The Wigner-Eckart Theorem for Reducible Symmetric Cartesian Tensor Operators

Antonio O. Bouzas *
Departamento de Física Aplicada, CINVESTAV-IPN
Carretera Antigua a Progreso Km. 6, Apdo. Postal 73 “Cordemex”
Mérida 97310, Yucatán, México
February 17, 2016

Abstract
We explicitly establish a unitary correspondence between spherical irreducible tensor operators and cartesian tensor operators of any rank. That unitary relation is implemented by means of a basis of integer-spin wave functions that constitute simultaneously a basis of the spaces of cartesian and spherical irreducible tensors. As a consequence, we extend the Wigner–Eckart theorem to cartesian irreducible tensor operators of any rank, and to totally symmetric reducible ones. We also discuss the tensorial structure of several standard spherical irreducible tensors such as ordinary, bipolar and tensor spherical harmonics, spin-polarization operators and multipole operators. As an application, we obtain an explicit expression for the derivatives of any order of spherical harmonics in terms of tensor spherical harmonics.

Keywords: spherical tensor, cartesian tensor, spherical harmonic, angular momentum, Wigner-Eckart

*E-mail: abouzas@mda.cinvestav.mx
1 Introduction

The Wigner–Eckart theorem is one of the fundamental results in quantum angular-momentum theory. As is well known, it states that the dependence on magnetic quantum numbers of the matrix elements of spherical irreducible tensor operators (henceforth sitos) between angular–momentum eigenstates, is factorizable into a Clebsch–Gordan (henceforth CG) coefficient. This leads to a drastic simplification of the calculation of tensor-operator matrix elements, such as those appearing in perturbative computations in molecular, atomic and nuclear systems (and more generally in rotationally invariant many-body problems), and a vast array of other quantum-mechanical systems such as, e.g., the theory of anisotropic liquids [1]. By now standard textbook material, the Wigner–Eckart theorem was first formulated by Eckart [2] for rank-1 sitos and generalized by Wigner [3] to sitos of any rank. Wigner’s treatment is based on group–theoretic methods involving finite rotation operators. The definition of sitos and the proof of the Wigner–Eckart theorem based on angular-momentum commutation relations (i.e., on infinitesimal rotation operators), as usually found in textbooks [4, 5, 6, 7], is due to Racah [8].

In this paper we consider the relationship between sitos and cartesian irreducible tensor operators (henceforth citos). We explicitly establish a unitary correspondence between them valid for any rank. The precise relation between spherical and cartesian tensors allows us to apply the technical machinery of tensor algebra to spherical tensors and, conversely, the techniques of quantum angular–momentum theory to cartesian tensors. That interplay is, in fact, the main subject of this paper. In this respect, our results are a significant extension of the classic work of Zemach [10] and complementary to more recent results (e.g., [11] and references cited there).

Another important feature of our approach is that the coefficients of the unitary transformation relating sitos and citos have a well-defined physical meaning: they are an orthonormal, complete set of standard spin wave–functions, satisfying the eigenvalue equations, phase conventions and complex–conjugation properties expected of angular–momentum eigenstates and eigenfunctions which, furthermore, form a Clebsch–Gordan series of angular–momentum states. They transform under rotations either as cartesian or as spherical tensors, which explains their role in relating both types of tensors. By means of the relation between spherical and cartesian irreducible tensor operators we extend the Wigner–Eckart theorem to citos of any rank. Remarkably, such an extension has not been considered before in the literature. We discuss also the cartesian tensorial form of several commonly occurring sitos (ordinary spherical harmonics, as well as bipolar and tensor ones, among others). Those cartesian expressions provide a viewpoint complementary to the usual analytical one, by making the tensorial structure of sitos completely explicit, which makes possible to obtain relations that would otherwise be more difficult to find. Furthermore, writing sitos in tensorial form is of interest in the context of relativistic theories, for example in connection with covariant partial–wave expansions. The converse case is also true, since by mapping cartesian tensors into spherical ones their angular–momentum properties become apparent.

Reducible cartesian tensors occur frequently in physics, so the evaluation of the angular-momentum matrix elements of reducible tensor operators is clearly of interest. We obtain in this paper a further extension of the Wigner–Eckart theorem to a limited class of reducible tensor operators of any rank, namely, that of totally symmetric ones. This allows us to compute the matrix elements of tensor powers of the position and of the momentum operators. As an application, we obtain an explicit expression for the gradients of spherical harmonics to all orders in terms of tensor spherical harmonics. That result is a generalization of the well-known gradient formula [12, 7, 13] for first derivatives to derivatives of any order.

The paper is organized as follows. In the following section we introduce the spin operator for cartesian tensors and briefly discuss our notation and conventions for tensors. In section 3 we construct a standard basis of spin wave–functions for any integer spin and establish their main properties both as angular–momentum eigenfunctions and as a basis of the space of cartesian irreducible tensors. By means of that basis, in section 4 we obtain the unitary relation between sitos and citos. In section 5 we establish the Wigner–Eckart theorem for citos. In section 6 we analyze several sitos commonly used in the literature, including ordinary, bipolar, and tensor spherical harmonics, spin–polarization operators, and electric multipole operators, from the point of view of their relation to citos. The Wigner–Eckart theorem for totally symmetric reducible tensors is discussed in section 7. Its application to the computation of derivatives of spherical harmonics to any order is worked out in section 8. In section 9 we discuss partially irreducible cartesian tensors, provide the extension of the Wigner-Eckart theorem to them, and discuss the magnetic multipole expansion. Finally, in section 10

\footnote{A more detailed historical account is given in [9].}
are hermitian and, as expected, satisfy angular-momentum commutation relations

This equality is consistent with the fact that a rank-

orthogonal matrices \( R \) with \( \det R = 1 \), so we will not need to distinguish between tensors and pseudo-tensors. Given a fixed orthogonal coordinate frame, we denote coordinate versors either by \( \hat{x}, \hat{y}, \hat{z} \) or by \( \hat{e}^i \) (\( i = 1, 2, 3 \)), with components \( \hat{e}^i_j = \delta_{ij} \) so that \( \hat{e}^{i,2,3} = \hat{x}, \hat{y}, \hat{z} \). An infinitesimal rotation is of the form

This equality is consistent with the fact that a rank-

orthogonal matrices \( R \) with \( \det R = 1 \), so we will not need to distinguish between tensors and pseudo-tensors. Given a fixed orthogonal coordinate frame, we denote coordinate versors either by \( \hat{x}, \hat{y}, \hat{z} \) or by \( \hat{e}^i \) (\( i = 1, 2, 3 \)), with components \( \hat{e}^i_j = \delta_{ij} \) so that \( \hat{e}^{i,2,3} = \hat{x}, \hat{y}, \hat{z} \). An infinitesimal rotation is of the form

The spin operator for cartesian tensors.

We include here for later reference the relation

the powers in each term. Both procedures are straightforward, though somewhat tedious, so we omit the
details for brevity. We include here for later reference the relation

as the tensor product of

important consequence of the definition (1) and use (4) to obtain a binomial expansion for

doing this, one can expand the exponentials on both sides of (5) or (6) in powers of \( \theta \) and use (4) to obtain a binomial expansion for

powers in each term. Both procedures are straightforward, though somewhat tedious, so we omit the
details for brevity. We include here for later reference the relation

which gives the expression for the matrix of the squared spin operator.

\[ (S_{(n)})^2_{i_1...i_n} = 2n \prod_{q=1}^n \delta_{i_q h_q} + \sum_{p,t=1}^n (\delta_{i_p h_p} \delta_{i_t h_t} - \delta_{i_p h_t} \delta_{i_t h_p}) \prod_{q=1}^n \delta_{i_q h_q}, \]
The set of all rank-\( n \) complex irreducible (i.e., totally symmetric and traceless [14]) tensors is a \( 2n + 1 \)-dimensional linear subspace of the space of complex rank-\( n \) tensors. That subspace is invariant under \( \hat{S}_r \) for any vector \( \vec{v} \) since, as can be seen from (2), \( v_k (S_{\alpha \beta})_{ij} ... ) \) are totally symmetric and traceless in their free indices if the tensor \( A_{k_1 ... k_n} \) is irreducible. Similarly, \( \hat{R}_1 \) is irreducible if \( A_{k_1 ... k_n} \) is. Given a tensor \( A_{i_1 ... i_n} \) we define its associated totally symmetrized tensor as

\[
A_{\{i_1 ... i_n\}} = \frac{1}{n!} \sum_{\sigma} A_{i_{\sigma 1} ... i_{\sigma n}},
\]

where the sum extends over all permutations \( i_{\sigma 1} ... i_{\sigma n} \) of \( i_1 ... i_n \). The totally symmetric part of \( A_{i_1 ... i_n} \) is then \( 1/n A_{\{i_1 ... i_n\}} \). Similarly, we denote by \( A_{(i_1 ... i_n)} \) the traceless part of \( A_{i_1 ... i_n} \) (for example, \( r_i r_j - 1/3 r^2 \delta_{ij} \)). The traceless part of the totally symmetrized tensor associated to \( A_{i_1 ... i_n} \) is therefore \( 1/n A_{\{i_1 ... i_n\}} \). We provide a practical method to compute the irreducible part of any tensor in the following section (see equation (24) below).

3 A basis for irreducible tensors and integer–spin wave–functions

In this section we construct an orthonormal basis for the \((2s + 1)\)-dimensional space of irreducible rank-\( s \) tensors, \( s \geq 0 \) integer. The basis irreducible tensors are eigenfunctions of \( \hat{S}_r^2 \) and \( \hat{S} \cdot \hat{S}_r \) and satisfy the phase conventions required of standard angular–momentum eigenfunctions (see appendix A). They are, therefore, also a basis of spin-\( s \) wave–functions. Furthermore, as shown in the following section, those basis tensors are the matrix elements of the unitary transformation mapping spherical irreducible tensor operators into cartesian ones.

The basis of spin-1 wave functions consists of the simultaneous eigenvectors of \( \hat{S}_{r}^2 \) and \( \hat{S} \cdot \hat{S}_r \). We choose their global phase so as to obtain the usual polarization unit vectors

\[
\hat{\epsilon}(1)(\pm 1) = \frac{1}{\sqrt{2}} (\hat{\epsilon} \pm i \hat{\gamma}), \quad \hat{\epsilon}(1)(0) = \hat{\zeta}.
\]

(9a)

We can also write, more compactly,

\[
\hat{\epsilon}(1)(m) = \sqrt{4\pi / 3} Y_{1m}(\hat{\epsilon}), \quad m = 0, \pm 1,
\]

(9b)

with \( Y_{1m} \) a spherical harmonic, an equality that can easily be checked and whose origins are explained below in section 6. The basis vectors (9) possess the following orthonormality, complex conjugation, and completeness properties

\[
\hat{\epsilon}(1)(m')^* \cdot \hat{\epsilon}(1)(m) = \delta_{m'm}, \quad \hat{\epsilon}(1)(m)^* = (-1)^m \hat{\epsilon}(1)(-m), \quad \sum_{m=-1}^{1} \hat{\epsilon}(1)(m) \hat{\epsilon}(1)(m)^* = \delta_{ij}.
\]

(10)

From (9a) and (A.1b) we find that

\[
\langle 1, m' | S_k | 1, m \rangle = \hat{\epsilon}(1)(m')^* (S_{1k})_{ij} \hat{\epsilon}(1)(m) \],
\]

(11)

so the vectors (9) do satisfy the standard conventions for angular-momentum wave-functions, and in particular the Condon–Shortley phase convention [15, 3, 16, 7] (see Appendix A).

Before discussing the general case of rank-\( s \) tensors it is convenient to briefly consider first the case \( s = 2 \). Thus, we look for a basis of spin-2 wave functions consisting of rank-2 tensors \( \hat{\epsilon}(2)_{ij}(m) \), \(-2 \leq m \leq 2\). Because those basis wave-functions must be eigenfunctions of \( \hat{S}_r^2 \) with quantum number \( s = 2 \), without admixture of states with other \( s \), the tensor \( \hat{\epsilon}(2)_{ij}(m) \) must be irreducible. Otherwise, some nonvanishing linear combination of its components would exist that transforms as a lower-rank tensor, therefore representing states of spin 1 or 0. Furthermore, the tensors \( \hat{\epsilon}(2)_{ij}(m) \) must be orthonormal and satisfy the usual conventions (A.1a) for angular-momentum eigenstates. Given our spin-1 wave functions (9), the general theory of angular momentum indicates that the sought–for rank-2 tensors are given by

\[
\hat{\epsilon}(2)_{ij}(m) = \sum_{m_1, m_2 = -1}^{1} \langle 1, m_1; 1, m_2 | 2, m \rangle \hat{\epsilon}(1)(m_1) \hat{\epsilon}(1)(m_2).
\]

(12)
Explicit evaluation of the r.h.s. of this equation shows that \( \hat{e}_{(2)}(m) \) are symmetric and traceless, therefore irreducible. The spin operator \( \hat{S} \) is represented in the space of rank-2 tensors by the spin matrix \( \hat{S}^2(2) \) from (4), with
\[
(S^2(2))_{i_1i_2;k_1k_2} = 4 \delta_{i_1k_1} \delta_{i_2k_2} - 2 \delta_{i_1i_2} \delta_{k_1k_2} + 2 \delta_{i_1k_2} \delta_{i_2k_1}.
\] (13)
We see from (13) that irreducible tensors are eigenstates of \( \hat{S}^2(2) \) with eigenvalue \( s(s + 1) = 6 \), or \( s = 2 \), antisymmetric tensors are eigenstates with \( s = 1 \) and tensors that are multiples of the identity correspond to \( s = 0 \). This decomposition of rank-2 tensor space corresponds, of course, to the usual decomposition into traceless symmetric, antisymmetric, and trace parts.

We now turn to the general case \( s \geq 2 \). The basis spin wave-functions must be \( 2s + 1 \) rank-\( s \) irreducible tensors \( \hat{e}_{(s)i_1...i_s}(m) \), \( -s \leq m \leq s \), constituting an orthonormal set satisfying the conventions (A.1b) for angular-momentum states. Furthermore, as functions of the spin \( s \), they should be members of a Clebsch–Gordan series of angular-momentum states. Having already found the basis tensors for \( s = 1, 2 \), we proceed recursively to define
\[
\hat{e}_{(s)i_1...i_s}(m) = \sum_{m_1 = -s-1}^{s+1} \sum_{m_2 = -s-1}^{s+1} \langle s-1, m_1; 1, m_2 | s, m \rangle \hat{e}_{(s-1)i_1...i_{s-1}}(m_1) \hat{e}_{(1)i_2}(m_2), \quad -s \leq m \leq s.
\] (14)
From this definition and the standard properties of CG coefficients [7, 13], we can easily derive the orthonormality and complex-conjugation relations
\[
\hat{e}^\ast_{(n)i_1...i_n}(m) \hat{e}_{(n)i_1...i_n}(m) = \delta_{m'm}, \quad \hat{e}^\ast_{(n)i_1...i_n}(m) = (-1)^m \hat{e}_{(n)i_1...i_n}(-m).
\] (15)
From the first equality we see that the tensors (14) do form an orthonormal set which is, therefore, a basis of a \( (2s + 1) \)-dimensional subspace of the space of rank-\( s \) complex tensors. In order to identify that subspace with the subspace of irreducible tensors, which has the same dimension, we have to prove that the basis tensors are irreducible. For that purpose, we notice that (14) is a recursion relation with known coefficients and initial condition (9). Exploiting the fact that the explicit expression for CG coefficients [7, 13] coupling angular momenta that differ by one unit, as in (14), is rather simple, we can solve the recursion by iteration to find
\[
\hat{e}_{(n)i_1...i_n}(m) = \left( \frac{(n + m)!}{(n - m)!} \right)^{\frac{1}{2}} \sum_{s_1+...+s_n = m} (\sqrt{2})^{n-\sum_{h=1}^{n} |s_h|} \hat{e}_{(1)i_1}(|s_1|) ... \hat{e}_{(1)i_n}(|s_n|).
\] (16)
This expression provides an explicit definition of \( \hat{e}_{i_1...i_n} \), equivalent to (14). It also shows that \( \hat{e}_{(n)i_1...i_n} \) is totally symmetric. Thus, in order to prove that it is also totally traceless it is enough to show that it is traceless with respect to the first pair of indices. That follows by induction, since \( \hat{e}_{(2)jj}(m) = 0 \) as follows by explicit computation, and since \( \hat{e}_{(s-1)ji...ij}(m) = 0 \) implies \( \hat{e}_{(s)ji...ij}(m) = 0 \), by (14). Besides the recursive and explicit definitions (14) and (16), an implicit definition of \( \hat{e}_{(s)} \) can also be given
\[
\hat{e}_{(s)i_1...i_s}(m) = \sqrt{\frac{4\pi}{s!(2s + 1)!}} \partial_{i_1} \cdot \partial_{i_s} (\hat{r}^s Y_{sm}(\hat{r})).
\] (17)
This equality will be proved below, in section 6.1. The total symmetry of \( \hat{e}_{(s)i_1...i_s}(m) \) is apparent in (17), and its tracelessness follows because \( |\hat{r}^s Y_{sm}(\hat{r})| \) is a solution to the Laplace equation.

Since the set of \( (2s + 1) \) spin-\( s \) wave functions (14) is an orthonormal basis of the subspace of irreducible tensors, the orthogonal projector from the space of rank-\( s \) tensors onto that subspace must be given by
\[
X_{i_1...i_s;j_1...j_s} = \sum_{m=-s}^{s} \hat{e}_{(s)i_1...i_s}(m) \hat{e}_{(s)j_1...j_s}(m)^\ast = \sum_{m=-s}^{s} \hat{e}_{(s)i_1...i_s}(m)^\ast \hat{e}_{(s)j_1...j_s}(m).
\] (18)
If the left-hand side of this equality is computed explicitly, (18) constitutes a completeness relation for the standard tensors (14). In [17] an explicit expression is given for \( s = 2, 3 \), as well as an algebraic expression valid for any \( s \). Those expressions are not particularly useful for the purposes of this paper, however, so we omit them for brevity. Rather, we shall regard (18) as an explicit expression for the projector \( X_{i_1...i_s;j_1...j_s} \).

Its usefulness is illustrated below in (24).
From (16) we find the two simple relations
\begin{equation}
\varrho_{(s)i_1\ldots i_n}(\pm s) = \varrho_{(1)i_1}(\pm 1)\ldots \varrho_{(1)i_n}(\pm 1).
\end{equation}

These equalities are useful, together with standard recoupling identities, to compute reduced matrix elements. Furthermore, they imply \( \varrho_{(n_1+n_2)i_1\ldots i_{n_1+n_2}}(\pm (n_1+n_2)) = \varrho_{(n_1)i_1\ldots i_{n_1}}(\pm n_1)\varrho_{(n_2)i_{n_1+1}\ldots i_{n_1+n_2}}(\pm n_2) \), so the basis spin wave-functions (14) comply also with the Condon–Shortley phase convention for coupled angular momentum states \( [15, 16] \), \( |j_1,j_2,j_1+j_2,j_1+j_2\rangle = |j_1,j_1;j_2,j_2\rangle \). Another important property of the basis tensors (14) is the equality
\begin{equation}
\varrho_{(n_1+n_2)k_1\ldots k_{n_1}h_1\ldots h_{n_2}}(m) = \sum_{m_1=-n_1}^{n_1} \sum_{m_2=-n_2}^{n_2} \langle n_1,m_1;n_2,m_2|n_1+n_2,m\rangle \varrho_{(n_1)k_1\ldots k_{n_1}}(m_1)\varrho_{(n_2)h_1\ldots h_{n_2}}(m_2),
\end{equation}
which shows that the maximal coupling of two standard tensors is again a standard tensor, and of which (14) is the particular case \( n_1 = 1 \) or \( n_2 = 1 \). It is possible to derive (20) directly by substituting (14) on its right-hand side and using recoupling identities [17]. Here we give a less direct proof. Both sides of the equality (20) are by construction eigenstates of \( \hat{S}^2 \) and \( \hat{\varepsilon} \cdot \hat{S} \) with the same eigenvalues. Thus, for \( m < n_1 + n_2 \) both sides are obtained by repeated application of \( S_- \) to their \( m = n_1 + n_2 \) values. Since for \( m = n_1 + n_2 \) both sides are seen to be equal by (19), the equality holds for \( m < n_1 + n_2 \) as well.

The spin operator \( \hat{S} \) is represented in the space of rank-\( n \) tensors by the spin matrix (2). Notice that (4) means that \( \hat{S}_n = \hat{S}_{(n-1)} \otimes I_1 + I_{n-1} \otimes \hat{S}_{(1)} \), which is consistent with the inductive definition (14). From (14) and (2) we can show the fundamental relation
\begin{equation}
\langle n,m'|S_k|n,m\rangle = \varrho_{(n)i_1\ldots i_n}(m') (S_{(n)k})_{i_1\ldots i_n;j_1\ldots j_n} \varrho_{(n)j_1\ldots j_n}(m),
\end{equation}
where the left-hand side is a standard angular-momentum matrix element as given by (A.1b). A detailed proof of (21) is given at the end of appendix A. Multiplying both sides of (21) by \( \varrho_{(n)}(m') \) and summing over \( m' \) we derive the equivalent relation
\begin{equation}
(S_{(n)k})_{i_1\ldots i_n;j_1\ldots j_n} \varrho_{(n)j_1\ldots j_n}(m) = \sum_{m'=-n}^{n} \varrho_{(n)i_1\ldots i_n}(m') (S_{(n)k})_{h_1\ldots h_n;j_1\ldots j_n} \varrho_{(n)j_1\ldots j_n}(m') (S_{(n)k})^*_{h_1\ldots h_n;i_1\ldots i_n} \varrho_{(n)i_1\ldots i_n}(m),
\end{equation}
where in the first equality we used the fact that the tensor on the left-hand side is irreducible, therefore invariant under the projector (18). From (21) and (22) we can inductively prove a generalization of (21) to any number of spin-operator components
\begin{equation}
\langle n,m'|S_{k_1}\ldots S_{k_p}|n,m\rangle = \varrho_{(n)i_1\ldots i_n}(m') (S_{(n)k_1})_{i_1\ldots i_n;j_1\ldots j_n} \varrho_{(n)j_1\ldots j_n}(m), \quad p \geq 1,
\end{equation}
and from this relation the corresponding generalization of (22) follows. The squared spin operator is represented by (7). It is not difficult to verify from that equation that any rank-\( n \) irreducible tensor is an eigenfunction of \( S^2_{(n)} \) with eigenvalue \( n(n+1) \). Lower eigenvalues correspond to tensors with less symmetry or with non-vanishing traces.

Lastly, we notice that, since the standard tensors (14) or their complex conjugates constitute an orthonormal basis of the linear space of rank-s irreducible tensors, given any rank-\( n \) complex tensor \( A_{i_1\ldots i_n} \) its irreducible part can be written as
\begin{equation}
\frac{1}{n!} A_{i_1\ldots i_n} = \sum_{m=-n}^{n} \varrho_{(n)i_1\ldots i_n}(m)^* \varrho_{(n)j_1\ldots j_n}(m) A_{j_1\ldots j_n}.
\end{equation}
In fact, (24) provides a practical method to obtain the irreducible part of a reducible tensor. If the tensor \( A_{i_1\ldots i_n} \) under consideration is irreducible, then the left-hand side of (24) is equal to \( A_{i_1\ldots i_n} \).
3.1 Finite rotations

We turn next to the transformation properties of \( \tilde{e}_{(s)} \) under finite rotations. The theory of finite rotations in quantum mechanics is well known (see [3, 4, 5, 6, 7, 9, 13, 16]). The generator of infinitesimal rotations is the total angular–momentum operator \( \hat{J} \). Thus, in terms of the normal parameters \( \tilde{\theta} \) the unitary rotation operator is given by \( U(\mathcal{R}(\tilde{\theta})) = \exp(-i\tilde{\theta} \cdot \hat{J}) \). Similarly, in terms of Euler angles we have \( U(\mathcal{R}(\alpha, \beta, \gamma)) = \exp(-i\alpha J_3)\exp(-i\beta J_2)\exp(-i\gamma J_3) \). The matrix representation of the rotation operator \( U(\mathcal{R}) \) in the eigenspace of total angular momentum \( j \) is defined as

\[
U(\mathcal{R}) |j, m\rangle = \sum_{m'} |j, m'\rangle D^j_{m' m}(\mathcal{R}), \quad D^j_{m' m}(\mathcal{R}) = \langle j, m' | U(\mathcal{R}) | j, m \rangle. \tag{25}
\]

If the rotation matrix \( \mathcal{R} \) is parameterized as a function of the Euler angles, the resulting rotation matrices \( D^j_{m' m}(\alpha, \beta, \gamma) \) are the Wigner \( D \)-matrices [3, 9, 13, 16]. Normal parameters may also be used, and the resulting unitary rotation matrices \( D^j_{m' m}(\tilde{\theta}) \) (sometimes denoted \( U^j_{m' m}(\tilde{\theta}) \) [13]) and their relation to Wigner \( D \)-matrices have been extensively studied [9, 13]. The generic notation \( D^j_{m' m}(\mathcal{R}) \) used here refers to any such parameterization.

From the definition (25), by using (21) and (6), for \( D^j_{m' m}(\mathcal{R}) \) with integer \( j \) we get

\[
D^j_{m' m}(\mathcal{R}) = \tilde{e}(\ell) h_{\ell h_{\ell+1}}(m')^* \mathcal{R}_{h_{\ell+2} \ldots \mathcal{R}_{h_{\ell+j} \ldots \mathcal{R}_{h_{\ell+j}}}(m), \quad 0 \leq \ell \in \mathbb{Z}, \tag{26}
\]

which expresses \( D^j_{m' m}(\mathcal{R}) \) as the spherical components of the cartesian rotation matrix \( (\mathcal{R} \otimes \ldots \otimes \mathcal{R})_{h_{\ell} \ldots \mathcal{R}_{h_{\ell+j}} \ldots \mathcal{R}_{h_{\ell+j}}}(m) \).

Substituting (16) into (26) leads to an expression of \( D^n(\mathcal{R}) \) with integer \( n \) in terms of \( D^1(\mathcal{R}) \)

\[
D^n_{m' m}(\mathcal{R}) = \frac{2n}{(2n)!} \sqrt{(n + m')!(n - m')!(n + m)!} \sqrt{(n + m)! (n - m)!} \times \sum_{s'_n \ldots s'_1 = -1}^{1} \sum_{s_1 + \ldots + s_n = m}^{1} \prod_{s'_k = r_{|s'_k|+|s_k|}}^{1} D^1_{s'_k, s_k}(\mathcal{R}) \tag{27}
\]

which is formally analogous to (40) and which, like (26), holds for any parameterization used for \( \mathcal{R} \). The relations (26) and (27) have not been given in the previous literature.

The transformation rules of the basis tensors \( \tilde{e}_{(s)} \) under finite rotations are summarized by the equalities

\[
(e^{-i\tilde{\theta} (s)})_{i_1 \ldots i_n j_1 \ldots j_n} \tilde{e}_{(s)}(m) = \mathcal{R}_{i_1 j_1} (\tilde{\theta}) \ldots \mathcal{R}_{i_n j_n} (\tilde{\theta}) \tilde{e}_{(s)}(m) = \sum_{m'} \tilde{e}_{(m')} (m') D^m_{m' m}(\mathcal{R}), \tag{28}
\]

where the first equality is (6) and the second one is a direct consequence of (26). We see from (28) that under rotations the basis tensors \( \tilde{e}_{(s)} \) transform equally well as cartesian or as spherical tensors. This property is the basis of the unitary relation between spherical and cartesian irreducible tensor operators discussed in the following section.

4 Cartesian and spherical irreducible tensor operators

Let \( \hat{J} \) be an angular-momentum operator, and \( |j, m\rangle \) the simultaneous eigenstates of \( \hat{J}^2 \) and \( \hat{J} \cdot \hat{J} \), satisfying the standard conventions (see appendix A). An operator \( O_{i_1 \ldots i_n} \) is a rank-\( n \) cartesian tensor operator relative to \( \hat{J} \) if it satisfies the commutation relation

\[
[J_k, O_{i_1 \ldots i_n}] = -(S_{(n)k})_{i_1 \ldots i_n j_1 \ldots j_n} O_{j_1 \ldots j_n}, \tag{29}
\]

with \( S_{(n)} \) defined in (2). We say that \( O_{i_1 \ldots i_n} \) is a cartesian irreducible tensor operator (henceforth cito) if it is totally symmetric and traceless. If \( O_{i_1 \ldots i_n} \) is a generic tensor operator, its irreducible component is
1/n!O_{i_1...i_n}=0$. An operator $O_{nm}$, with integer $n, m$ ($n \geq 0, -n \leq m \leq n$) is a spherical irreducible tensor operator (henceforth SITO) relative to $\hat{J}$ if

$$[J_z, O_{nm}] = \sum_{m'=-n}^{n} \langle n, m'|J_z|n, m\rangle O_{nm'}.$$  \hfill (30a)

From this equation and (A.3a) we get the equivalent statement that $O_{nm}$ is a SITO if

$$[\hat{\varepsilon}(\lambda) \cdot \hat{J}, O_{nm}] = \sqrt{n(n+1)}\langle n, m; 1, \epsilon|n, m + \epsilon\rangle O_{n(m+\epsilon)}, \quad \epsilon = 0, \pm 1.$$ \hfill (30b)

If $O_{nm}$ is a SITO, then $O^\dagger_{nm}$ is not (unless $n = 0$) but $(-1)^m O^\dagger_{n(-m)}$ is. We call $O_{nm}$ hermitian if $O_{nm} = (-1)^m O^\dagger_{n(-m)}$.

It is well known [4, 7, 13, 16] that if $a_i$ is a vector operator then $A_{1m}$ with $A_{1m}(\pm 1) = \mp (1/\sqrt{2})(a_1 + ia_3)$, $A_{10} = a_3$ is a rank-1 SITO, and if $b_{ij}$ is a rank-2 cartesian tensor operator then $B_{2m}$ with $B_{2m}(\pm 2) = (1/2)(b_{11} - b_{22} \pm 2ib_{12})$, $B_{20} = \sqrt{3/2}b_{33}$ is a rank-2 SITO. It is clear that $A_{1m} = \hat{\varepsilon}(\lambda)(m)a_i$ and $B_{2m} = \hat{\varepsilon}(\lambda)(m)\hat{J}$.

The following Lemma generalizes those relations to tensors of any rank.

**Lemma 4.1.** Let $O_{i_1...i_n}$ be a rank-$n$ cartesian tensor operator, not necessarily irreducible, relative to the angular-momentum operator $\hat{J}$. Then $O_{nm} = \hat{\varepsilon}(n)(i_1...i_n)(m)O_{i_1...i_n}$ is a rank-$n$ SITO relative to $\hat{J}$.

**Proof.**

$$[J_k, O_{nm}] = \hat{\varepsilon}(n)(i_1...i_n)(m)[J_k, O_{i_1...i_n}] = \frac{1}{n!} \hat{\varepsilon}(n)(i_1...i_n)(m)[J_k, O_{i_1...i_n}]_0$$

$$= \hat{\varepsilon}(n)(i_1...i_n)(m) \sum_{p=1}^{n} i\varepsilon_{kp,r} \frac{1}{n!} O_{(i_1...i_p-1r_p+1...i_n)}_0$$

$$= \hat{\varepsilon}(n)(i_1...i_n)(m) \sum_{p=1}^{n} i\varepsilon_{kp,r} \sum_{m'=-n}^{n} \hat{\varepsilon}(n)(i_1...i_p-1r_p+1...i_n)(m')^{*} \hat{\varepsilon}(n)(q_1...q_n)(m')O_{q_1...q_n}$$

$$= \sum_{m'=-n}^{n} \langle n, m'|S_k|n, m\rangle \hat{\varepsilon}(n)(q_1...q_n)(m')O_{q_1...q_n} = \sum_{m'=-n}^{n} \langle n, m'|J_k|n, m\rangle O_{nm'},$$

where the second equality holds because $\hat{\varepsilon}(n)$ is irreducible, the third one because $O_{(i_1...i_n)}_0$ is a cartesian tensor operator, the fourth one because of (24), and the fifth one by (21). In the last equality we used the fact that $\hat{S}$ and $\hat{J}$ are both angular-momentum operators and, therefore, their matrix elements are both given by (A.1b).

Reciprocally, by means of the spin wave–functions of section 3, CITOS can be obtained from SITOS.

**Lemma 4.2.** Let $O_{nm}$ be a rank-$n$ SITO relative to the angular-momentum operator $\hat{J}$. Then $O_{i_1...i_n} = \sum_{m=-n}^{n} \hat{\varepsilon}(n)(i_1...i_n)(m)^*O_{nm}$ is a rank-$n$ CITO relative to $\hat{J}$.

**Proof.**

$$[J_k, O_{i_1...i_n}] = \sum_{m=-n}^{n} \hat{\varepsilon}(n)(i_1...i_n)(m)^*[J_k, O_{nm}] = \sum_{m=-n}^{n} \hat{\varepsilon}(n)(i_1...i_n)(m)^* \sum_{m'=-n}^{n} \langle n, m'|J_k|n, m\rangle O_{nm'}$$

$$= \sum_{m'=-n}^{n} O_{nm'} \sum_{m=-n}^{n} \langle n, m'|S_k|n, m\rangle \hat{\varepsilon}(n)(i_1...i_n)(m)^*$$

$$= \sum_{m'=-n}^{n} O_{nm'} \sum_{m=-n}^{n} \hat{\varepsilon}(n)(q_1...q_n)(m')^{*} i\varepsilon_{kq_1...q_n} \hat{\varepsilon}(n)(q_1...q_n)(m')^{*} \hat{\varepsilon}(n)(i_1...i_n)(m)^*$$

$$= \sum_{l=1}^{l} i\varepsilon_{kq_1...q_n} \sum_{m=-n}^{n} \hat{\varepsilon}(n)(i_1...i_n)(m)^* \hat{\varepsilon}(n)(q_1...q_n)(m)O_{q_1...q_n}(q_1...q_n)}$$
where the second equality holds because $O_{nm}$ is a sito, the third one by (A.1b) and the fourth one by (21). Notice that, in the next-to-last equality, the sum in the last parentheses is totally symmetric in $q_1 \ldots q_n$, because $O_{rgq}$ is. It is traceless in, say, $q_j$, $q_i$ because $\varepsilon_{rkq}$ is antisymmetric in $q_i$, $r$. Thus, by total symmetry it is totally traceless, therefore irreducible (with respect to $q_1 \ldots q_n$). It is therefore left unchanged by contraction with the first factor, which is a projector onto the subspace of irreducible tensors. The last equality then follows. We have, thus, proved that $O_{11 \ldots 1}$ is a cartesian tensor operator relative to $\vec{J}$. Since its irreducibility is obvious by construction, it is a cito. 

Furthermore, the sitos obtained from Lemma 4.1 and the citos from Lemma 4.2 are actually all possible ones. As we now show, there are no more sitos and citos than those described in the Lemmas.

**Corollary 4.1.** $O_{nm}$ is a rank-$n$ sito relative to $\vec{J}$ if and only if there exists a rank-$n$ cartesian tensor operator $O_{i_1 \ldots i_n}$ relative to $\vec{J}$, not necessarily irreducible, such that $O_{nm} = \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n}$. If $O_{i_1 \ldots i_n}$ is required to be irreducible, it is unique.  

**Proof.** If $O_{i_1 \ldots i_n}$ is a cartesian tensor operator and $O_{nm} = \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n}$, then $O_{nm}$ is a sito by Lemma 4.1. On the other hand, if $O_{nm}$ is a sito then $O_{i_1 \ldots i_n} = \sum_{m'} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m')O_{nm'}$ is a sito by Lemma 4.2, and $O_{nm} = \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n}$ by the orthonormality of $\tilde{\varepsilon}_{(n)i_1 \ldots i_n}(\mu)$ with $-n \leq \mu \leq n$. The existence statement is therefore proved.

Now let $O_{nm}$ and $O'_{nm}$ be as in the Corollary, $A_i \neq 0$ such that $A_{\{i_1 \ldots i_n\}} = 0$, and $O'_{i_1 \ldots i_n} = O_{i_1 \ldots i_n} + A_{i_1 \ldots i_n}$. Clearly, $O'_{i_1 \ldots i_n} \neq O_{i_1 \ldots i_n}$ and $\tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n} = \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O'_{i_1 \ldots i_n}$, so $O_{i_1 \ldots i_n}$ is in general not unique. If $O_{i_1 \ldots i_n}$ and $O'_{i_1 \ldots i_n}$ both satisfy the hypothesis and are irreducible, however, then their difference is also irreducible and $\tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)(O_{i_1 \ldots i_n} - O'_{i_1 \ldots i_n}) = O_{nm} - O_{nm} = 0$ for all $-n \leq m \leq n$, so by completeness $O_{i_1 \ldots i_n} - O'_{i_1 \ldots i_n} = 0$ and therefore $O_{i_1 \ldots i_n}$ is unique. 

**Corollary 4.2.** $O_{i_1 \ldots i_n}$ is a rank-$n$ sito relative to $\vec{J}$ if and only if there exists a (unique) rank-$n$ sito $O_{nm}$ relative to $\vec{J}$ such that $O_{nm} = \sum_{m=-n}^{n} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)^*O_{nm}$.  

**Proof.** If $O_{nm}$ is a sito then $O_{i_1 \ldots i_n} = \sum_{m} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)^*O_{nm}$ is a rank-$n$ sito relative to $\vec{J}$, by Lemma 4.1. Conversely, if $O_{i_1 \ldots i_n}$ is a sito then $O_{nm} = \sum_{m} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n}$ is a sito, by Lemma 4.1, and $O_{nm} = \sum_{m} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)^*O_{nm} = \sum_{m} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n}$, where the last equality follows by completeness. Thus, existence of $O_{nm}$ is necessary and sufficient, as stated.

If $O_{nm}$ and $O'_{nm}$ are sitos both satisfying the statement, then $O_{nm} = \sum_{m=-n}^{n} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)O_{i_1 \ldots i_n} = O'_{nm}$ for all $-n \leq m \leq n$.  

We call a sito $O_{i_1 \ldots i_n}$ and a sito $O_{nm}$ related to each other as described in the Lemmas “dual” to each other. It is easily shown, using Corollaries 4.1 and 4.2, that $O_{i_1 \ldots i_n} = O_{i_1 \ldots i_n}$ if and only if $O_{nm} = (-1)^m O_{i_1 \ldots i_n}^\dagger$. 

As a simple illustration of the results presented in this section, consider a single spinless particle moving in a central potential. For that system any rank-$n$ tensor operator must be a linear combination of the operators

$$T^{(n,r_p,n_L)}_{i_1 \ldots i_n} = r_{i_1} \cdots r_{i_n} L_{i_{n+1}} \cdots L_i \cdots L_{i_{n+1}} \cdots \cdots L_{i_n}, \quad n_r, n_p, n_L \geq 0, \quad n_r + n_p + n_L = n.$$  

For each triple $(n_r, n_p, n_L)$ we have a different cartesian tensor operator relative to $\vec{L}$. None of them is irreducible if $n \geq 2$. Thus, every rank-$n$ sito is a linear combination of $T^{(n,r_p,n_L)}_{i_1 \ldots i_n}$, and every rank-$n$ sito $O_{nm}$ can be expressed as a linear combination of $\tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m) T^{(n,r_p,n_L)}_{i_1 \ldots i_n}$. In section 6 below we briefly describe the tensor structure of the most common sitos.
5 The Wigner–Eckart theorem for irreducible cartesian tensor operators

If $O_{nk}$ is a rank-$n$ sito relative to $\vec{J}$ the Wigner–Eckart theorem states that its matrix elements are given by

$$\langle j', m'|O_{nk}|j, m \rangle = \langle j'||O_n||j\rangle \langle j, m; n, k|j', m' \rangle,$$

where the reduced matrix element $\langle j'||O_n||j\rangle$ is independent of $m, m'$. From the Wigner–Eckart theorem for sitos (32) and Corollary 4.2 we immediately obtain

**Theorem** (Wigner–Eckart theorem for sitos). Let $O_{i_1...i_n}$ be a rank-$n$ sito relative to $\vec{J}$. Then, its matrix elements are given by

$$\langle j', m'|O_{i_1...i_n}|j, m \rangle = \langle j'||\tilde{\epsilon}_{(n)} \cdot O||j\rangle \langle j, m; n, m'-m|j', m'\rangle \tilde{\epsilon}_{(n)i_1...i_n}(m'-m)*,$$

where the reduced matrix element $\langle j'||\tilde{\epsilon}_{(n)i_1...i_n} O_{k_1...k_n}|j\rangle$ depends on the operator $O$ and on $n, j', j$, but is independent of $m', m$, and of $i_1...i_n$.

If the sito $O_{nm}$ and the sito $O_{i_1...i_n}$ are dual to each other in the sense of section 4, then it is clear that $\langle j'||O_n||j\rangle = \langle j'||\tilde{\epsilon}_{(n)} \cdot O||j\rangle$. The Wigner–Eckart theorem for sitos applies to any scalar and cartesian vector operators, since for those the irreducibility requirement is moot. It can be extended to rank-$n \geq 2$ reducible tensor operators by expanding them in their irreducible components of rank $\tilde{n}$ with $0 \leq \tilde{n} \leq n$ and applying the theorem to each irreducible component separately. To the best of our knowledge, however, no such general decomposition theorem has been given in the literature. The simplest example is, of course, that of rank-2 cartesian tensors, whose decomposition is trivial to obtain,

$$\langle j', m'|O_{h_1h_2}|j, m \rangle = \langle j'||O_{(2)}||j\rangle \langle j, m; 2, m'-m|j', m'\rangle \tilde{\epsilon}_{(2)h_1h_2}(m'-m)*$$

$$+ \langle j'||O_{(1)}||j\rangle \langle j, m; 1, m'-m|j', m'\rangle \tilde{\epsilon}_{h_1h_2k}(m'-m)* + \langle j||O_{(0)}||j\rangle \delta_{j'} \delta_{m'm} \delta_{h_1h_2}, \tag{33}$$

$$O_{(2)i_1i_2} = \frac{1}{2} O_{(i_1i_2)0}, \quad O_{(1)k} = \frac{1}{2} \tilde{\epsilon}_{h_1h_2k} O_{k_1k_2}, \quad O_{(0)} = \frac{1}{3} O_{kk}.$$ 

Here, the operators $O_{(q)}, 0 \leq q \leq 2$, are rank-$q$ sitos relative to $\vec{J}$. We wrote their reduced matrix elements without $\tilde{\epsilon}$ tensors for brevity, since no notational ambiguity may arise in this case. A generalization of the above theorem to the case of totally–symmetric reducible tensor operators of any rank is given below in section 7, and to partially irreducible tensor operators in section 9.

6 Standard spherical irreducible tensor operators

In this section we consider some standard sitos from the point of view of the preceding sections, and discuss their relation to sitos. As a by-product, some relations among standard sitos are found that may be more difficult to obtain by other methods, as shown in this section and in section 8.

6.1 Spherical harmonics

Spherical harmonics, as is easy to prove [17], can be written as

$$Y_{\ell m}(\vec{r}) = N_{\ell} \tilde{\epsilon}(\ell)_{i_1...i_\ell} (m) \hat{r}_{i_1} \cdots \hat{r}_{i_\ell}, \quad N_{\ell} = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{(2\ell + 1)!!}{\ell!}}. \tag{34}$$

This equation shows that the sito dual to $Y_{\ell m}$ in the sense of Lemma 4.1 is $\tilde{\epsilon}_{(i_1...i_\ell)m}$, up to a multiplicative constant. The reduced matrix element of $Y_{\ell m}$ is well-known from the literature [7, 13], so from (34) we find

$$\langle \ell'||\tilde{\epsilon}_{(n)i_1...i_n} \hat{r}_{i_1} \cdots \hat{r}_{i_n}||\ell \rangle = \frac{1}{N_n} \langle \ell'||Y_n||\ell \rangle, \quad \langle \ell'||Y_n||\ell \rangle = \sqrt{\frac{(2\ell + 1)(2n + 1)}{4\pi(2\ell + 1)^3}} \langle \ell, 0; n, 0|\ell', 0 \rangle, \tag{35}$$
From (34) and the second equality in (15) we recover the familiar relation \( Y_{\ell m}(\hat{\mathbf{r}})^* = (-1)^m Y_{-\ell -m}(\hat{\mathbf{r}}) \).
We notice that (17) follows immediately from (34). The relation inverse to (34) is given by (67) below. Substituting (34) in the addition theorem for spherical harmonics leads to
\[
P_{\ell}(\hat{\mathbf{r}} \cdot \hat{\mathbf{r}}') = \frac{(2\ell - 1)!!}{\ell!} \hat{r}_{(i_1 \cdots i_{\ell})} \hat{r}'_{(i_1 \cdots i_{\ell})},
\]
which gives a multilinear representation for Legendre polynomials.

The expressions (34) for \( Y_{\ell m} \) and (36) for \( P_{\ell} \) as multilinear forms on the unit sphere have useful applications, some of which we discuss below. Here, we briefly mention that (34) yields the numerical coefficients in Stevens’ operator-equivalent method [18], as shown by the relation
\[
\langle j, m' | \hat{\mathbf{r}}_{(n)j_1 \cdots j_n} r_{i_1} \cdots r_{i_n} | j, m \rangle = \frac{\langle j | \hat{\mathbf{r}}_{(n)j_1 \cdots j_n} r_{j_1} \cdots r_{j_n} | j \rangle}{\langle j | \hat{\mathbf{r}}_{(n)j_1 \cdots j_n} J_{i_1} \cdots J_{i_n} | j \rangle} \langle j, m' | \hat{\mathbf{r}}_{(n)h_1 \cdots h_n} (k) J_{h_1} \cdots J_{h_n} | j, m \rangle,
\]
with the reduced matrix elements given by (35) and (17)
\[
\langle j | \hat{\mathbf{r}}_{(n)k_1 \cdots k_n} J_{k_1} \cdots J_{k_n} | j \rangle = 2^{-n} \sqrt{n!} \sqrt{(2j + n + 1)!} \sqrt{(2j + 1)(2j - n)!}. \tag{38}
\]
In the simplest case \( n = 2 \) (\( n = 1 \) being trivial) from (37) we get
\[
2z^2 - (x^2 + y^2) = 3z^2 - r^2 = r^2 C(j, 2)(2J^2 - J_x^2 - J_y^2) = C(j, 2)(3J^2 - j(j + 1)),
\]
\[
r_{i_1} r_{j_1} = r^2 C(j, 2) \frac{1}{2} (J_i J_j + J_j J_i), \quad i \neq j,
\]
\[
C(j, 2) = -4 \sqrt{j(j + 1)} \sqrt{\frac{2j + 1}{(2j - 1)(2j + 3)}} \sqrt{\frac{2j - 2}{(2j + 3)!}}. \tag{39}
\]
Further discussion of the operator-equivalent method is outside the scope of this paper, however, so we refer to [18, 19].

### 6.1.1 An explicit expression for \( Y_{\ell m} \)

Taking (34) as a definition of spherical harmonics leads to an explicit expression for them. From (34) we easily obtain \( Y_{1m}(\hat{\mathbf{r}}) \) in terms of the spherical coordinates \( \theta, \varphi \) of \( \hat{\mathbf{r}} \). On the other hand, from (34) and (16) we obtain
\[
Y_{\ell m}(\hat{\mathbf{r}}) = \sqrt{\frac{2\ell + 1}{4\pi}} \left( \frac{4\pi}{3} \right)^{\frac{\ell}{2}} \frac{1}{\ell!} \sqrt{\ell + m)!/(\ell - m)!} \sum_{s_1, \ldots, s_n = -1}^{1} \frac{1}{(\sqrt{2})^{\sum_{k=1}^{n} |s_k|}} Y_{1s_1}(\hat{\mathbf{r}}) \cdots Y_{1s_n}(\hat{\mathbf{r}}). \tag{40}
\]
This expression for \( Y_{\ell m} \) in terms of \( Y_{1s} \) can be put in a more explicit form by exploiting the total symmetry of the summand under permutations of the summation indices. We temporarily assume \( m > 0 \) for concreteness, and define \( N_{\pm 1, 0} \) as the number of 1s, -1s and 0s, respectively, in the summation multiindex \( (s_1, \ldots, s_\ell) \) in (40). Thus, \( N_1 + N_{-1} + N_0 = \ell, N_1 - N_{-1} = m, \) and therefore \( N_0 = \ell + m - 2N_1. \) It is also easy to see, by considering a few particular cases, that \( m \leq N_1 \leq [(\ell + m)/2], \) where \([(\ldots)]\) denotes integer part. There are \( (\ell) \) ways of distributing \( N_1 \) 1s among \( \ell \) indices \( s_i \), and there are \( (\ell - N_1) \) ways to distribute \( N_{-1} = N_1 - m - 1s \) among the remaining \( \ell - N_1 \) indices, and the remaining \( N_0 \) indices must take the value 0. Thus, for given \( \ell, m \) we can reduce the sum in (40) to a single sum over \( N_1. \) By using the explicit form of \( Y_{1s}, \) from (40) we obtain
\[
Y_{\ell m}(\hat{\mathbf{r}}) = \sqrt{\frac{2\ell + 1}{4\pi}} \left( \frac{\ell - m)!}{\ell + m)!} \right) e^{im\varphi} P_{\ell m}(\cos \theta),
\]
\[
P_{\ell m}(x) = \frac{(\ell + m)!}{\ell!} \sum_{N_1=m}^{[(\ell + m)/2]} \left( \frac{\ell}{N_1} \right) \left( \ell - N_1 \right) (-1)^{N_1} 2^{2N_1 - m} (\sqrt{1 - x^2})^{2N_1 - m} x^{\ell - 2N_1 + m}, \tag{41}
\]
valid for integer \( \ell \geq 0 \) and \(-\ell \leq m \leq \ell. \) We see that starting from (34) we not only recovered the standard expression (A.4) but also obtained an explicit expression for the associated Legendre function \( P_{\ell m} \) by purely tensorial considerations without reference to the Legendre differential equation. (For further expressions for \( P_{\ell m} \) and \( Y_{\ell m} \) see [13, 20]. See [21] for related recent results.)
6.2 Bipolar spherical harmonics

Consider a system formed by two spinless particles moving in a central potential, with orbital angular momenta $\vec{L}_{1,2}$ coupled to total angular momentum $\vec{J}$. Its angular wave function is given by a bipolar spherical harmonic $Y_{j m}^{\ell_1 \ell_2}(\vec{r}_1, \vec{r}_2)$, defined as \cite{13}

$$Y_{j m}^{\ell_1 \ell_2}(\vec{r}_1, \vec{r}_2) = \langle \vec{r}_1, \vec{r}_2|\ell_1, \ell_2; j, m \rangle = \sum_{\mu_1=-\ell_1}^{\ell_1} \sum_{\mu_2=-\ell_2}^{\ell_2} \langle \ell_1, \mu_1; \ell_2, \mu_2|j, m \rangle Y_{\ell_1 \mu_1}(\vec{r}_1)Y_{\ell_2 \mu_2}(\vec{r}_2). \quad (42)$$

Its complex conjugation properties follow from (42), $Y_{j m}^{\ell_1 \ell_2}(\vec{r}_1, \vec{r}_2)^* = (-1)^{\ell_1+\ell_2-\ell}(-1)^m Y_{j m}^{\ell_1 \ell_2}(\vec{r}_2, \vec{r}_1) = (-1)^m Y_{j m}^{\ell_1 \ell_2}(\vec{r}_2, \vec{r}_1)$. From the Clebsch–Gordan coupling of two spherical harmonics \cite{13} we have the equality

$$Y_{j m}^{\ell_1 \ell_2}(\vec{r}, \vec{\hat{r}}) = \sqrt{\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2j+1)}} \langle \ell_1, 0; \ell_2, 0|j, 0 \rangle Y_{jm}(\vec{r}), \quad (43)$$

that we will need below. Bipolar spherical harmonics define operators in the Hilbert state–space of the two–particle system, acting multiplicatively in the coordinate representation $\langle \vec{r}_1, \vec{r}_2|Y_{j m}^{\ell_1 \ell_2}|\psi \rangle = Y_{j m}^{\ell_1 \ell_2}(\vec{r}_1, \vec{r}_2)\psi(\vec{r}_1, \vec{r}_2)$. An analogous, but different, operator is obtained in the momentum representation by the multiplicative action of $Y_{j m}^{\ell_1 \ell_2}(\vec{p}_1, \vec{p}_2)$. As operators, bipolar spherical harmonics are sitos of rank $j$ relative to $\vec{J} = \vec{L}_1 + \vec{L}_2$.

If the coupling in (42) is maximal, $j = \ell + \ell'$, then $Y_{j m}^{\ell \ell'}$ has a tensorial representation analogous to (34) that follows from (20)

$$Y_{(\ell+\ell')m}^{\ell \ell'}(\vec{r}, \vec{\hat{r}}') = N_{\ell \ell'}\hat{\varepsilon}_{(j)i_1 \ldots i_j j_{\ell'}}(m)\vec{r}_{i_1} \ldots \vec{r}_{i_{\ell}} \vec{\hat{r}}'_{i_{\ell+1}} \ldots \vec{\hat{r}}'_{i_{j_{\ell'}}}. \quad (44)$$

Thus, a maximally-coupled bipolar spherical harmonic is dual to the cartesian irreducible tensor operator

$$N_{\ell \ell'}\hat{\varepsilon}_{(j)i_1 \ldots i_j j_{\ell'}}(m)\vec{r}_{i_1} \ldots \vec{r}_{i_{\ell}} \vec{\hat{r}}'_{i_{\ell+1}} \ldots \vec{\hat{r}}'_{i_{j_{\ell'}}}. \quad (45)$$

which is the rank-2 analog of (9b).

If the angular-momentum coupling in $Y_{j m}^{\ell \ell'}(\vec{r}, \vec{\hat{r}}')$ is not maximal its tensorial expression is more complicated. It has been derived in the general case $|\ell'-\ell| \leq j \leq \ell + \ell'$ in \cite{22} using the methods of \cite{17}, which are beyond the scope of this paper. We quote the result without proof in (B.1) for completeness, and because we need some of its consequences below. From that expression we can read off the cartesian irreducible tensor dual to $Y_{j m}^{\ell \ell'}(\vec{r}, \vec{\hat{r}}')$, which is the irreducible part of the tensor contracted with $\hat{\varepsilon}_{(j)i_1 \ldots i_j}$ there.

6.2.1 The binomial expansion for spherical harmonics

Given two position vectors $\vec{r}_a$, $a = 1, 2$, it may be of interest to compute $Y_{\ell m}(\vec{r})$, with $\vec{r}$ a linear combination of $\vec{r}_{1,2}$, in terms of $Y_{\ell m}(\vec{r}_{1,2})$. For instance, $\vec{r}$ may be the center-of-mass of $\vec{r}_{1,2}$ or their associated relative position vector $\vec{r}_1 - \vec{r}_2$, or, in the momentum representation, the total or relative momentum of two particles. Setting $\vec{r} = (\alpha \vec{r}_1 + \beta \vec{r}_2)/(\alpha \vec{r}_1 + \beta \vec{r}_2)$ in (34), with $\alpha, \beta$ real numbers, applying the binomial expansion for the multiple product of $\vec{r}$ there, and using (20), leads to the binomial expansion for spherical harmonics

$$Y_{\ell m} \left( \frac{\alpha \vec{r}_1 + \beta \vec{r}_2}{|\alpha \vec{r}_1 + \beta \vec{r}_2|} \right) = \sqrt{\frac{4\pi}{\sqrt{2(\ell-n)+1}}} \sum_{n=0}^{\ell} \frac{1}{\sqrt{2(\ell-n)+1}} Y_{\ell m} \left( \frac{\alpha \vec{r}_1 + \beta \vec{r}_2}{|\alpha \vec{r}_1 + \beta \vec{r}_2|} \right) Y_{\ell m} \left( \frac{(\alpha \vec{r}_1 + \beta \vec{r}_2)^{\ell-n}}{|\alpha \vec{r}_1 + \beta \vec{r}_2|^{\ell-n}} \right). \quad (46)$$

Notice that the bipolar spherical harmonic in (46) is maximally coupled. The binomial expansion can be extended to a multinomial expansion for $Y_{\ell m}(\vec{R}/|\vec{R}|)$ with $\vec{R} = \sum_{k=1}^{k} \alpha_k \vec{r}_a$, $k \geq 2$. In that case, because all angular-momentum couplings are maximal as in (46), all coupling schemes lead to the same result.
6.3 Tensor spherical harmonics

Tensor spherical harmonics are simultaneous eigenfunctions of $\hat{L}^2$, $\hat{S}^2$, $\hat{J}^2$, and $J_3$, as is appropriate to the wave functions of a particle with spin $\vec{S}$ and orbital angular-momentum $\hat{L}$ coupled to total angular-momentum $\vec{J}$. They are defined as [22]

$$
(Y_{jm}^{\ell n}(\vec{r}))_{i_1 \ldots i_n} = \sum_{\mu=-\ell}^{\ell} \sum_{\nu=-n}^{n} \langle \ell, \mu; n, \nu|j, m \rangle Y_{\mu \nu}(\vec{r}) \hat{c}_{(n)j} \ldots \hat{c}_{(n)\mu} (\nu). \tag{47}
$$

From the second equality in (15) and the conjugation of spherical harmonics we derive the conjugation relation $(Y_{jm}^{\ell n}(\vec{r}))_{i_1 \ldots i_n} = (-1)^{\ell+s-j}(1-m)Y_{jm}^{\ell n}(\vec{r})_{i_1 \ldots i_n}$. The quantities $Y_{jm}^{\ell n}(\vec{r})$ are tensor functions defined on the unit sphere, known as spin-$n$ spherical harmonics or rank-$n$ tensor spherical harmonics. If $n = 0$ we have that $Y_{0m}^{\ell n} = Y_{\ell m}$ is an ordinary, scalar spherical harmonic. For $n = 1$, $Y_{1m}^{\ell 1}(\vec{r})$ is a vector spherical harmonic. In that case (47) agrees with the definition given in [7, 23], agrees with [24] up to a factor of $i$, and differs from those in [5, 13] in the choice of spin wave-function basis. $Y_{jm}^{\ell n}(\vec{r})$ transforms as a rank-$s$ cartesian tensor relative to $\vec{J}$. Its total contraction with an orbital rank-$s$ tensor operator transforms as a rank-$l$ sito relative to $\vec{L}$, scalar relative to $\vec{S}$.

Maximally coupled tensor spherical harmonics ($j = \ell + n$) have a simple tensorial expression analogous to (34). By substituting (34) in (47) and using (20) we get

$$
(Y_{(\ell+n)m}^{\ell n}(\vec{r}))_{i_1 \ldots i_n} = N_{\ell} \hat{c}_{(n)\ell} \hat{c}_{(n)n+1} \ldots \hat{c}_{(n)\ell+1}.
$$

In particular we have the relations

$$(Y_{sm}^{\ell s}(\vec{r}))_{i_1 \ldots i_s} = \frac{1}{\sqrt{4\pi}} \hat{c}_{(s)\ell} \ldots \hat{c}_{(s)s}(m), \quad (Y_{(\ell+s)m}^{\ell s}(\vec{r}))_{i_1 \ldots i_s} = \sqrt{\frac{\ell + 1}{2\ell + 3}} (Y_{(\ell+s)m}^{\ell+1(s-1)}(\vec{r}))_{i_1 \ldots i_{s-1}},
$$

and $(Y_{(\ell+n)m}^{\ell n}(\vec{r}))_{i_1 \ldots i_n} \hat{c}_{i_1} \ldots \hat{c}_{i_n} = (N_{\ell}/N_{\ell+n})Y_{(\ell+n)m}(\vec{r})$ is an ordinary spherical harmonic. The tensorial expression of non-maximally coupled tensor spherical harmonics is more involved than that of maximally coupled ones. We can get some insight into it by relating tensor spherical harmonics to bipolar ones and using (B.1). From (34), (42) and (47) we obtain the bipolar spherical harmonics as

$$
Y_{jm}^{\ell n}(\vec{r}, \vec{r}') = N_s (Y_{jm}^{\ell n}(\vec{r}))_{i_1 \ldots i_s} \hat{c}_{(s)i_1} \ldots \hat{c}_{(s)i_s}.
$$

This relation can be inverted to write tensor spherical harmonics in terms of bipolar ones

$$
(Y_{jm}^{\ell n}(\vec{r}))_{i_1 \ldots i_s} = \sqrt{4\pi} \sqrt{\frac{1}{s!(2s+1)!}} (-1)^{\ell+s-j} \partial'_{i_1} \ldots \partial'_{i_s} \langle |r'|^s |Y_{jm}^{\ell n}(\vec{r}', \vec{r}) \rangle. \tag{50}
$$

From this equation and (B.1) the tensorial expressions of non-maximally coupled tensor spherical harmonics can be obtained. More interestingly, by writing the cartesian tensors appearing in (B.1) as maximally coupled tensor spherical harmonics, through (48), we can express non-maximally-coupled tensor spherical harmonics in terms maximally coupled ones. Once those relations have been obtained, use of (48) yields the sought-for tensorial expressions. We will restrict ourselves here to quoting the results for next– and next–to–next–to–maximal coupling. For $j = \ell + s - 1$ we have

$$
Y_{(\ell+s-1)m}^{\ell s}(\vec{r}) = \sqrt{\frac{2\ell + 1}{s!(\ell + s)}} (\vec{r} \cdot \vec{S}(s)) Y_{(\ell+s-1)m}^{\ell(s-1)}(\vec{r}), \tag{51}
$$

Notice that in the momentum representation the matrix on the right-hand side would be the helicity operator $\vec{p} \cdot \vec{S}$. Similarly, for $j = \ell + s - 1$ and $s \geq 2$ we have

$$
Y_{(\ell+s-2)m}^{\ell s}(\vec{r}) = \sqrt{\frac{2\ell - 1}{s!(2s - 1)}} \sqrt{\frac{2\ell + 1}{\ell - 1}} \frac{1}{\sqrt{2\ell + s - 1}} \frac{1}{\sqrt{\ell + s - 1}} \times \left( (\vec{r} \cdot \vec{S}(s)) \cdot (\vec{r} \cdot \vec{S}(s)) - \frac{s!(\ell + s - 1)}{2\ell - 1} \right) Y_{(\ell+s-2)m}^{\ell(s-1)}(\vec{r}). \tag{52a}
$$

14
and, if \( s = 1 \),
\[
Y_{(\ell - 1)m}^{\ell}(\vec{r}) = \sqrt{\frac{\ell - 1}{\ell}} Y_{(\ell - 2)m}^{\ell}(\vec{r}) - \sqrt{\frac{2\ell - 1}{\ell}} Y_{(\ell - 1)m}^{\ell}(\vec{r}) \tag{52b}
\]

Analogous relations can be obtained for \( j = \ell + s - \nu \) with \( \nu \geq 3 \). Additionally, such relations as (51) and (52) are of interest because they are independent of the spin wave-function basis used to define the tensor spherical harmonics. For brevity, however, we will not dwell longer on those issues here.

### 6.4 Spin polarization operators

In the \((2s + 1)\)-dimensional space of spin states of a spin-\( s \) particle, the spin operator \( \vec{S} \) may be viewed as a \((2s + 1) \times (2s + 1)\) matrix and \( \vec{S}^2 = s(s + 1)I \), with \( I \) the identity matrix. A complete set of \((2s + 1)^2\) matrices in that space is given by the polarization operators defined in section 2.4 of [13] as

\[
T_{\ell m}(s) = \kappa_\ell(s) \left( \vec{S} \cdot \vec{S} \right)^\ell \langle |\vec{r}|^\ell \gamma_{\ell m}(\vec{r}) \rangle, \quad \kappa_\ell(s) = \frac{2\ell}{\ell!} \sqrt{\frac{4\pi(2s - \ell)!}{(2s + \ell + 1)!}}, \quad 0 \leq \ell \leq 2s, \quad -\ell \leq m \leq \ell. \tag{53}
\]

From this equation and (17) we immediately obtain the equivalent expression

\[
T_{\ell m}(s) = \kappa_\ell'(s) \bar{\gamma}_{(\ell)_{i_1 \ldots i_\ell}}(m)S_{i_1} \ldots S_{i_\ell}, \quad \kappa_\ell'(s) = \frac{2\ell}{\ell!} \sqrt{\frac{(2s - \ell)!(2\ell + 1)!}{\ell!(2s + \ell + 1)!}}. \tag{54}
\]

Thus, \( T_{\ell m}(s) \) is a rank-\( \ell \) sito relative to \( \vec{S} \), dual to the cito \( 1/\ell!S_{i_1} \ldots S_{i_\ell} \) (i.e., the irreducible component of the cartesian tensor operator \( S_{i_1} \ldots S_{i_\ell} \)) introduced in [10]. The reduced matrix element of \( T_{\ell m}(s) \) is \( \langle s|T_{\ell m}(s)|s \rangle = \sqrt{(2\ell + 1)(2s + 1)} \). The operator \( T_{\ell m}(s) \) is hermitian, \( T_{\ell m}(s)^\dagger = (-1)^m T_{\ell(-m)}(s) \), and satisfies the orthonormality relation

\[
\text{Tr} \left( T_{\ell m'}(s) T_{\ell m}(s) \right) = \sum_\mu \langle s, \mu|T_{\ell m'}(s)^\dagger T_{\ell m}(s)|s, \mu \rangle = \delta_{\ell \ell'} 6_\ell 6_{m'm}, \tag{55}
\]

which can be readily verified by inserting \( \sum_{m'} |s, \mu'\rangle \langle s, \mu'| \) between the two operators and applying the Wigner–Eckart theorem to the resulting matrix elements. A more detailed description of the properties of the operators \( T_{\ell m}(s) \) is given in the reference cited above.

### 6.5 Electric multipole moments

As an application of the results of section 6.1, we derive in this section a general expression for the cartesian \( 2^n \)-pole electric tensor and its relation to the spherical one. The magnetic multipoles are discussed below in section 9.1. The electric potential is given by [25]

\[
\phi(\vec{r}', t) = \frac{1}{4\pi \varepsilon_0} \int_V d^3r' \rho(\vec{r}', t) |\vec{r} - \vec{r}'|^{-1} \tag{56}
\]

where \( \rho(\vec{r}, t) \) is the charge density, assumed to vanish for all \( t \) outside a bounded volume \( V \). The Coulomb integral (56) gives the potential \( \phi(\vec{r}) \) in electrostatics, and in electrodynamics in the Coulomb gauge with \( \rho(\vec{r}, t) \) the instantaneous charge density. More generally, (56) holds when retardation effects can be neglected.

Assuming \( |\vec{r}| > |\vec{r}'| \) for all \( \vec{r}' \) in \( V \), we can substitute the well-known expansion of \( 1/|\vec{r} - \vec{r}'| \) in spherical harmonics [25] in (56) to obtain the spherical multipole expansion

\[
\phi(\vec{r}) = \frac{1}{4\pi \varepsilon_0} \sum_{n=0}^\infty \frac{4\pi}{2n + 1} \frac{1}{|\vec{r}|^{n+1}} \sum_{m=-n}^n q_{nm} Y_{nm}(\vec{r}), \quad q_{nm} = \int_V d^3r' \rho(\vec{r}') |\vec{r}'|^{n} Y_{nm}(\vec{r}'). \tag{57}
\]

In this equation and in what follows we omit the temporal coordinate in \( \phi(\vec{r}, t) \), \( \rho(\vec{r}, t) \) and \( q_{nm}(t) \) for brevity. For \( n \geq 0 \) fixed, the \( 2n + 1 \) quantities \( q_{nm} \) are called “spherical \( 2^n \)-pole moments” [25]. In the coordinate representation in quantum mechanics \( q_{nm} \) is a rank-\( n \) sito, as is apparent from the first equality in (57).
since $Y_{nm}$ is a rank-$n$ sito and $\phi$ is a scalar. (Notice that our $q_{nm}$ is the complex conjugate of the one in [25].) A cartesian multipole expansion, on the other hand, is of the form

$$\phi(\mathbf{r}) = \frac{1}{4\pi\varepsilon_0} \sum_{n=0}^{\infty} \frac{1}{n!} \frac{1}{|\mathbf{r}|^{2n+1}} Q_{i_1 \ldots i_n} r_{i_1} \cdots r_{i_n},$$  

(58)

where $Q_{i_1 \ldots i_n}$ is the cartesian $2^n$-pole tensor. Clearly, $Q_{i_1 \ldots i_n}$ must be a rank-$n$ cartesian tensor, since $\phi$ in (58) is a scalar, and it must be completely symmetric since any antisymmetric part would not contribute to (58). It must also be traceless, because otherwise the traces of $Q_{i_1 \ldots i_n}$ would make contributions of $\mathcal{O}(1/r^{k+1})$ with $k < n$. Thus, $Q_{i_1 \ldots i_n}$ is a rank-$n$ cartesian irreducible tensor in the classical theory, and a rank-$n$ cite to in the quantum theory. To obtain (58) and the expression for $Q_{i_1 \ldots i_n}$ from (56), we start from the expansion of $1/|\mathbf{r} - \mathbf{r}'|$ in Legendre polynomials [25] written in the form

$$\frac{1}{|\mathbf{r} - \mathbf{r}'|} = \sum_{n=0}^{\infty} \frac{|\mathbf{r}'|^n}{|\mathbf{r}|^{n+1}} P_n(\mathbf{r} \cdot \mathbf{r}'),$$  

(59)

which we substitute in (56). By using the expression (36) for the Legendre polynomial $P_n$ we are led to (58) with

$$\frac{1}{(2n-1)!!} Q_{i_1 \ldots i_n} = \int_V d^3r' \rho(\mathbf{r}') r'_{i_1} \cdots r'_{i_n} = \sum_{m=-n}^{n} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m) \tilde{\varepsilon}_{(n)j_1 \ldots j_n}(m) \int_V d^3r' \rho(\mathbf{r}') r'_{j_1} \cdots r'_{j_n}. $$

(60)

As is easy to check, for $n = 0, 1, 2$, $Q_{i_1 \ldots i_n}$ is the total charge, dipole vector, and quadrupole tensor, respectively, of the charge distribution $\rho$. We can make contact with the notation of [26] by substituting

$$\tilde{r}_{(i_1} \cdots \tilde{r}_{i_n)} = (-1)^n \frac{r_{i_1} \cdots r_{i_n}}{(2n-1)!!} \partial_{i_1} \cdots \partial_{i_n} \frac{1}{|\mathbf{r}|}$$

(61)

in (60). From (60) and (34) we get

$$q_{nm} = \frac{1}{\sqrt{4\pi}} \sqrt{\frac{2n + 1}{n!(2n-1)!!}} Q_{i_1 \ldots i_n} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m), \quad Q_{i_1 \ldots i_n} = \sqrt{4\pi} \sqrt{\frac{n!(2n-1)!!}{2n + 1}} \sum_{m=-n}^{n} q_{nm} \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)^*. $$

(62)

We see that the rank-$n$ spherical and cartesian multipole tensors are related to each other according to the general results of section 4, up to a normalization constant. Equation (62) reproduces the expressions for $q_{nm}$ in terms of $Q_{i_1 \ldots i_n}$ given in equations (4.4)—(4.6) of [25] (taking into account that our $q_{nm}$ is the complex conjugate of the one in that reference) for $n = 0, 1, 2$, and generalizes them to any natural $n$, making completely explicit the analogous relations obtained in [27].

7 The Wigner-Eckart theorem for reducible symmetric cartesian tensor operators

The results of the previous sections, and in particular the Wigner–Eckart theorem, can in principle be extended to generic reducible tensors and tensor operators by decomposing them into their irreducible components. In this section we consider the extension to the case of totally symmetric reducible cartesian tensors.

We introduce a basis of totally symmetric rank-$n$ tensors as the set of tensors $\tilde{\varepsilon}_{(n,s)}(m)$ of rank $n$ and spin $s$, with $s = 0, 2, \ldots n$ if $n$ is even and $s = 1, 3, \ldots n$ if it is odd, and $-s \leq m \leq s$, defined as

$$\tilde{\varepsilon}_{(n,s)i_1 \ldots i_n}(m) = \lambda_{(n,s)} \frac{1}{n!} \tilde{\varepsilon}(s)_{i_1 \ldots i_n}(m) \delta_{i_1 i_2} \cdots \delta_{i_{n-1} i_n}. $$

(63a)

It is clear from this definition that for $s = n$ the basis tensor is irreducible and $\tilde{\varepsilon}_{(n,n)i_1 \ldots i_n}(m) = \tilde{\varepsilon}_{(n)i_1 \ldots i_n}(m)$. Furthermore, if $n$ is even and $s = 0$ then $\tilde{\varepsilon}_{(0)}(0) = 1$. The normalization constant in (63a) is given by

$$\lambda_{(n,s)} = \sqrt{\frac{1}{2^s s! n!} \frac{(2s + 1)!!}{(n + s + 1)!!}}. \quad n\delta = \frac{n - s}{2}. $$

(63b)
From (63) the basis tensors are seen to satisfy the normalization and complex conjugation relations
\[
\tilde{e}_{(n,s')}(m')^* \cdot \tilde{e}_{(n,s)}(m) = \delta_{s',s} \delta_{m'm}, \quad \tilde{e}_{(n,s)}(m)^* = (-1)^m \tilde{e}_{(n,s)}(-m),
\]
where the dot stands for total index contraction. The definition (63) is far from arbitrary; from it and (17) we obtain the equality
\[
\tilde{e}_{(n,s)}(m) = \lambda'_{(n,s)} \partial_{i_1} \ldots \partial_{i_n} (|\vec{r}|^n Y_{sm}(\vec{r})), \quad \lambda'_{(n,s)} = \left(4\pi \frac{1}{2^n n_\delta n! n!(n+s+1)!}\right)^{1/2},
\]
valid for 0 \leq n - s even, generalizing (17) to the case of totally symmetric reducible tensors, and which can be taken as a definition of \(\tilde{e}_{(n,s)}\) equivalent to (63). It is clear from (63) that for \(n\) fixed there are \((n+1)(n+2)/2\) basis tensors, spanning the subspace of totally symmetric tensors. It is straightforward to show from (2), (7) that the basis tensors \(\tilde{e}_{(n,s)}(m)\) are eigenfunctions of \(\hat{S}^2_{(n)}\) and \(\hat{S} \cdot \hat{S}_{(n)}\) with eigenvalues \(s\) and \(m\).

Given any totally symmetric rank-\(n\) complex tensor \(A_{i_1 \ldots i_n}\) we have the expansion
\[
A_{i_1 \ldots i_n} = \sum_{(n-s)\text{even}}^{n} \lambda_{(n,s)} \sum_{m=-s}^{s} \left(\text{Tr}(s)(A) \cdot \tilde{e}_{(s)}(m)\right) \tilde{e}_{(n,s)}(i_1 \ldots i_n)(m)^*, \quad \text{Tr}(s)(A)_{i_1 \ldots i_s} \equiv A_{i_1 \ldots i_s k_1 \ldots k_n},
\]
with \(n_\delta\) as in (63b). As a particular case of (66) we have
\[
\hat{r}_{i_1} \ldots \hat{r}_{i_n} = \sum_{(n-s)\text{even}}^{n} \lambda'_{(n,s)} \sum_{m=-s}^{s} Y_{sm}(\vec{r}) \tilde{e}_{(n,s)}(i_1 \ldots i_n)(m)^*,
\]
with \(\lambda'_{(n,s)}\) as in (65), which is the relation inverse to (34). From the expansion (66) and the Wigner–Eckart theorem for \(\text{cito}\) we obtain

**Theorem** (Wigner–Eckart theorem for totally symmetric tensor operators). Let \(O_{i_1 \ldots i_n}\) be a totally symmetric cartesian tensor operator relative to \(\hat{J}\). Then, its matrix elements are given by
\[
\langle j', \mu'| O_{i_1 \ldots i_n} | j, \mu \rangle = \sum_{(n-s)\text{even}}^{n} \lambda_{(n,s)} \langle j'| \tilde{e}_{(s)}(m) \cdot \text{Tr}(s)(O) | j \rangle \sum_{m=-s}^{s} \langle j, \mu; s, m| j', \mu' \rangle \tilde{e}_{(n,s)}(i_1 \ldots i_n)(m)^*,
\]
Among the most commonly–occurring totally symmetric tensor operators we have \(r_{i_1} \ldots r_{i_n}\) and \(p_{i_1} \ldots p_{i_n}\). The former is the simplest possible example, since its traces are trivial to compute. We have
\[
\langle \ell', \mu'| r_{i_1} \ldots r_{i_n} | \ell, \mu \rangle = |\vec{r}|^n \sum_{(n-s)\text{even}}^{n} \lambda_{(n,s)} \langle \ell'| \tilde{e}_{(s)}(k_1 \ldots k_s \hat{r}_{k_1} \ldots \hat{r}_{k_s}) | \ell \rangle \sum_{m=-s}^{s} \langle \ell, \mu; s, m| \ell', \mu \rangle \tilde{e}_{(n,s)}(i_1 \ldots i_n)(m)^*,
\]
with the reduced matrix element given by (35). From this matrix element we obtain a related result involving spherical harmonics
\[
\sum_{\mu', \mu} Y_{\ell' \mu'}(\hat{q}') \langle \ell', \mu'| \hat{r}_{i_1} \ldots \hat{r}_{i_n} | \ell, \mu \rangle Y_{\ell \mu}(\hat{q})^* = \sum_{(n-s)\text{even}}^{n} (-1)^{-s} \sqrt{\frac{2\ell' + 1}{2s + 1}} \lambda_{(n,s)} \langle \ell'| \tilde{e}_{(s)}(k_1 \ldots k_s \hat{r}_{k_1} \ldots \hat{r}_{k_s}) | \ell \rangle \times \sum_{m=-s}^{s} \tilde{e}_{(n,s)}(i_1 \ldots i_n)(m)^* Y_{\ell \mu}(\hat{q}),
\]
Notice that the left-hand side of this equality is just the matrix element \(\langle \hat{q}'| P_{\ell'} \hat{r}_{i_1} \ldots \hat{r}_{i_n} P_{\ell}\hat{q}\rangle\), with \(P_{\ell}\) the angular-momentum projector operator [17]. Setting \(\hat{q}' = \hat{q}\) in this last equality and using (43) on its right-hand side, we obtain the expansion in spherical harmonics of \(\langle \hat{q}| P_{\ell'} \hat{r}_{i_1} \ldots \hat{r}_{i_n} P_{\ell}\hat{q}\rangle\). This simple example illustrates the power of our approach; the case of tensor powers of the momentum operator, \(p_{i_1} \ldots p_{i_n}\), is discussed in detail in the following section.
8 Derivatives of spherical harmonics to all orders

The gradient of \( Y_{\ell m}(\vec{r}) \) can be expressed as a linear combination of vector spherical harmonics, a widely known result going back to [12] and now standard textbook material [7, 13, 16]. In this section we generalize that result to the derivatives of \( Y_{\ell m}(\vec{r}) \) of all orders, expressed in terms of tensor spherical harmonics, as an application of (68). For that purpose, we would like to write equalities of the form

\[
\partial_{i_1} \ldots \partial_{i_s} Y_{\ell m}(\vec{r}) \neq \langle \vec{r} | \partial_{i_1} \ldots \partial_{i_s} | \ell, m \rangle \neq \sum_{\ell', m'} Y_{\ell' m'}(\vec{r}) \langle \ell', m' | \partial_{i_1} \ldots \partial_{i_s} | \ell, m \rangle.
\]

The reason why we cannot use equal signs in these relations is that, whereas \( Y_{\ell m}(\vec{r}) \) is independent of \( |\vec{r}| \), \( \partial_{\ell} Y_{\ell m}(\vec{r}) \) and higher derivatives are not. We remark, however, that \( \langle \vec{r} | n \partial_{i_1} \ldots \partial_{i_s} Y_{\ell m}(\vec{r}) \rangle \) and \( (|\vec{r}| | \partial_{i_1} \ldots | \partial_{i_s} Y_{\ell m}(\vec{r}) \rangle \) do not depend on \( |\vec{r}| \). We are thus led to define the operator

\[
\Omega_{n_1 \ldots n_s} = \langle \vec{r} | \partial_{i_1} \ldots \partial_{i_s} | \ell, m \rangle - \langle \vec{r} | \partial_{i_1} \ldots \partial_{i_s} | \ell, m \rangle - \langle \vec{r} | \partial_{i_1} \ldots \partial_{i_s} | \ell, m \rangle,
\]

satisfying the relation

\[
\langle \vec{r} | n \partial_{i_1} \ldots \partial_{i_s} Y_{\ell m}(\vec{r}) \rangle = \langle \vec{r} | \Omega_{n_1 \ldots n_s} | \ell, m \rangle = \sum_{\ell', m'} Y_{\ell' m'}(\vec{r}) \langle \ell', m' | \Omega_{n_1 \ldots n_s} | \ell, m \rangle.
\]

Since \( \Omega_{n_1 \ldots n_s} \) is totally symmetric by (70), we can apply the theorem (68) to the right-hand side of (71). By using (68) and (47), from (71) we get

\[
\langle \vec{r} | n \partial_{i_1} \ldots \partial_{i_s} Y_{\ell m}(\vec{r}) \rangle = \sum_{\ell'=\ell-n}^{\ell+n} \sum_{n=s \text{ even}}^{n} \sqrt{\frac{2\ell'+1}{2\ell+1}} (-1)^{s} \frac{1}{n!} \langle \ell' | \hat{\varepsilon}(\ell) \cdot \text{Tr}(s) \rangle |\ell, n, s \rangle \times \left( \Omega_{n_1 \ldots n_s} \right)_{\{i_1 \ldots i_s \} \ldots \delta_{i_{s+1}i_{s+2}} \ldots \delta_{i_{n-1}i_n}},
\]

where we assume \( \ell \geq n \), \( \lambda_{n,s} \) is defined in (63b) and \( \text{Tr}(s) \) in (66). In order to make this expression more explicit we need to evaluate the traces. We do so by going back to (70), with \( f = Y_{\ell m} \), and using the fact that \( Y_{\ell m} \) is an eigenfunction of the Laplace operator, to get²

\[
\langle \vec{r} | n \partial_{i_1} \ldots \partial_{i_{2k+1}} \partial_{i_{2k+2}} \ldots \partial_{i_{n}} Y_{\ell m}(\vec{r}) \rangle = (-1)^k \ell(\ell+1) \frac{(\ell-1)!!}{(\ell-2k+1)!!} \Omega_{n_1 \ldots n_s},
\]

where \( \Omega_{n,q} \) is the rank-(\( n-q+1 \)) tensor operator defined as

\[
\Omega_{n,q} = (-n-1)\hat{r}_n + |\vec{r}| \partial_{i_s} (-n-2)\hat{r}_{n-1} + |\vec{r}| \partial_{i_{n-1}} \ldots (q-1)\hat{r}_{i_q} + |\vec{r}| \partial_{i_q}.
\]

The operator \( \Omega_{n,q} \) is a generalization of \( \Omega_{n} \) defined in (69), with \( \Omega_{n,1} = \Omega_{n} \). From (73) we obtain the sought–for traces of \( \Omega_{n,q} \) as

\[
\text{Tr}(s) \langle \Omega_{n,q} \rangle_{i_1 \ldots i_s} = (-1)^{(n-s)/2} \ell(\ell+1) \frac{(\ell-1)!!}{(\ell-n+s+1)!!} \Omega_{n,q},
\]

with \( \text{Tr}(s) \) as defined in (66). The reduced matrix elements of \( \Omega_{n,q} \) appearing in (72) through the relation (74) can be evaluated with (19) by means of the usual recoupling techniques [16, 13]. We omit the algebra for brevity and state here the result

\[
\langle \ell' | \hat{\varepsilon}_r \cdot \Omega_{n,q} | \ell \rangle = (-1)^{(\ell' - \ell + r)/2} \frac{r!}{(2r-1)!} \frac{2\ell'+1}{2\ell'+1} \frac{(\ell - q + 2)!!}{(\ell' + n - 2)!!} \frac{(\ell + n - s - 2)!!}{(\ell - n + s + 1)!!} \langle \ell, 0, r, 0 | \ell', 0 \rangle,
\]

²We define double factorials for odd integers \( n = 2k-1 \) as \( n!! = \Pi_{h=1}^{k}(2h-1) \) and for even integers \( n = 2k \) as \( n!! = \Pi_{h=1}^{k}(2h) \) so that \( n!! = n!!((n-1)!!) \).
with $r = n - q + 1$ the rank of $\Omega_{(n,q)}$. Notice that the CG coefficient on the right–hand side vanishes unless $\ell + r - \ell'$ is even.

Putting together (72), (74) and (75) finally leads to

$$|\vec{r}|^n \partial_{i_1} \ldots \partial_{i_n} Y_{\ell m}(\vec{r}) = \sum_{\ell' = |\ell| - n}^{\ell + n} \sum_{s = 0}^{n} \Theta_{n s}(\ell, \ell')(\ell', 0; 0|\ell', 0) \left( Y_{\ell' m}(\vec{r}) \right)_{\{i_1 \ldots i_n\}} \delta_{i_{s+1}i_{s+2}} \ldots \delta_{i_{n-1}i_n},$$

$$\Theta_{n s}(\ell, \ell') = (-1)^{\frac{s+1}{2}} (-1)^{\eta s} \frac{2s + 1}{2^{n+\eta s}(n + s + 1)!} \sqrt{\frac{(2s - 1)!!}{(\ell + 1)!!} \frac{(\ell' + n - 2)!!}{(\ell - 2)!!}} \frac{n!}{(\ell - n + 1)!!}$$

(76)

To the best of our knowledge, this general result has not been given in the previous literature. It is certainly not to be found in the references listed in the bibliography.

Equation (76) gives an explicit expression for the $n^{th}$ derivatives of $Y_{\ell m}$ in terms of tensor spherical harmonics. For each $s$, $\ell$, $m$, equation (76) can be inverted to give $Y_{\ell' m}^{s}(\vec{r})$ as a linear combination of derivatives of $Y_{\ell m}(\vec{r})$. Those relations can, in fact, be taken as the definition of tensor spherical harmonics. For instance, in the case $n = 1$ from (76) and (51) we get

$$Y_{\ell m}^{(\ell - 1)}(\vec{r}) = \frac{|\vec{r}|^{-1} Y_{\ell m}(\vec{r})}{\sqrt{\ell (2\ell + 1)}} \nabla \left( |\vec{r}|^{\ell - 1} Y_{\ell m}(\vec{r}) \right),$$

$$Y_{\ell m}^{(\ell + 1)}(\vec{r}) = \frac{|\vec{r}|^{\ell + 2}}{\sqrt{(\ell + 1)(2\ell + 1)}} \nabla \left( |\vec{r}|^{-(\ell + 1)} Y_{\ell m}(\vec{r}) \right).$$

(77)

which allows us to make contact with vector spherical harmonics as defined in electromagnetism [25, 28].

We mention, finally, that from (76) we can obtain an expression for the matrix elements of momentum operators $(\ell', m' | p_{i_1} \ldots p_{i_n} | \ell, m)$. Indeed, multiplying (76) by $Y_{\ell' m'}(\vec{r})^*$ and integrating over the unit sphere, with the help of (47) we get

$$\int d^2 \vec{r} Y_{\ell' m'}(\vec{r})^* \partial_{i_1} \ldots \partial_{i_n} Y_{\ell m}(\vec{r}) = |\vec{r}|^{-n} \sum_{(n-s) \text{ even}}^{n} \Theta_{n s}(\ell, \ell') \frac{n!}{\lambda(n,s)} \left( \ell, 0; 0|\ell', 0 \right) \langle \ell', m'; s, m - m' | \ell, m \rangle$$

$$\times \hat{\varepsilon}_{i_1 \cdots i_n} (m - m'),$$

(78)

with $\Theta_{n s}$ as defined in (76) and $\lambda(n,s)$ in (63b).

9 The Wigner-Eckart theorem for partially irreducible tensors

The last class of reducible tensors we consider is that of partially irreducible tensors, defined as those tensors $T_{i_1 \cdots i_{n+1}}$ of rank $n + 1$ totally symmetric and traceless in their first $n$ indices. They play a rôle in the cartesian multipole expansion of the electromagnetic vector potential discussed in section 9.1. A rank-$n + 1$ partially irreducible tensor possesses $6n + 3$ independent components: $2n + 3$ corresponding to the irreducible part of spin $s = n + 1$, $2n + 1$ to the parts antisymmetric in some pair $i_k i_{n+1}$ $(1 \leq k \leq n)$ of spin $s = n$, and $2n - 1$ to the trace parts of spin $s = n - 1$. A basis of the space of rank-$n + 1$ partially irreducible tensor is then given by

$$B_{i_1 \cdots i_{n+1}}^{(j)}(m) = \sum_{\mu, \nu} (n, \mu; 1, \nu | j, m) \hat{\varepsilon}_{(n,i_1 \cdots i_n}(\mu) \hat{\varepsilon}_{(1)i_{n+1)}(\nu), \quad j = n - 1, n, n + 1, \quad -j \leq m \leq j.$$  

(79)

From (15) and standard properties of the Clebsch-Gordan coefficients the basis tensors (79) are found to satisfy the orthonormality and complex conjugation relations

$$B_{i_1 \cdots i_{n+1}}^{(j)}(m) B_{i_1 \cdots i_{n+1}}^{(j')} (m')^* = \delta_{jj'} \delta_{mm'}, \quad B_{i_1 \cdots i_{n+1}}^{(j)}(m)^* = (-1)^{n+1-j} (-1)^m B_{i_1 \cdots i_{n+1}}^{(j)} (-m).$$

(80)

In order to obtain matrix elements of partially irreducible tensor operators we need to express the reducible rank-$n + 1$ basis tensors (79) as (linear combinations of) direct products of an irreducible tensor of rank $s$, with $s = n + 1$, $n$, $n - 1$, with a rank-$(n + 1 - s)$ spin-0 (i.e., isotropic) tensor:

$$B_{i_1 \cdots i_{n+1}}^{(n+1)}(m) = \hat{\varepsilon}_{(n+1)i_1 \cdots i_{n+1}},$$

(81a)
\[ B^{(n)}_{i_1 \ldots i_{n+1}}(m) = \frac{i}{\sqrt{n(n+1)}} \sum_{k=1}^{n} \varepsilon_{i_k n+1} h \varepsilon_{(n)h i_1 \ldots i_k \ldots i_n}, \]  
\[ B^{(n-1)}_{i_1 \ldots i_{n+1}}(m) = \frac{1}{n \sqrt{(2n-1)(2n+1)}} \left( 2 \sum_{1 \leq k < h \leq n} \varepsilon_{(n-1)i_1 \ldots i_k \ldots i_h \ldots i_{n+1}} \delta_{i_k h} \right) \]  
where the caret over a subscript indicates that it is to be omitted. Equation (81b) is just (14); proofs of (81b), (81c) as direct consequences of (77) are given in Appendix C.

Given a partially irreducible tensor \( T_{i_1 \ldots i_{n+1}} \), from (79)-(81) we have,
\[ T_{i_1 \ldots i_{n+1}} = \sum_{j=n-1}^{n+1} \sum_{m=-j}^{j} T^{(j)}(m) B^{(j)}_{i_1 \ldots i_{n+1}}(m)^*, \]  
with
\[ T^{(n+1)}(m) = B^{(n+1)}_{i_1 \ldots i_{n+1}}(m) T_{i_1 \ldots i_{n+1}} = \varepsilon_{(n+1)i_1 \ldots i_{n+1}}(m) T_{i_1 \ldots i_{n+1}}, \]  
\[ T^{(n)}(m) = B^{(n)}_{i_1 \ldots i_{n+1}}(m) T_{i_1 \ldots i_{n+1}} = i \sqrt{\frac{n}{n+1}} \varepsilon_{(n)i_1 \ldots i_{n-1}h}(m) \varepsilon_{h i_1 \ldots i_{n+1}} T_{i_1 \ldots i_{n+1}}, \]  
\[ T^{(n-1)}(m) = B^{(n-1)}_{i_1 \ldots i_{n+1}}(m) T_{i_1 \ldots i_{n+1}} = -\sqrt{\frac{2n-1}{2n+1}} \varepsilon_{(n-1)i_1 \ldots i_{n-1}}(m) T_{i_1 \ldots i_{n-1}j}, \]  
Notice that, due to the symmetry properties of \( T_{i_1 \ldots i_{n+1}} \), the tensor contraction on the r.h.s. of (83b) can also be written as \( \varepsilon_{(n)i_1 \ldots i_{k-1}h i_{k+1} \ldots i_{n+1}}(m) \varepsilon_{h i_1 \ldots i_{n+1}} T_{i_1 \ldots i_{n+1}}, \) with \( 1 \leq k \leq n \). Similarly, the tensor contraction on the r.h.s. of (83c) can be written as \( \varepsilon_{(n-1)i_1 \ldots i_{k-1}h i_{k+1} \ldots i_{n+1}}(m) T_{i_1 \ldots i_{n-1}j}, \) with \( 1 \leq k \leq n \). The forms used in (83) were chosen for notational convenience.

The components \( T^{(j)}(m) \) defined in (83) are srsos, by Corollary 4.1, so from (82) and the Wigner-Eckart theorem (32) we obtain the equality
\[ \langle j', m'|T_{i_1 \ldots i_{n+1}}|j, m \rangle = \sum_{s=n-1}^{n+1} \langle j'||T^{(s)}||j \rangle \sum_{s_z=-s}^{s} \langle j, m; s, s_z|j', m' \rangle B^{(s)}_{i_1 \ldots i_{n+1}}(s_z)^*, \]  
which is the Wigner-Eckart theorem for partially irreducible cartesian tensor operators.

### 9.1 Magnetic multipole moments

In this section we derive the spherical and cartesian multipole expansions for the magnetic vector potential, and the relation between them to all orders. We restrict ourselves here to the case where time-retardation effects can be neglected. In that case the magnetic potential is given by [25]
\[ A_k(\vec{r}, t) = \frac{\mu_0}{4\pi} \int d^3\vec{r}' j_k(\vec{r}', t) = \frac{\mu_0}{4\pi} \int d^3\vec{r}' \sum_{\ell=0}^{\infty} \frac{4\pi}{2\ell+1} |\vec{r}|^{\ell+1} \sum_{\mu=-\ell}^{\ell} Y_{\ell\mu}(\vec{r}') Y_{\ell\mu}(\vec{r}) \delta_{ik} \delta_{\mu\mu'}, \]  
where in the last equality we substituted the expansion of \( 1/|\vec{r} - \vec{r}'| \) in spherical harmonics [25]. In (85) we can rewrite
\[ \sum_{\mu=-\ell}^{\ell} Y_{\ell\mu}(\vec{r}') Y_{\ell\mu}(\vec{r}) = \sum_{\mu=-\ell}^{\ell} \sum_{\mu'=-\ell}^{\ell} Y_{\ell\mu'}(\vec{r}') Y_{\ell\mu'}(\vec{r}) \delta_{ik} \delta_{\mu\mu'}, \]  
with
\[ \delta_{ik} \delta_{\mu\mu'} = \sum_{\nu=-1}^{1} \varepsilon_{(1)i}(\nu)^* \varepsilon_{(1)k}(\nu) \delta_{\mu\mu'} = \sum_{\nu=-1}^{1} \sum_{\nu'=-1}^{1} \varepsilon_{(1)i}(\nu)^* \varepsilon_{(1)k}(\nu) \delta_{\mu\mu'} \delta_{\nu\nu'}, \]  
\[ = \sum_{j=|\ell-1|}^{\ell+1} \sum_{m=-j}^{j} \sum_{\nu,\nu'=-1}^{1} \varepsilon_{(1)i}(\nu)^* \varepsilon_{(1)k}(\nu)(j, \ell, \mu; 1, \nu | j, m)(\ell, \mu; 1, \nu | j, m). \]  
(86b)
By inserting (86b) in (86a) and the result in (85) we obtain

$$\vec{A}(\vec{r}, t) = \frac{\mu_0}{4\pi} \sum_{\ell=0}^{\infty} \frac{4\pi}{2\ell + 1} \frac{1}{|\vec{r}|^{\ell+1}} \sum_{j=-\ell}^{\ell} \sum_{m=-j}^{j} m_{\ell m}^{(1)}(t)^* Y_{\ell m}^{(1)}(\vec{r}), \quad m_{\ell m}^{(1)}(t) = \int_V d^3 r' |\vec{r}'|^\ell \vec{A}(\vec{r}', t) \cdot Y_{\ell m}^{(1)}(\vec{r}').$$

(87)

This expression is a spherical multipole expansion, but it must be simplified since it contains redundant terms. We consider first the term in (87) with $j = \ell - 1 \ (\ell \geq 1)$. From the third equality in (77) this term is seen to be a gradient that does not contribute to the magnetic field. Furthermore, since the argument of the gradient is a harmonic function, it is divergenceless. This term plays a role in setting boundary conditions such as $\vec{A}(R, \theta, \phi) = \vec{v}(\theta, \phi)$ or $\vec{r} \cdot \vec{A}(R, \theta, \phi) = 0$ for some finite value $r = R$. We restrict ourselves here to the case $\vec{A} \rightarrow 0$ as $r \rightarrow \infty$, so we will set $m_{(\ell-1)m}^{(1)} = 0$ from here on.

The term with $j = \ell + 1 \ (\ell \geq 0)$ in (87) is related to the time derivative of the electric multipole moment $q_{(\ell+1)m}$ given in (57). To show this we adopt the method used in [26]. We consider a closed surface $S$ with exterior normal $\hat{n}$ containing the volume $V$ and its boundary in its interior, so that $\vec{j} = 0$ on $S$. By means of Gauss’ divergence theorem and the continuity equation $\partial \vec{A} / \partial t = 0 = \hat{\rho}$ we obtain

$$0 = \oint_S d^2 r' \tilde{\vec{A}}(\vec{r}) r'_1 \ldots r'_n = \int_V d^3 r' \left( \vec{A}(\vec{r}) \partial_r (r'_1 \ldots r'_n) - \hat{\rho}(\vec{r}) r'_1 \ldots r'_n \right).$$

Multiplication of this equation by $\delta_{(n)1\ldots n}(m)$ and use of (34) leads to

$$\int_V d^3 r' \vec{A}(\vec{r}) \partial_r (|\vec{r}'|^m Y_{nm}(\vec{r})) = \hat{q}_{nm}.$$

(88)

with $q_{nm}$ the electric multipole moments defined in (57). The gradient in the integrand in (88) is given by the first equality in (77), which yields

$$\sqrt{(\ell + 1)(2\ell + 3)} m_{(\ell+1)m}^{(1)} = \hat{q}_{(\ell+1)m}.$$

(89)

We then have

$$\vec{A}(\vec{r}, t) = \frac{\mu_0}{4\pi} \sum_{\ell=1}^{\infty} \frac{4\pi}{2\ell + 1} \frac{1}{|\vec{r}|^{\ell+1}} \sum_{m=-\ell}^{\ell} m_{\ell m}^{(1)}(t) Y_{\ell m}^{(1)}(\vec{r})$$

$$+ \frac{\mu_0}{4\pi} \sum_{\ell=0}^{\infty} \frac{4\pi}{2\ell + 1} \frac{1}{\sqrt{(\ell + 1)(2\ell + 3)}} \frac{1}{|\vec{r}|^{\ell+1}} \sum_{m=-(\ell+1)}^{(\ell+1)} \hat{q}_{(\ell+1)m} Y_{(\ell+1)m}^{(1)}(\vec{r}).$$

(90)

with $m_{\ell m}^{(1)}$, $q_{(\ell+1)m}$ as defined in (87), (57), respectively. Equation (90) is the spherical multipole expansion of the vector potential. We notice that in the magnetostatic case $\partial_k j_k = 0 = \hat{\rho}$, only the first line in (90) is non-vanishing. In that case (90) yields a vector potential that is transverse both in momentum and coordinate space, $\vec{\nabla} \times \vec{A} = 0 = \vec{r} \cdot \vec{A}$.

In order to obtain the cartesian multipole expansion of the magnetic potential, and its relation to the spherical one, we could proceed as in the case of the electric potential, with (59) as a starting point, to obtain [26]

$$A_i(\vec{r}) = \frac{\mu_0}{4\pi} \sum_{\ell=0}^{\infty} \frac{1}{\ell! |\vec{r}|^{\ell+1}} \tilde{M}_{i_1\ldots i_{\ell+1}} r_{i_1} \ldots r_{i_{\ell+1}}, \quad \tilde{M}_{i_1\ldots i_{\ell+1}} = (2\ell - 1)!! \int_V d^3 r' r'_{(i_1} \ldots r'_{i_{\ell+1})} j_k(\vec{r}).$$

This cartesian multipole expansion is given in terms of the partially irreducible magnetic multipole tensor $\tilde{M}_{i_1\ldots i_{\ell+1}}$, thus, it may further unraveled into irreducible components by means of the decomposition (82), (83) for $\tilde{M}$ [26]. Equivalently, we will derive the cartesian expansion from the spherical one (90) to take advantage of the simplifications already carried out on it.

We consider first the terms on the first line of (90). The vector spherical harmonic $Y_{(\ell+1)m}^{(1)}(\vec{r})$, as defined by (47), can be expanded in tensorial form by multiplying (81b) by $\vec{r}_{i_1} \ldots \vec{r}_{i_{\ell+1}}$, as done below in (C.3). Inserting
that tensorial expansion in the first line of (90), after some rearrangements we get,

$$A_j^{(1)}(\vec{r},t) = \frac{\mu_0}{4\pi} \sum_{\ell=1}^{\infty} \sum_{k_1, \ldots, k_{\ell-1}} \frac{1}{r^{2\ell+1}} r_{k_1} \cdots r_{k_{\ell-1}} \varepsilon_{jk_1k_2} M_{h_kk_1 \ldots k_{\ell-1}}(t)^*,$$

$$M_{k_1 \ldots k_{\ell}}(t) = \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell + 1} \frac{\ell}{\ell + 1} \sqrt{\frac{\ell + 1}{\ell}} m_{\ell m}(t) \hat{e}_{(t)k_1 \ldots k_{\ell}} M_{k_1 \ldots k_{\ell}}(t).$$

(91)

This equality gives the cartesian multipole expansion of the first line of (90). $M_{k_1 \ldots k_{\ell}}(t)$ is the magnetic $2\ell$-multipole irreducible tensor, given in (91) in terms of the spherical one $m_{\ell m}(t)$. Multiplication of the second line of (91) by $\hat{e}_{(t)k_1 \ldots k_{\ell-1}}(m)$ yields the inverse relation:

$$m_{\ell m}(t) = -\frac{2\ell + 1}{4\pi} \frac{1}{\ell} \sqrt{\frac{\ell + 1}{\ell}} \hat{e}_{(t)k_1 \ldots k_{\ell}} M_{k_1 \ldots k_{\ell}}(t).$$

(92)

Furthermore, by replacing in the second line of (91) the definition (87) of $m_{\ell m}(t)$ and using (C.3) again, we have

$$M_{k_1 \ldots k_{\ell}}(t) = \frac{4\pi}{2\ell + 1} \frac{\ell}{\ell + 1} \sum_{m=-\ell}^{\ell} \hat{e}_{(t)k_1 \ldots k_{\ell}}(m) \hat{e}_{(t)k'_1 \ldots k'_{\ell-1}}(m) \int_V d^3r' \left( \vec{r}(\vec{r}', t) \wedge \vec{r}' \right) \cdot \vec{r}'_1 \cdots \vec{r}'_{\ell-1}.$$  

(93)

This equation gives the irreducible magnetic multipole tensor $M_{k_1 \ldots k_{\ell}}$, up to a normalization, as the irreducible component of the integral on the right-hand side.

We turn next to the second line in (90). Since $Y_{\ell+1}^{(1)}(\vec{r})$ is maximally coupled, we can use (14) (or, equivalently, (20)) and (34) in (47) to write

$$Y_{\ell+1}^{(1)}(\vec{r}, (\ell+1)m) = N_{\ell} \hat{e}_{(t)j_1 \ldots j_{\ell+1}}(m) \hat{r}_{j_1} \cdots \hat{r}_{j_{\ell}}.$$  

(94)

With this expression, and equation (62) expressing the spherical electric multipoles $q_{\ell m}$ in terms of the cartesian ones $Q_{i_1 \ldots i_{\ell}}$, the second line of (90) can be written as

$$A_j^{(2)}(\vec{r}, t) = \frac{\mu_0}{4\pi} \sum_{\ell=1}^{\infty} \sum_{k_1, \ldots, k_{\ell-1}} \frac{1}{r^{2\ell+1}} r_{k_1} \cdots r_{k_{\ell-1}} \left( \varepsilon_{jk_1k_2} M_{h_kk_1 \ldots k_{\ell-1}}(t)^* + \frac{1}{(\ell + 1)(2\ell + 1)} \hat{Q}_{j_1 \ldots j_{\ell+1}}(t)^* \right),$$

(95)

where we have used the fact that $Q_{j_1 \ldots j_{\ell+1}}$ is a rank-$(\ell + 1)$ irreducible tensor. From (90), (91), (95) we get the complete, fully reduced magnetic cartesian multipole expansion

$$A_j(\vec{r}, t) = \frac{\mu_0}{4\pi |\vec{r}|} \hat{Q}_j(t)^* + \frac{\mu_0}{4\pi} \sum_{\ell=1}^{\infty} \sum_{k_1, \ldots, k_{\ell-1}} \frac{1}{r^{2\ell+1}} r_{k_1} \cdots r_{k_{\ell-1}} \left( \varepsilon_{jk_1k_2} M_{h_kk_1 \ldots k_{\ell-1}}(t)^* + \frac{1}{(\ell + 1)(2\ell + 1)} \hat{Q}_{k_1 \ldots k_{\ell+1}}(t)^* \right),$$

(96)

where we have separated the time derivative of the electric dipole moment which is the only $O(1/r)$ term. The expansion (96) has been previously given in [26]. Here we recover that result and extend it by giving the relations (91), (92) between the spherical magnetic moments (87), (90) and the cartesian ones (93), (96) to all orders in the multipole expansion. Equations (91), (92) give an explicit form for the analogous relations found in [27].

10 Final remarks

In this paper we have established in full generality the explicit form of the unitary correspondence between spherical and cartesian irreducible tensor operators relative to a generic angular-momentum operator $\hat{J}$. The matrix elements of that unitary transformation are the standard rank-$s$ tensors $\hat{e}_{(s)}(m)$ defined in section 3, which constitute an orthonormal basis for the space of rank-$s$ irreducible tensors, and also a standard basis of spin-$s$ wave functions. We defined $\hat{e}_{(s)}(m)$ in three equivalent ways, namely, recursively (14), explicitly (16) and implicitly (17). The tensors $\hat{e}_{(s)}(m)$ satisfy all of the usual phase and coupling conventions required to make them bona-fide angular-momentum wave functions. Furthermore, they transform under rotations...
equivalently as cartesian or spherical tensors. We remark here that an analogous basis of cartesian irreducible spinors can be constructed along the same lines [17, 10, 29]. Both the tensor and spinor bases are of the (non-relativistic) Rarita-Schwinger [29] type. With the spin wave functions $\tilde{\gamma}_x(m)$ as matrix elements of a unitary change of basis, we establish the relation between cartesian and spherical irreducible tensors of any rank in section 4.

The unitary mapping described in 4 is important because it allows us to apply the methods and technical tools of quantum angular–momentum theory to tensor algebra and vice versa. The interrelation of tensor and angular–momentum methods is used in section 5 to extend the Wigner–Eckart theorem to cartesian irreducible tensor operators of any rank, thus determining the form of their matrix elements. In principle, this result can be applied to any cartesian tensor operator, by linearly decomposing it into its irreducible components. In section 7 we take a step towards that goal by extending the Wigner–Eckart theorem to totally symmetric reducible tensors, which is the main result of this paper. Such an extension allows us to obtain matrix elements for arbitrary tensor powers of the position or momentum operators. This is exploited in section 8 to give an explicit expression for the gradients of any order of spherical harmonics. An additional extension of the Wigner-Eckart theorem to partially irreducible cartesian tensor operators is given in section 9. Partially irreducible tensors occur in some applications, such as the magnetic multipole expansion discussed in 9.1.

On the other hand, the results of section 3 and 4 also allow us to find the cartesian form of standard spherical tensors. Such cartesian tensorial forms provide a complementary approach to the usual analytic methods often based on differential equations. In section 3.1 we show that Wigner $D$-matrices are the spherical components of three-dimensional rotation matrices, which leads to an expression of $D_\ell$ as a linear combination of products of $D_1$ matrices. In section 6 we obtain the cartesian tensorial form of ordinary, bipolar and tensor spherical harmonics, and spin-polarization operators. We find some relations between those standard functions that are of interest, like the decomposition of $D$-matrices mentioned above, the binomial expansion for spherical harmonics, and the relation between tensor and bipolar spherical harmonics, based on the tensorial representations for them. We discuss also the relation between spherical and cartesian multipoles of any rank, both for the scalar electric (section 6.5) and vector magnetic (9.1) potentials. The best illustration of the kind of relations referred to here, and of the power of our approach, is the explicit expression for gradients of any order of spherical harmonics found in section 8.

Acknowledgements

The author has been partially supported by Sistema Nacional de Investigadores de México.

References

[1] M. Kröger: Models for Polymeric and Anisotropic Liquids, Springer, New York 2005.
[2] C. Eckart: Reviews of Modern Physics 2, 305 (1930).
[3] E. Wigner: Group Theory and its Application to the Quantum Mechanics of Atomic Spectra, Academic Press, New York 1959.
[4] L. D. Landau, E. M. Lifshitz: Quantum Mechanics, Butterworth–Heinemann, New York 2003.
[5] A. Messiah: Quantum Mechanics, Vol. 2, Elsevier, Amsterdam 1961.
[6] C. Cohen-Tannoudji, B. Diu, F. Laloë: Quantum Mechanics, Vol. 2, John Wiley, New York 1977.
[7] A. Galindo, P. Pascual: Quantum Mechanics I, Springer-Verlag, New York 1990.
[8] G. Racah: Physical Review 62, 438 (1942).
[9] L. C. Biedenharn, J. D. Louck: Angular Momentum in Quantum Physics, in Encyclopedia of Mathematics and its Applications, G. C. Rota editor, Cambridge University Press, New York 2009.
[10] C. Zemach: Phys. Rev. 140, B97 (1965).
A Angular momentum: notation and conventions

In this appendix we state our conventions for quantum angular-momentum theory \([3, 4, 5, 6, 7, 9, 13, 15, 16]\). Throughout this paper we follow the convention of [4] that angular-momentum operators are dimensionless. In particular, the orbital angular-momentum operator for a single particle is \(\vec{L} = (1/\hbar)\vec{r} \wedge \vec{p} = -i\vec{r} \wedge \vec{\nabla}\). In order to switch to the alternate convention in which angular-momentum operators have units of \(\hbar\) it suffices to replace \(\vec{J}\) (resp. \(\vec{L}, \vec{S}\)) in our equations by \(\vec{J}/\hbar\) (resp. \(\vec{L}/\hbar, \vec{S}/\hbar\)).

Let \(\vec{J}\) be a generic angular-momentum operator, \([J_h, J_l] = i\varepsilon_{hik}J_k\). The simultaneous eigenstates of \(\vec{J}^2\) and \(J_3\) are denoted \(|j, m\rangle\), with \(j \geq 0\) and \(-j \leq m \leq j\) integer or half-odd-integer. The state vectors \(|j, m\rangle\) are assumed to be normalized, therefore orthonormal, and their relative phases are chosen so that they satisfy the usual convention

\[
\langle j, m'| J_\pm | j, m \rangle = \sqrt{(j + m)(j + m + 1)} \delta_{m'(m+1)}, \quad \langle j, m'| J_3 | j, m \rangle = m \delta_{m'(m+1)}. \tag{A.1a}
\]

In particular, they satisfy the Condon–Shortley phase convention \(\langle j, m'| J_\pm | j, m \rangle \geq 0\) [15, 16, 7]. For the cartesian components of \(\vec{J}\) we then have

\[
\langle j, m'| J_{\perp} | j, m \rangle = \frac{1}{2} \sqrt{j(j + 1) - mm'}(\delta_{m'(m+1)} \pm \delta_{m'(m-1)}), \tag{A.1b}
\]
and the matrix element of $J_3$ as in (A.1a). By using the relation

$$
\langle j, m; 1, \epsilon | j, m' \rangle = \frac{1}{\sqrt{j(j+1)}} \times \left( \frac{\sqrt{2} \sqrt{(j-\epsilon m)(j+\epsilon m+1)}}{m \delta_{mm'}} \right) \delta_{m(m+\epsilon)} \quad \text{if} \quad \epsilon = \pm 1 \\
= \frac{1}{\sqrt{j(j+1)}} \times \left( \frac{\sqrt{2} \sqrt{(j-\epsilon m)(j+\epsilon m+1)}}{m \delta_{mm'}} \right) \quad \text{if} \quad \epsilon = 0
$$

(A.2)
equation (A.1a) can be written more compactly as

$$
\langle j, m'; | \vec{J} | j, m \rangle = \sqrt{j(j+1)} \langle j, m; 1, \epsilon | j, m' \rangle, \quad \epsilon = 0, \pm 1,
\text{ with } \vec{c}(\epsilon) \text{ defined in (9), from whence we obtain}
$$

(A.3a)

$$
\langle j, m' | J_k | j, m \rangle = \sqrt{j(j+1)} \langle j, m; 1, m' - m | j, m' \rangle \vec{c}(m' - m)^*,
\text{ which is equivalent to (A.1b)}.
$$

(A.3b)

For integer $j$ the spatial wave–function associated with the orbital angular–momentum eigenstates is given by the spherical harmonics, for which we follow the modern conventions [6, 7, 13, 25] (a different phase convention for $Y_{\ell m}$ is used in older texts [4, 15, 16])

$$
Y_{\ell m} = \sqrt{\frac{2\ell + 1}{4\pi}} \frac{(\ell - m)!}{(\ell + m)!} P_{\ell m} \exp \left[ \frac{i\theta}{2} \right], \quad P_{\ell m}(x) = (-1)^{m} \frac{\ell^m}{\ell!} \frac{x^m}{(1 - x^2)^{\ell/2}} \frac{d^m}{dx^m} (1 - x^2)^{\ell/2},
$$

(A.4)

where $\theta$, $\varphi$ are the polar coordinates of $\vec{r}$, and where $P_{\ell m}(x)$ is an associated Legendre function of the first kind (as defined, e.g., in [7, 25]) that for $m = 0$ reduces to a Legendre polynomial $P_{\ell}(x)$. An explicit expression for $P_{\ell m}(x)$ is given in section 6.1.1.

We turn next to the coupling of angular momenta. Consider two subsystems with angular-momentum operators $\vec{J}_a$, $a = 1, 2$, each one acting on the Hilbert space of states $H_a$ of its subsystem. Let $H = H_1 \otimes H_2$ be the state space of the total system, on which the total angular-momentum operator $\vec{J} = \vec{J}_1 \otimes I_2 + I_1 \otimes \vec{J}_2$ acts, where $I_a$ is the identity operator on $H_a$. The definition of $\vec{J}$ is usually written in the abbreviated form $\vec{J} = \vec{J}_1 + \vec{J}_2$. If each subsystem $a$ is in a state $| \mu_a \rangle$, simultaneous eigenstate of $(\vec{J}_a^2)$ and $(\vec{J}_a)$, the state of the total system is the tensor product state $| j_1, \mu_1; j_2, \mu_2 \rangle = | j_1, \mu_1 \rangle \otimes | j_2, \mu_2 \rangle$. On the other hand, the states with definite total angular momentum $| j_1, j_2, j, m \rangle$ are chosen to be simultaneous eigenstates of $(\vec{J}_1^2)$, $(\vec{J}_2^2)$, and $\vec{J}_3$. The unitary transformation relating the two orthonormal bases of $H$ is given by the CG coefficients, which we denote as

$$
| j_1, j_2, j, m \rangle = \sum_{\mu_1, \mu_2} \langle j_1, \mu_1; j_2, \mu_2 | j, m \rangle | j_1, \mu_1; j_2, \mu_2 \rangle.
$$

(A.5)

A global complex factor in the CG coefficients is determined by the normalization condition and the Condon–Shortley [15] phase convention $(j_1, j_1; j_2, j - j_1 | j_1, j)$ $\geq 0$, which implies in particular that all CG coefficients are real. Since $| j_1, j_2, j, m \rangle$ is by definition an eigenstate of $\vec{J}_1^2$ and $\vec{J}_3$, the matrix elements of $\vec{J}$ between those states do not depend on $j_2$,

$$
\langle j_1, j_2, j', m' | \vec{J} | j_1, j_2, j, m \rangle = \langle j', m' | \vec{J} | j, m \rangle = \langle j, m' | \vec{J} | j, m \rangle \delta_{j', j},
$$

(A.6)

where the last matrix element is the standard one as given in (A.1b) or (A.3b).

**Proof of (21)** To prove (21) we proceed by induction on $n$. The case $n = 1$ is (11), which is seen to be true by exhaustive evaluation of all possible cases $m', m = 0, \pm 1$. Assuming (21) to be true, we have to prove that

$$
\langle n + 1, m' | S_k | n + 1, m \rangle = \delta_{n, -1} \langle n + 1, m' | \hat{S}_n | n + 1, m \rangle = \delta_{m', 1} \langle n + 1, m' | \hat{S}_n | n + 1, m \rangle + \delta_{m', 1} \langle n + 1, m' | \hat{S}_n | n + 1, m \rangle
$$

(A.7)

with $-n - 1 \leq m', m \leq n + 1$. From (4), the matrix $\hat{S}_{(n+1)}$ can be written as

$$
\hat{S}_{(n+1)} = \hat{S}_n \hat{S}_{(1)} + \hat{S}_n \hat{S}_{(2)} + \cdots + \hat{S}_n \hat{S}_{(n+1)}.
$$

Substituting this equality together with (14) into the right-hand side of (A.7) leads to

$$
\hat{c}_{i_1 \cdots i_{n+1}} (m')^* (S_{(n+1)} k_{i_1 \cdots i_{n+1}:j_1 \cdots j_{n+1}}) = \sum_{\mu', \mu = -n, \nu'} \sum_{\nu' = -1} \langle n, \mu'; 1, \nu' | n + 1, m' \rangle \langle n, \mu; 1, \nu | n + 1, m \rangle
$$
where in the last equality we used the case \( n = 1 \) given by (11) and the inductive hypothesis (21) to express the matrix elements of \( S_A(k) \) and \( S_B(k) \) on the second line in terms of the matrix elements of a spin operator \( \hat{S}_A \) for a spin-n system \( A \) and a spin operator \( \hat{S}_B \) for a spin-1 system \( B \), respectively. \( \hat{S}_{A,B} \) being both angular-momentum operators, their matrix elements are given by (A.1b). The total angular-momentum operator for the total system \( A + B \) is \( \hat{S} = \hat{S}_A \otimes I_B + I_A \otimes \hat{S}_B \), and we have

\[
\begin{align*}
&\sum_{\mu',\mu = -n}^{n} \sum_{n',\nu = -1}^{1} \langle n, \mu'; 1, \nu'|n + 1, m'\rangle \langle n, \mu; 1, \nu|n + 1, m\rangle \left(\langle n, \mu'|[S_A(k)|n, \mu]\delta_{\nu', \nu} + \delta_{\mu', \mu}(1, \nu'|[S_B(k)|1, \nu]\right) \\
&= \langle n, 1, n + 1, m'|[S_k(n)|n, 1, n + 1, m\rangle = \langle n + 1, m'|[S_k(n)|n + 1, m\rangle,
\end{align*}
\]

where the last equality is (A.6).

## B Non–maximally–coupled bipolar spherical harmonics

The bipolar spherical harmonics \([13]\) defined in (42) have been given an explicit tensorial expression in \([22]\). Here we quote that expression for \( Y_{j,m}^{(\ell', \nu')} (\hat{r}, \hat{r}') \) with a slightly different notation that is more appropriate to the purposes of this paper. We assume \( \ell' \geq \ell \) for notational simplicity. The case \( \ell' < \ell \) results from the relation \( Y_{j,m}^{(\ell', \nu')} (\hat{r}, \hat{r}') = (-1)^{\ell' + \ell - j} Y_{j,m}^{(\ell, \nu)} (\hat{r}', \hat{r}) \) that follows from the definition (42). Thus, for \( \ell' \geq \ell \) from \([22]\) we find

\[
Y_{j,m}^{(\ell', \nu')} (\hat{r}, \hat{r}') = \frac{i^\nu}{4\pi} \sqrt{2\nu'!} \binom{2j + 1}{j + n} \binom{2\ell' + 1}{\ell' + \ell + j + 1} \sum_{k_1 = k_{1\min}}^{k_{2\max}} \sum_{k_2 = 0}^{2n} (-1)^{k_2} \binom{n}{k_1} \binom{q_{\max}}{q_{\min}} \times (2q - 1)!! \sum_{k = k_{1\min}}^{k_{2\max}} \frac{t}{2q!} \sum_{j'_{k_1+q}, \cdots, j_k} \sum_{h_1, \cdots, h_{2q} = 0} P_{(\ell', j', \nu')}^{(k, q)} (\hat{r}, \hat{r}'),
\]

where the following notations have been used

\[
\nu = \ell' + \ell - j, \quad n = \ell' - \ell, \quad t = j - n, \quad \nu = \nu' - \ell,
\]

\[
k_{1\min} = \max \left\{ 0, n - \frac{\nu}{2} \right\}, \quad k_{2\max} = \min \left\{ \frac{\nu}{2}, n \right\}, \quad q_{\min} = \max \left\{ 0, \ell + k_2 - \nu \right\}, \quad q_{\max} = \min \left\{ \ell + \frac{\nu}{2}, n \right\}, \quad \nu \text{ even,}
\]

and where \( P_n^{(k)} (x) \) is the \( k \)-th derivative of the Legendre polynomial \( P_n(x) \). In (B.1a) it is understood that the factor \( r_{i_1} \cdots r_{i_{k_2+q}} \) is to be replaced by 1 if \( k_2 + q < 1 \), and analogously the other products of \( r_{i'} \) and \( \nu' \). It is not difficult to check that (B.1) reduces to (44) in the case of maximal coupling \( \nu = 0 \). In the case \( \nu > 0 \) of non-maximally coupled \( Y_{j,m}^{(\ell', \nu')} \), (B.1) gives its dual cartesian irreducible tensor just as (44) does for maximally coupled ones.

## C Proof of (81)

To derive (81b) we start from the second equality in (77) written in the form

\[
(Y_{\ell m} (\hat{r}))_j = \sqrt{\ell(\ell + 1)} N_{\ell j a b} \partial_a \partial_b \langle \hat{r} (\ell) k_1 \cdots k_2 \rangle (\hat{r}_{k_1} \cdots \hat{r}_{k_2}),
\]

(81c)
where we have used (34). By multiplying both sides of (C.1) by \( r^f \), substituting in it definition (47) for \( Y_{nm}^{f} \) and using the relation \( \varepsilon_{j\alpha \beta \gamma} r^f \partial_\alpha (f(r^f)) = \varepsilon_{j \alpha \beta \gamma} r^f \partial_\alpha (r^f(f(r^f))) \) on its right-hand side, we get

\[
\sum_{\mu, \nu} (\ell, \mu; 1, \nu | \ell, m) \varepsilon_{(\ell)i_{1} \ldots i_{\ell}}(\mu)\varepsilon_{(1)j}(\nu) r_{i_1} \ldots r_{i_{\ell}} = -i \frac{\ell}{\sqrt{\ell(\ell + 1)}} \varepsilon_{j \alpha \beta \gamma} r^f \partial_\alpha \varepsilon_{(\ell)k_1 \ldots k_{\ell}}(m) r_{k_1} \ldots r_{k_{\ell}}, \tag{C.2}
\]

where in the second equality we made use of the total symmetry of \( \varepsilon_{(\ell)} \). Division of both sides of (C.2) by \( r^f \) yields its useful form

\[
(Y_{\ell m}^{f}(r))_{j} = -i \frac{\ell}{\ell + 1} \varepsilon_{j h \ell} \varepsilon_{(\ell)j_{1} \ldots j_{\ell - 1}}(m) \hat{r}_{j_{1}} \ldots \hat{r}_{j_{\ell - 1}}. \tag{C.3}
\]

Differentiation of both sides of (C.2) with respect to \( \partial_{j_1} \ldots \partial_{j_{\ell}} \) leads to

\[
\ell! \sum_{\mu, \nu} (\ell, \mu; 1, \nu | \ell, m) \varepsilon_{(\ell)i_{1} \ldots i_{\ell}}(\mu)\varepsilon_{(1)j}(\nu) = -i \frac{\ell}{\ell + 1} (\ell - 1)! \sum_{h=1}^{\ell} \varepsilon_{j_{h}b} \varepsilon_{(\ell)b_{1} \ldots b_{h-1} i_{1} \ldots i_{\ell}}(m), \tag{C.4}
\]

which is (81b). We see that (77), (81b) and (C.1)–(C.3) are different ways of rewriting the same equality. The derivation of (81c) starts with the third equality in (77) written in the form

\[
r^n (Y_{(n-1)m}^{n1}(\hat{r}))_{i} = \frac{1}{\sqrt{n(2n-1)}} (\partial_{i} (r^{n+1} Y_{(n-1)m}(\hat{r})) - (2n + 1) r^{n-1} Y_{(n-1)m}(\hat{r}) r_{i}). \tag{C.5}
\]

Differentiation of both sides of this equality with respect to \( \partial_{j_1} \ldots \partial_{j_n} \) and use of (47) and (65) leads to

\[
\sum_{\mu, \nu} (n, \mu; 1, \nu | n - 1, m) \varepsilon_{(n,n)j_{1} \ldots j_{n}}(\mu)\varepsilon_{(1)i}(\nu) = \frac{1}{\sqrt{n(2n-1)}} \left( \lambda'_{(n,n)} \varepsilon_{(\ell+1)j_{1} \ldots j_{n}}(m) - (2n + 1) \frac{\lambda'_{(n,n)}}{\lambda'_{(n-1,n-1)}} \sum_{k=1}^{n} \varepsilon_{(n-1,n-1)j_{1} \ldots j_{n}}(m) \delta_{j_{k} i} \right), \tag{C.6}
\]

where, as above, a caret over a subindex indicates that it is omitted. Substitution of (63) in (C.6) finally leads to

\[
\sum_{\mu, \nu} (n, \mu; 1, \nu | n - 1, m) \varepsilon_{(n,n)j_{1} \ldots j_{n}}(\mu)\varepsilon_{(1)i}(\nu) = \frac{1}{\sqrt{n(2n-1)(2n+1)}} \left( \frac{1}{(n-1)!} \varepsilon_{(n-1)j_{1} \ldots j_{n}}(m) \delta_{j_{n} i} - (2n + 1) \sum_{k=1}^{n} \varepsilon_{(n-1)j_{1} \ldots j_{n}}(m) \delta_{j_{k} i} \right)
\]

\[
= \frac{1}{n \sqrt{(2n-1)(2n+1)}} \left( 2 \sum_{1 \leq k < h \leq n} \varepsilon_{(n-1)j_{1} \ldots j_{k} \ldots j_{n}}(m) \delta_{j_{k} j_{h}} - (2n - 1) \sum_{k=1}^{n} \varepsilon_{(n-1)j_{1} \ldots j_{k} \ldots j_{n}}(m) \delta_{j_{k} i} \right), \tag{C.7}
\]

the last equality being (81c).