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The Second Orthogonality Conditions in the Theory of Proper and Improper Rotations. I. Derivation of the Conditions and of Their Main Consequences*

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A new set of orthogonality conditions is derived for real three-by-three orthogonal matrices which describe transformations in Euclidean three-dimensional space. The principal consequences of these conditions are obtained. These are: (1) the existence and construction of the intrinsic vector of the transformation, (2) an equation connecting the trace of a transformation matrix with that of its square, which, for rotations, can be solved to give the well-known trace formula analytically, (3) a simple formula for the determinant of a transformation matrix directly in terms of the relative handedness of the two coordinate systems connected by the transformation, (4) the secular equation for a transformation matrix.

Key Words: Matrices; orthogonal transformations; rotation.

1. Introduction

There are several ways to represent proper and improper rotations in three-dimensional space. They can be represented by dyadics, which are linear operators on the vectors of Euclidean three-dimensional space [1].[1] Quaternions offer a more abstract and more elegant means of representation [2]. The quaternion representation leads to, and is equivalent to, a representation in terms of the group $SU(2)$ of two-dimensional unitary matrices with determinant unity [3]. The simplest representation to work with, and by means of which to visualize proper and improper rotations, is in terms of real, three-by-three orthogonal matrices [4]. This is the representation which we will be concerned with in this series of papers. In this series of papers the word "transformation," will generically denote the kind of transformation which is described by a general, real, three-by-three, orthogonal matrix, without regard to the value of the determinant of the matrix. When it is necessary to take the value of the determinant into account we will speak of the transformations with determinant plus one as "rigid rotations," or "proper rotations," or simply "rotations," and the transformations with determinant minus one as "improper rotations."

The usual definition of orthogonality of the underlying coordinate systems in three-dimensional Euclidean space, leads to a well-known set of conditions on the elements of the transformation matrices. We will refer to these conditions [eqs (7)] as the first orthogonality conditions. The properties of the matrices cannot, however, be deduced directly from these conditions. Instead, specific properties must be deduced analytically or geometrically. For example, the axis of a proper rotation is usually found from Euler's theorem [5], while the angle of rotation may be found by considering the action of the rotation matrix on specific vectors.

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

By considering an alternative but equivalent definition of orthogonality of the underlying coordinate systems, it is possible to derive a new set of orthogonality conditions on the transformation matrices. We will refer to these new conditions as the second orthogonality conditions [eqs (9)]. They have the important quality of being working relations. From them, one can deduce, for example, all of the well-known properties of rotation matrices, in most cases more elegantly and concisely than with the usual methods of deducing these properties. One can also deduce some new properties.

The purpose of this paper is to derive the second orthogonality conditions (sec. 2), and to deduce their main consequences (sec. 3). Discussion of some of the consequences will be presented in subsequent papers in this series. It is hoped that the series as a whole offers a unified and simple presentation of the theory of proper and improper rotations which will be practically and pedagogically useful.

As is well known, transformations can be regarded as either passive or active. In a passive transformation all physical objects are regarded as being fixed in space while the transformations are carried out on coordinate systems. In an active transformation, there is a single coordinate system which is thought of as being unaffected, while the transformations act on physical objects in space. Although the two interpretations are equivalent for the purposes of this series of papers, it is nevertheless useful in visualizing transformations, to favor one interpretation. For the most part we will regard them as passive transformations.

2. The Second Orthogonality Conditions

We consider the transformation between a Cartesian coordinate system S, whose axes are specified by a triad of mutually orthogonal unit vectors $\mathbf{b}_1$, $\mathbf{b}_2$, $\mathbf{b}_3$, and a system S' which is co-original with S, specified by the triad $\mathbf{b}_1'$, $\mathbf{b}_2'$, $\mathbf{b}_3'$. In this transformation, which is illustrated in figures 1, we take into account the possibility that the handedness of S' might differ from that of S. The customary way to express the unit normalization and mutual orthogonality of the vectors in each triad is by means of the relations

$$\mathbf{b}_i \cdot \mathbf{b}_j = \delta_{ij}, \tag{1a}$$

$$\mathbf{b}_i' \cdot \mathbf{b}_j' = \delta_{ij}, \tag{1b}$$

where δ_{ij} is the Kronecker delta, equal to zero for $i \neq j$ and equal to one when $i=j$. There is an alternative expression of orthogonality of basis vectors of a coordinate system which has the advantage over the expressions (1) that it allows for the explicit inclusion of the handedness of the particular coordinate system. This expression of orthogonality, for the coordinate systems S and S', respectively, is [2]

$$\mathbf{b}_i \times \mathbf{b}_j = p\epsilon_{ijk}\mathbf{b}_k, \tag{2a}$$

$$\mathbf{b}_i' \times \mathbf{b}_j' = p'\epsilon_{ijk}\mathbf{b}_k', \tag{2b}$$

where ϵ_{ijk} is the Levi-Civita symbol, which is antisymmetric in the interchange of any two of its indices (implying that it vanishes when any two of its indices are equal), and is equal to one when (i, j, k) is equal to (1, 2, 3) or to any cyclic permutation of (1, 2, 3). The factors p and p' are the "handedness" factors, which are equal to one for a right handed coordinate system, and to minus one for a left handed system. The choice of handedness that is associated with $p=+1$ is dictated by the fact that we are using the conventional right handed cross product in eqs (2).

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[2] In eqs (2) and subsequently in this series of papers, we use the customary convention that a repeated index on any one side of an equation is to be summed over its range.

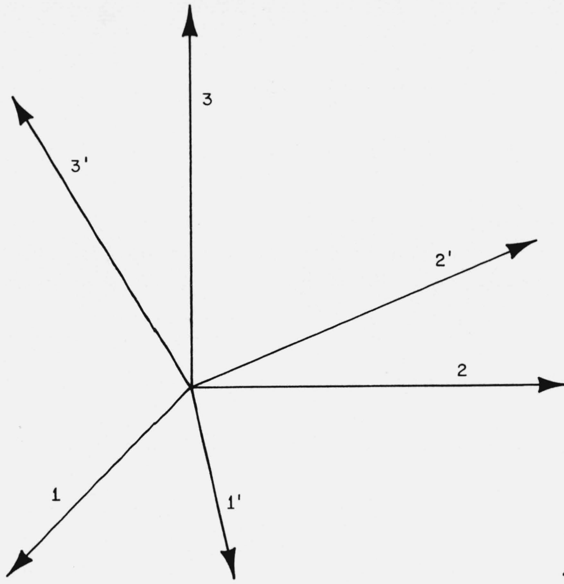

FIGURE 1a. *An orthogonal transformation which does not bring about a change of handedness.*

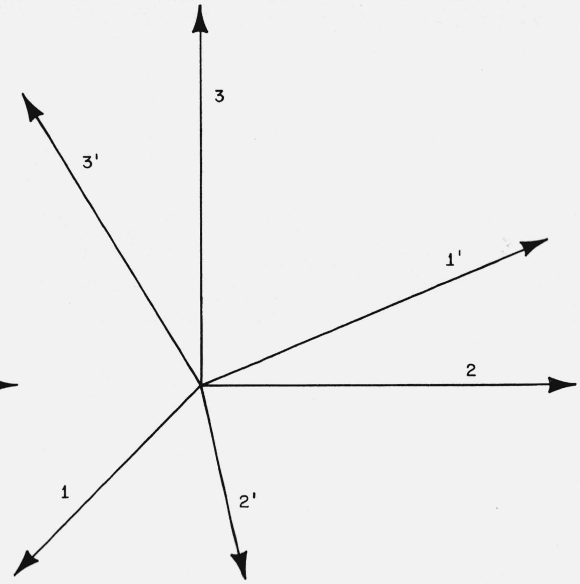

FIGURE 1b. *An orthogonal transformation which brings about a change in handedness.*

The eqs (2) as they stand do not guarantee the unit normalization of the vectors in each triad. To insure such normalization, one adds the supplementary requirements

$$\mathbf{b}_1 \cdot \mathbf{b}_2 \times \mathbf{b}_3 = p, \tag{3a}$$

$$\mathbf{b}_1' \cdot \mathbf{b}_2' \times \mathbf{b}_3' = p'. \tag{3b}$$

Equations (2) and (3) immediately lead to eqs (1). In addition to being orthonormal, the $\mathbf{b}$ and $\mathbf{b}'$ triads are each separately complete. This is expressed by

$$\mathbf{b}_i \mathbf{b}_i = \mathsf{I}, \tag{4a}$$

$$\mathbf{b}_i' \mathbf{b}_i' = \mathsf{I}, \tag{4b}$$

where I, the unit dyadic, has the property that $\mathsf{I} \cdot \mathbf{F} = \mathbf{F} \cdot \mathsf{I} = \mathbf{F}$ for any vector $\mathbf{F}$.

The matrix of transformation $A = (A_{ij})$ between S and S' is constructed from the cosines of the angles between the $\mathbf{b}$ and $\mathbf{b}'$ vectors. To be specific we define

$$A_{ij} \equiv \mathbf{b}_i' \cdot \mathbf{b}_j. \tag{5}$$

The elements of A then appear as the coefficients of expansion of the vectors of either triad in terms of the other triad as basis. These expansions are obtained by using the completeness relations (4),

$$\mathbf{b}_i' = \mathbf{b}_i' \cdot \mathsf{I} = \mathbf{b}_i' \cdot \mathbf{b}_j \mathbf{b}_j = (\mathbf{b}_i' \cdot \mathbf{b}_j) \mathbf{b}_j = A_{ij} \mathbf{b}_j, \tag{6a}$$

$$\mathbf{b}_i = \mathbf{b}_i \cdot \mathsf{I} = \mathbf{b}_i \cdot \mathbf{b}_j' \mathbf{b}_j' = (\mathbf{b}_j' \cdot \mathbf{b}_i) \mathbf{b}_j' = A_{ji} \mathbf{b}_j'. \tag{6b}$$

As a result of the orthonormality and completeness of the $\mathbf{b}$ and $\mathbf{b}'$ vectors, the matrix A satisfies the well known orthogonality relations

$$A_{ij}A_{kj}=(\mathbf{b}_i'\cdot\mathbf{b}_j)(\mathbf{b}_k'\cdot\mathbf{b}_j)=\mathbf{b}_i'\cdot(\mathbf{b}_j\mathbf{b}_j)\cdot\mathbf{b}_k'=\mathbf{b}_i'\cdot\mathbf{b}_k'=\delta_{ik}, \tag{7a}$$

$$A_{ji}A_{jk}=(\mathbf{b}_j'\cdot\mathbf{b}_i)(\mathbf{b}_j'\cdot\mathbf{b}_k)=\mathbf{b}_i\cdot(\mathbf{b}_j'\mathbf{b}_j')\cdot\mathbf{b}_k=\mathbf{b}_i\cdot\mathbf{b}_k=\delta_{ik}. \tag{7b}$$

We will refer to these as the first orthogonality conditions.

The second orthogonality relations are derived by requiring that the transformation of either of the cross product relations (2) by the transformations (6), reproduces the other one of the relations (2). If eq (6a) is inserted for $\mathbf{b}'$ everywhere in eq (2b), we get

$$A_{ir}A_{jm}\mathbf{b}_r\times\mathbf{b}_m=p'\epsilon_{ijk}A_{kn}\mathbf{b}_n.$$

Equation (2a) is now used for the cross product on the left side of this equation. The result may be written

$$\left(A_{ir}A_{jm}\epsilon_{rmn}-\frac{p'}{p}\epsilon_{ijk}A_{kn}\right)\mathbf{b}_n=0. \tag{8a}$$

Alternatively, we could have transformed the relation (2a) using the transformation (6b). We would then have found

$$\left(A_{ri}A_{mj}\epsilon_{rmn}-\frac{p}{p'}\epsilon_{ijk}A_{nk}\right)\mathbf{b}_n'=0. \tag{8b}$$

In eqs (8) we have vanishing linear combinations of each set of basis vectors. Since the vectors in each set are linearly independent, the coefficients in each linear combination must vanish identically. This leads to

$$A_{ir}A_{jm}\epsilon_{rmn}=\frac{p'}{p}\epsilon_{ijk}A_{kn}, \tag{9a}$$

$$A_{ri}A_{mj}\epsilon_{rmn}=\frac{p}{p'}\epsilon_{ijk}A_{nk}. \tag{9b}$$

These equations, which we shall refer to as the second orthogonality conditions, appear to be new, or at any rate do not appear to have been discussed before. In the next section we will work out their main consequences.

3. Consequences of the Second Orthogonality Conditions

As a first consequence of eqs (9), we construct a vector which is not altered by the transformation represented by A. To do this, we contract on i and n in eq (9a), that is, we set $i=n$ and sum on the repeated index so formed. Now the Levi-Civita symbol has the same value for any cyclic permutation of its indices. For example

$$\epsilon_{njk}=\epsilon_{jkn}. \tag{10}$$

Therefore we may write the contracted form of eq (9a) as

$$A_{jm}(\epsilon_{mnr}A_{nr})=\frac{p'}{p}\epsilon_{jkn}A_{kn}. \tag{11}$$

By defining the three component quantity $\mathbf{V}_m$ as

$$\mathbf{V}_m \equiv \epsilon_{mnr} A_{nr}, \tag{12}$$

we may write eq (11) in the form

$$A_{jm}\mathbf{V}_m = \frac{p'}{p}\mathbf{V}_j. \tag{13a}$$

This equation says that unless it is identically zero, the "vector" $\mathbf{V}$ is an eigenvector of A belonging to the eigenvalue p'/p. Similarly, contracting on i and n in eq (9b), and observing that $p/p' = p'/p$, we find

$$A_{mj}\mathbf{V}_m = (\tilde{A})_{jm}\mathbf{V}_m = \frac{p'}{p}\mathbf{V}_j. \tag{13b}$$

so that $\mathbf{V}$ is also an eigenvector of the matrix $\tilde{A}$, the transpose of A, belonging to the same eigenvalue p'/p.

Of course $\mathbf{V}$ is not the only real eigenvector of A and of $\tilde{A}$ belonging to the eigenvalue p'/p. Because of the homogeneity of eqs (13) any non-null vector parallel or antiparallel to $\mathbf{V}$ is an eigenvector. For example if $\mathbf{V}$ is not identically zero, a unit vector may be formed from it by dividing $\mathbf{V}$ by its length. In the case of rigid rotations, for which $p'/p = 1$, this unit vector specifies the direction of the axis of rotation, and the development embodied in eqs (11) through (13) can be taken as a new proof of Euler's theorem [5]. The significance of the particular vector $\mathbf{V}$ for rigid rotations is that is gives not only the axis of rotation but the sine of the angle of rotation as well. When combined with the cosine of the angle of rotation as derived from the trace of A, this gives directly the complete, unambiguous correlation between the axis and angle of rotation. This will be seen in the second paper in this series, where eqs (13) and the vector $\mathbf{V}$ are considered in detail. In particular, it will be shown that $\mathbf{V}$ can be expressed as

$$\mathbf{V} = 2\mathbf{n} \sin \alpha,$$

where $\mathbf{n}$ is a unit vector giving the direction and the chosen sense of the axis of rotation, and α is the angle of rotation whose sense of description about the axis agrees with the handedness of the coordinate system which is rotated by A.

Although the derivations of eqs (12) and (13) from the second orthogonality relations are new, most of the results of those equations are not new. In particular, the fact that the ratios of the components of any vector which specifies the axis of a rigid rotation are identical to the ratios of the components of $\mathbf{V}$, has been known for a long time [6, 7]. This result has unfortunately not been adequately stressed in the literature. We would like to call attention to it here and to emphasize the slightly more general conclusion that eqs (12) and (13) form a prescription for writing down real eigenvectors of a transformation matrix without in fact solving the eigenvalue equation for the matrix. The prescription fails of course when $\mathbf{V}$ vanishes identically. As can be seen from eq (12), this occurs whenever A is symmetric in addition to being orthogonal. In paper II we shall see that a symmetric A corresponds to a rigid rotation of either 0° or 180° for the proper rotations ($p'/p = 1$), and to either a reflection in a plane or to an inversion of the coordinate system with respect to the origin, for the improper rotations ($p'/p = -1$). In such instances one must solve the eigenvalue equation for A to find its real eigenvectors.

We have been referring to $\mathbf{V}$ as a vector since it is a three-component object. However, it is not a vector in the sense in which the physicist usually understands that word. He would think of a vector as a one-to-one correspondence between coordinate systems and sets of three numbers, which under a transformation of coordinates obeys the transformation law of coordinate intervals.[3] Strictly speaking, **V** has relevance to the transformation between two coordinate systems, rather than as an object germane to individual coordinate systems. For convenience, however, we will continue to refer to **V** as a vector, keeping in mind its limitations under the transformation definition. For want of a better name, we shall henceforth call **V** the intrinsic vector.

The second consequence of eqs (9) that we shall derive is a new equation which connects the trace of A, tr A, with tr (A^2). To find it, we multiply eq (9a) by ϵ_{ijn}, and sum on i, j, and n. With the aid of the identities [4]

$$\epsilon_{ijn}\epsilon_{rmn} = \delta_{ir}\delta_{jm} - \delta_{im}\delta_{jr}, \tag{14a}$$

$$\epsilon_{ijn}\epsilon_{ijk} = 2\delta_{nk}, \tag{14b}$$

we arrive at

$$A_{ii}A_{jj} - A_{ij}A_{ji} = 2\frac{p'}{p}A_{nn}.$$

In trace notation this equation appears as

$$(\mathrm{tr}\, A)^2 - \mathrm{tr}\,(A^2) = 2\frac{p'}{p}\mathrm{tr}\, A. \tag{15}$$

Equation (15) can also be derived by similar operations on eq (9b).

The trace of a transformation matrix is primarily important for rigid rotations, where it furnishes the cosine of the angle α of rotation by means of the well known formula

$$\mathrm{tr}\, A = 1 + 2\cos\alpha. \tag{16}$$

The standard derivation of this formula [5] makes use of the special form of a rotation matrix when the axis of rotation is one of the coordinate axes, say the z axis. By direct calculation of the underlying two-dimensional transformation, this matrix is seen to be

$$\begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \equiv R_z(\alpha). \tag{17}$$

The trace of this matrix is given by eq (16). It is then noted that *any* rotation matrix may be put into the form (17) by an appropriate similarity transformation. The result (16) for an arbitrary rotation matrix then follows from the fact that the trace of a matrix is invariant under a similarity transformation.[5]

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[3] I am indebted to Robert Richtmeyer, from whom I first heard this particular wording of the transformation definition of a vector.

[4] An elementary and very lucid introduction to the use of the Levi-Civita symbol can be found in ref. [8]. This includes a derivation of the identity (14a), from which the identity (14b) may be derived by further contraction.

[5] In the language of group theory, real three-by-three orthogonal matrices belong to the vector representation, or the irreducible representation corresponding to $l=1$, of the rotation group. The characters of a representation are the traces of its matrices. Equation (16) is true only for the characters of the vector representation. For the matrices of the irreducible representation belonging to integral $l \geqslant 1$ the characters are given by $1+2\cos\alpha + \ldots + 2\cos l\alpha$, where α is the angle of rotation.

It is possible to derive the formula for the trace analytically from eq (15) using only general properties of rotations, and without the need to consider special forms of the rotation matrix. The derivation is interesting because it shows that the formula (16) is a direct consequence of the algebraic properties of rotation matrices, and so gives an insight into the structure of that formula which one does not get from the standard derivation. The details of the derivation of eq (16) from eq (15) will be presented in paper IV.

As a third consequence of eqs (9) we deduce a transparent expression for the determinant of A, det A. We first note that the properties of determinants furnish the identities [6]

$$A_{ir}A_{jm}A_{sn}\epsilon_{rmn}=(\det A)\,\epsilon_{ijs}, \tag{18a}$$

$$A_{ri}A_{mj}A_{ns}\epsilon_{rmn}=(\det A)\,\epsilon_{ijs}. \tag{18b}$$

If we then multiply either eq (9a) by A_{sn} or eq (9b) by A_{ns} and sum on s then the left side of either of the resulting equations is, by eqs (18), equal to (det A) ϵ_{ijs}. The right sides each lead to (p'/p) ϵ_{ijs}, with the help of the first orthogonality conditions (7). Equating these two expressions we have

$$\det A=\frac{p'}{p}. \tag{19}$$

This equation states in a concise form the result that the determinant of a real three-by-three orthogonal transformation matrix is equal to $+1$ when the transformation does not cause a change in handedness, and equal to -1 when it does. This result is of course well known but does not emerge quite as concisely in the customary way of deriving it. There, one uses the first orthogonality conditions to arrive at the result $(\det A)^2=1$, from which it follows that $\det A=\pm 1$. One then argues that only for the proper rotations is A continuously connected to the identity matrix, for which the determinant is $+1$. This leaves the value -1 of the determinant to account for the improper rotations. The second orthogonality conditions lead to these conclusions in a single succinct equation.

The final result of this section is a derivation of the secular equation for a transformation matrix, directly from the second orthogonality conditions. A word of clarification is in order. By the phrase "secular equation" of a matrix, one usually means the polynomial equation obeyed by the eigenvalues of the matrix. The Cayley-Hamilton theorem [10] asserts that the matrix itself obeys its own polynomial equation. For this reason we refer to the polynomial equation satisfied by a transformation matrix as its secular equation. It is in this form that the secular equation for A comes out of eqs (9).

We multiply eq (9a) by ϵ_{stn}, and sum on n using the identity (14a). This gives

$$A_{is}A_{jt}-A_{it}A_{js}=\frac{p'}{p}\,\epsilon_{ijk}\epsilon_{stn}A_{kn}. \tag{20}$$

We now contract this equation on s and j. To evaluate the right side of the contracted equation we use the cyclic property (10) of ϵ and the identity (14a). The result is

$$(A^2)_{it}-(\operatorname{tr}A)A_{it}=\frac{p'}{p}\,[A_{ti}-(\operatorname{tr}A)\delta_{it}].$$

The matrix form of this equation is

$$A^2-(\operatorname{tr}A)A=\frac{p'}{p}\,[\tilde{A}-(\operatorname{tr}A)I], \tag{21}$$

[6] A derivation of these identities may be found in ref. [9]. In the theory of Cartesian tensors, these identities constitute the proof that the Levi-Civita symbol is a pseudotensor of the third rank.

where $\tilde{A}$ is the transpose of A, and I is the identity matrix. Upon multiplying eq (21) by A, either from the left or from the right, and noting that $A\tilde{A}=\tilde{A}A=I$ from the first orthogonality relations, we have

$$A^3-(\mathrm{tr}\,A)A^2+\frac{p'}{p}(\mathrm{tr}\,A)A-\frac{p'}{p}I=0. \tag{22}$$

This is the secular equation for A.

For the special case of rigid rotations, we can set $p'/p=1$, and use eq (16) for $\mathrm{tr}\,A$, in eq (22). The secular equation for a rotation matrix is then

$$A^3-(1+2\cos\alpha)A^2+(1+2\cos\alpha)A-I=0. \tag{23}$$

This may be written in the factored form

$$(A-I)[A^2-(2\cos\alpha)A+I]=0. \tag{24}$$

If A in eq (23) (or eq (24)) is replaced by a numerical variable representing the eigenvalues of A, then the solution of the resulting equation gives the usual result that the eigenvalues are 1, $e^{i\alpha}$, and $e^{-i\alpha}$. The fact that one of the eigenvalues is unity may be taken as yet another direct proof from eqs (9) of Euler's theorem. This proof has the advantage over the one based on eqs (13) in that it remains valid even when the intrinsic vector vanishes.

A more powerful use of eq (23) is in finding a closed-form expression for A as a function of the axis and angle of rotation. On the basis of very general properties of rotation matrices, the solution of eq (23) is

$$A(\alpha)=I-N\sin\alpha+N^2(1-\cos\alpha). \tag{25}$$

Here, N is a matrix which is formed from the components of $\mathbf{n}$, the unit vector along the sense of the axis of rotation, by the prescription

$$N_{ik}\equiv\epsilon_{ijk}n_j. \tag{26}$$

In explicit matrix form, N appears as

$$N=\begin{pmatrix}0 & -n_3 & n_2\\ n_3 & 0 & -n_1\\ -n_2 & n_1 & 0\end{pmatrix}. \tag{27}$$

Equation (25) is probably more familiar in its exponential form.[7]

$$A(\alpha)=e^{-N\alpha}. \tag{28}$$

Since eq (23) is independent of the axis of rotation, it is to be expected that it has to be supplemented by a condition which introduces the axis. The appropriate condition is the eigenvalue equation for A corresponding to the eigenvalue $+1$.

The details of how eq (23) is solved to give eq (25) are interesting in their own right, and are given in paper IV. As with the solution of eq (15) to yield the trace formula, the process of solving

[7] The reader who is familiar with the dyadic representation of rotations will recognize the similarity between eq (25) and the rotation dyadic [11]. The matrix N is replaced by the dyadic $-\mathbf{n}\times\mathbf{I}$, where $\mathbf{I}$ is the unit dyadic, the minus sign entering because a dyadic is generally used to describe an active transformation, whereas eq (25) is meant to describe a passive transformation. The matrix N^2 is replaced by the dyadic $\mathbf{n}\times(\mathbf{n}\times\mathbf{I})$ which is just $(-\mathbf{n}\times\mathbf{I})\cdot(-\mathbf{n}\times\mathbf{I})=(-\mathbf{n}\times\mathbf{I})^2$. One can check that the matrix form of $\mathbf{n}\times\mathbf{I}$ is given by the right side of eq (26).

eq (23) from general properties of rotations shows the intimate connection between the result, eq (25), and the algebraic properties of rotation matrices. As will be seen in paper IV, the same general properties of rotations are invoked to solve both eqs (15) and (23). These are the group property, and the periodicity property.

In all of the results derived in this section, it can be seen that the only way in which p and p' occur is in the ratio p'/p. This is an expression of the fact that only the relative handedness of two coordinate systems is of any significance. To emphasize this fact we shall continue to write the ratio as p'/p, rather than define a new symbol for it.

We have already indicated the contents of papers II and IV of this series. Paper III will be concerned with the proof of the theorem of conjugacy, from the second orthogonality conditions. This theorem makes statements about the axes and angles of rotation of two rotation matrices connected by an orthogonal similarity transformation.

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