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General expressions for Stevens operators and spin operator equivalents

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Several definitions of the crystal electric field (CEF) have been used over time and their variety has lead to many misunderstandings, in both theoretical and experimental literature. Two categories of definitions can be mentioned, the first being the operators equivalents introduced by Stevens in 1952 and the second being the crystal-field operators, introduced later by Wybourne and expanded on the Racah spherical tensors. This paper aims at providing some clarification in this field. We first make a review of several expressions introduced in various references to compute crystal-field operators and we make connections between them. Then, we introduce an explicit way to compute crystal-field operators, in terms of j and m as well as in terms of J^2 and J_z . We eventually give some connections between the Stevens operators equivalents and the crystal-field operators.

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I. INTRODUCTION

Operator equivalents O_n^m were introduced in 1952 by Stevens¹ to parametrize the Hamiltonian describing magnetic properties of rare earths. Indeed the 4f shell of most rare earths can be described by a spectroscopic term $^{2S+1}L_J$, where J is a good quantum number. As a result, its ground state belongs to the vector space generated by state vectors $|JM\rangle$ (where $M = -J, \dots, J$) and the action of the crystal field can be written as a linear combination of operators O_n^m that can be expressed as a polynomial in the spin operators J_x, J_y and J_z . These Stevens operators were then widely used to analyze spectroscopic experiments in EPR, ESR, ENDOR, UV-visible spectroscopy, Mössbauer spectroscopy² as well as neutron scattering and x-ray absorption spectroscopy. Explicit expressions for O_n^m were given in several tables and, because of the complexity of these expressions, each new table listed the misprints in the previous ones².

On the other hand, it was later realized³ that the transformation properties of O_n^m under rotation are very complicated. By contrast, spherical tensors⁴ T_μ^k (with $\mu = -k, \dots, k$) enjoy the same transformation properties as spherical harmonics and are linked by the relation⁵ (p. 90): $[J_-, T_\mu^k] = \sqrt{(k+\mu)(k-\mu+1)}T_{\mu-1}^k$ whereas O_n^m of different m have no simple relations. Moreover, any $(2j+1) \times (2j+1)$ matrix can be written as a linear combination of T_μ^k for $k = 0, \dots, 2j^6$. In particular, spherical tensors can be used to express any finite dimensional Hamiltonian. For all these reasons, many authors replaced Stevens operators by spherical tensors or combinations thereof, leading to new tables. Besides, additional confusion arises from the fact that spherical tensors come with various normalizations in the literature.

The operator equivalents were introduced in 1952 by Stevens¹ for O_2^0, O_4^0 and O_6^0 . Then, $O_6^6 + O_6^{-6}$ was given by Bleaney and Stevens⁷. It was later realized³ that the transformation properties of O_n^m would be much simpler if spherical tensors⁴ were used. This lead to the introduction of a large number of more or less similar operators, that were reviewed by Rudowicz and coll.^{2,8}

The absence of an analytical expression for these operator equivalents imposed the publication of extensive tables running over many pages and scattered in several articles and books. Moreover, each single entry can be quite complicated (for example the expression for O_{12}^1 is 11 lines long in²).

To avoid egregious mistakes some authors proposed to derive these results with a computer through recursion methods^{9,10}.

To solve these problems, several closed form expressions were proposed¹¹. In this paper we make a critical review of these expressions and we present a new method to translate an analytical expression in terms of the angular momentum quantum number j into an analytical expression in terms of the angular momentum operator J^2 . Finally, we describe the connection between the parameters of the effective Hamiltonian and the parameters of the crystal-field Hamiltonian.

The plan of the paper is the following. We start from the definition of spherical tensors T_μ^k and we introduce the operator P_μ^k which has the advantage of having only diagonal matrix elements ($\langle jm|P_\mu^k|jm'\rangle = 0$ if $m \neq m'$) and from which T_μ^k can be easily computed. Then, we review the different expressions for P_μ^k proposed in the literature and we

make connections between them. We also provide a way to go from an expression of $\langle jm|P_\mu^k|jm\rangle$ in terms of j and m to an expression of P_μ^k in terms of J^2 and J_z . Finally, we give some applications to checking tables, connecting with various Stevens operators and linking effective Hamiltonians to crystal field operators.

II. SPHERICAL TENSORS AND THEIR MATRIX ELEMENTS

A. Definition and main properties

General (Irreducible) spherical tensors \mathcal{T}_μ^k (with $\mu = -k, \dots, k$) are defined by the relations⁵ (p. 157)

$$\mathcal{T}_k^k = a_k J_+^k, \quad (1)$$

$$[J_-, \mathcal{T}_\mu^k] = \sqrt{(k+\mu)(k-\mu+1)} \mathcal{T}_{\mu-1}^k, \quad (2)$$

where a_k is a real constant, $J_\pm = J_x \pm iJ_y$ and $J_+^k = (J_+)^k$ (i.e. k is a true exponent and not an upper index as in T_μ^k).

These operators satisfy the important properties⁵ (p. 656)

$$(\mathcal{T}_\mu^k)^\dagger = (-1)^\mu \mathcal{T}_{-\mu}^k, \quad (3)$$

and

$$\sum_{\mu=-k}^k (\mathcal{T}_\mu^k)^\dagger \mathcal{T}_\mu^k = a_k^2 \frac{(k!)^2}{(2k)!} \prod_{s=1}^k (4J^2 + 1 - s^2), \quad (4)$$

where $J^2 = J_x^2 + J_y^2 + J_z^2$.

Moreover if, for a given j , we denote by M_μ^k the $(2j+1) \times (2j+1)$ matrix defined by the matrix elements $(M_\mu^k)_{mm'} = \langle jm|\mathcal{T}_\mu^k|jm'\rangle$, then we have the orthogonality relation⁶:

$$\text{Tr}((M_\mu^k)^\dagger M_{\mu'}^k) = \delta_{k,k'} \delta_{\mu,\mu'} \frac{(k!)^2 a_k^2}{(2k+1)!} \frac{(2j+k+1)!}{(2j-k)!}, \quad (5)$$

where the adjoint \dagger can be replaced by a transpose since the matrix elements are real. This property can be used for instance to determine the expansion of a Hamiltonian over spherical tensors. Indeed, if H is a $(2j+1) \times (2j+1)$ Hamiltonian matrix, then the parameters B_k^μ of

$$H = \sum_{k,\mu} B_k^\mu \mathcal{T}_\mu^k,$$

are given by

$$B_k^\mu = \frac{(2k+1)!}{(k!)^2 a_k^2} \frac{(2j-k)!}{(2j+k+1)!} \text{Tr}((M_\mu^k)^\dagger H).$$

B. Common conventions

We denote by T_μ^k the spherical tensor corresponding to⁵

$$a_k = (-1)^k \frac{\sqrt{(2k)!}}{k!}.$$

Another frequently used convention¹² is

$$a_k = (-1)^k 2^{-k/2}.$$

Let us finally define Racah's unit tensor operators^{4,13} $u_q^k(j)$, for which a_k depends on the value of j on which the tensor operators are applied:

$$a_k = \frac{(-1)^k}{k!} \left(\frac{(2k)!(2j-k)!}{(2j+k+1)!} \right)^{1/2}.$$

C. Matrix elements

Any Hamiltonian acting within a vector space generated by $|jm\rangle_{m=-j,\dots,j}$ can be written as a sum

$$H = \sum_{k,\mu} B_k^\mu \mathcal{T}_\mu^k.$$

Please note that the position of the angular momentum quantum number k and the magnetic quantum number μ are traditionally at a different position in B_k^μ or O_k^μ and \mathcal{T}_μ^k .

The matrix elements of the Hamiltonian can be derived from the matrix elements of \mathcal{T}_μ^k , which are given by the Wigner-Eckart theorem:

$$\langle jm' | \mathcal{T}_\mu^k | jm \rangle = (-1)^{j-m'} \begin{pmatrix} j & k & j \\ -m' & \mu & m \end{pmatrix} \langle j || \mathcal{T}^k || j \rangle.$$

To compute the reduced matrix element $\langle j || \mathcal{T}^k || j \rangle$ we only need

$$\mathcal{T}_k^k | jm \rangle = a_k J_+^k | jm \rangle = a_k \left(\frac{(j-m)!(j+m+k)!}{(j-m-k)!(j+m)!} \right)^{1/2} | jm+k \rangle, \quad (6)$$

and the explicit expression¹⁴ (p. 268)

$$\begin{pmatrix} j & k & j \\ -m' & k & m \end{pmatrix} = \delta_{m',m+k} (-1)^{j-m} \left(\frac{(2k)!(2j-k)!(j+m+k)!(j-m)!}{(2j+k+1)!(k!)^2(j-m-k)!(j+m)!} \right)^{1/2},$$

which give us

$$\langle j || \mathcal{T}^k || j \rangle = (-1)^k a_k k! \left(\frac{(2j+k+1)!}{(2k)!(2j-k)!} \right)^{1/2}. \quad (7)$$

In particular, we see that Racah's unit operators derive their names from the reduced matrix element $\langle j || u^k(j) || j \rangle = 1$. Note that Eq. (7) differs from the reduced matrix element given in⁵ (p. 157) by a factor of $\sqrt{2j+1}$ due to the fact that these authors use a Wigner-Eckart theorem involving Clebsch-Gordan coefficients instead of $3j$ -symbols. Note that the orthogonality relation (5) follows from the Wigner-Eckart theorem and the orthogonality of $3-j$ symbols.

III. EXPLICIT EXPRESSIONS FOR \mathcal{T}_μ^k

In this section we assume that $\mu \geq 0$. The first step to obtain an explicit expression is to write \mathcal{T}_μ^k as the product of J_+^μ times a polynomial in J^2 and J_z . This polynomial will only have non-zero matrix elements between vector states with the same m and j . The second step is to obtain explicit expressions for this polynomial.

A. P_μ^k and its properties

To derive an explicit expression for \mathcal{T}_μ^k we first define P_μ^k for $\mu \geq 0$ by⁵ (p. 658)

$$\mathcal{T}_\mu^k = a_k \sqrt{\frac{(k+\mu)!(k-\mu)!}{(2k)!}} J_+^\mu P_\mu^k, \quad (8)$$

with $P_k^k = 1$. We first show that P_μ^k is a polynomial of J^2 and J_z . Indeed, the recursive relation (2) for \mathcal{T}_μ^k leads to the recursive expression for P_μ^k

$$(k-\mu+1)P_{\mu-1}^k = P_{\mu-1}^\mu P_\mu^k + J_+ [J_-, P_\mu^k],$$

where

$$P_{\mu-1}^\mu = -\mu(\mu-1) - 2\mu J_z.$$

To give a recursive proof of the polynomial nature of P_μ , we start from the fact that $P_k^k = 1$ is a polynomial in J^2 and J_z . Assume now that P_μ^k is a polynomial in J^2 and J_z . Then, by using⁹

$$[J_-, J_z^n] = J_- \nabla J_z^n,$$

where $\nabla J_z^n = J_z^n - (J_z - 1)^n$ is the backward difference, we see that $[J_-, P_\mu^k]$ is the product of J_- by a polynomial in J^2 and J_z . It follows that $J_+ [J_-, P_\mu^k]$ and $P_{\mu-1}^k$ are also polynomials of this form because $J_+ J_- = J^2 - J_z^2 - J_z$. As a consequence, the operator P_μ^k is a polynomial in J^2 and J_z for all μ such that $k \geq \mu \geq 0$, which implies that its matrix elements are diagonal in j and m : $\langle jm | P_\mu^k | j' m' \rangle = \delta_{jj'} \delta_{mm'} \langle jm | P_\mu^k | jm \rangle$.

To be more explicit, if $P_\mu^k(J^2, J_z)$ is the operator P_μ^k whose dependence on J^2 and J_z is made explicit, we denote by $P_\mu^k(J^2, \nabla J_z)$ the operator $P_\mu^k(J^2, J_z)$ where each monomial J_z^n is replaced by ∇J_z^n . Then, the recursive expression becomes

$$(k - \mu + 1) P_{\mu-1}^k(J^2, J_z) = -(\mu(\mu - 1) + 2\mu J_z) P_\mu^k(J^2, J_z) + (J^2 - J_z^2 - J_z) P_\mu^k(J^2, \nabla J_z).$$

Finally, we give the formula for $\mathcal{T}_{-\mu}^k$ following Ryabov¹⁰

$$\mathcal{T}_{-\mu}^k = (-1)^k a_k \sqrt{\frac{(k + \mu)!(k - \mu)!}{(2k)!}} J_-^\mu P_\mu^k(J^2, -J_z).$$

If we combine this with $(\mathcal{T}_\mu^k)^\dagger = (-1)^\mu \mathcal{T}_{-\mu}^k$, $J_+^\dagger = J_-$ and the fact that $P_\mu^k(J^2, J_z)$ is self-adjoint, we obtain the remarkably simple intertwining formula

$$P_\mu^k(J^2, J_z) J_-^\mu = (-1)^{k-\mu} J_-^\mu P_\mu^k(J^2, -J_z).$$

We now list the existing closed-form expressions for the matrix elements of P_μ^k . Note that each expression corresponds to a formula for the corresponding Clebsch-Gordan coefficients.

B. Coala

The first closed-form expression was given by Coala¹⁵

$$\begin{aligned} \langle jm' | \mathcal{T}_\mu^k | jm \rangle &= (-1)^k \left(\frac{(2j+1)(k!)^2(2j-k)!}{(2j+k+1)!} \right)^{1/2} \sqrt{(k+\mu)!(k-\mu)!} \\ &\sum_{p=\mu}^k (-1)^p \frac{(j-\mu-m)!(j+m)!}{(j-m-p)!(j-k+m+p)!p!(k-p)!(p-\mu)!(k+\mu-p)!} \langle jm' | J_+^\mu | jm \rangle, \end{aligned}$$

where we corrected a misprint. By comparing this expression with Eq. (3.170) in⁵ (p. 79) for the Clebsch-Gordan coefficients $(jmk\mu | jm')$ we see that

$$\langle jm' | \mathcal{T}_\mu^k | jm \rangle = (jmk\mu | jm'),$$

so that

$$a_k = \frac{(-1)^k}{k!} \left(\frac{(2j+1)(2k)!(2j-k)!}{(2j+k+1)!} \right)^{1/2}.$$

Therefore,

$$\langle jm | P_\mu^k | jm \rangle = (-1)^k (k!)^2 \sum_{p=\mu}^k (-1)^p \frac{(j-\mu-m)!(j+m)!}{(j-m-p)!(j-k+m+p)!p!(k-p)!(p-\mu)!(k+\mu-p)!}.$$

By using the descending Pochhammer symbol $[a]_p$ defined for $p \geq 0$ by By using the descending Pochhammer symbol $[a]_p$ defined for $p \geq 0$ by

$$[a]_p = \frac{a!}{(a-p)!}, \quad (9)$$

we can rewrite this as

$$\langle jm | P_\mu^k | jm \rangle = (-1)^k \sum_{p=\mu}^k (-1)^p \binom{k}{p} \binom{k}{p-\mu} [j+m]_{k-p} [j-m-\mu]_{p-\mu}. \quad (10)$$

C. Biedenharn and Louck

Table 6 of⁵ gives the following relation for the non-zero matrix elements of P_μ^k :

$$\langle jm|P_\mu^k|jm\rangle = \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} [j+m]_p [j-m-\mu]_{k-\mu-p}. \quad (11)$$

where $[a]_p$ is the descending Pochhammer symbol for $p \geq 0$

$$[a]_p = \frac{a!}{(a-p)!}. \quad (12)$$

Note that, in the rest of their book Biedenharn and Louck use the ascending Pochhammer symbol⁵ (p. 352). We notice that the expressions given by Coala and by Biedenharn and Louck become identical if we write $q = k - p$.

D. Grenet and Kibler

Again for $\mu \geq 0$, the formula given by Grenet and Kibler is⁶

$$\langle jm|P_\mu^k|jm\rangle = \frac{k!}{(2j-k)!(k+\mu)!} \sum_{z=\mu}^k (-1)^{\mu+z} \frac{(2j-z)!(k+z)!}{z!(k-z)!(z-\mu)!} \frac{(j+m)!}{(j+m+\mu-z)!},$$

that we rewrite

$$\langle jm|P_\mu^k|jm\rangle = \frac{(k!)^2}{(k+\mu)!} \sum_{p=0}^{k-\mu} \frac{(-1)^p}{p!} \binom{k+\mu+p}{k} \binom{2j-\mu-p}{2j-k} [j+m]_p. \quad (13)$$

A remarkable aspect of this formula is that m appears only in one term $[j+m]_p$. This allows us to obtain a relatively simple expression for P_μ^k as a function of J_z . Indeed, if we expand the Pochhammer symbol in terms of (signed) Stirling numbers of the first kind $s(p, n)$:

$$[a]_p = \sum_{q=0}^p s(p, q) a^q. \quad (14)$$

Hence

$$[j+m]_p = \sum_{q=0}^p s(p, q) (j+m)^q = \sum_{n=0}^p m^n \sum_{q=0}^{p-n} \binom{n+q}{n} s(p, n+q) j^q \quad (15)$$

And we obtain an explicit expression of P_μ^k in terms of j and J_z :

$$P_\mu^k = \sum_{n=0}^{k-\mu} \alpha_{\mu n}^k(j) J_z^n, \quad (16)$$

where

$$\alpha_{\mu n}^k(j) = \frac{(k!)^2}{(k+\mu)!} \sum_{p=n}^{k-\mu} \frac{(-1)^p}{p!} \binom{k+\mu+p}{k} \binom{2j-\mu-p}{2j-k} \sum_{q=0}^{p-n} \binom{n+q}{n} s(p, n+q) j^q. \quad (17)$$

E. Other expressions

Since matrix elements of T_μ^k are directly related to Clebsch-Gordan coefficients, every Clebsch-Gordan coefficient formula gives an expression for the matrix elements of T_μ^k . A large number of such formulas are given in¹⁴ and

Shimpuku gives 168 different formulas in¹⁶. The formulas used in the literature to calculate T_μ^k correspond to the cases where there are a small number of terms using the variable m , so that the expression in terms of J_z is (relatively) simple. From that point of view, the formula given by Grenet and Kibler cannot be improved.

There are also several semi-explicit expressions using iterated forward differences, quasi-powers or hypergeometric functions¹⁴. Within this semi-explicit family, a series of authors¹⁷⁻²¹ used a connection between some Clebsch-Gordan coefficients and Chebyshev polynomials of a discrete real variable (not to be confused with the Chebyshev polynomials $T_n(x)$ and $U_n(x)$ of the first and second kind). Then, they used iterated forward differences of these polynomials to obtain the Clebsch-Gordan coefficients required to calculate the matrix elements of T_μ^k . We do not elaborate because semi-explicit formulas are not the subject of this paper and because a very nice and extensive article was recently published on this topic²¹.

F. From matrix elements to operators

We proved that P_μ^k is a polynomial of J^2 and J_z . We gave an explicit expression for P_μ^k as a polynomial of J_z with coefficients $\alpha_{\mu m}^k(j)$ which are polynomials of j . It is interesting to use expressions for P_μ^k as a polynomial of J_z and J^2 because these expressions are independent of j and some tables are given in terms of J^2 instead of j . To replace the dependence on j by a dependence on J^2 , we need to find polynomials $\beta_{\mu m}^k(J^2)$ such that

$$\beta_{\mu m}^k(J^2)|jm\rangle = \beta_{\mu m}^k(j(j+1))|jm\rangle = \alpha_{\mu m}^k(j)|jm\rangle.$$

We treat this problem in a general way and for notational convenience we replace j by x and we solve the following problem: let P and Q be polynomials related by $P(x) = Q(x(x+1))$, calculate the coefficients of Q from the coefficients of P . Assume that

$$P(x) = \sum_{i=0}^n a_i x^i = Q(x(x+1)) = \sum_{j=0}^m b_j (x(x+1))^j.$$

We expand

$$Q(x(x+1)) = \sum_{j=0}^m \sum_{k=0}^j b_j \binom{j}{k} x^{2k} x^{j-k} = \sum_{j=0}^m \sum_{k=0}^j b_j \binom{j}{k} x^{j+k}.$$

In the last expression we define $i = j + k$, so that $k = i - j$. We know that $j \geq k \geq 0$ so that $i/2 \leq j \leq i$. But we also know that $0 \leq j \leq m$. Thus

$$Q(x(x+1)) = \sum_{i=0}^{2m} x^i \sum_{j=\lceil i/2 \rceil}^{\min(m,i)} b_j \binom{j}{i-j},$$

and

$$a_i = \sum_{j=\lceil i/2 \rceil}^{\min(m,i)} b_j \binom{j}{i-j}.$$

The term of maximum degree is $a_{2m} = b_m$, so that $n = 2m$. If we want to express b_j in terms of a_i , we need only the first $m+1$ values a_i . Moreover, we have $a_0 = b_0$ and the interesting cases are

$$a_i = \sum_{j=1}^m M_{ij} b_j,$$

where the $m \times m$ matrix $M = (M_{ij})$

$$M_{ij} = \binom{j}{i-j} \text{ for } i \geq j \geq \lceil i/2 \rceil,$$

$$M_{ij} = 0 \text{ otherwise,}$$

is invertible because it is lower diagonal with diagonal $M_{ii} = 1$. Since M is a lower triangular matrix with unit diagonal, its inverse is also a lower triangular matrix with unit diagonal. To prove this, write $M = 1 - K$, where K is lower triangular with zero diagonal so that $K^m = 0$ and note that $M^{-1} = I + \sum_{k=1}^{m-1} K^k$. Moreover, the first k lines of the inverse of a triangular matrix M depend only on the first k lines of M . In this sense, the inverse of M does not depend on the dimension of M .

It turns out that this problem is solved a theorem given by Riordan²² (p. 50) : If

$$\alpha_i = \sum_j (-1)^j \beta_j \binom{p+qj-j}{i-j},$$

then

$$\beta_i = \sum_j (-1)^j \alpha_j \frac{p+qj-j}{p+qi-j} \binom{p+qi-j}{i-j}.$$

In the case $\alpha_i = a_i$, $\beta_j = (-1)^j b_j$, $p = 0$ and $q = 2$ we recover our equation

$$a_i = \sum_j b_j \binom{j}{i-j},$$

and Riordan's theorem gives the inverse relation:

$$\begin{aligned} b_0 &= a_0, \\ b_i &= \sum_{j=1}^i (-1)^{i-j} \frac{j}{2i-j} \binom{2i-j}{i-j} a_j \text{ for } i \geq 1. \end{aligned}$$

G. Explicit expressions in terms of j and m

As an application of the formulae presented in this paper, we give explicit expressions for P_μ^k in terms of j and m for $k = 0$ to 6.

$$P_0^0 = 1.$$

$$P_0^1 = -2m,$$

$$P_1^1 = 1.$$

$$P_0^2 = -2j^2 - 2j + 6m^2,$$

$$P_1^2 = -4m - 2,$$

$$P_2^2 = 1.$$

$$P_0^3 = 12j^2m + 12jm - 20m^3 - 4m,$$

$$P_1^3 = -3j^2 - 3j + 15m^2 + 15m + 6,$$

$$P_2^3 = -6m - 6,$$

$$P_3^3 = 1.$$

$$P_0^4 = 6j^4 + 12j^3 - 60j^2m^2 - 6j^2 - 60jm^2 - 12j + 70m^4 + 50m^2,$$

$$P_1^4 = 24j^2m + 12j^2 + 24jm + 12j - 56m^3 - 84m^2 - 76m - 24,$$

$$P_2^4 = -4j^2 - 4j + 28m^2 + 56m + 36,$$

$$P_3^4 = -8m - 12,$$

$$P_4^4 = 1.$$

$$\begin{aligned}
P_0^5 &= -60j^4m - 120j^3m + 280j^2m^3 + 140j^2m + 280jm^3 + 200jm - 252m^5 - 420m^3 - 48m, \\
P_1^5 &= 10j^4 + 20j^3 - 140j^2m^2 - 140j^2m - 70j^2 - 140jm^2 - 140jm - 80j + 210m^4 \\
&\quad + 420m^3 + 630m^2 + 420m + 120, \\
P_2^5 &= 40j^2m + 40j^2 + 40jm + 40j - 120m^3 - 360m^2 - 480m - 240, \\
P_3^5 &= -5j^2 - 5j + 45m^2 + 135m + 120, \\
P_4^5 &= -10m - 20, \\
P_5^5 &= 1.
\end{aligned}$$

$$\begin{aligned}
P_0^6 &= -20j^6 - 60j^5 + 420j^4m^2 + 100j^4 + 840j^3m^2 + 300j^3 - 1260j^2m^4 - 1680j^2m^2 - 80j^2 \\
&\quad - 1260jm^4 - 2100jm^2 - 240j + 924m^6 + 2940m^4 + 1176m^2, \\
P_1^6 &= -120j^4m - 60j^4 - 240j^3m - 120j^3 + 720j^2m^3 + 1080j^2m^2 + 1200j^2m + 420j^2 + 720jm^3 \\
&\quad + 1080jm^2 + 1320jm + 480j - 792m^5 - 1980m^4 - 4320m^3 - 4500m^2 - 2808m - 720, \\
P_2^6 &= 15j^4 + 30j^3 - 270j^2m^2 - 540j^2m - 375j^2 - 270jm^2 - 540jm - 390j + 495m^4 + 1980m^3 \\
&\quad + 4095m^2 + 4230m + 1800, \\
P_3^6 &= 60j^2m + 90j^2 + 60jm + 90j - 220m^3 - 990m^2 - 1790m - 1200, \\
P_4^6 &= -6j^2 - 6j + 66m^2 + 264m + 300, \\
P_5^6 &= -12m - 30, \\
P_6^6 &= 1.
\end{aligned}$$

H. Explicit expressions in terms of J^2 and J_z

As an application of the formulae presented in this paper, we give explicit expressions for P_μ^k in terms of J^2 and J_z for $k = 0$ to 6.

$$P_0^0 = 1.$$

$$\begin{aligned}
P_0^1 &= -2J_z, \\
P_1^1 &= 1.
\end{aligned}$$

$$\begin{aligned}
P_0^2 &= -2J^2 + 6J_z^2, \\
P_1^2 &= -2(2J_z + 1), \\
P_2^2 &= 1.
\end{aligned}$$

$$\begin{aligned}
P_0^3 &= 3J_z(4J^2J_z - 5J_z^2 - 1), \\
P_1^3 &= -3J^2 + 3(5J_z^2 + 5J_z + 2), \\
P_2^3 &= -6(J_z + 1), \\
P_3^3 &= 1.
\end{aligned}$$

$$\begin{aligned}
P_0^4 &= 6(J^2)^2 - 12J^2(5J_z^2 + 1) + 10J_z^2(7J_z^2 + 5), \\
P_1^4 &= 3(2J_z + 1)(J^2 - 7J_z^2 - 7J_z - 6), \\
P_2^4 &= -4J^2 + 4(7J_z^2 + 14J_z + 9), \\
P_3^4 &= -4(2J_z + 3), \\
P_4^4 &= 1.
\end{aligned}$$

$$\begin{aligned}
P_0^5 &= -4J_z(15(J^2)^2 + 10J^2(7J_z^2 + 5) - 3(21J_z^4 + 35J_z^2 + 4)), \\
P_1^5 &= 10(J^2)^2 - 20J^2(7J_z^2 + 7J_z + 4) + 30(7J_z^4 + 14J_z^3 + 21J_z^2 + 14J_z + 4), \\
P_2^5 &= 40(J_z + 1)(J^2 - 3(J_z^2 + 2J_z + 2)), \\
P_3^5 &= -5J^2 + 15(3J_z^2 + 9J_z + 8), \\
P_4^5 &= -10(J_z + 2), \\
P_5^5 &= 1.
\end{aligned}$$

$$\begin{aligned}
P_0^6 &= -20(J^2)^3 + 20(J^2)^2(21J_z^2 + 8) - 60J^2(21J_z^4 + 35J_z^2 + 4) + 84J_z^2(11J_z^4 + 35J_z^2 + 14), \\
P_1^6 &= -12(2J_z + 1)(5(J^2)^2 + 10J^2(4 + 3J_z + 3J_z^2) - 3(11J_z^4 + 22J_z^3 + 49J_z^2 + 38J_z + 20)), \\
P_2^6 &= 15(J^2)^2 - 30J^2(9J_z^2 + 18J_z + 13) + 45(11J_z^4 + 44J_z^3 + 91J_z^2 + 94J_z + 40), \\
P_3^6 &= 10(2J_z + 3)(3J^2 - 11J_z^2 - 33J_z - 40), \\
P_4^6 &= -6J^2 + 6(11J_z^2 + 44J_z + 50), \\
P_5^6 &= -6(2J_z + 5), \\
P_6^6 &= 1.
\end{aligned}$$

We can notice that $P_{2\nu+1}^{2m}$ is proportional to $2J_z + 2\nu + 1$ and $P_{2\nu}^{2m+1}$ is proportional to $J_z + \nu$. As far as we know, this observation is new and we ignore whether it can be extended to all values of k . As a consequence, $P_{2\nu+1}^{2m}|j, -\frac{2\nu+1}{2}\rangle = 0$ and $P_{2\nu}^{2m+1}|j, -\nu\rangle = 0$ for all values of j . This restricts the influence of the corresponding crystal field parameters.

IV. FROM CRYSTAL FIELD PARAMETERS TO OPERATOR EQUIVALENTS

When investigating rare earths, neutron scattering generally uses operator equivalents whereas x-ray absorption spectroscopy uses crystal field parameters. More precisely, the crystal field acting on the angular part of the 4f shell is described by

$$H_L = \sum_{k,\mu} B_k^\mu C_\mu^k(L),$$

whereas operator equivalents are

$$H_J = \sum_{k,\mu} C_k^\mu \mathcal{T}_\mu^k(J).$$

A. One-electron case

As a simple case, we consider the case where the shell ℓ is occupied by a single electron. We use formula (40) of¹⁴ (p. 481)

$$\langle LSjm' | C_\mu^k \otimes 1 | LSjm \rangle = (-1)^{j-m'} \begin{pmatrix} j & k & j \\ -m' & \mu & m \end{pmatrix} (-1)^{j+L+S-k} (2j+1) \begin{Bmatrix} L & S & j \\ j & k & L \end{Bmatrix} \langle L || C^k || L \rangle.$$

Moreover,

$$\langle \ell || C^k || \ell \rangle = (-1)^\ell (2\ell + 1) \begin{pmatrix} \ell & k & \ell \\ 0 & 0 & 0 \end{pmatrix},$$

where¹⁴ (p. 251)

$$\begin{pmatrix} \ell & k & \ell \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{\sqrt{2k+1}} C_{\ell 0 \ell 0}^{k 0} = (-1)^{\ell-k/2} \frac{k!(\ell+k/2)!}{(k/2)!(k/2)!(\ell-k/2)!} \left(\frac{(2\ell-k)!}{(2\ell+k+1)!} \right)^{1/2}$$

The relation between C_μ^k acting on $|\ell m\rangle$ and \mathcal{T}_μ^k is

$$C_\mu^k(\ell) = (-1)^{k/2} \frac{(2\ell+1)(\ell+k/2)!(2\ell-k)!\sqrt{(2k!)}}{(k/2)!(k/2)!(\ell-k/2)!(2\ell+k+1)!a_k} \mathcal{T}_\mu^k.$$

B. Many-electron case

We consider now the case where shell ℓ is occupied by n electrons ($0 \leq n \leq 2(2\ell + 1)$). For the case of a shell ℓ containing n electrons, we use Eq. (11.53)¹³ (p. 317)

$$\langle \ell^n \alpha LS || U^{(k)} || \ell^n \alpha' L' S' \rangle = \delta_{SS'} n (-1)^{\ell+L+k} \sqrt{(2L+1)(2L'+1)} \\ \sum_{\bar{\alpha}\bar{L}\bar{S}} (-1)^{\bar{L}} \left\{ \begin{matrix} \ell & k & \ell \\ L & \bar{L} & L' \end{matrix} \right\} (\ell^n \alpha LS \{ | \ell^{n-1} \bar{\alpha} \bar{L} \bar{S} \rangle \langle \ell^{n-1} \bar{\alpha} \bar{L} \bar{S} | \} \ell^n \alpha' L' S').$$

The coefficients of fractional parentage were obtained from the table computed by Velkov in his PhD thesis^{23,24}.

V. CONCLUSION

In this paper, we reviewed the existing expressions for the spherical tensor form of Stevens or spin operator equivalents. We gave explicit proofs of these forms, which were not available in the literature and we devised a way to transform expressions in terms of j and m into expressions in terms of J^2 and J_z . Along the way, we discovered factorization properties of some of the spherical tensors which seem to be new.

We hope that the present paper will enable the physics and chemistry communities to avoid having recourse to cumbersome (and generally not fully correct) tables.

Among the perspectives of this work, we might mention the question whether or not the factorization properties extend to general values of k . We also want to mention that some analytical expressions were given for non-diagonal tensor-equivalent operators²⁵⁻²⁷, i.e. for the case of matrix elements between different values of j . However, the generalization of our results to the non-diagonal case seems non trivial.

VI. ACKNOWLEDGEMENTS

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VII. PROOFS

As far as we know, no proof of the formulas given by Biedenharn and Louck and by Grenet and Kibler were published, although Geneviève Grenet provides a proof in her PhD thesis. Since these proofs depend on rather unusual expressions for the Clebsch-Gordan coefficients, we find it useful to make them explicit. In this section we use the spherical tensors T_μ^k normalized by⁵

$$a_k = (-1)^k \frac{\sqrt{(2k)!}}{k!}.$$

A. Proof of Coala's formula

Equation (14) of Ref.¹⁵ is, in our notation,

$$\langle jm' | \mathcal{T}_\mu^k | jm \rangle = \delta_{m', m+\mu} (-1)^k \left(\frac{(2j+1)(k!)^2 (2j-k)!}{(2j+k+1)!} \right)^{1/2} \sqrt{(k+\mu)!(k-\mu)!} \\ \sum_{p=\mu}^k (-1)^p \frac{(j-\mu-m)!(j+m)!}{(j-m-p)!(j-k+m+p)!p!(k-p)!(p-\mu)!(k+\mu-p)!} \langle jm' | J_+^\mu | jm \rangle.$$

We recall that

$$J_+^\mu |\ell m - \mu\rangle = \left(\frac{(\ell - m + \mu)!(\ell + m)!}{(\ell - m)!(\ell + m - \mu)!} \right)^{1/2} |\ell m\rangle,$$

so that

$$\langle jm' | J_+^\mu | jm \rangle = \delta_{m', m+\mu} \left(\frac{(j-m)!(j+m+\mu)!}{(j-m-\mu)!(j+m)!} \right)^{1/2}.$$

Therefore,

$$\begin{aligned} \langle jm' | \mathcal{T}_\mu^k | jm \rangle &= \delta_{m', m+\mu} (-1)^k \left(\frac{(2j+1)(k!)^2(2j-k)!}{(2j+k+1)!} \right)^{1/2} \left(\frac{(j-m)!(j+m+\mu)!}{(j-m-\mu)!(j+m)!} \right)^{1/2} \sqrt{(k+\mu)!(k-\mu)!} \\ &\quad \sum_{p=\mu}^k (-1)^p \frac{(j-\mu-m)!(j+m)!}{(j-m-p)!(j-k+m+p)!p!(k-p)!(p-\mu)!(k+\mu-p)!}. \end{aligned}$$

For $\mu = k$ this is

$$\begin{aligned} \langle jm' | \mathcal{T}_k^k | jm \rangle &= (-1)^k \left(\frac{(2j+1)(k!)^2(2j-k)!}{(2j+k+1)!} \right)^{1/2} \sqrt{(2k)!} (-1)^k \frac{(j-k-m)!(j+m)!}{(j-m-k)!(j+m)!k!k!} \langle jm' | J_+^k | jm \rangle \\ &= \left(\frac{(2j+1)(2k)!(2j-k)!}{(k!)^2(2j+k+1)!} \right)^{1/2} \langle jm' | J_+^k | jm \rangle. \end{aligned}$$

To check Coala's formula, we notice that the reference he uses seems to be the symmetric form, Eq. (3.170) in⁵. Let us check that. According to Eq. (3.170) in⁵ (p. 79).

$$\begin{aligned} (j_1 m_1 j_2 m_2 | jm) &= \delta_{m, m_1+m_2} \left(\frac{(2j+1)(j_1+j_2-j)!(j+j_1-j_2)!(j+j_2-j_1)!}{(j_1+j_2+j+1)!} \right)^{1/2} \\ &\quad \sum_z (-1)^z \frac{((j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(j+m)!(j-m)!)^{1/2}}{z!(j_1+j_2-j-z)!(j_1-m_1-z)!(j_2+m_2-z)!(j-j_2+m_1+z)!(j-j_1-m_2+z)!} \end{aligned}$$

The relevant coefficient is $\langle jmk\mu | jm + \mu \rangle$, so that

$$\begin{aligned} \langle jmk\mu | jm + \mu \rangle &= \left(\frac{(2j+1)(2j-k)!k!k!}{(2j+k+1)!} \right)^{1/2} \\ &\quad \sum_z (-1)^z \frac{((j+m)!(j-m)!(k+\mu)!(k-\mu)!(j+m+\mu)!(j-m-\mu)!)^{1/2}}{z!(k-z)!(j-m-z)!(k+\mu-z)!(j-k+m+z)!(z-\mu)!} \end{aligned}$$

B. Proof of the Biedenharn and Louck formula

We want to prove the expression for $\langle jm | P_\mu^k | jm \rangle$. For this we need an expression for the Clebsch-Gordan coefficient which is adapted to what we want. Recall that,

$$T_\mu^k = (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} J_+^\mu P_\mu^k,$$

and that

$$\langle jm + \mu | T_\mu^k | jm \rangle = (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} \langle jm + \mu | J_+^\mu P_\mu^k | jm \rangle = C_{m\mu, m+\mu}^{jkj} \left(\frac{(2j+k+1)!}{(2j+1)(2j-k)!} \right)^{1/2}.$$

The formula for the matrix element of P_μ^k given by Eq. (11) is

$$\begin{aligned} P_\mu^k | jm \rangle &= \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \frac{(j+m)!}{(j+m-p)!} \frac{(j-m-\mu)!}{(j-m-k+p)!} | jm \rangle \\ &= \frac{(j+m)!(j-m-\mu)!}{(2j-k)!} \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p} | jm \rangle. \end{aligned}$$

Then,

$$\begin{aligned} \langle j, m + \mu | J_+^\mu P_\mu^k | jm \rangle &= \left(\frac{(j-m)!(j+m+\mu)!}{(j-m-\mu)!(j+m)!} \right)^{1/2} \frac{(j+m)!(j-m-\mu)!}{(2j-k)!} \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p} \\ &= \frac{((j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!)^{1/2}}{(2j-k)!} \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p}. \end{aligned}$$

Hence

$$\begin{aligned} \langle jm + \mu | T_\mu^k | jm \rangle &= (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} \langle jm + \mu | J_+^\mu P_\mu^k | jm \rangle \\ &= (-1)^k \frac{((k+\mu)!(k-\mu)!(j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!)^{1/2}}{(2j-k)!k!} \\ &\quad \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p} \\ &= C_{m\mu, m+\mu}^{jkj} \left(\frac{(2j+k+1)!}{(2j+1)(2j-k)!} \right)^{1/2}. \end{aligned}$$

This gives us the Clebsch-Gordan coefficient

$$\begin{aligned} C_{m\mu, m+\mu}^{jkj} &= (-1)^k \left(\frac{(2j+1)(k+\mu)!(k-\mu)!(j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!}{(2j+k+1)!(2j-k)!(k!)^2} \right)^{1/2} \\ &\quad \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{k-\mu-p} \binom{2j-k}{j+m-p}. \end{aligned}$$

We need to find a place where this expression for the Clebsch-Gordan coefficient is given. We first use

$$C_{m\mu, m+\mu}^{jkj} = (-1)^k C_{\mu m, m+\mu}^{kjj}.$$

The coefficients of Shimpuku's expression becomes

$$\begin{aligned} a_1 &= 2j - k, & a_2 &= k, & a_3 &= k, \\ b_1 &= k - \mu, & b_2 &= j - m, & b_3 &= j + m + \mu, \\ c_1 &= k + \mu, & c_2 &= j + m, & c_3 &= j - m - \mu. \end{aligned}$$

Then the sum (p. 413)

$$\sum_{\alpha} (-1)^{\alpha} \binom{a_3}{\alpha} \binom{a_2}{b_1 - \alpha} \binom{a_1}{c_2 - \alpha} = \sum_{\alpha} (-1)^{\alpha} \binom{k}{\alpha} \binom{k}{k - \mu - \alpha} \binom{2j - k}{j + m - \alpha},$$

is exactly what we need. We must check that the overall factors agree. Indeed:

$$\begin{aligned} \frac{\binom{b_1+c_1}{a_3} \binom{b_2+c_2}{a_3}}{\binom{J+1}{a_3} \binom{b_1+c_1}{b_1} \binom{b_2+c_2}{c_2} \binom{b_3+c_3}{c_3}} &= \frac{\binom{2k}{k} \binom{2j}{k}}{\binom{2j+k+1}{k} \binom{2k}{k-\mu} \binom{2j}{j+m} \binom{2j}{j-m-\mu}} \\ &= \left(\frac{(2j+1)(k+\mu)!(k-\mu)!(j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!}{(2j+k+1)!(2j-k)!(k!)^2} \right)^{1/2}. \end{aligned}$$

To summarize. The expression for P_μ^k cannot be obtained from the usual formulas for the Clebsch-Gordan coefficients. Among the 168 expressions for the Clebsch-Gordan coefficients proposed by Shimpuku¹⁶, only the first one of p. 413 provides the proper result

$$C_{\mu m, m+\mu}^{kjj} = \left(\frac{\binom{2k}{k} \binom{2j}{k}}{\binom{2j+k+1}{k} \binom{2k}{k-\mu} \binom{2j}{j+m} \binom{2j}{j-m-\mu}} \right)^{1/2} \sum_p (-1)^p \binom{k}{p} \binom{k}{k-\mu-p} \binom{2j-k}{j+m-p}.$$

By using $C_{m\mu, m+\mu}^{jkj} = (-1)^k C_{\mu m, m+\mu}^{kjj}$ we obtain

$$C_{m\mu, m+\mu}^{jkj} = (-1)^k \left(\frac{(2j+1)(k+\mu)!(k-\mu)!(j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!}{(2j+k+1)!(2j-k)!(k!)^2} \right)^{1/2} \\ \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{k-\mu-p} \binom{2j-k}{j+m-p}.$$

The Wigner-Eckart theorem for T_μ^k is expressed by

$$\langle jm + \mu | T_\mu^k | jm \rangle = C_{m\mu, m+\mu}^{jkj} \left(\frac{(2j+k+1)!}{(2j+1)(2j-k)!} \right)^{1/2} \\ = (-1)^k \frac{((k+\mu)!(k-\mu)!(j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!)^{1/2}}{(2j-k)!k!} \\ \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p}$$

From the relation

$$T_\mu^k = (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} J_+^\mu P_\mu^k,$$

we obtain

$$\langle jm + \mu | J_+^\mu P_\mu^k | jm \rangle = \frac{((j-m)!(j+m+\mu)!(j+m)!(j-m-\mu)!)^{1/2}}{(2j-k)!} \\ \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p}$$

From the standard formula

$$\langle jm + \mu | J_+^\mu | jm \rangle = \langle jm | \left(\frac{(j-m)!(j+m+\mu)!}{(j-m-\mu)!(j+m)!} \right)^{1/2},$$

we get

$$\langle jm | P_\mu^k | jm \rangle = \frac{(j+m)!(j-m-\mu)!}{(2j-k)!} \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \binom{2j-k}{j+m-p} \\ = \sum_{p=0}^{k-\mu} (-1)^p \binom{k}{p} \binom{k}{\mu+p} \frac{(j+m)!(j-m-\mu)!}{(j+m-p)!(j-k-m+p)!}.$$

C. Proof of the Grenet and Kibler

Majumdar proved the following expression for the Clebsch-Gordan coefficients^{29,30}:

$$C_{a\alpha b\beta}^{c\gamma} = \delta_{\gamma, \alpha+\beta} \left(\frac{(2c+1)(-a+b+c)!}{(a+b-c)!(a-b+c)!(a+b+c+1)!} \right)^{1/2} \left(\frac{(a+\alpha)!(a-\alpha)!(b-\beta)!(c+\gamma)!}{(b+\beta)!(c-\gamma)!} \right)^{1/2} \\ \sum_z (-1)^{b+\beta+z} \frac{(2c-z)!(a+b-c+z)!}{z!(c+\gamma-z)!(-a+b+c-z)!(a-c-\beta+z)!}.$$

Therefore,

$$C_{jm k \mu}^{j m + \mu} = \left(\frac{(2j+1)}{(2j-k)!(2j+k+1)!} \right)^{1/2} \left(\frac{(j+m)!(j-m)!(k-\mu)!(j+m+\mu)!}{(k+\mu)!(j-m-\mu)!} \right)^{1/2} \\ \sum_z (-1)^{k+\mu+z} \frac{(2j-z)!(k+z)!}{z!(j+m+\mu-z)!(k-z)!(z-\mu)!},$$

We saw that

$$\langle j, m + \mu | T_\mu^k | jm \rangle = C_{jmk\mu}^{j+m+\mu} \left(\frac{(2j+k+1)!}{(2j+1)(2j-k)!} \right)^{1/2}.$$

Therefore,

$$\begin{aligned} \langle j, m + \mu | T_\mu^k | jm \rangle &= \frac{1}{(2j-k)!} \left(\frac{(j+m)!(j-m)!(k-\mu)!(j+m+\mu)!}{(k+\mu)!(j-m-\mu)!} \right)^{1/2} \\ &\quad \sum_z (-1)^{k+\mu+z} \frac{(2j-z)!(k+z)!}{z!(j+m+\mu-z)!(k-z)!(z-\mu)!}. \end{aligned}$$

We know that

$$T_\mu^k = (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} J_+^\mu P_\mu^k,$$

so that

$$\begin{aligned} \langle j, m + \mu | T_\mu^k | jm \rangle &= (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} \langle j, m + \mu | J_+^\mu P_\mu^k | jm \rangle \\ &= (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} \sum_{j'm'} \langle j, m + \mu | J_+^\mu | j'm' \rangle \langle j'm' | P_\mu^k | jm \rangle \end{aligned}$$

By using Eq. (6) and the orthonormality of the basis vectors we obtain

$$\langle j, m + \mu | T_\mu^k | jm \rangle = (-1)^k \frac{\sqrt{(k+\mu)!(k-\mu)!}}{k!} \left(\frac{(j-m)!(j+m+\mu)!}{(j-m-\mu)!(j+m)!} \right)^{1/2} \langle jm | P_\mu^k | jm \rangle.$$

Our final result is now, for $\mu \geq 0$ and $k \geq 2j$

$$\langle jm | P_\mu^k | jm \rangle = \frac{k!}{(2j-k)!(k+\mu)!} \sum_z (-1)^{\mu+z} \frac{(2j-z)!(k+z)!}{z!(k-z)!(z-\mu)!} \frac{(j+m)!}{(j+m+\mu-z)!},$$

that we rewrite

$$\langle jm | P_\mu^k | jm \rangle = \sum_{z=\mu}^k (-1)^{\mu+z} \binom{k}{z} \binom{k+z}{z-\mu} \frac{(2j-z)!}{(2j-k)!} \frac{(j+m)!}{(j+m+\mu-z)!},$$

or

$$\langle jm | P_\mu^k | jm \rangle = \sum_{s=0}^{k-\mu} (-1)^s \binom{k}{\mu+s} \binom{k+\mu+s}{s} \frac{(2j-\mu-s)!}{(2j-k)!} \frac{(j+m)!}{(j+m-s)!}.$$

The identity of Eqs. (11) and (13) was checked with Mathematica for $k = 0$ to 12. This can be rewritten

$$\langle jm | P_\mu^k | jm \rangle = \frac{(k!)^2}{(k+\mu)!} \sum_{s=0}^{k-\mu} (-1)^s \binom{k+\mu+s}{k} \binom{2j-\mu-s}{k-\mu-s} \binom{j+m}{s}.$$

On the other hand, Eq. (11) can be rewritten

$$\begin{aligned} \langle jm | P_\mu^k | jm \rangle &= \sum_{s=0}^{k-\mu} (-1)^s \binom{k}{s} \binom{k}{\mu+s} \frac{(j+m)!}{(j+m-s)!} \frac{(j-m-\mu)!}{(j-m-k+s)!} \\ &= \sum_{s=0}^{k-\mu} (-1)^s \binom{k}{s} \binom{k}{\mu+s} \binom{j+m}{s} s! \binom{j-m-\mu}{k-\mu-s} (k-\mu-s)! \\ &= \frac{(k!)^2}{(k+\mu)!} \sum_{s=0}^{k-\mu} (-1)^s \binom{k+\mu}{\mu+s} \binom{j+m}{s} \binom{j-m-\mu}{k-\mu-s}. \end{aligned}$$

The two formulas are identical if

$$\sum_{s=0}^{k-\mu} (-1)^s \binom{k+\mu+s}{k} \binom{2j-\mu-s}{k-\mu-s} \binom{j+m}{s} = \sum_{s=0}^{k-\mu} (-1)^s \binom{k+\mu}{\mu+s} \binom{j+m}{s} \binom{j-m-\mu}{k-\mu-s}.$$

This can be rewritten

$$\sum_{s=0}^{k-\mu} (-1)^s \binom{k+\mu+s}{k} \binom{b}{s} \binom{b+c-s}{k-\mu-s} = \sum_{s=0}^{k-\mu} (-1)^s \binom{k+\mu}{\mu+s} \binom{b}{s} \binom{c}{k-\mu-s}.$$

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