degenerate case one of the eigenvalues is -1 and the other two are $+1$. The A for this case is a matrix for pure reflection in a plane perpendicular to the characteristic direction which belongs to the eigenvalue -1. The eigenvalues $+1$ correspond to any pair of mutually orthogonal directions in the plane of reflection. In the three-fold degenerate case all of the eigenvalues are -1, and A is the inversion matrix.

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