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SIX-DIMENSIONAL ORTHOGONAL TENSOR REPRESENTATION OF THE ROTATION ABOUT AN AXIS IN THREE DIMENSIONS

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Abstract—The representation of the classical formula that contains Euler's theorem on three-dimensional rigid body rotations, as an orthogonal tensor in three dimensions, is extended to a six-dimensional representation as a tool for accomplishing coordinate transformations of the anisotropic elasticity tensor.

1. INTRODUCTION

Euler's theorem on the representation of rigid body rotations (Brand, 1947; Lamb, 1929; Goldstein, 1950; Pars, 1979; Whittaker, 1937) has many forms. The theorem concerns the characterization of a three-dimensional rotation by an angle θ about a specific axis, here indicated by the unit vector $\mathbf{p}$. This theorem is represented by the action of a three-dimensional orthogonal tensor $\mathbf{Q}$ determined from the angle θ and the unit vector $\mathbf{p}$ by the formula (Beatty, 1966, 1977; Finger, 1892; Gurtin, 1976; Truesdell and Toupin, 1960)

$$\mathbf{Q} = \mathbf{1} + \sin\theta\mathbf{P} + (1-\cos\theta)\mathbf{P}^2 = e^{\theta\mathbf{P}}, \tag{1}$$

where the three-dimensional skew-symmetric tensor $\mathbf{P}$ with components P_{ij} is introduced to represent the unit vector $\mathbf{p}$,

$$\mathbf{P} = \begin{bmatrix} 0 & -p_3 & p_2 \\ p_3 & 0 & -p_1 \\ -p_2 & p_1 & 0 \end{bmatrix} \quad \text{or} \quad P_{ij} = -e_{ijk}p_k, \tag{2}$$

and $e^{\theta\mathbf{P}}$ is the exponential matrix function. An elementary derivation of the result (1) using the exponential matrix function $e^{\theta\mathbf{P}}$ is given in the Appendix. The exponential representation (1) is also of interest in computational solid mechanics for integrating incremental constitutive relations (Balendran and Nemat Nasser, 1994). It is easy to show that $\mathbf{P}$ has the following properties:

$$\mathbf{P} = -\mathbf{P}^{\mathrm{T}}, \quad \mathbf{Pp} = \mathbf{0}, \quad \mathbf{P}^2 = \mathbf{p}\otimes\mathbf{p} - \mathbf{1}, \quad \mathbf{P}^3 = -\mathbf{P}. \tag{3}$$

In this paper we show that, in a space of six dimensions, the representation of a three-dimensional rotation by an angle θ about a specific axis, characterized by the unit vector $\mathbf{p}$, is represented as a six-dimensional orthogonal tensor by the formula

$$\hat{\mathbf{Q}} = \hat{\mathbf{1}} + \sin\theta\hat{\mathbf{P}} + (1-\cos\theta)\hat{\mathbf{P}}^2 + \tfrac{1}{3}\sin\theta(1-\cos\theta)(\hat{\mathbf{P}}+\hat{\mathbf{P}}^3) + \tfrac{1}{6}(1-\cos\theta)^2(\hat{\mathbf{P}}^2+\hat{\mathbf{P}}^4) = e^{\theta\hat{\mathbf{P}}}, \tag{4}$$

where the six-dimensional skew-symmetric tensor $\hat{\mathbf{P}}$ with components

$$\hat{\mathbf{P}} = \begin{bmatrix} 0 & 0 & 0 & 0 & \sqrt{2}p_2 & -\sqrt{2}p_3 \\ 0 & 0 & 0 & -\sqrt{2}p_1 & 0 & \sqrt{2}p_3 \\ 0 & 0 & 0 & \sqrt{2}p_1 & -\sqrt{2}p_2 & 0 \\ 0 & \sqrt{2}p_1 & -\sqrt{2}p_1 & 0 & p_3 & -p_2 \\ -\sqrt{2}p_2 & 0 & \sqrt{2}p_2 & -p_3 & 0 & p_1 \\ \sqrt{2}p_3 & -\sqrt{2}p_3 & 0 & p_2 & -p_1 & 0 \end{bmatrix} \tag{5}$$

satisfies the following conditions:

$$\hat{\mathbf{P}} = -\hat{\mathbf{P}}^{\mathrm{T}}, \quad \hat{\mathbf{P}}^5 + 5\hat{\mathbf{P}}^3 + 4\hat{\mathbf{P}} = 0, \quad \hat{\mathbf{P}}^6 + 5\hat{\mathbf{P}}^4 + 4\hat{\mathbf{P}}^2 = 0. \tag{6}$$

Matrices of six-dimensional tensor components are distinguished with circumflexes. Note that formulae (1) and (4) show that a change in the sense of $\mathbf{p}$ is the same as a reversal of the direction of the angle of rotation θ; thus formulae (1) and (4) are invariant under the change of variables from $\mathbf{p}$, θ to $-\mathbf{p}$, $-\theta$.

Formula (4) is of interest in anisotropic elasticity because the elasticity tensor can be expressed as a second rank tensor in six dimensions (Mehrabadi and Cowin, 1990) as well as in its more traditional representation as a fourth rank tensor in three dimensions. Orthogonal transformations in six dimensions can then be used to represent orthogonal transformations in three dimensions as described in section 2. Formula (4) connects the geometric operation in three dimensions to the matrix algebra of six dimensions. Since the tensor transformation rules for a second rank tensor rather than a fourth rank tensor apply, transformations of the reference coordinate system for the elasticity tensor may be accomplished in a very straightforward fashion using matrix multiplication. It follows that one of the contemporary symbolic algebra computational programs (Maple, Mathematica, MacSyma, Matlab, etc.) may easily be employed to accomplish coordinate transformations. In these programs, transformations in the six-dimensional space are six-by-six matrix multiplications that are quickly entered and computed with the symbolic algebra software. The fact that it is neither notationally nor computationally easy to do specific fourth rank tensor transformations in three dimensions has hindered the presentation of this material in the past.

The derivation of formula (4) is given in section 3 and an example of its application is given in section 4. The example is the development of a matrix representation for monoclinic symmetry.

2. THE SIX-DIMENSIONAL NOTATION

The anisotropic form of Hooke's law is often written in indicial notation as $T_{ij} = C_{ijkm}E_{km}$, where the C_{ijkm} are the components of the three-dimensional fourth rank elasticity tensor. There are three important symmetry restrictions on the fourth rank tensor components C_{ijkm}. These restrictions, which require that components with the subscripts *ijkm*, *jikm* and *kmij* be equal, follow from the symmetry of the stress tensor, the symmetry of the strain tensor, and the requirement that no work be produced by the elastic material in a closed loading cycle, respectively. Written as a linear transformation in six dimensions, Hooke's law has the representation $\mathbf{T} = \mathbf{cE}$ or

$$\begin{bmatrix} T_{11} \\ T_{22} \\ T_{33} \\ T_{23} \\ T_{13} \\ T_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ 2E_{23} \\ 2E_{13} \\ 2E_{12} \end{bmatrix} \tag{7}$$

in the two subscript notation of Voigt (1910) for the components of C_{ijkm}. In the Voigt notation the components of **c** and C_{ijkm} are related by replacing the six-dimensional indices 1, 2, 3, 4, 5 and 6 by the pairs of three-dimensional indices 1, 2 and 3; thus, 1, 2, 3, 4, 5 and 6 become 11, 22, 33, 23 or 32, 13 or 31, 12 or 21, respectively. The members of the paired indices 23 or 32, 13 or 31, 12 or 21 are equivalent because of the symmetry of the tensors of stress and strain. The matrix **c** in eqn (7) is not a matrix of tensor components in six dimensions, although it is formed from the components of a three-dimensional fourth rank tensor.

Six-dimensional vector bases and notations are introduced so that stress and strain can be considered as vectors in a six-dimensional vector space as well as second rank tensors in three-dimensional Cartesian reference systems. The six-dimensional quantities will be indicated by a circumflex; thus, the six-dimensional vectors of stress and strain will be denoted by $\hat{\mathbf{T}}$ and $\hat{\mathbf{E}}$, respectively, whereas the three-dimensional second rank tensors of stress and strain are denoted by **T** and **E**, respectively. The direct relationship between the components of $\hat{\mathbf{T}}$ and **T**, and $\hat{\mathbf{E}}$ and **E**, are the dual representations given by

$$\hat{\mathbf{T}} = \begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \hat{T}_3 \\ \hat{T}_4 \\ \hat{T}_5 \\ \hat{T}_6 \end{bmatrix} = \begin{bmatrix} T_{11} \\ T_{22} \\ T_{33} \\ \sqrt{2}T_{23} \\ \sqrt{2}T_{13} \\ \sqrt{2}T_{12} \end{bmatrix}, \quad \hat{\mathbf{E}} = \begin{bmatrix} \hat{E}_1 \\ \hat{E}_2 \\ \hat{E}_3 \\ \hat{E}_4 \\ \hat{E}_5 \\ \hat{E}_6 \end{bmatrix} = \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ \sqrt{2}E_{23} \\ \sqrt{2}E_{13} \\ \sqrt{2}E_{12} \end{bmatrix}, \tag{8}$$

where the shearing components of these new six-dimensional stress and strain vectors are the shearing components of these three-dimensional stress and strain tensors multiplied by $\sqrt{2}$. This $\sqrt{2}$ factor ensures that the scalar product of the two six-dimensional vectors is equal to the trace of the product of the corresponding second rank tensors, $\hat{\mathbf{T}} \cdot \hat{\mathbf{E}} = \mathrm{tr}\,\mathbf{TE}$. Introducing the new notation of eqn (8) into eqn (7), eqn (7) can be rewritten in the form

$$\hat{\mathbf{T}} = \hat{\mathbf{c}}\hat{\mathbf{E}}, \tag{9}$$

where $\hat{\mathbf{c}}$ is a new six-by-six matrix. The matrix form of eqn (9) is given by

$$\begin{bmatrix} T_{11} \\ T_{22} \\ T_{33} \\ \sqrt{2}T_{23} \\ \sqrt{2}T_{13} \\ \sqrt{2}T_{12} \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} & c_{13} & \sqrt{2}c_{14} & \sqrt{2}c_{15} & \sqrt{2}c_{16} \\ c_{12} & c_{22} & c_{23} & \sqrt{2}c_{24} & \sqrt{2}c_{25} & \sqrt{2}c_{26} \\ c_{13} & c_{23} & c_{33} & \sqrt{2}c_{34} & \sqrt{2}c_{35} & \sqrt{2}c_{36} \\ \sqrt{2}c_{14} & \sqrt{2}c_{24} & \sqrt{2}c_{34} & 2c_{44} & 2c_{45} & 2c_{46} \\ \sqrt{2}c_{15} & \sqrt{2}c_{25} & \sqrt{2}c_{35} & 2c_{45} & 2c_{55} & 2c_{56} \\ \sqrt{2}c_{16} & \sqrt{2}c_{26} & \sqrt{2}c_{36} & 2c_{46} & 2c_{56} & 2c_{66} \end{bmatrix} \begin{bmatrix} E_{11} \\ E_{22} \\ E_{33} \\ \sqrt{2}E_{23} \\ \sqrt{2}E_{13} \\ \sqrt{2}E_{12} \end{bmatrix} \tag{10}$$

or

$$\begin{bmatrix} \hat{T}_1 \\ \hat{T}_2 \\ \hat{T}_3 \\ \hat{T}_4 \\ \hat{T}_5 \\ \hat{T}_6 \end{bmatrix} = \begin{bmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{bmatrix} \begin{bmatrix} \hat{E}_1 \\ \hat{E}_2 \\ \hat{E}_3 \\ \hat{E}_4 \\ \hat{E}_5 \\ \hat{E}_6 \end{bmatrix}.$$

The relationship between the non-tensorial Voigt notation $\mathbf{c}$ and the six-dimensional second rank tensor components $\hat{\mathbf{c}}$ is easily constructed from eqn (10); a table of this relationship is given in Mehrabadi and Cowin (1990).

The symmetric matrix $\hat{\mathbf{c}}$ can be shown (Mehrabadi and Cowin, 1990) to represent the components of a second rank tensor in a six-dimensional space, whereas the components of the matrix $\mathbf{c}$ appearing in eqn (7) do not form a tensor. Two reference bases or coordinate systems will be employed in three-dimensional space; these two systems have equivalent bases in six-dimensional space. The first basis is called the Latin basis or coordinate system because Latin letters are used to indicate indices associated with the system; it has base vectors $\mathbf{e}_i$, $i = 1, 2, 3$. The second basis is exactly like the first but a slightly different notation is employed in order to distinguish it from the first. For the other system Greek indices are employed and the base vectors are $\mathbf{e}_\alpha$, $\alpha = \mathrm{I, II, III}$. The orthogonal transformation from the Greek to the Latin system in three dimensions is represented by the matrix $\mathbf{Q}$ with components $Q_{i\alpha} = \mathbf{e}_i \cdot \mathbf{e}_\alpha$. The orthogonal transformation from the Greek to the Latin bases in six dimensions is represented by $\hat{\mathbf{Q}}$, where $\hat{\mathbf{Q}}$ is a six-by-six matrix of tensor components,

$$\hat{\mathbf{Q}} = \begin{bmatrix} \hat{Q}_{1\mathrm{I}} & \hat{Q}_{1\mathrm{II}} & \hat{Q}_{1\mathrm{III}} & \hat{Q}_{1\mathrm{IV}} & \hat{Q}_{1\mathrm{V}} & \hat{Q}_{1\mathrm{VI}} \\ \hat{Q}_{2\mathrm{I}} & \hat{Q}_{2\mathrm{II}} & \hat{Q}_{2\mathrm{III}} & \hat{Q}_{2\mathrm{IV}} & \hat{Q}_{2\mathrm{V}} & \hat{Q}_{2\mathrm{VI}} \\ \hat{Q}_{3\mathrm{I}} & \hat{Q}_{3\mathrm{II}} & \hat{Q}_{3\mathrm{III}} & \hat{Q}_{3\mathrm{IV}} & \hat{Q}_{3\mathrm{V}} & \hat{Q}_{3\mathrm{VI}} \\ \hat{Q}_{4\mathrm{I}} & \hat{Q}_{4\mathrm{II}} & \hat{Q}_{4\mathrm{III}} & \hat{Q}_{4\mathrm{IV}} & \hat{Q}_{4\mathrm{V}} & \hat{Q}_{4\mathrm{VI}} \\ \hat{Q}_{5\mathrm{I}} & \hat{Q}_{5\mathrm{II}} & \hat{Q}_{5\mathrm{III}} & \hat{Q}_{5\mathrm{IV}} & \hat{Q}_{5\mathrm{V}} & \hat{Q}_{5\mathrm{VI}} \\ \hat{Q}_{6\mathrm{I}} & \hat{Q}_{6\mathrm{II}} & \hat{Q}_{6\mathrm{III}} & \hat{Q}_{6\mathrm{IV}} & \hat{Q}_{6\mathrm{V}} & \hat{Q}_{6\mathrm{VI}} \end{bmatrix}. \tag{11}$$

The six-dimensional bases, $\hat{\mathbf{e}}_I$, $I, J, K = 1, 2, 3, 4, 5, 6$ and $\hat{\mathbf{e}}_\Lambda$, $\Lambda = \mathrm{I, II, III, IV, V, VI}$, are associated with the three-dimensional bases $\mathbf{e}_i$, $i = 1, 2, 3$ and $\mathbf{e}_\alpha$, $\alpha = \mathrm{I, II, III}$, respectively. Using these bases, the components of a six-dimensional second rank tensor $\hat{B}_{JK}$ are related to the components of the three-dimensional fourth rank tensor B_{ijkm} by

$$\hat{\mathbf{B}} = \hat{B}_{JK}\hat{\mathbf{e}}_J \otimes \hat{\mathbf{e}}_K = B_{ijkm}\mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k \otimes \mathbf{e}_m. \tag{12}$$

In the special case of the orthogonal tensors $\mathbf{Q}$ and $\hat{\mathbf{Q}}$, which are both second rank and two-space tensors, the relationship (12) between the components of the two-space, six-dimensional second rank tensor $\hat{Q}_{K\Lambda}$ and the two-space, three-dimensional fourth rank tensor $Q_{ik\alpha\beta}$ is written as

$$\hat{\mathbf{Q}} = \hat{Q}_{K\Lambda}\hat{\mathbf{e}}_K \otimes \hat{\mathbf{e}}_\Lambda = Q_{ik\alpha\beta}\mathbf{e}_i \otimes \mathbf{e}_k \otimes \mathbf{e}_\alpha \otimes \mathbf{e}_\beta, \tag{13}$$

where the fourth rank two-space tensor in three dimensions is formed using the tensor transformation law for fourth rank tensors in three dimensions as a guide, thus

$$Q_{ik\alpha\beta} = \tfrac{1}{2}(Q_{i\alpha}Q_{k\beta} + Q_{i\beta}Q_{k\alpha}). \tag{14}$$

The detailed relationship between components is as follows (Mehrabadi and Cowin, 1990): the elements in the upper left hand three-by-three matrix of eqn (11) are given in terms of the elements of $\mathbf{Q}$ by

$$\hat{Q}_{K\Lambda} = Q_{i\alpha}Q_{i\alpha}, \quad \text{no sum on } \alpha,\ K = i = 1,2,3\,;\ \Lambda = \alpha = \text{I, II, III}\,; \tag{15}$$

the elements in the upper right hand three-by-three matrix of eqn (11) are given in terms of the elements of **Q** by

$$\hat{Q}_{K\text{IV}} = \sqrt{2}Q_{i\text{II}}Q_{i\text{III}}, \quad \hat{Q}_{K\text{V}} = \sqrt{2}Q_{i\text{I}}Q_{i\text{III}}, \quad \hat{Q}_{K\text{VI}} = \sqrt{2}Q_{i\text{I}}Q_{i\text{II}},$$
$$\text{no sum on } i,\ K = i = 1,2,3\,; \tag{16}$$

the elements in the lower left hand three-by-three matrix of eqn (11) are given in terms of the elements of **Q** by

$$\hat{Q}_{4\Lambda} = \sqrt{2}Q_{2\alpha}Q_{3\alpha}, \quad \hat{Q}_{5\Lambda} = \sqrt{2}Q_{1\alpha}Q_{3\alpha}, \quad \hat{Q}_{6\Lambda} = \sqrt{2}Q_{1\alpha}Q_{2\alpha},$$
$$\text{no sum on } \alpha,\ \Lambda = \alpha = \text{I, II, III}\,; \tag{17}$$

and the elements in the lower right hand three-by-three matrix of eqn (11) are given in terms of the elements of **Q** by

$$\hat{Q}_{4\text{IV}} = Q_{2\text{II}}Q_{3\text{III}} + Q_{3\text{II}}Q_{2\text{III}}, \quad \hat{Q}_{4\text{V}} = Q_{2\text{I}}Q_{3\text{III}} + Q_{3\text{I}}Q_{2\text{III}}, \quad \hat{Q}_{4\text{VI}} = Q_{2\text{I}}Q_{3\text{II}} + Q_{3\text{I}}Q_{2\text{II}}$$
$$\hat{Q}_{5\text{IV}} = Q_{1\text{II}}Q_{3\text{III}} + Q_{3\text{II}}Q_{1\text{III}}, \quad \hat{Q}_{5\text{V}} = Q_{1\text{I}}Q_{3\text{III}} + Q_{3\text{I}}Q_{1\text{III}}, \quad \hat{Q}_{5\text{VI}} = Q_{1\text{I}}Q_{3\text{II}} + Q_{3\text{I}}Q_{1\text{II}}$$
$$\hat{Q}_{6\text{IV}} = Q_{1\text{II}}Q_{2\text{III}} + Q_{2\text{II}}Q_{1\text{III}}, \quad \hat{Q}_{6\text{V}} = Q_{1\text{I}}Q_{2\text{III}} + Q_{2\text{I}}Q_{1\text{III}}, \quad \hat{Q}_{6\text{VI}} = Q_{1\text{I}}Q_{2\text{II}} + Q_{2\text{I}}Q_{1\text{II}}. \tag{18}$$

To see that $\hat{\mathbf{Q}}$ is an orthogonal matrix in six dimensions requires some algebraic manipulation. The proof rests on the orthogonality of the three-dimensional **Q**:

$$\mathbf{QQ}^{\mathrm{T}} = \mathbf{Q}^{\mathrm{T}}\mathbf{Q} = \mathbf{1} \Rightarrow \hat{\mathbf{Q}}\hat{\mathbf{Q}}^{\mathrm{T}} = \hat{\mathbf{Q}}^{\mathrm{T}}\hat{\mathbf{Q}} = \hat{\mathbf{1}}. \tag{19}$$

It should be noted that, while it is always possible to find $\hat{\mathbf{Q}}$ given **Q** by use of eqns (15)–(18), it is not possible to determine **Q** unambiguously given $\hat{\mathbf{Q}}$ because the components of **Q** are squared to determine the components of $\hat{\mathbf{Q}}$ and this fact introduces a sign ambiguity in the inverse calculation. To see this non-uniqueness note that both $\mathbf{Q} = \mathbf{1}$ and $\mathbf{Q} = -\mathbf{1}$ correspond to $\hat{\mathbf{Q}} = \hat{\mathbf{1}}$. Mehrabadi and Cowin (1990) show that $\hat{\mathbf{c}}$ transforms as a second rank tensor in a six-dimensional space,

$$\hat{c}_{KJ} = \hat{Q}_{K\Lambda}\hat{c}_{\Lambda\Psi}\hat{Q}_{\Psi J} \quad \text{or} \quad [\hat{c}_{KJ}] = \hat{\mathbf{Q}}[\hat{c}_{\Lambda\Psi}]\hat{\mathbf{Q}}^{\mathrm{T}}. \tag{20}$$

3. THE SIX-DIMENSIONAL REPRESENTATION OF THREE-DIMENSIONAL ROTATION

The six-dimensional representation [formula (4)] for the rotation will be derived in this section. This derivation simplifies a great deal if we introduce the notation

$$[\mathbf{A},\mathbf{B}]_{ijkm} = \tfrac{1}{2}(A_{ik}B_{jm} + A_{im}B_{jk} + A_{jm}B_{ik} + A_{jk}B_{im}), \tag{21}$$

where **A** and **B** are any two second-rank tensors in three dimensions and [**A**, **B**] is a fourth rank tensor in three dimensions. Note that the fourth rank tensor [**A**, **B**] introduced in eqn (21) has the following properties:

$$[\mathbf{A},\mathbf{B}] = [\mathbf{B},\mathbf{A}], \quad [\mathbf{A},-\mathbf{B}] = -[\mathbf{A},\mathbf{B}], \tag{22}$$

and the following multiplication formula

$$[\mathbf{A},\mathbf{B}]_{ijrs}[\mathbf{C},\mathbf{D}]_{rskm} = [\mathbf{AC},\mathbf{BD}]_{ijkm}+[\mathbf{AD},\mathbf{BC}]_{ijkm} \tag{23a}$$

or simply

$$[\mathbf{A},\mathbf{B}][\mathbf{C},\mathbf{D}] = [\mathbf{AC},\mathbf{BD}]+[\mathbf{AD},\mathbf{BC}]. \tag{23b}$$

In this new notation formula (14) may be written as

$$Q_{ik\alpha\beta} = \tfrac{1}{2}(Q_{i\alpha}Q_{k\beta}+Q_{i\beta}Q_{k\alpha}) = \tfrac{1}{2}[\mathbf{Q},\mathbf{Q}]_{ik\alpha\beta}. \tag{24}$$

The first step in the derivation of formula (4) is to substitute for $\mathbf{Q}$ from formula (1) into eqn (24), thus

$$\begin{aligned}\tfrac{1}{2}[\mathbf{Q},\mathbf{Q}]_{ik\alpha\beta} &= \tfrac{1}{2}[\mathbf{1},\mathbf{1}]_{ik\alpha\beta}+\sin\theta[\mathbf{1},\mathbf{P}]_{ik\alpha\beta}+(1-\cos\theta)[\mathbf{1},\mathbf{P}^2]_{ik\alpha\beta}\\ &\quad+\tfrac{1}{2}\sin^2\theta[\mathbf{P},\mathbf{P}]_{ik\alpha\beta}+\sin\theta(1-\cos\theta)[\mathbf{P},\mathbf{P}^2]_{ik\alpha\beta}+\tfrac{1}{2}(1-\cos\theta)^2[\mathbf{P}^2,\mathbf{P}^2]_{ik\alpha\beta}.\end{aligned} \tag{25}$$

The second step is to employ eqn (13) and (24) in eqn (25), thus

$$\begin{aligned}\hat{\mathbf{Q}} &= \hat{\mathbf{1}}+\sin\theta\langle\mathbf{1},\mathbf{P}\rangle+(1-\cos\theta)\langle\mathbf{1},\mathbf{P}^2\rangle+\tfrac{1}{2}\sin^2\theta\langle\mathbf{P},\mathbf{P}\rangle\\ &\quad+\sin\theta(1-\cos\theta)\langle\mathbf{P},\mathbf{P}^2\rangle+\tfrac{1}{2}(1-\cos\theta)^2\langle\mathbf{P}^2,\mathbf{P}^2\rangle,\end{aligned} \tag{26}$$

where

$$\langle\mathbf{A},\mathbf{B}\rangle = \langle\mathbf{A},\mathbf{B}\rangle_{IJ}\hat{\mathbf{e}}_I\otimes\hat{\mathbf{e}}_J \equiv [\mathbf{A},\mathbf{B}]_{ijkm}\mathbf{e}_i\otimes\mathbf{e}_j\otimes\mathbf{e}_k\otimes\mathbf{e}_m, \tag{27}$$

and it is easily shown that

$$\hat{\mathbf{1}} = \tfrac{1}{2}\langle\mathbf{1},\mathbf{1}\rangle. \tag{28}$$

The third step is to note that, from its location as the term proportional to $\sin\theta$ in eqn (26), it may be seen that the six-dimensional analog of the tensor $\mathbf{P}$ is $\langle\mathbf{1},\mathbf{P}\rangle$, thus $\langle\mathbf{1},\mathbf{P}\rangle$ is defined as $\hat{\mathbf{P}}$:

$$\hat{\mathbf{P}} \equiv \langle\mathbf{1},\mathbf{P}\rangle. \tag{29}$$

The fourth step is to obtain an expression for $\hat{\mathbf{Q}}$ in terms of $\hat{\mathbf{P}}$. Thus the four quantities $\langle\mathbf{1},\mathbf{P}^2\rangle$, $\langle\mathbf{P},\mathbf{P}\rangle$, $\langle\mathbf{P},\mathbf{P}^2\rangle$ and $\langle\mathbf{P}^2,\mathbf{P}^2\rangle$ appearing in eqn (26) must be calculated as polynomials of $\hat{\mathbf{P}}$. To this end the formula (23) and the identity $(3)_4$ are employed, thus

$$\hat{\mathbf{P}}^2 = \langle\mathbf{1},\mathbf{P}\rangle\langle\mathbf{1},\mathbf{P}\rangle = \langle\mathbf{1},\mathbf{P}^2\rangle+\langle\mathbf{P},\mathbf{P}\rangle \tag{30}$$

$$\hat{\mathbf{P}}^3 = -\langle\mathbf{1},\mathbf{P}\rangle+3\langle\mathbf{P},\mathbf{P}^2\rangle \tag{31}$$

$$\hat{\mathbf{P}}^4 = -\langle\mathbf{1},\mathbf{P}^2\rangle-4\langle\mathbf{P},\mathbf{P}\rangle+3\langle\mathbf{P}^2,\mathbf{P}^2\rangle. \tag{32}$$

Solving for the three quantities $\langle\mathbf{1},\mathbf{P}^2\rangle$, $\langle\mathbf{P},\mathbf{P}^2\rangle$ and $\langle\mathbf{P}^2,\mathbf{P}^2\rangle$ in terms of the powers of $\hat{\mathbf{P}}$ and $\langle\mathbf{P},\mathbf{P}\rangle$, it follows from eqns (30), (31) and (32) that

$$\langle\mathbf{1},\mathbf{P}^2\rangle = \hat{\mathbf{P}}^2-\langle\mathbf{P},\mathbf{P}\rangle \tag{33}$$

$$\langle\mathbf{P},\mathbf{P}^2\rangle = \tfrac{1}{3}(\hat{\mathbf{P}}+\hat{\mathbf{P}}^3) \tag{34}$$

$$\langle \mathbf{P}^2, \mathbf{P}^2 \rangle = \tfrac{1}{3}(\hat{\mathbf{P}}^2 + \hat{\mathbf{P}}^4) + \langle \mathbf{P}, \mathbf{P} \rangle. \tag{35}$$

The final step, that of obtaining formula (4), is accomplished by substituting eqns (33), (34) and (35) into eqn (26) and observing that all the terms involving $\langle \mathbf{P}, \mathbf{P} \rangle$ cancel out.

For the proof of the exponential matrix function representation (4) of $\hat{\mathbf{Q}}$, expressions for higher powers of $\hat{\mathbf{P}}$ are needed. An expression for $\hat{\mathbf{P}}^5$ can be found from eqns (29) and (32), thus

$$\hat{\mathbf{P}}^5 = \hat{\mathbf{P}} - 15\langle \mathbf{P}, \mathbf{P}^2 \rangle, \tag{36}$$

and it follows from eqn (31) that

$$\hat{\mathbf{P}}^5 + 5\hat{\mathbf{P}}^3 + 4\hat{\mathbf{P}} = 0 \tag{37}$$

when $\langle \mathbf{P}, \mathbf{P}^2 \rangle$ is eliminated and eqn (29) employed. This result is given as the property $(6)_2$ of $\hat{\mathbf{P}}$. The Cayley–Hamilton theorem for $\hat{\mathbf{P}}$ is given by

$$\hat{\mathbf{P}}^6 + 5\hat{\mathbf{P}}^4 + 4\hat{\mathbf{P}}^2 = 0. \tag{38}$$

This shows that $\hat{\mathbf{P}}$ has eigenvalues 0, 0, $2i$, $-2i$, i, $-i$. Using eqns (3), (29), (33), (34), (35), (37) and (38), it follows that

$$\operatorname{tr}\hat{\mathbf{P}} = 0, \quad \operatorname{tr}\hat{\mathbf{P}}^3 = 0, \quad \operatorname{tr}\hat{\mathbf{P}}^5 = 0, \quad \operatorname{tr}\hat{\mathbf{P}}^2 = -10, \quad \operatorname{tr}\hat{\mathbf{P}}^4 = 34, \quad \operatorname{tr}\hat{\mathbf{P}}^6 = -130. \tag{39}$$

For comparison, the Cayley–Hamilton theorem (Finkbiner, 1960; Frazer *et al.*, 1960; Mirsky, 1990) for a six-by-six skew-symmetric matrix $\hat{\mathbf{W}}$ is

$$\hat{\mathbf{W}}^6 - \tfrac{1}{2}(\operatorname{tr}\hat{\mathbf{W}}^2)\hat{\mathbf{W}}^4 + \tfrac{1}{4}(\tfrac{1}{2}(\operatorname{tr}\hat{\mathbf{W}}^2)^2 - \operatorname{tr}\hat{\mathbf{W}}^4)\hat{\mathbf{W}}^2 - \tfrac{1}{12}(\tfrac{1}{4}(\operatorname{tr}\hat{\mathbf{W}}^2)^3 - \tfrac{3}{2}(\operatorname{tr}\hat{\mathbf{W}}^2)(\operatorname{tr}\hat{\mathbf{W}}^4) + 2\operatorname{tr}\hat{\mathbf{W}}^6)\hat{\mathbf{1}} = 0. \tag{40}$$

The formulae for the powers of $\hat{\mathbf{P}}$ are found using eqn (37),

$$\hat{\mathbf{P}}^{2n+3} = (-1)^n[\tfrac{1}{3}(2^{2n+2} - 1)(\hat{\mathbf{P}} + \hat{\mathbf{P}}^3) - \hat{\mathbf{P}}], \quad n \geqslant 0 \tag{41}$$

and

$$\hat{\mathbf{P}}^{2n+4} = (-1)^n[\tfrac{1}{3}(2^{2n-2} - 1)(\hat{\mathbf{P}}^2 + \hat{\mathbf{P}}^4) - \hat{\mathbf{P}}^2], \quad n \geqslant 0. \tag{42}$$

The proof of the exponential matrix function representation formula [(4)] of $\hat{\mathbf{Q}}$ now parallels the derivation in the Appendix of the analogous three-dimensional (1) exponential matrix function formula. Employing the properties of exponential functions of matrices given in the Appendix, it is easy to see that if $\mathbf{W}$ is an N-dimensional skew-symmetric matrix and $\mathbf{B} = e^{x\mathbf{W}}$ is an N-by-N matrix, then $\mathbf{B}$ is orthogonal. Here we wish to prove that the orthogonal tensor associated with the skew-symmetric tensor $\hat{\mathbf{P}}$, i.e. $e^{\theta\hat{\mathbf{P}}}$, is the orthogonal tensor $\hat{\mathbf{Q}}$ given by eqn (4). To this end we employ the definition of the exponential matrix series in the special form

$$e^{\theta\hat{\mathbf{P}}} = \sum_{n=1}^{\infty} \frac{\theta^n\hat{\mathbf{P}}^n}{n!} = \mathbf{1} + \theta\hat{\mathbf{P}} + \frac{\theta^2}{2}\hat{\mathbf{P}}^2 + \sum_{n=0}^{\infty} \frac{(\theta\hat{\mathbf{P}})^{2n+3}}{(2n+3)!} + \sum_{n=0}^{\infty} \frac{(\theta\hat{\mathbf{P}})^{2n+4}}{(2n+4)!} \tag{43}$$

and observe that the last two terms have the representations

$$\sum_{n=0}^{\infty} \frac{(\theta\hat{\mathbf{P}})^{2n+3}}{(2n+3)!} = \tfrac{1}{6}(8\sin\theta - \sin 2\theta - 6\theta)\hat{\mathbf{P}} + \tfrac{1}{6}(2\sin\theta - \sin 2\theta)\hat{\mathbf{P}}^3 \tag{44}$$

$$\sum_{n=0}^{\infty} \frac{(\theta\hat{\mathbf{P}})^{2n+4}}{(2n+4)!} = \tfrac{1}{12}(15 - 6\theta^2 - 16\cos\theta + \cos 2\theta)\hat{\mathbf{P}}^2 + \tfrac{1}{12}(3 - 4\cos\theta + \cos 2\theta)\hat{\mathbf{P}}^4, \tag{45}$$

which follow from eqns (41), (42) and the series expansions for $\sin\theta$, $\cos\theta$, $\sin 2\theta$ and $\cos 2\theta$. Combining these last three results, it follows that

$$e^{\theta\hat{\mathbf{P}}} = \mathbf{1} + \tfrac{1}{6}(8\sin\theta - \sin 2\theta)\hat{\mathbf{P}} + \tfrac{1}{12}(15 - 16\cos\theta + \cos 2\theta)\hat{\mathbf{P}}^2 + \tfrac{1}{6}(2\sin\theta - \sin 2\theta)\hat{\mathbf{P}}^3 + \tfrac{1}{12}(3 - 4\cos\theta + \cos 2\theta)\hat{\mathbf{P}}^4. \tag{46}$$

Using the trigonometric double-angle formulae, eqn (46) becomes

$$e^{\theta\hat{\mathbf{P}}} = \hat{\mathbf{1}} + \sin\theta\hat{\mathbf{P}} + (1-\cos\theta)\hat{\mathbf{P}}^2 + \tfrac{1}{3}\sin\theta(1-\cos\theta)(\hat{\mathbf{P}} + \hat{\mathbf{P}}^3) + \tfrac{1}{6}(1-\cos\theta)^2(\hat{\mathbf{P}}^2 + \hat{\mathbf{P}}^4), \tag{47}$$

and it follows from formula (4) that

$$\hat{\mathbf{Q}} = e^{\theta\hat{\mathbf{P}}}. \tag{48}$$

4. EXAMPLE: APPLICATION OF THE SIX-DIMENSIONAL FORMULA TO MONOCLINIC MATERIAL SYMMETRY

The monoclinic crystal system has exactly one plane of reflective symmetry (Cowin and Mehrabadi, 1987; Gurtin, 1972; Hearmon, 1961; Lekhnitskii, 1963; Fedorov, 1968). A material is said to have a *plane of reflective symmetry* or a *mirror plane* at a point if the structure of the material has reflective or mirror symmetry with respect to a plane passing through the point. The formulae (1) and (4) apply to the planes of reflective symmetry; one has only to set the angle of rotation equal to π. The reflection transformation in three dimensions is denoted by $\mathbf{R}$ and defined by

$$\mathbf{R} = -\mathbf{Q}(\pi, \mathbf{p}) = -e^{\pi\mathbf{P}}; \tag{49}$$

it follows from eqns (1) and (3) that $\mathbf{R}$ has the representation

$$\mathbf{R} = -\mathbf{1} - 2\mathbf{P}^2 = \mathbf{1} - 2\mathbf{p}\otimes\mathbf{p} = \mathbf{R}^{\mathrm{T}}, \quad \mathbf{R}^2 = \mathbf{1}. \tag{50}$$

The reflection transformation in six dimensions is denoted by $\hat{\mathbf{R}}$ and defined by

$$\hat{\mathbf{R}} = \hat{\mathbf{Q}}(\pi, \mathbf{p}) = e^{\pi\hat{\mathbf{P}}}. \tag{51}$$

The fact that the definition of $\mathbf{R}$ contains a minus sign and that for $\hat{\mathbf{R}}$ does not, stems from the fact noted at the end of section 2, namely that the components of $\mathbf{Q}$ are squared to determine the components of $\hat{\mathbf{Q}}$. It follows from eqn (5) that $\hat{\mathbf{R}}$ has the representation

$$\hat{\mathbf{R}} = \hat{\mathbf{1}} + \tfrac{8}{3}\hat{\mathbf{P}}^2 + \tfrac{2}{3}\hat{\mathbf{P}}^4 = \hat{\mathbf{R}}^{\mathrm{T}}, \quad \hat{\mathbf{R}}^2 = \hat{\mathbf{1}}. \tag{52}$$

The normal to the plane of mirror symmetry is taken to be in the $\mathbf{e}_1$ direction; thus $\mathbf{p} = \mathbf{e}_1$ and from eqns (5) and (52) it follows that

$$\hat{\mathbf{R}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix}. \tag{53}$$

Monoclinic material symmetry requires that the matrix of tensor components of the elasticity tensor,

$$\hat{\mathbf{c}} = \begin{bmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{bmatrix}, \tag{54}$$

be invariant under a reflection. By invariant we mean that the components of $\hat{\mathbf{c}}$ referred to the original and the reflected coordinate system must be the same, that is to say

$$\hat{\mathbf{c}} = [\hat{c}_{KJ}] = [\hat{c}_{\Lambda\Psi}]; \tag{55}$$

thus the components of $\hat{\mathbf{c}}$ must satisfy the condition

$$\hat{\mathbf{c}} = \hat{\mathbf{R}}\hat{\mathbf{c}}\hat{\mathbf{R}}. \tag{56}$$

Substitution of eqns (53) and (54) into eqn (56) and the subsequent matrix multiplication yield

$$\hat{\mathbf{c}} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & \hat{c}_{15} & \hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & \hat{c}_{25} & \hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & \hat{c}_{35} & \hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & \hat{c}_{45} & \hat{c}_{46} \\ \hat{c}_{15} & \hat{c}_{25} & \hat{c}_{35} & \hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ \hat{c}_{16} & \hat{c}_{26} & \hat{c}_{36} & \hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{bmatrix} = \begin{bmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & -\hat{c}_{15} & -\hat{c}_{16} \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & -\hat{c}_{25} & -\hat{c}_{26} \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & -\hat{c}_{35} & -\hat{c}_{36} \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & -\hat{c}_{45} & -\hat{c}_{46} \\ -\hat{c}_{15} & -\hat{c}_{25} & -\hat{c}_{35} & -\hat{c}_{45} & \hat{c}_{55} & \hat{c}_{56} \\ -\hat{c}_{16} & -\hat{c}_{26} & -\hat{c}_{36} & -\hat{c}_{46} & \hat{c}_{56} & \hat{c}_{66} \end{bmatrix}. \tag{57}$$

From eqn (57) it is clear that $\hat{\mathbf{c}}$ is not invariant under the reflection $\hat{\mathbf{R}}$ unless

$$\hat{c}_{15} = \hat{c}_{25} = \hat{c}_{35} = \hat{c}_{45} = \hat{c}_{16} = \hat{c}_{26} = \hat{c}_{36} = \hat{c}_{46} = 0; \tag{58}$$

thus $\hat{\mathbf{c}}$ is given by

$$\hat{\mathbf{c}} = \begin{bmatrix} \hat{c}_{11} & \hat{c}_{12} & \hat{c}_{13} & \hat{c}_{14} & 0 & 0 \\ \hat{c}_{12} & \hat{c}_{22} & \hat{c}_{23} & \hat{c}_{24} & 0 & 0 \\ \hat{c}_{13} & \hat{c}_{23} & \hat{c}_{33} & \hat{c}_{34} & 0 & 0 \\ \hat{c}_{14} & \hat{c}_{24} & \hat{c}_{34} & \hat{c}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \hat{c}_{55} & \hat{c}_{56} \\ 0 & 0 & 0 & 0 & \hat{c}_{56} & \hat{c}_{66} \end{bmatrix}. \tag{59}$$

There are 13 distinct elements of $\hat{\mathbf{c}}$ for monoclinic symmetry in the representation (59), but an arbitrary rotation in the plane of reflection can be used to eliminate one of the 13 elements (Fedorov, 1968).

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APPENDIX. AN ALGEBRAIC DERIVATION OF THE REPRESENTATION OF RIGID OBJECT ROTATION IN THREE DIMENSIONS

The representation (1) of a three-dimensional rotation by an angle θ about the axis $\mathbf{p}$ is developed here using algebraic methods of functions of matrices. It is known (Finkbiner, 1960; Frazer *et al.*, 1960; Mirsky, 1990) that if $\mathbf{A}$ and $\mathbf{B}$ are square matrices of scalars, then the exponential function of matrices

$$e^{\mathbf{A}} = \sum_{n=1}^{\infty} \frac{\mathbf{A}^n}{n!} \tag{A1}$$

has the following properties:

$$\mathbf{B} = \mathbf{Q}^{\mathrm{T}}\mathbf{A}\mathbf{Q} \Rightarrow e^{\mathbf{B}} = \mathbf{Q}^{\mathrm{T}}e^{\mathbf{A}}\mathbf{Q}, \quad \mathbf{BA} = \mathbf{AB} \Rightarrow e^{\mathbf{A}+\mathbf{B}} = e^{\mathbf{A}}e^{\mathbf{B}} \tag{A2}$$

$$e^{-\mathbf{A}} = \{e^{\mathbf{A}}\}^{-1}, \quad e^{\mathbf{A}^{\mathrm{T}}} = \{e^{\mathbf{A}}\}^{\mathrm{T}}, \quad \frac{de^{t\mathbf{A}}}{dt} = \mathbf{A}e^{t\mathbf{A}} = e^{t\mathbf{A}}\mathbf{A}, \quad \mathbf{A} = \text{constant}. \tag{A3}$$

Using these properties it is easy to show that if $\mathbf{W}$ is skew-symmetric and $\mathbf{B} = e^{\chi\mathbf{W}}$, then $\mathbf{B}$ is orthogonal. Since the rotation matrix $\mathbf{Q}$ is orthogonal, it can be written as an exponential matrix function of a product of a skew-symmetric matrix, say $\mathbf{P}$, and the angle θ,

$$\mathbf{Q} = e^{\theta \mathbf{P}}. \tag{A4}$$

It follows from eqn (A1) that $\mathbf{Q}$ may be expressed as an infinite series,

$$\mathbf{Q} = \mathbf{1} + \frac{\theta}{1!}\mathbf{P} + \frac{\theta^2}{2!}\mathbf{P}^2 + \frac{\theta^3}{3!}\mathbf{P}^3 + \cdots + \frac{\theta^n}{n!}\mathbf{P}^n + \ldots \tag{A5}$$

and since, from eqn (3), $\mathbf{P}^3 = -\mathbf{P}$, it follows that

$$\mathbf{P}^{2n+1} = (-1)^n\mathbf{P}, \quad \mathbf{P}^{2n+2} = (-1)^n\mathbf{P}^2. \tag{A6}$$

The infinite series (A5) may be reduced to a sum of a finite number of terms,

$$\mathbf{Q} = \mathbf{1} + \left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} + \ldots\right)\mathbf{P} + \left(\frac{\theta^2}{2!} - \frac{\theta^4}{4!} + \frac{\theta^6}{6!} + \ldots\right)\mathbf{P}^2 = \mathbf{1} + \sin\theta\mathbf{P} + (1 - \cos\theta)\mathbf{P}^2, \tag{A7}$$

recovering the representation (1) again.