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Irreducible Cartesian tensors of highest weight, for arbitrary order

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ABSTRACT

A closed form expression is presented for the irreducible Cartesian tensor of highest weight, for arbitrary order. Two proofs are offered, one employing bookkeeping of indices and, after establishing the connection with the so-called natural tensors and their projection operators, the other one employing purely coordinate-free tensor manipulations. Some theorems and formulas in the published literature are generalized from SO(3) to SO(n), for dimensions $n \geq 3$.

1. Introduction

The study of spin polarized beams in accelerators (in fact, ensembles of polarized particles in general) leads naturally to the study of irreducible representations of the rotation group. A review of spin dynamics in accelerators can be found in [1]. An important text on group representation theory is that by Weyl [2], with many important results for the classical groups in general. The most widely employed formalism in this regard (for the rotation group) is that of irreducible spherical tensors. The theory of spherical harmonics is very well developed and is described in many texts. For example, the text by Jackson [3] gives a detailed application for problems in electrodynamics. In this context, one should note that, given the connection to group representation theory, the subject of irreducible tensors is of relevance to a wide variety of academic disciplines. In fact, the major references cited below come from theoretical chemistry. For this reason, the results and proofs below will be placed in a general setting. It is the author's hope that by so doing, just as he found important results in papers on theoretical chemistry, so also the material in this paper may prove to be of interest beyond specialized applications to spin polarized beams in accelerators.

In addition to spherical harmonics, it is also of interest to employ Cartesian coordinates and irreducible Cartesian tensors. This paper presents a closed form expression for the irreducible Cartesian tensor of highest weight, for tensors of arbitrary order. To avoid confusion of terminology, let us clarify the use of the terms 'rank' and 'order.' Spherical harmonics are usually classified as being of 'rank n' for $n = 0, 1, 2$, etc. For a square matrix, the rank denotes the number of linearly independent rows or columns. For a tensor, we employ the term 'order' to denote the number of indices attached to the tensor. This usage follows the practice in the text by Snider [4]. I shall denote the order by 'p' below because the use of 'r' might be confusing and 'o' is an obviously poor choice. For $p=2$, the answer is well known to be a symmetric traceless 3×3 matrix. Although specific results for higher orders have been derived, e.g. $p=3$ and 4, what about a *general* formula for all higher orders? In this context, Coope et al. [5] and Coope and Snider [6] published significant papers with results of immediate relevance to the current paper. Many of the theorems and formulas in the above papers in fact generalize naturally to SO (n) for dimensions $n \geq 3$. The relevant expressions for SO (n) will be presented in Section 6. The formulas involve Gegenbauer polynomials, which are the generalizations of the Legendre polynomials to higher dimensions.

The literature on applications of irreducible tensors to problems in atomic, molecular and particle physics, and also chemistry, is vast. In fact, the major references for our purposes are from theoretical chemistry [5–9]. Results from [10–12] will also be cited. As in all of the above papers, we are concerned with the three-dimensional representation of SO(3), denoted by $\mathbf{1}$ below. The p-fold tensor product can be decomposed into a direct sum of irreducible representations of SO(3)

$$\underbrace{\mathbf{1} \otimes \cdots \otimes \mathbf{1}}_{p} = \mathbf{p} \oplus \cdots \tag{1.1}$$

The direct sum on the right hand side consists of tensors of weights w, where $0 \leq w \leq p$. The object of interest in this paper is the tensor of highest weight, i.e. $w=p$. It is known that this tensor is unique and is totally symmetric under an arbitrary permutation of the indices, and is traceless under the contraction of any pair of

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indices. The well known case of $p=2$ will clarify the notion of weight and order: $\mathbf{1}\otimes\mathbf{1}=\mathbf{2}\oplus\mathbf{1}\oplus\mathbf{0}$. The right hand side consists of a direct sum of tensors of weights 2, 1 and 0, respectively. In component notation, with an obvious notation,

$$T_{ij}=\frac{\delta_{ij}}{3}T^{(0)}+\varepsilon_{ijk}T_k^{(1)}+T_{ij}^{(2)}. \tag{1.2}$$

(Unless otherwise stated, the indices run from 1 through 3 in this paper.) The Einstein summation convention is employed in this paper. It is well known that the tensor of highest weight $T_{ij}^{(2)}$ is a symmetric traceless matrix ($p=2$ and weight $w=p=2$ in this case). The tensor of weight 0 is essentially an irreducible tensor of order 0 and the tensor of weight 1 is essentially an irreducible tensor of order 1. They are multiplied (or contracted) with Kronecker deltas or the Levi–Civita tensor ε_{ijk} to raise them to a higher order, but their information content is of a lower order $w<p$. Following the terminology in [5], we shall use the term *natural tensor* to denote the irreducible Cartesian tensor of order p and highest weight $w=p$. It is clear from Eq. (1.2) that the tensors of lower weight are also natural tensors, but of lower order. For example, for $p=3$, we can form third order tensors of weights 0, 1 and 2 via $\varepsilon_{ijk}T^{(0)}$, $\delta_{ij}T_k^{(1)}$ and $\varepsilon_{ija}T_{ak}^{(2)}$, respectively, and obvious permutations of the indices. Note that, unlike the tensor of highest weight, the tensors of lower weight are in general not unique.

2. Natural tensor of order *p*

The natural tensor of order p will be denoted by $\mathbf{T}^{(p)}$ in coordinate-free notation and by $T_{i_1\ldots i_p}^{(p)}$ in terms of indices $i_1,\ldots i_p$. Since we shall need to symmetrize over the indices in many of the formulas below,we introduce some notation for brevity. The notation $\sum_{\rm symm}$ denotes a symmetrized sum of the arguments, while curly braces $\{\cdots\}$ denote a *normalized* symmetrized sum. For example,for distinct vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, $\sum_{\rm symm}\boldsymbol{uv}=u_iv_j+u_jv_i$ and $\{\boldsymbol{uv}\}=\frac{1}{2}\sum_{\rm symm}\boldsymbol{uv}$. Next,for three vectors, $\sum_{\rm symm}\boldsymbol{uvv}=u_iv_jv_k+u_jv_iv_k+u_kv_iv_j$ and $\{\boldsymbol{uvw}\}=\frac{1}{3}\sum_{\rm symm}\boldsymbol{uvv}$. In general,the normalized symmetrization requires a division by the number of distinct combinations. The expression for the natural tensor of order p is then as follows. For spin polarized particles in accelerators,we are typically interested in tensors referenced to a quantization axis,say $\boldsymbol{n}$. (Note that $\boldsymbol{n}$ is in general a function of the phase space location $(\boldsymbol{q},\boldsymbol{p})$ of the canonical coordinates and conjugate momenta. See [1] for details concerning the spin eigenstates in accelerators. Such issues are not pertinent in this paper.) It is perhaps easier to visualize if the expression is first displayed using indices. It has long been known that $T^{(0)}=1$, $T_i^{(1)}=n_i$ and $T_{ij}^{(2)}=n_in_j-\frac{1}{3}\delta_{ij}$. For higher orders, in fact $p\ge 2$,

$$\begin{aligned}T_{i_1\ldots i_p}^{(p)}(\boldsymbol{n})&=n_{i_1}n_{i_2}\ldots n_{i_p}\\&-\frac{1}{2p-1}\sum_{\rm symm}\delta_{i_1i_2}n_{i_3}\ldots n_{i_p}\\&+\frac{1}{(2p-1)(2p-3)}\sum_{\rm symm}\delta_{i_1i_2}\delta_{i_3i_4}n_{i_5}\ldots n_{i_p}\\&-\frac{1}{(2p-1)(2p-3)(2p-5)}\sum_{\rm symm}\delta_{i_1i_2}\delta_{i_3i_4}\delta_{i_5i_6}n_{i_7}\ldots n_{i_p}+\cdots\end{aligned} \tag{2.1}$$

The permutations span all distinct combinations of the indices. There are in total $1+\lfloor(p/2)\rfloor$ rows. If p is odd, the last row will contain $n_{i_1}\delta_{i_2i_3}\ldots\delta_{i_{p-1}i_p}$ + permutations, while if p is even the last row will contain only products of Kronecker deltas, viz. $\delta_{i_1i_2}\ldots\delta_{i_{p-1}i_p}+$ permutations. A proof of the above expression will be given below. The literature contains many papers on irreducible Cartesian tensors, but they mostly derive explicit solutions for low orders, with prescriptions to go to higher orders, but not a general expression for arbitrary order p. The solutions for $p=3$ and 4 were derived by Stone [9] and Eq. (2.1) agrees with his expressions.

In coordinate-free notation, let $\mathsf{T}^{(1)}$ be a natural tensor of order 1 (a vector, not necessarily of unit length). Following [5], U denotes the second order unit tensor with components δ_{ij}. A dot product denotes a contraction below. Then

$$\mathsf{T}^{(p)}=\sum_{t=0}^{\lfloor(p/2)\rfloor}(-1)^t\frac{(2p-2t-1)!!}{(2p-1)!!}(\mathsf{T}^{(1)}\cdot\mathsf{T}^{(1)})^t\sum_{\rm symm}(\mathsf{T}^{(1)})^{p-2t}(\mathsf{U})^t. \tag{2.2}$$

Note that Coope et al. derived the following elegant formula [5, Eq. (17)]. Starting from a natural tensor of order j and a natural tensor of order 1 (a vector), they showed how to construct a natural tensor of order $j+1$

$$\mathsf{T}^{(j+1)}=[\mathsf{T}^{(j)}\otimes\mathsf{T}^{(1)}]^{(j+1)}=\left\{\mathsf{T}^{(j)}\mathsf{T}^{(1)}-\frac{j}{2j+1}(\mathsf{T}^{(j)}\cdot\mathsf{T}^{(1)})\mathsf{U}\right\}. \tag{2.3}$$

Since a natural tensor is totally symmetric in all of its indices, on the right hand side $\mathsf{T}^{(1)}$ can be contracted with any index of $\mathsf{T}^{(j)}$. The above procedure can be applied recursively, starting from $j=1$, up to any desired value, say p. The expression in Eq. (2.2) can therefore be viewed as the solution of the recurrence relation in Eq. (2.3).

3. Proof

The proof of Eq. (2.1) will now be given. A copy of the proof below was sent to Coope and Snider. Snider very kindly replied [13] with a derivation of Eq. (2.2) using purely coordinate-free Cartesian tensor manipulations. Subsequently, Coope also replied [14] with a derivation using the projection operator $\mathsf{E}^{(j)}$ derived in 1970 by Coope and Snider [6, Eq. (6)]. The details of Coope's elegant and succint derivation, which also employs purely coordinate-free Cartesian tensor manipulations, will be presented in Section 5.

The present proof makes explicit use of the bookkeeping of indices. First, by construction the expression in Eq. (2.1) is a tensor of order p and totally symmetric under an arbitrary permutation of its indices. The presence of the first term $n_{i_1}\ldots n_{i_p}$ makes it unique: any other candidate solution must contain the same term. To demonstrate that the expression is irreducible, it suffices to show that it vanishes identically under the contraction of any pair of indices. Without loss of generality, we contract i_1 and i_2. We must show that $\delta_{i_1i_2}T_{i_1i_2i_3\ldots i_p}^{(p)}$ vanishes identically. The proof proceeds by analyzing the terms in Eq. (2.1) line by line, keeping track of the bookkeeping as we proceed. The contraction of the first line in Eq. (2.1) with $\delta_{i_1i_2}$ yields (L_1 for "line 1") $L_1=n_{i_3}\ldots n_{i_p}$. The second line in Eq. (2.1)contains a sum of terms with exactly one Kronecker delta in each term. (The tth line in Eq. (2.1) consists of a sum of terms with exactly t Kronecker deltas in each term, counting from t=0.) One term contains a factor $\delta_{i_1i_2}$, there are $p-2$ terms which contain a factor δ_{i_1j} (where $3\le j\le p$), there are $p-2$ terms which contain a factor δ_{i_2k} (where $3\le k\le p$), and the remaining terms each contain a factor $n_{i_1}n_{i_2}$. The contraction of the first three sets of terms with $\delta_{i_1i_2}$ all yield the product $n_{i_3}\ldots n_{i_p}$. Consider these terms first and denote their sum by L_{2a}. Then

$$\begin{aligned}L_{2a}&=-\frac{\delta_{i_1i_2}}{2p-1}\Big[\delta_{i_1i_2}n_{i_3}\ldots n_{i_p}+\underbrace{\delta_{i_1j}n_{i_2}n_{i_3}\ldots n_j\ldots n_{i_p}}_{3\le j\le p}+\underbrace{\delta_{i_2k}n_{i_1}n_{i_3}\ldots n_k\ldots n_{i_p}}_{3\le k\le p}\Big]\\&=-\frac{3+p-2+p-2}{2p-1}n_{i_3}\ldots n_{i_p}\\&=-\frac{2p-1}{2p-1}n_{i_3}\ldots n_{i_p}\\&=-n_{i_3}\ldots n_{i_p}\end{aligned}$$