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On three-dimensional rotational averages

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In theories which describe the response of freely rotating molecules to externally imposed stimuli it is frequently necessary to average rotationally a product of direction cosines relating space-fixed and molecular coordinate frames. In this paper a systematic method for deriving the required tensor averages is presented, and results up to the seventh rank are explicitly shown. Where appropriate both reducible and irreducible expressions are given and their equivalence is demonstrated. Finally, some useful identities relating rotational averages of different ranks are noted.

I. INTRODUCTION

In the study of several physical processes such as the interaction of radiation with matter, experiments are frequently performed upon matter in a fluid phase. In order to relate the results of such experiments with theory, it is necessary to take random orientation of the molecules into account when deriving expressions for observables. This is usually accomplished by deriving the relevant result for a system with fixed orientation and then performing a rotational average. In general, the first step leads to an expression for an observable T of the form

$$T=A_{i_1\cdots i_n}P_{i_1\cdots i_n}\ , \qquad (1)$$

where $P_{i_1\cdots i_n}$ is the tensor associated with the response of a molecule to external conditions represented by $A_{i_1\cdots i_n}$. For example, in a dipole-allowed one-photon absorption calculation where T refers to the transition rate, **A** and **P** are second rank tensors related to the polarization of the radiation and the square of the transition moment, respectively. The tensor components of **A** and **P** in Eq. (1) are specified with respect to a common frame, say a space-fixed frame. This frame is usually chosen so that the components of the tensor **A** can be expressed in a simple manner. For a randomly oriented system it is convenient to re-express the components of the molecular property tensor **P** with respect to a molecule-fixed frame through the relation

$$P_{i_1\cdots i_n}=l_{i_1\lambda_1}\cdots l_{i_n\lambda_n}P_{\lambda_1\cdots\lambda_n}\ , \qquad (2)$$

where $l_{i_p\lambda_p}$ refers to the direction cosine of the angle between the space-fixed and molecule-fixed axes i_p and λ_p. The problem of obtaining the rotationally averaged result for T then reduces to that of finding the rotational average of the direction cosine product $l_{i_1\lambda_1}\cdots l_{i_n\lambda_n}$. For this purpose it is convenient to specify the direction cosines in Eq. (2) in terms of Euler angles, so that $l_{i_p\lambda_p}$ refers to the (i_p, λ_p) element of the Euler angle matrix.[1] Denoting the rotational average of $l_{i_1\lambda_1}\cdots l_{i_n\lambda_n}$ by $I^{(n)}_{i_1\cdots i_n;\lambda_1\cdots\lambda_n}$, we have

$$I^{(n)}_{i_1\cdots i_n;\lambda_1\cdots\lambda_n}=\frac{1}{8\pi^2}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi} l_{i_1\lambda_1}\cdots l_{i_n\lambda_n}\sin\theta\, d\varphi\, d\theta\, d\psi, \qquad (3)$$

where φ, θ, and ψ are the Euler angles relating the space-fixed and molecule-fixed frames. For low values of n these averages are easily worked out and are well known; recent applications include studies on higher multipole contributions to circular dichroism[2] and optical rotation.[3] Results for high n, however, are increasingly in demand for use in the theory of nonlinear optical processes. For example, the lowest order calculation on the hyper-Raman effect, which is a three-photon process, calls for the sixth rank average.[4,5] Calculations[6] on the differential hyper-Raman scattering by optically active molecules require rotational averages for even higher n. The trigonometric averaging procedure, though simple to use for low n, can be tedious for high n because a large number of integrals have to be evaluated. It is further complicated by the problem of reducibility, since for high n the tensor components are, in general, linearly dependent. Hence, a straightforward application of the trigonometric procedure to such cases does not lead to unique expressions for the averages.

In this paper we present a systematic method of calculating $I^{(n)}$ which does not rely on the explicit integration of Eq. (3). Results up to $n=7$ are given, and the relationship between the so-called reducible and irreducible forms are discussed. Finally, we note a few useful identities relating the rotational averages of different ranks.

II. METHOD

Since $I^{(n)}_{i_1\cdots i_n;\lambda_1\cdots\lambda_n}$ is rotationally invariant, it is possible to express it as a linear combination of isotropic tensors. According to an important theorem of Weyl[7] (see also Jeffreys[8]), each member of the sum is a product of two isotropic tensors—one with Latin suffices and the other with Greek suffices. An important feature of these products is that the Latin and Greek indices do not mix. For even n these isotropic tensors are products of $n/2$ Kronecker deltas such as $\delta_{i_1i_2}\cdots\delta_{i_{n-1}i_n}$; for odd n they are products of one Levi-Civita antisymmetric tensor and $(n-3)/2$ Kronecker deltas as for example $\epsilon_{i_1i_2i_3}\delta_{i_4i_5}\cdots\delta_{i_{n-1}i_n}$. In each case isomers of these tensors may be formed by permutation of the indices $i_1\cdots i_n$, and the total number of isomers is given by

$$\left.\begin{aligned} N_n&=\frac{n!}{2^{n/2}(n/2)!} && (n\ \text{even})\\ &=\frac{n!}{3\cdot 2^{(n-1)/2}((n-3)/2)!} && (n\ \text{odd})\end{aligned}\right\}\ . \qquad (4)$$

Let us denote the rth member of the set of isomers in the space-fixed frame by $f_r^{(n)}$, and the corresponding isomer in the molecular frame by $g_r^{(n)}$. We have suppressed the tensor indices for convenience. $I^{(n)}_{i_1\cdots i_n;\lambda_1\cdots\lambda_n}$

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TABLE I. The number of isotropic tensor isomers N_n and the size Q_n of the linearly independent basis set for rank n.

n	2	3	4	5	6	7	8	9	10
N_n	1	1	3	10	15	105	105	1260	945
Q_n	1	1	3	6	15	36	91	232	603

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is then a linear combination of the products $f_r^{(n)} g_s^{(n)}$:

$$I^{(n)} = \sum_{r,s} m_{rs}^{(n)} f_r^{(n)} g_s^{(n)} . \tag{5}$$

The problem thus reduces to finding the numerical coefficients $m_{rs}^{(n)}$.

Using the well-known relationships

$$\delta_{i_1 i_2} l_{i_1\lambda_1} l_{i_2\lambda_2} = \delta_{\lambda_1\lambda_2} , \tag{6}$$

$$\epsilon_{i_1 i_2 i_3} l_{i_1\lambda_1} l_{i_2\lambda_2} l_{i_3\lambda_3} = \epsilon_{\lambda_1\lambda_2\lambda_3} , \tag{7}$$

we write down the general equation

$$f_q^{(n)} l_{i_1\lambda_1} \cdots l_{i_n\lambda_n} = g_q^{(n)} . \tag{8}$$

A rotational average of Eq. (8) leads directly to

$$f_q^{(n)} I^{(n)} = g_q^{(n)} . \tag{9}$$

Combining Eqs. (5) and (9) and multiplying by $g_t^{(n)}$ we have

$$\sum_{r,s} f_q^{(n)} f_r^{(n)} m_{rs}^{(n)} g_s^{(n)} g_t^{(n)} = g_q^{(n)} g_t^{(n)} . \tag{10}$$

Let us denote the index-contracted product of two isomers $f_u^{(n)}$ and $f_v^{(n)}$ by $s_{uv}^{(n)}$. Then,

$$f_u^{(n)} f_v^{(n)} = g_u^{(n)} g_v^{(n)} = s_{uv}^{(n)} , \tag{11}$$

and Eq. (10) yields the important result

$$\mathbf{M}^{(n)} = (\mathbf{S}^{(n)})^{-1} . \tag{12}$$

Here, $\mathbf{M}^{(n)}$ is the square matrix with elements $m_{rs}^{(n)}$ and $\mathbf{S}^{(n)}$ is the square matrix with elements $s_{rs}^{(n)}$. Equation (12) holds provided the inverse of $\mathbf{S}^{(n)}$ exists. In order to employ this method to find $I^{(n)}$, it is therefore clearly essential to use complete and linearly independent basis sets of the isotropic tensors $f_r^{(n)}$ and $g_r^{(n)}$. By a simple group theoretical argument[9] it is easily shown that the number of linearly independent tensor isomers of rank n is given by

formula

$$Q_n = \sum_{r=0}^{p} \frac{n!\,(3r-n+1)}{(n-2r)!\,r!\,(r+1)!} , \tag{13}$$

where p assumes the value $n/2$ if n is even, and $(n-1)/2$ if n is odd. For $n=2$ to 10 the number of isomers N_n and the size Q_n of the linearly independent set are tabulated in Table I. From this table it is clear that for even $n \leq 6$ or for odd $n \leq 3$ the full set of isotropic tensor isomers are linearly independent and therefore form a suitable basis set. However, for even $n > 6$ or odd $n > 3$ the full set is overcomplete. We therefore need to select a complete and linearly independent subset for our basis, and this may be done using Smith's standard tableau method[10] as outlined in the next section. The reader is referred to Ref. 10 for details.

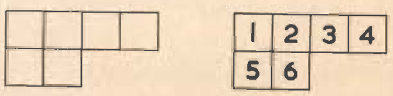
III. SMITH'S METHOD OF BASIS SET ENUMERATION

We first define a partition of n as a sequence of positive integers $(n_1 n_2 \cdots n_r)$ whose sum is n, with $n_1 \geq n_2 \cdots \geq n_r$. Corresponding to each partition we construct a frame of n squares in rows and columns, with n_i squares in row i the first elements of each row lying directly under one another. The partition (42) of $n=6$, for example, corresponds to the frame shown in Fig. 1(a). By entering the index numbers 1 to n in such a way that they increase in every row from left to right, and in every column reading downwards, we obtain what is termed a standard tableau; there are usually a number of these with different index ordering for each frame.[11] For a given n, it is in general possible to construct several frames; however, as Smith has shown, only certain frames can be used in the construction of the basis set. For convenience we discuss the even and odd rank cases separately.

Even rank. The construction of frames for even n is governed by two rules. First, the number of rows cannot exceed the dimensionality of the tensor, which in our case is three. Secondly, the frame columns must be in pairs with the two members of each pair having the same length, i.e., the same number of squares (see Fig. 2). The construction of standard tableaus from these frames is straightforward. With each pair of columns of a standard tableau is then associated a generalized Kronecker delta[12]

$$\delta^{i_\alpha \cdots i_\beta}_{i_\gamma \cdots i_\delta} = \begin{vmatrix} \delta_{i_\alpha i_\gamma} & \cdots & \delta_{i_\alpha i_\delta} \\ \vdots & & \\ \delta_{i_\beta i_\gamma} & \cdots & \delta_{i_\beta i_\delta} \end{vmatrix} , \tag{14}$$

where α to β are the successive entries down one column and γ to δ those down the other. For example, the standard tableau shown in Fig. 1(b) is associated with the tensor $\delta^{i_1 i_5}_{i_2 i_6} \delta^{i_3}_{i_4} = \delta_{i_1 i_2}\delta_{i_5 i_6}\delta_{i_3 i_4} - \delta_{i_1 i_6}\delta_{i_2 i_5}\delta_{i_3 i_4}$. It is useful to note that each type of frame used in constructing standard tableaus is associated with a different representation,[11] and the restrictions upon the types of frame permitted here limit the number of different types to $p(n/2, 3)$, which is the number of partitions of $n/2$ into at most three parts.[13] The total number of standard tableaus obtainable from these frames is precisely Q_n and the tensors they represent, or suitable linear combinations



(a) (b)

FIG. 1. (a) A typical frame, and (b) a typical standard tableau of rank 6.

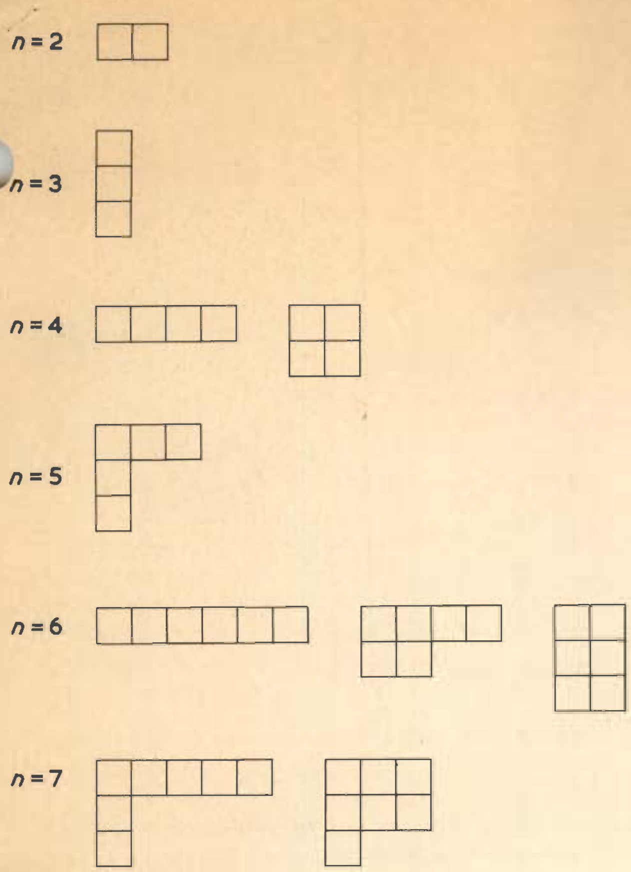


FIG. 2. Frames for tensors of rank n.

of these tensors, constitute a complete and linearly independent set.

Odd rank. For odd n we have an additional rule that the first column must contain three squares. The construction of the rest of the frame with $(n-3)$ squares is subject to the same rules as for the even n case discussed above. For example, when $n=7$ we have two possible frames (see Fig. 2). The first column of a standard tableau for odd n represents the antisymmetric tensor $\epsilon_{i_\alpha i_\beta i_\gamma}$, where α, β, and γ are the entries in this column, and the remaining pairs of columns are interpreted as generalized Kronecker deltas. The restrictions limit the number of permitted frames to $p[(n-3)/2, 3]$, and the standard tableaus again represent a complete set of Q_n linearly independent isotropic tensors.

Having outlined the procedure for determining suitable basis sets for construction of $S^{(n)}$ and use in the matrix inversion method to find $M^{(n)}$, we now explicitly evaluate the rotational averages for ranks $n=2$ to 7; for convenience, we again discuss the even and odd rank cases separately.

IV. ROTATIONAL AVERAGES OF EVEN RANK

A. $n=2$

There is only one isotropic tensor of rank 2, namely, $\delta_{i_1 i_2}$. Therefore,

TABLE II. The isotropic tensor isomers of rank 6.

r	$f_r^{(6)}$	r	$f_r^{(6)}$	r	$f_r^{(6)}$
1	$\delta_{i_1i_2}\delta_{i_3i_4}\delta_{i_5i_6}$	6	$\delta_{i_1i_3}\delta_{i_2i_6}\delta_{i_4i_5}$	11	$\delta_{i_1i_5}\delta_{i_2i_4}\delta_{i_3i_6}$
2	$\delta_{i_1i_2}\delta_{i_3i_5}\delta_{i_4i_6}$	7	$\delta_{i_1i_4}\delta_{i_2i_3}\delta_{i_5i_6}$	12	$\delta_{i_1i_5}\delta_{i_2i_6}\delta_{i_3i_4}$
3	$\delta_{i_1i_2}\delta_{i_3i_6}\delta_{i_4i_5}$	8	$\delta_{i_1i_4}\delta_{i_2i_5}\delta_{i_3i_6}$	13	$\delta_{i_1i_6}\delta_{i_2i_3}\delta_{i_4i_5}$
4	$\delta_{i_1i_3}\delta_{i_2i_4}\delta_{i_5i_6}$	9	$\delta_{i_1i_4}\delta_{i_2i_6}\delta_{i_3i_5}$	14	$\delta_{i_1i_6}\delta_{i_2i_4}\delta_{i_3i_5}$
5	$\delta_{i_1i_3}\delta_{i_2i_5}\delta_{i_4i_6}$	10	$\delta_{i_1i_5}\delta_{i_2i_3}\delta_{i_4i_6}$	15	$\delta_{i_1i_6}\delta_{i_2i_5}\delta_{i_3i_4}$

$$\mathbf{S}^{(2)} = \delta_{i_1 i_2}\delta_{i_1 i_2} = 3 , \tag{15}$$

which, together with Eqs. (5) and (12), leads directly to the well-known result

$$I^{(2)}_{i_1 i_2;\lambda_1\lambda_2} = \tfrac{1}{3}\delta_{i_1 i_2}\delta_{\lambda_1\lambda_2} . \tag{16}$$

B. $n=4$

The three independent isotropic tensors of rank 4 are

$$\left.\begin{aligned} f_1^{(4)} &= \delta_{i_1 i_2}\delta_{i_3 i_4} \\ f_2^{(4)} &= \delta_{i_1 i_3}\delta_{i_2 i_4} \\ f_3^{(4)} &= \delta_{i_1 i_4}\delta_{i_2 i_3} \end{aligned}\right\} . \tag{17}$$

Using them we find

$$\mathbf{S}^{(4)} = \begin{pmatrix} 9 & 3 & 3 \\ 3 & 9 & 3 \\ 3 & 3 & 9 \end{pmatrix} \tag{18}$$

hence

$$I^{(4)}_{i_1 i_2 i_3 i_4;\lambda_1\lambda_2\lambda_3\lambda_4} = \frac{1}{30}\begin{pmatrix} \delta_{i_1 i_2}\delta_{i_3 i_4} \\ \delta_{i_1 i_3}\delta_{i_2 i_4} \\ \delta_{i_1 i_4}\delta_{i_2 i_3} \end{pmatrix}^T \begin{pmatrix} 4 & -1 & -1 \\ -1 & 4 & -1 \\ -1 & -1 & 4 \end{pmatrix} \begin{pmatrix} \delta_{\lambda_1\lambda_2}\delta_{\lambda_3\lambda_4} \\ \delta_{\lambda_1\lambda_3}\delta_{\lambda_2\lambda_4} \\ \delta_{\lambda_1\lambda_4}\delta_{\lambda_2\lambda_3} \end{pmatrix} , \tag{19}$$

where T denotes transpose. This result has previously been obtained in a similar form by Keilich,[14] Monson and McClain,[15] and Power and Thirunamachandran.[2]

C. $n=6$

There are 15 tensor isomers for this case, as shown in Table II, and these form a linearly independent set. The matrix $\mathbf{S}^{(6)}$ may be constructed in the usual way, and the inverse gives

$$\mathbf{M}^{(6)}=\frac{1}{210}\begin{bmatrix}
16 & -5 & -5 & -5 & 2 & 2 & -5 & 2 & 2 & 2 & 2 & -5 & 2 & 2 & -5\\
-5 & 16 & -5 & 2 & -5 & 2 & 2 & 2 & -5 & -5 & 2 & 2 & 2 & -5 & 2\\
-5 & -5 & 16 & 2 & 2 & -5 & 2 & -5 & 2 & 2 & -5 & 2 & -5 & 2 & 2\\
-5 & 2 & 2 & 16 & -5 & -5 & -5 & 2 & 2 & 2 & -5 & 2 & 2 & -5 & 2\\
2 & -5 & 2 & -5 & 16 & -5 & 2 & -5 & 2 & -5 & 2 & 2 & 2 & 2 & -5\\
2 & 2 & -5 & -5 & -5 & 16 & 2 & 2 & -5 & 2 & 2 & -5 & -5 & 2 & 2\\
-5 & 2 & 2 & -5 & 2 & 2 & 16 & -5 & -5 & -5 & 2 & 2 & -5 & 2 & 2\\
2 & 2 & -5 & 2 & -5 & 2 & -5 & 16 & -5 & 2 & -5 & 2 & 2 & 2 & -5\\
2 & -5 & 2 & 2 & 2 & -5 & -5 & -5 & 16 & 2 & 2 & -5 & 2 & -5 & 2\\
2 & -5 & 2 & 2 & -5 & 2 & -5 & 2 & 2 & 16 & -5 & -5 & -5 & 2 & 2\\
2 & 2 & -5 & -5 & 2 & 2 & 2 & -5 & 2 & -5 & 16 & -5 & 2 & -5 & 2\\
-5 & 2 & 2 & 2 & 2 & -5 & 2 & 2 & -5 & -5 & -5 & 16 & 2 & 2 & -5\\
2 & 2 & -5 & 2 & 2 & -5 & -5 & 2 & 2 & -5 & 2 & 2 & 16 & -5 & -5\\
2 & -5 & 2 & -5 & 2 & 2 & 2 & 2 & -5 & 2 & -5 & 2 & -5 & 16 & -5\\
-5 & 2 & 2 & 2 & -5 & 2 & 2 & -5 & 2 & 2 & 2 & -5 & -5 & -5 & 16
\end{bmatrix} . \tag{20}$$

The result for $I^{(6)}$ now follows from Eq. (5), and in this form it has also been obtained by Kielich,[14] McClain,[5] and Healy.[3]

We conclude this section by noting that in the results discussed above, the number of independent coefficients in the matrices $\mathbf{M}^{(n)}$ in each case equals the number of permitted frames. This result is in general only applicable if the full set of tensor isomers is used for the basis.

V. ROTATIONAL AVERAGES OF ODD RANK

A. $n=3$

As for $n=2$, there is just one isotropic tensor of rank 3, namely, the Levi-Civita antisymmetric tensor $\epsilon_{i_1i_2i_3}$. Thus,

$$\mathbf{S}^{(3)}=\epsilon_{i_1i_2i_3}\epsilon_{i_1i_2i_3}=6 \tag{21}$$

and

$$I^{(3)}_{i_1i_2i_3;\lambda_1\lambda_2\lambda_3}=\tfrac{1}{6}\epsilon_{i_1i_2i_3}\epsilon_{\lambda_1\lambda_2\lambda_3} . \tag{22}$$

B. $n=5$

This is the first instance where we have to choose a linearly independent subset from the full isomer set, as $Q_n < N_n$ (see Table I). For $n=5$ there is only one allowed frame, corresponding to the partition (311), from which six standard tableaus may be constructed. They correspond to the tensors

$$\left.\begin{aligned}
f_1^{(5)}&=\epsilon_{i_1i_2i_3}\delta_{i_4i_5}\\
f_2^{(5)}&=\epsilon_{i_1i_2i_4}\delta_{i_3i_5}\\
f_3^{(5)}&=\epsilon_{i_1i_2i_5}\delta_{i_3i_4}\\
f_4^{(5)}&=\epsilon_{i_1i_3i_4}\delta_{i_2i_5}\\
f_5^{(5)}&=\epsilon_{i_1i_3i_5}\delta_{i_2i_4}\\
f_6^{(5)}&=\epsilon_{i_1i_4i_5}\delta_{i_2i_3}
\end{aligned}\right\} . \tag{23}$$

Using this basis set we find the following result for $I^{(5)}$, in agreement with Kielich[16]:

$$I^{(5)}_{i_1i_2i_3i_4i_5;\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5}=\frac{1}{30}\begin{bmatrix}\epsilon_{i_1i_2i_3}\,\delta_{i_4i_5}\\ \epsilon_{i_1i_2i_4}\,\delta_{i_3i_5}\\ \epsilon_{i_1i_2i_5}\,\delta_{i_3i_4}\\ \epsilon_{i_1i_3i_4}\,\delta_{i_2i_5}\\ \epsilon_{i_1i_3i_5}\,\delta_{i_2i_4}\\ \epsilon_{i_1i_4i_5}\,\delta_{i_2i_3}\end{bmatrix}^T\begin{bmatrix}3 & -1 & -1 & 1 & 1 & 0\\ -1 & 3 & -1 & -1 & 0 & 1\\ -1 & -1 & 3 & 0 & -1 & -1\\ 1 & -1 & 0 & 3 & -1 & 1\\ 1 & 0 & -1 & -1 & 3 & -1\\ 0 & 1 & -1 & 1 & -1 & 3\end{bmatrix}\begin{bmatrix}\epsilon_{\lambda_1\lambda_2\lambda_3}\,\delta_{\lambda_4\lambda_5}\\ \epsilon_{\lambda_1\lambda_2\lambda_4}\,\delta_{\lambda_3\lambda_5}\\ \epsilon_{\lambda_1\lambda_2\lambda_5}\,\delta_{\lambda_3\lambda_4}\\ \epsilon_{\lambda_1\lambda_3\lambda_4}\,\delta_{\lambda_2\lambda_5}\\ \epsilon_{\lambda_1\lambda_3\lambda_5}\,\delta_{\lambda_2\lambda_4}\\ \epsilon_{\lambda_1\lambda_4\lambda_5}\,\delta_{\lambda_2\lambda_3}\end{bmatrix} . \tag{24}$$

This result is, however, also expressible in terms of the overcomplete set of N_n tensor isomers. We shall refer to such results as reducible, to distinguish them from the irreducible type involving only the Q_n isomers. We shall also denote the tensors and matrices associated with such reducible results with primes henceforth.

For the fifth rank case the full set of ten tensor isomers consists of the six given in Eq. (23), with $f_r^{(5)}$ read as $f_r'^{(5)}$, and the four listed below, each of which is expressible in terms of the original six tensors as shown:

$$f_7'^{(5)} = \epsilon_{i_2 i_3 i_4}\delta_{i_1 i_5} = f_1^{(5)} - f_2^{(5)} + f_4^{(5)} , \tag{25}$$

$$f_8'^{(5)} = \epsilon_{i_2 i_3 i_5}\delta_{i_1 i_4} = f_1^{(5)} - f_3^{(5)} + f_5^{(5)} , \tag{26}$$

$$f_9'^{(5)} = \epsilon_{i_2 i_4 i_5}\delta_{i_1 i_3} = f_2^{(5)} - f_3^{(5)} + f_6^{(5)} , \tag{27}$$

$$f_{10}'^{(5)} = \epsilon_{i_3 i_4 i_5}\delta_{i_1 i_2} = f_4^{(5)} - f_5^{(5)} + f_6^{(5)} . \tag{28}$$

We can now deduce from symmetry considerations[17] that the reducible matrix $\mathbf{M}'^{(5)}$ can be written in the form

$$\mathbf{M}'^{(5)} = \begin{bmatrix} a & b & b & -b & -b & 0 & b & b & 0 & 0 \\ b & a & b & b & 0 & -b & -b & 0 & b & 0 \\ b & b & a & 0 & b & b & 0 & -b & -b & 0 \\ -b & b & 0 & a & b & -b & b & 0 & 0 & b \\ -b & 0 & b & b & a & b & 0 & b & 0 & -b \\ 0 & -b & b & -b & b & a & 0 & 0 & b & b \\ b & -b & 0 & b & 0 & 0 & a & b & -b & b \\ b & 0 & -b & 0 & b & 0 & b & a & b & -b \\ 0 & b & -b & 0 & 0 & b & -b & b & a & b \\ 0 & 0 & 0 & b & -b & b & b & -b & b & a \end{bmatrix} , \tag{29}$$

where a and b are undetermined coefficients. Explicit integration of Eq. (3) yields just one equation relating a and b, namely,

$$a + 2b = 1/30 . \tag{30}$$

This agrees with the observation that as the full set of tensor isomers is used, the number of independent coefficients must equal the number of allowed frames for $n=5$, i.e., one. The overcompleteness of the basis set precludes unique solutions, and any pair of values satisfying Eq. (30) can be used to express $I^{(5)}$. One such pair, $a=1/30$, $b=0$, leads to the following particularly simple form[2]:

$$\begin{aligned} I^{(5)}_{i_1 i_2 i_3 i_4 i_5;\lambda_1\lambda_2\lambda_3\lambda_4\lambda_5} = \tfrac{1}{30}(&\epsilon_{i_1 i_2 i_3}\delta_{i_4 i_5}\epsilon_{\lambda_1\lambda_2\lambda_3}\delta_{\lambda_4\lambda_5} + \epsilon_{i_1 i_2 i_4}\delta_{i_3 i_5}\epsilon_{\lambda_1\lambda_2\lambda_4}\delta_{\lambda_3\lambda_5} + \epsilon_{i_1 i_2 i_5}\delta_{i_3 i_4}\epsilon_{\lambda_1\lambda_2\lambda_5}\delta_{\lambda_3\lambda_4} + \epsilon_{i_1 i_3 i_4}\delta_{i_2 i_5}\epsilon_{\lambda_1\lambda_3\lambda_4}\delta_{\lambda_2\lambda_5} \\ &+ \epsilon_{i_1 i_3 i_5}\delta_{i_2 i_4}\epsilon_{\lambda_1\lambda_3\lambda_5}\delta_{\lambda_2\lambda_4} + \epsilon_{i_1 i_4 i_5}\delta_{i_2 i_3}\epsilon_{\lambda_1\lambda_4\lambda_5}\delta_{\lambda_2\lambda_3} + \epsilon_{i_2 i_3 i_4}\delta_{i_1 i_5}\epsilon_{\lambda_2\lambda_3\lambda_4}\delta_{\lambda_1\lambda_5} + \epsilon_{i_2 i_3 i_5}\delta_{i_1 i_4}\epsilon_{\lambda_2\lambda_3\lambda_5}\delta_{\lambda_1\lambda_4} \\ &+ \epsilon_{i_2 i_4 i_5}\delta_{i_1 i_3}\epsilon_{\lambda_2\lambda_4\lambda_5}\delta_{\lambda_1\lambda_3} + \epsilon_{i_3 i_4 i_5}\delta_{i_1 i_2}\epsilon_{\lambda_3\lambda_4\lambda_5}\delta_{\lambda_1\lambda_2}) . \end{aligned} \tag{31}$$

To demonstrate the equivalence[18] of the irreducible form (24) and the reducible form following from Eq. (29) we write

$$\left.\begin{aligned} f_r'^{(5)} &= \sum_{s=1}^{6} h_{rs} f_s^{(5)} \\ g_r'^{(5)} &= \sum_{s=1}^{6} h_{rs} g_s^{(5)} \end{aligned}\right\} , \tag{32}$$

where the coefficients h_{rs} are easily obtained with the aid of Eqs. (25)–(28). The reducible 10×10 matrix $\mathbf{M}'^{(5)}$ is then related to the irreducible 6×6 matrix $\mathbf{M}^{(5)}$ through the equation

$$\mathbf{M}^{(5)} = \mathbf{H}^T \mathbf{M}'^{(5)} \mathbf{H} , \tag{33}$$

where the matrix elements of the 10×6 matrix $\mathbf{H}$ are h_{rs}. A straightforward multiplication shows that Eq. (33) holds provided Eq. (30) is satisfied.

[illegible]. $n = 7$

Of the 105 isotropic tensor isomers for $n=7$, it is possible to choose a linearly independent set of 36 isomers by writing down the standard tableaus corresponding to the frames (331) and (511) shown in Fig. 2. These isomers are given in Table III. Construction of the matrix $\mathbf{S}^{(7)}$ then leads directly to the result, Eq. (34), for $\mathbf{M}^{(7)}$, and hence $I^{(7)}$ is obtained.

TABLE III. The irreducible set of rank 7 isomers.

r	$f_r^{(7)}$	r	$f_r^{(7)}$	r	$f_r^{(7)}$
1	$\epsilon_{i_1 i_2 i_3}\delta_{i_4 i_5}\delta_{i_6 i_7}$	13	$\epsilon_{i_1 i_2 i_7}\delta_{i_3 i_4}\delta_{i_5 i_6}$	25	$\epsilon_{i_1 i_3 i_7}\delta_{i_2 i_4}\delta_{i_5 i_6}$
2	$\epsilon_{i_1 i_2 i_3}\delta_{i_4 i_6}\delta_{i_5 i_7}$	14	$\epsilon_{i_1 i_2 i_7}\delta_{i_3 i_5}\delta_{i_4 i_6}$	26	$\epsilon_{i_1 i_3 i_7}\delta_{i_2 i_5}\delta_{i_4 i_6}$
3	$\epsilon_{i_1 i_2 i_3}\delta_{i_4 i_7}\delta_{i_5 i_6}$	15	$\epsilon_{i_1 i_2 i_7}\delta_{i_3 i_6}\delta_{i_4 i_5}$	27	$\epsilon_{i_1 i_3 i_7}\delta_{i_2 i_6}\delta_{i_4 i_5}$
4	$\epsilon_{i_1 i_2 i_4}\delta_{i_3 i_5}\delta_{i_6 i_7}$	16	$\epsilon_{i_1 i_3 i_4}\delta_{i_2 i_5}\delta_{i_6 i_7}$	28	$\epsilon_{i_1 i_4 i_5}\delta_{i_2 i_3}\delta_{i_6 i_7}$
5	$\epsilon_{i_1 i_2 i_4}\delta_{i_3 i_6}\delta_{i_5 i_7}$	17	$\epsilon_{i_1 i_3 i_4}\delta_{i_2 i_6}\delta_{i_5 i_7}$	29	$\epsilon_{i_1 i_4 i_5}\delta_{i_2 i_7}\delta_{i_3 i_6}$
6	$\epsilon_{i_1 i_2 i_4}\delta_{i_3 i_7}\delta_{i_5 i_6}$	18	$\epsilon_{i_1 i_3 i_4}\delta_{i_2 i_7}\delta_{i_5 i_6}$	30	$\epsilon_{i_1 i_4 i_6}\delta_{i_2 i_3}\delta_{i_5 i_7}$
7	$\epsilon_{i_1 i_2 i_5}\delta_{i_3 i_4}\delta_{i_6 i_7}$	19	$\epsilon_{i_1 i_3 i_5}\delta_{i_2 i_4}\delta_{i_6 i_7}$	31	$\epsilon_{i_1 i_4 i_6}\delta_{i_2 i_7}\delta_{i_3 i_5}$
8	$\epsilon_{i_1 i_2 i_5}\delta_{i_3 i_6}\delta_{i_4 i_7}$	20	$\epsilon_{i_1 i_3 i_5}\delta_{i_2 i_6}\delta_{i_4 i_7}$	32	$\epsilon_{i_1 i_4 i_7}\delta_{i_2 i_3}\delta_{i_5 i_6}$
9	$\epsilon_{i_1 i_2 i_5}\delta_{i_3 i_7}\delta_{i_4 i_6}$	21	$\epsilon_{i_1 i_3 i_5}\delta_{i_2 i_7}\delta_{i_4 i_6}$	33	$\epsilon_{i_1 i_4 i_7}\delta_{i_2 i_6}\delta_{i_3 i_5}$
10	$\epsilon_{i_1 i_2 i_6}\delta_{i_3 i_4}\delta_{i_5 i_7}$	22	$\epsilon_{i_1 i_3 i_6}\delta_{i_2 i_4}\delta_{i_5 i_7}$	34	$\epsilon_{i_1 i_5 i_6}\delta_{i_2 i_3}\delta_{i_4 i_7}$
11	$\epsilon_{i_1 i_2 i_6}\delta_{i_3 i_5}\delta_{i_4 i_7}$	23	$\epsilon_{i_1 i_3 i_6}\delta_{i_2 i_5}\delta_{i_4 i_7}$	35	$\epsilon_{i_1 i_5 i_7}\delta_{i_2 i_3}\delta_{i_4 i_6}$
12	$\epsilon_{i_1 i_2 i_6}\delta_{i_3 i_7}\delta_{i_4 i_5}$	24	$\epsilon_{i_1 i_3 i_6}\delta_{i_2 i_7}\delta_{i_4 i_5}$	36	$\epsilon_{i_1 i_6 i_7}\delta_{i_2 i_3}\delta_{i_4 i_5}$

$$M^{(7)}=\frac{1}{420}\left[\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr}
51 & -28 & -13 & -35 & 22 & 7 & -5 & -8 & 7 & 1 & 16 & -15 & 1 & 16 & -15 & 15 & -16 & -1 & 15 & -1 & -16 & -7 & -7 & 20 & -7 & -7 & 20 & -15 & 15 & 9 & -15 & 9 & -15 & -6 & -6 & 0 \\
-28 & 66 & -28 & 32 & -40 & 6 & -4 & 26 & -16 & -10 & 2 & 6 & 12 & -34 & 12 & -6 & 40 & -32 & -12 & -12 & 34 & 10 & -6 & -2 & 4 & 16 & -26 & 24 & -30 & 0 & 0 & -24 & 30 & 6 & 12 & 6 \\
-13 & -28 & 51 & 1 & 16 & -15 & 7 & -20 & 7 & 7 & -20 & 7 & -15 & 16 & 1 & -7 & -22 & 35 & -1 & 15 & -16 & -1 & 15 & -16 & 5 & -7 & 8 & -9 & 15 & -9 & 15 & 15 & -15 & 0 & -6 & -6 \\
-35 & 32 & 1 & 67 & -42 & -11 & -19 & 28 & -3 & 9 & -28 & 11 & 9 & -28 & 11 & -15 & 24 & -7 & -9 & -7 & 24 & 5 & 7 & -18 & 5 & 7 & -18 & 37 & -31 & -19 & 25 & -19 & 25 & 14 & 14 & 0 \\
22 & -40 & 16 & -42 & 62 & -10 & 14 & -38 & 12 & -14 & 18 & -2 & -2 & 20 & -14 & 4 & -30 & 24 & 10 & 12 & -32 & -4 & -2 & 10 & -6 & -4 & 16 & -34 & 40 & 22 & -16 & 14 & -20 & -14 & -12 & 2 \\
7 & 6 & -15 & -11 & -10 & 27 & 3 & 6 & -9 & 3 & 6 & -9 & -9 & 4 & 3 & 5 & 4 & -15 & -1 & -3 & 6 & -1 & -3 & 6 & 1 & -1 & 0 & -1 & -5 & -1 & -5 & 7 & -1 & 0 & -2 & -2 \\
-5 & -4 & 7 & -19 & 14 & 3 & 27 & -16 & -5 & -9 & 8 & 1 & -9 & 8 & 1 & 1 & -6 & 5 & -5 & 5 & -6 & 1 & -1 & 2 & 1 & -1 & 2 & -17 & 11 & 7 & -5 & 7 & -5 & -6 & -6 & 0 \\
-8 & 26 & -20 & 28 & -38 & 6 & -16 & 50 & -16 & 8 & -22 & 8 & 6 & -6 & -4 & 0 & 16 & -18 & -6 & -16 & 28 & 4 & 2 & -10 & 2 & 0 & -4 & 28 & -34 & -16 & 14 & -10 & 10 & 18 & 6 & 2 \\
7 & -16 & 7 & -3 & 12 & -9 & -5 & -16 & 27 & 1 & 8 & -9 & 3 & -8 & 3 & -1 & -4 & 7 & 5 & 5 & -16 & -3 & -1 & 6 & -1 & 1 & 0 & -5 & 11 & 5 & -5 & -1 & -1 & -6 & 6 & -2 \\
1 & -10 & 7 & 9 & -14 & 3 & -9 & 8 & 1 & 27 & -16 & -5 & -9 & 6 & 3 & -1 & -4 & 5 & 1 & -1 & 2 & -5 & 5 & -6 & 1 & -3 & 4 & 7 & -5 & -17 & 11 & 7 & -5 & 6 & 0 & -6 \\
16 & 2 & -20 & -28 & 18 & 6 & 8 & -22 & 8 & -16 & 50 & -16 & 6 & -14 & 4 & 6 & 10 & -18 & 4 & 2 & -10 & -6 & -16 & 28 & 2 & 6 & -10 & -16 & 14 & 28 & -34 & -10 & 10 & -18 & 2 & 6 \\
-15 & 6 & 7 & 11 & -2 & -9 & 1 & 8 & -9 & -5 & -16 & 27 & 3 & 4 & -9 & -3 & -2 & 7 & -3 & -1 & 6 & 5 & 5 & -16 & -1 & -1 & 2 & 5 & -5 & -5 & 11 & -1 & -1 & 6 & -2 & 6 \\
1 & 12 & -15 & 9 & -2 & -9 & -9 & 6 & 3 & -9 & 6 & 3 & 27 & -16 & -5 & -1 & 10 & -9 & 1 & -3 & 4 & 1 & -3 & 4 & -5 & 5 & -6 & 7 & -5 & 7 & -5 & -17 & 11 & 0 & 6 & 6 \\
16 & -34 & 16 & -28 & 20 & 4 & 8 & -6 & -8 & 6 & -14 & 4 & -16 & 50 & -16 & 6 & -32 & 24 & 4 & 4 & -12 & 2 & 6 & -10 & -6 & -16 & 28 & -16 & 14 & -10 & 10 & 28 & -34 & 2 & -18 & -6 \\
-15 & 12 & 1 & 11 & -14 & 3 & 1 & -4 & 3 & 3 & 4 & -9 & -5 & -16 & 27 & -3 & 12 & -7 & -3 & 1 & 4 & -1 & -1 & 2 & 5 & 5 & -16 & 5 & -5 & -1 & -1 & -5 & 11 & -2 & 6 & -6 \\
15 & -6 & -7 & -15 & 4 & 5 & 1 & 0 & -1 & -1 & 6 & -3 & -1 & 6 & -3 & 27 & -10 & -11 & -9 & 3 & 4 & 3 & -9 & 6 & 3 & -9 & 6 & 7 & -1 & -1 & -5 & -1 & -5 & 2 & 2 & 0 \\
-16 & 40 & -22 & 24 & -30 & 4 & -6 & 16 & -4 & -4 & 10 & -2 & 10 & -32 & 12 & -10 & 62 & -42 & -2 & -14 & 20 & -14 & -2 & 18 & 14 & 12 & -38 & 14 & -20 & 22 & -16 & -34 & 40 & -2 & 12 & 14 \\
-1 & -32 & 35 & -7 & 24 & -15 & 5 & -18 & 7 & 5 & -18 & 7 & -9 & 24 & -7 & -11 & -42 & 67 & 9 & 11 & -28 & 9 & 11 & -28 & -19 & -3 & 28 & -19 & 25 & -19 & 25 & 37 & -31 & 0 & -14 & -14 \\
15 & -12 & -1 & -9 & 10 & -1 & -5 & -6 & 5 & 1 & 4 & -3 & 1 & 4 & -3 & -9 & -2 & 9 & 27 & -5 & -16 & -9 & 3 & 6 & -9 & 3 & 6 & -17 & 11 & 7 & -5 & 7 & -5 & -6 & -6 & 0 \\
-1 & -12 & 15 & -7 & 12 & -3 & 5 & -16 & 5 & -1 & 2 & -1 & -3 & 4 & 1 & 3 & -14 & 11 & -5 & 27 & -16 & 3 & -9 & 4 & 1 & 3 & -4 & -5 & 11 & -1 & -1 & 5 & -5 & 6 & -6 & 2 \\
-16 & 34 & -16 & 24 & -32 & 6 & -6 & 28 & -16 & 2 & -10 & 6 & 4 & -12 & 4 & 4 & 20 & -28 & -16 & -16 & 50 & 6 & 4 & -14 & 8 & -8 & -6 & 28 & -34 & -10 & 10 & -16 & 14 & 6 & 18 & -2 \\
-7 & 10 & -1 & 5 & -4 & -1 & 1 & 4 & -3 & -5 & -6 & 5 & 1 & 2 & -1 & 3 & -14 & 9 & -9 & 3 & 6 & 27 & -5 & -16 & -9 & 1 & 8 & 7 & -5 & -17 & 11 & 7 & -5 & 6 & 0 & -6 \\
-7 & -6 & 15 & 7 & -2 & -3 & -1 & 2 & -1 & 5 & -16 & 5 & -3 & 6 & -1 & -9 & -2 & 11 & 3 & -9 & 4 & -5 & 27 & -16 & 1 & -9 & 8 & -1 & -1 & -5 & 11 & 5 & -5 & -6 & 2 & -6 \\
20 & -2 & -16 & -18 & 10 & 6 & 2 & -10 & 6 & -6 & 28 & -16 & 4 & -10 & 2 & 6 & 18 & -28 & 6 & 4 & -14 & -16 & -16 & 50 & 8 & 8 & -22 & -10 & 10 & 28 & -34 & -16 & 14 & -6 & -2 & 18 \\
-7 & 4 & 5 & 5 & -6 & 1 & 1 & 2 & -1 & 1 & 2 & -1 & -5 & -6 & 5 & 3 & 14 & -19 & -9 & 1 & 8 & -9 & 1 & 8 & 27 & -5 & -16 & 7 & -5 & 7 & -5 & -17 & 11 & 0 & 6 & 6 \\
-7 & 16 & -7 & 7 & -4 & -1 & -1 & 0 & 1 & -3 & 6 & -1 & 5 & -16 & 5 & -9 & 12 & -3 & 3 & 3 & -8 & 1 & -9 & 8 & -5 & 27 & -16 & -1 & -1 & 5 & -5 & -5 & 11 & 2 & -6 & 6 \\
20 & -26 & 8 & -18 & 16 & 0 & 2 & -4 & 0 & 4 & -10 & 2 & -6 & 28 & -16 & 6 & -38 & 28 & 6 & -4 & -6 & 8 & 8 & -22 & -16 & -16 & 50 & -10 & 10 & -16 & 14 & 28 & -34 & -2 & -6 & -18 \\
-15 & 24 & -9 & 37 & -34 & -1 & -17 & 28 & -5 & 7 & -16 & 5 & 7 & -16 & 5 & 7 & 14 & -19 & -17 & -5 & 28 & 7 & -1 & -10 & 7 & -1 & -10 & 51 & -33 & -21 & 15 & -21 & 15 & 18 & 18 & 0 \\
15 & -30 & 15 & -31 & 40 & -5 & 11 & -34 & 11 & -5 & 14 & -5 & -5 & 14 & -5 & -1 & -20 & 25 & 11 & 11 & -34 & -5 & -1 & 10 & -5 & -1 & 10 & -33 & 45 & 15 & -15 & 15 & -15 & -12 & -12 & 0 \\
9 & 0 & -9 & -19 & 22 & -1 & 7 & -16 & 5 & -17 & 28 & -5 & 7 & -10 & -1 & -1 & 22 & -19 & 7 & -1 & -10 & -17 & -5 & 28 & 7 & 5 & -16 & -21 & 15 & 51 & -33 & -21 & 15 & -18 & 0 & 18 \\
-15 & 0 & 15 & 25 & -16 & -5 & -5 & 14 & -5 & 11 & -34 & 11 & -5 & 10 & -1 & -5 & -16 & 25 & -5 & -1 & 10 & 11 & 11 & -34 & -5 & -5 & 14 & 15 & -15 & -33 & 45 & 15 & -15 & 12 & 0 & -12 \\
9 & -24 & 15 & -19 & 14 & 7 & 7 & -10 & -1 & 7 & -10 & -1 & -17 & 28 & -5 & -1 & -34 & 37 & 7 & 5 & -16 & 7 & 5 & -16 & -17 & -5 & 28 & -21 & 15 & -21 & 15 & 51 & -33 & 0 & -18 & -18 \\
-15 & 30 & -15 & 25 & -20 & -1 & -5 & 10 & -1 & -5 & 10 & -1 & 11 & -34 & 11 & -5 & 40 & -31 & -5 & -5 & 14 & -5 & -5 & 14 & 11 & 11 & -34 & 15 & -15 & 15 & -15 & -33 & 45 & 0 & 12 & 12 \\
-6 & 6 & 0 & 14 & -14 & 0 & -6 & 18 & -6 & 6 & -18 & 6 & 0 & 2 & -2 & 2 & -2 & 0 & -6 & 6 & 6 & 6 & -6 & -6 & 0 & 2 & -2 & 18 & -12 & -18 & 12 & 0 & 0 & 30 & -6 & 6 \\
-6 & 12 & -6 & 14 & -12 & -2 & -6 & 6 & 6 & 0 & 2 & -2 & 6 & -18 & 6 & 2 & 12 & -14 & -6 & -6 & 18 & 0 & 2 & -2 & 6 & -6 & -6 & 18 & -12 & 0 & 0 & -18 & 12 & -6 & 30 & -6 \\
0 & 6 & -6 & 0 & 2 & -2 & 0 & 2 & -2 & -6 & 6 & 6 & 6 & -6 & -6 & 0 & 14 & -14 & 0 & 2 & -2 & -6 & -6 & 18 & 6 & 6 & -18 & 0 & 0 & 18 & -12 & -18 & 12 & 6 & -6 & 30
\end{array}\right]. \tag{34}$$

Once again the result may be expressed in reducible form by adopting the overcomplete basis set comprising the 105 isotropic tensor isomers. These may be grouped into 35 sets of three, each set being associated with a particular epsilon; the three members of a given set differ only in their pairing of indices in the Kronecker deltas. The 35 epsilons are obtainable using the dictionary order, i.e., $\epsilon_{i_1 i_2 i_3}$, $\epsilon_{i_1 i_2 i_4}$, $\epsilon_{i_1 i_2 i_5}, \ldots$. For each epsilon, three successive isomers of rank 7 are obtained by multiplying by $f_1^{(4)}$, $f_2^{(4)}$, $f_3^{(4)}$ of Eq. (17), respectively, with the indices i_1, i_2, i_3, i_4 replaced by the four unused indices in ascending order. For example, the first three isomers are formed with the first epsilon and the unused indices i_4, i_5, i_6, and i_7; so we have

$$\left.\begin{aligned} f_1'^{(7)} &= \epsilon_{i_1 i_2 i_3}\delta_{i_4 i_5}\delta_{i_6 i_7} \\ f_2'^{(7)} &= \epsilon_{i_1 i_2 i_3}\delta_{i_4 i_6}\delta_{i_5 i_7} \\ f_3'^{(7)} &= \epsilon_{i_1 i_2 i_3}\delta_{i_4 i_7}\delta_{i_5 i_6} \end{aligned}\right\} . \tag{35}$$

The 105×105 matrix $M'^{(7)}$ can now be written in block diagonal form with one 3×3 block for each epsilon, as expressed by the direct product

$$M'^{(7)} = E \times A \ , \tag{36}$$

where E is the unit matrix of rank 35, and A is the 3×3 matrix

$$\mathrm{A} = \frac{1}{840}\begin{pmatrix} 6 & -1 & -1 \\ -1 & 6 & -1 \\ -1 & -1 & 6 \end{pmatrix} . \tag{37}$$

In this form the seventh rank average result appears attractively simple. However, it should be borne in mind that in the application to a particular physical problem the simplest result may follow from use of the irreducible form which involves a smaller number of basis tensors.[19] The equivalence of the reducible and irreducible forms may be demonstrated in a manner analogous to that described for $I^{(5)}$.

We conclude our discussion of the odd rank averages by noting that the number of independent coefficients in the reducible matrices $\mathrm{M}'^{(n)}$ is equal to the partition $p[(n-3)/2, 3]$, which in turn equals the number of independent coefficients for the average of even rank $n-3$. Moreover, there are N_{n-3} isotropic tensor isomers of rank n for each of the epsilons, e.g., $N_4 = 3$ isomers for each of the 35 epsilons in the rank 7 case. Consequently, it is always possible to write a rotational average of odd rank in a block diagonal form, where there is one block for each epsilon and each block has the same set of $p[(n-3)/2, 3]$ distinct coefficients. The reducible results given above for $I^{(5)}$ and $I^{(7)}$ are both in this diagonal form.

VI. RELATIONS BETWEEN ROTATIONAL AVERAGES OF DIFFERENT RANKS

We conclude with some useful identities involving the relations between the rotational averages of different ranks. First, using Eq. (6) we note that

$$l_{i_1\lambda_1} \cdots l_{i_{n-2}\lambda_{n-2}} l_{i_{n-1}\lambda_{n-1}} l_{i_n\lambda_n} \delta_{i_{n-1}i_n} \delta_{\lambda_{n-1}\lambda_n} = 3 l_{i_1\lambda_1} \cdots l_{i_{n-2}\lambda_{n-2}} , \tag{38}$$

which upon rotational averaging gives

$$\tfrac{1}{3} I^{(n)}_{i_1 \cdots i_n; \lambda_1 \cdots \lambda_n} \delta_{i_{n-1}i_n} \delta_{\lambda_{n-1}\lambda_n} = I^{(n-2)}_{i_1 \cdots i_{n-2}; \lambda_1 \cdots \lambda_{n-2}} . \tag{39}$$

Similarly, using Eq. (7), we can relate $I^{(n)}$ to $I^{(n-3)}$ by

$$\tfrac{1}{6} I^{(n)}_{i_1 \cdots i_n; \lambda_1 \cdots \lambda_n} \epsilon_{i_{n-2}i_{n-1}i_n} \epsilon_{\lambda_{n-2}\lambda_{n-1}\lambda_n} = I^{(n-3)}_{i_1 \cdots i_{n-3}; \lambda_1 \cdots \lambda_{n-3}} . \tag{40}$$

To relate $I^{(n)}$ to $I^{(n-1)}$ we start with the elementary relation

$$\tfrac{1}{2} l_{i_2\lambda_2} l_{i_3\lambda_3} \epsilon_{i_1 i_2 i_3} \epsilon_{\lambda_1\lambda_2\lambda_3} = l_{i_1\lambda_1} . \tag{41}$$

After multiplying both sides of this expression by a further $n-2$ direction cosines, rearranging indices, and averaging, we find that

$$\tfrac{1}{2} I^{(n)}_{i_1 \cdots i_{n-2} i_n i_{n+1}; \lambda_1 \cdots \lambda_{n-2}\lambda_n\lambda_{n+1}} \epsilon_{i_{n-1}i_n i_{n+1}} \epsilon_{\lambda_{n-1}\lambda_n\lambda_{n+1}} = I^{(n-1)}_{i_1 \cdots i_{n-1}; \lambda_1 \cdots \lambda_{n-1}} , \tag{42}$$

which in principle enables us to determine every rotational average of rank lower than n from the result for $I^{(n)}$. It is important to note that the above expressions involve index symmetry constraints, and hence they cannot be used to generate higher order rotational averages from those already known. However, these identities do represent conditions which such results must fulfil, and this knowledge should prove useful in checking new results.

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