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6-j symbols for SO($2l+1$) and a structural analysis in terms of atomic quasiparticles

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Abstract. Starting from a primitive 6-j symbol for SO($2l+1$) in which four elementary spinor irreducible representations (irreps) $(\frac{1}{2}\frac{1}{2}\ldots\frac{1}{2})$ appear, and using the properties of the Kronecker products of partially stretched irreps, we develop a bootstrap procedure, based on a generalisation of the Biedenharn-Elliott sum rule, for calculating other 6-j and 9-j symbols for SO($2l+1$). Several of our formulae can be expressed in terms of SO(3) 3-j symbols and rotation matrices $d^{j}_{mn}(\frac{1}{2}\pi)$. An explanation for this is found by using the complementary groups whose generators involve the spin S and quasispin Q of electrons in an atomic l shell. The relation between the two kinds of coupling, that of the irreps of SO($2l+1$) and that of the SO(3) angular momenta, is particularly fruitful if the quasiparticle description is employed for the electrons. A further bootstrap leads to a formula for an SO($2l+1$) 6-j symbol whose six irreps are all of the type $(11\ldots10\ldots0)$, and this is shown to be consistent with a formula for an Sp($2n$) 6-j symbol if we replace $2n$ by the negative dimension $-2l-1$.

1. Introduction

The quantum theory of angular momentum depends in a crucial way on the n-j symbols associated with the names of Wigner (1959, 1965) and Racah (1942). Among the many surveys that have been made over the years, those of Edmonds (1957), Jucys and Bandzaitis (1977), Biedenharn and Louck (1981), and Lindner (1984) are particularly useful. The fact that we live in a three-dimensional space gives the theory a structure determined by SO(3), the special orthogonal group in three dimensions. However, it was clear many years ago that much of the mathematics could be carried over to other groups. The first systematic generalisation of the n-j symbols was made by Griffith (1962) for point groups. This area of application was further developed by Butler (1981), who applied methods that he had previously worked out for an arbitrary compact Lie group (Butler 1975). The usefulness of the generalised n-j symbols to nuclear and particle physics is apparent from the work of Kramer (1967), Moshinsky and Chacón (1968), Hecht (1975) and Le Blanc and Hecht (1987), among others. Our own interest has derived from work on the Jahn-Teller effect (Judd *et al* 1986a) and the quasiparticle approach to atomic shell theory (Judd and Li 1989), areas where a knowledge of the n-j symbols for SO($2l+1$) and G_2 is important.

The study of group-subgroup structures brings the so-called isoscalar factors into play. They can be regarded as parts of factored Clebsch-Gordan (CG) coefficients or generalised 3-j symbols. The literature is awash with all kinds of expressions for special n-j symbols and isoscalar factors. General formulae (such as exist for SO(3)) are hard to come by for the general Lie group, mainly because of multiply occurring irreducible representations (irreps) in the reduction of the Kronecker products of pairs of irreps. Additional classificatory labels have to be defined—a procedure that is often difficult to do in an elegant and satisfying manner. Problems of this kind are not so awkward if a purely numerical approach is followed. Indeed, procedures for calculating the actual values of the generalised n-j symbols are well advanced (see, for example, Bickerstaff and Wybourne 1981, Searle and Butler 1988). The basic idea is to use a knowledge of a few simple cases to get others via the extension of the Biedenharn-Elliott sum rule. This bootstrap method does not lend itself very readily to a general algebraic approach. However, for many applications the irreps that enter the calculations tend to be of low dimensionality, or of a special kind, and the multiplicity problem may be either not severe or absent altogether. We can thus ask whether analytical expressions can be found in terms of the highest weights that define the irreps. Butler (1976) has described how the classic formulae for SO(3) can be derived from a bootstrap that takes as its starting point a few very simple cases.

We need not be limited to this kind of method. Generating functions can be devised in some special cases (Judd and Lister 1987); isoscalar factors can be constructively put to use (Ališauskas 1987); and we can sometimes use the mathematical structure inherent in a particular physical problem (Hecht 1975, Le Blanc and Hecht 1987). In the present paper we propose to use the bootstrap approach in conjunction with our knowledge of atomic quasiparticles. Such quasiparticles have already been used to provide a reason for the existence of a particularly simple expression for a 6-j symbol for SO($2l+1$) in which four elementary spinors appear (Judd 1987). Needless to say, we do not claim that our formulae for 6-j and 9-j symbols depend on the existence of electrons in atoms: our quasiparticles merely provide a framework that assists in the development of the mathematics and in getting an understanding of the formulae that the bootstrap approach leads to. However, our use of quasiparticles means that many of our results find an immediate application in atomic shell theory. As is indicated in sections 16 and 17, additional bootstraps produce results of a more general interest.

2. Definitions

It is often convenient to work with U coefficients as well as 6-j symbols. In analogy to the definition of Jahn (1951) for SO(3), we define

$$U\begin{pmatrix} W_1 & W_2 & W_3 \\ W_4 & W_5 & W_6 \end{pmatrix} = [\mathrm{Dim}(W_3)\,\mathrm{Dim}(W_6)]^{1/2}\begin{Bmatrix} W_1 & W_2 & W_3 \\ W_4 & W_5 & W_6 \end{Bmatrix} \tag{1}$$

where W_i is an irreducible representation (irrep) of SO($2l+1$) and Dim(W_i) its dimension. For all triads ($W_1 W_2 W_3$) of irreps considered in the present paper the triple Kronecker product $W_1 \times W_2 \times W_3$ does not contain the identity irrep ($\dot{0}$) more than once, so there is no need to include multiplicity labels in equation (1). The U coefficients possess the advantage that, for a given W_1, W_2, W_4, and W_5, they form a unitary matrix with rows and columns labelled by W_3 and W_6. On the other hand, the 6-j symbol displays better the symmetries involved in interchanging its third column with either of the other two.

Similar reasons prompt us to relate a 9-j symbol to another U coefficient by means of the equation

$$U\begin{pmatrix} W_1 & W_2 & W_3 \\ W_4 & W_5 & W_6 \\ W_7 & W_8 & W_9 \end{pmatrix}$$

$$=[\mathrm{Dim}(W_3)\,\mathrm{Dim}(W_6)\,\mathrm{Dim}(W_7)\,\mathrm{Dim}(W_8)]^{1/2}\begin{Bmatrix} W_1 & W_2 & W_3 \\ W_4 & W_5 & W_6 \\ W_7 & W_8 & W_9 \end{Bmatrix}. \quad (2)$$

Our present interest is limited to just a few kinds of irreps. Rather than spell out their highest weights every time they appear, it is convenient to make several abbreviations. We write

$$(\tfrac{3}{2}^{l-q}\ \tfrac{1}{2}^{q}) \equiv w_q \quad (3)$$

so the elementary spinor whose highest weight is $(\frac{1}{2}\frac{1}{2}\ldots\frac{1}{2})$ is denoted by w_l. To describe the irrep $(11\ldots10\ldots0)$ in which $l-m'$ ones and m' zeros appear, we introduce an associated variable m, defined by

$$m+\tfrac{1}{2}=(-1)^{m'}(m'+\tfrac{1}{2}) \quad (4)$$

and write

$$(1^{l-m'}0^{m'}) \equiv W(m). \quad (5)$$

The reason for working with m rather than m' is that m is more easily incorporated into analytical expressions for phase factors. To make the connections clear, we give the m and m' labels for all irreps $W(m)$ of SO(7) in table 1. We note that m is always an even number (possibly zero).

Table 1. Values of m, m' and associated quantities for the four irreps of SO(7) of the type $W(m)$. In terms of the number N of electrons in the atomic f shell, the fourth column gives values of the total spin S (for N odd) or the quasispin Q (for N even). The fifth column gives values of S (for N even) or Q (for N odd).

$W(m)$	m'	m	$\frac{1}{2}(l-m)$	$\frac{1}{2}(l+m+1)$
(000)	3	−4	$\frac{7}{2}$	0
(100)	2	2	$\frac{1}{2}$	3
(110)	1	−2	$\frac{5}{2}$	1
(111)	0	0	$\frac{3}{2}$	2

3. Phases

Standard techniques, as described by Wybourne (1970, ch 6), can be used to separate Kronecker squares into their symmetric and antisymmetric parts. By using such methods, we are led to make the following choices for 3-j phases:

$$\{w_q w_l W(m)\}=(-1)^{m/2} \quad (6)$$

$$\{W(m_1)\,W(m_2)\,W(m_3)\}=(-1)^{(m_1+m_2+m_3)/2+\tau} \quad (7)$$

where $\tau=0$ for $l=0, 3, 4, 7, \ldots$, and $\tau=1$ for $l=1, 2, 5, 6, \ldots$. Equations (6) and (7) are to a large extent arbitrary: their function is to guarantee that the correct phases are produced when $w_q = w_l$ and when two of the three possible m_i are equal.

1-*j* phases (or, as they are sometimes called, 2-*j* phases) are obtained when one of the irreps of the type $W(m_i)$ is set equal to the scalar irrep $(00\ldots0)$. In this case, $m_i = l$ (l even) and $m_i = -l-1$ (l odd). Substitution into equations (6) and (7) leads to the results

$$\{w_l\} = (-1)^\tau \qquad \{W(m)\} = 1$$

in agreement with the tabulation of Butler and King (1974).

The 3-*j* phases of equations (6) and (7) involve simple phase triads: that is, we can write

$$\{W_1 W_2 W_3\} = (-1)^{\varphi(W_1)}(-1)^{\varphi(W_2)}(-1)^{\varphi(W_3)} \tag{8}$$

for all cases if we take

$$\varphi(W(m_i)) = \tfrac{1}{2}m_i + \tau \qquad \varphi(w_q) = \tfrac{1}{2}\tau. \tag{9}$$

This simplification means that we can manipulate our particular irreps of SO($2l+1$) in a way that closely parallels the angular momentum quantum numbers of the traditional Racah-Wigner calculus. Thus columns of a 6-*j* symbol can be interchanged without introducing phase factors (see Piepho and Schatz 1983, p 348). More generally, the formulae of Edmonds (1957), for example, can be extended from SO(3) to SO($2l+1$) by the simple device of making the label replacements $j_i \to W_i$ in the *n*-*j* symbols and, in the formulae themselves, the substitutions

$$(2j_i+1) \to \mathrm{Dim}(W_i) \qquad (-1)^{j_i} \to (-1)^{\varphi(W_i)}. \tag{10}$$

This procedure works whenever all irrep triads occur an even number of times, since the so-called historical phases of angular momentum theory disappear. We have used the general formulae of Butler (1981) in the analysis that follows; however, the replacements (10) serve as useful checks.

4. Dimensions

Algebraic expressions for the dimensions of the various irreps of SO($2l+1$) of interest to us can be found from the general formula of Weyl (1925). This procedure can be shortened by noting first that the dimension of w_l, whose weights are $(\pm\frac{1}{2}, \pm\frac{1}{2}, \ldots, \pm\frac{1}{2})$ (with all combinations of signs) is 2^l. Since $W(m)$ coincides with the totally antisymmetric irrep $[1^{l-m'}0^{m'}]$ of U($2l+1$), we have

$$\mathrm{Dim}(W(m)) = \frac{(2l+1)!}{(l-m')!(l+m'+1)!} = \frac{(2l+1)!}{(l-m)!(l+m+1)!} \tag{11}$$

the last step (the removal of the primes from the m's) following from an application of equation (4). Finally, from the Kronecker product

$$w_q = w_l \times W(q) - w_l \times W(q-1)$$

we can deduce that

$$\begin{aligned}\mathrm{Dim}(\tfrac{3}{2}^{l-q}\tfrac{1}{2}^{q}) &= \mathrm{Dim}(w_q)\\ &= 2^{l+1}(q+1)(2l+1)!/(l+q+2)!(l-q)!.\end{aligned} \tag{12}$$

Numerical values for special cases of $W(m)$ and w_q can be found from Wybourne (1970, tables A-19 to A-26) or from McKay and Patera (1981).

5. Primitive 6-*j* symbols

The starting point for our analysis is the equation

$$U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_l & w_l & W(m_2) \end{pmatrix} = \varepsilon 2^{1/2} d^{l+1/2}_{m_1+1/2, m_2+1/2}(\tfrac{1}{2}\pi) \tag{13}$$

where the SO(3) rotation matrix is given by

$$d^j_{mn}(\tfrac{1}{2}\pi) = 2^{-j} \sum_t (-1)^t \frac{[(j+m)!(j-m)!(j+n)!(j-n)!]^{1/2}}{(j+m-t)!(j-n-t)!t!(t+n-m)!}. \tag{14}$$

In the original statement of equation (13) (Judd 1987), the phase factor ε was chosen to be +1. In the present analysis we prefer to have consistency with equation (3.3.22) of Butler (1981) (or its equivalent, equation (6.3.2) of Edmonds (1957)). That is, we ask that Butler's phase be reproduced when we set either $W(m_1)$ or $W(m_2)$ equal to the scalar irrep $(\dot{0})$. This can be achieved by taking

$$\varepsilon = (-1)^{(m_1+m_2)/2+\tau}.$$

6. Partially stretched weights

As a first extension to the U coefficient of equation (13), we consider

$$U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_l & w_q & W(m_2) \end{pmatrix} \qquad (q<l) \tag{15}$$

which, according to Butler (1981, equation (3.2.18)) and the phase choices of section 3, is equal to the recoupling coefficient

$$\langle (w_l w_l) W(m_2), w_l, w_q \,|\, w_l, (w_l w_l) W(m_1), w_q \rangle \tag{16}$$

times the phase factor $(-1)^\tau$. When $q<l$, the first weights of the irreps appearing in the expression (16) are stretched, in as much as $\frac{1}{2}+\frac{1}{2}=1$ for $(w_l w_l) W(m_i)$, $1+\frac{1}{2}=\frac{3}{2}$ for $(W(m_2)w_l)w_q$, and $\frac{1}{2}+1=\frac{3}{2}$ for $(w_l W(m_1))w_q$. In cases such as this, it is useful to consider the subgroup SO(2) × SO(2l − 1) of SO(2l + 1). The generators of this subgroup are those of SO(2l + 1) less the shift operators that change the first weight. When the first weights are stretched, every irrep $(\omega_1\omega_2 \ldots \omega_l)$ of SO(2l + 1) can be unambiguously replaced by the irrep $(\omega_1) \times (\omega_2\omega_3 \ldots \omega_l)$ of SO(2) × SO(2l − 1), with the result that the recoupling coefficient (16) factorises into a part referring to SO(2l − 1) and the part

$$\langle ((\tfrac{1}{2})(\tfrac{1}{2}))1, (\tfrac{1}{2}), \tfrac{3}{2} \,|\, \tfrac{1}{2}, ((\tfrac{1}{2})(\tfrac{1}{2}))1, \tfrac{3}{2} \rangle \tag{17}$$

containing the SO(2) labels. Its magnitude is 1, as is that of each of the isoscalar factors associated with the four triads in the coefficient (16). Rather than make specific phase choices at this point, we simply carry forward a phase ambiguity. We are left with the SO(2l − 1) recoupling coefficient: this is identical to (16) except that the first weights of every irrep appearing therein have been excised.

By repeating this procedure $l-q$ times, all the $\frac{1}{2}$ weights of the irrep w_q can be removed, and w_q becomes $(\frac{1}{2}^q)$ of SO$(2q+1)$. We write this irrep as $w_{l'}$. On converting the recoupling coefficient to a U coefficient, we arrive at the result

$$U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_q & w_l & W(m_2) \end{pmatrix} = \varepsilon_q U\begin{pmatrix} w_{l'} & w_{l'} & W(m_1) \\ w_{l'} & w_{l'} & W(m_2) \end{pmatrix} \tag{18}$$

where the primed symbols, as well as the irreps $W(m_i)$ in the U coefficient on the right, refer to SO$(2q+1)$. The SO$(2q+1)$ U coefficient can be evaluated by means of equation (13).

At present the phase ε_q is undetermined. In sections 7 and 8 it appears as ε_q^2 and lies dormant. However, the Racah back-coupling in section 12 enables it to be calculated as

$$\varepsilon_q = \{w_l\}\{w_{l'}\} = (-1)^{\tau-\tau'}. \tag{19}$$

It can be shown that this is what we could get if we took the recoupling coefficients (17) and all the isoscalar factors associated with the reduction

$$\mathrm{SO}(2l+1) \to \mathrm{SO}(2)\times\mathrm{SO}(2)\times\ldots\times\mathrm{SO}(2)\times\mathrm{SO}(2q+1) \tag{20}$$

equal to $+1$. As an illustration of how this truncation technique can be used to find an SO(7) 6-j symbol, we give the following equations:

$$\begin{Bmatrix} (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (111) \\ (\frac{3}{2}\frac{3}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (110) \end{Bmatrix}$$

$$= -(10/147)^{1/2}\begin{Bmatrix} (\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}) & (11) \\ (\frac{3}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}) & (10) \end{Bmatrix}$$

$$= -(3/735)^{1/2}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ \frac{1}{2} & \frac{1}{2} & 0 \end{Bmatrix} = -(3/2940)^{1/2}\{\tfrac{1}{2}\tfrac{1}{2}1\} = -(3/2940)^{1/2}.$$

7. First bootstrap

We can use our knowledge of the U coefficient (15) in an application of the Biedenharn–Elliott sum rule, as generalised by Butler (1981, equation (3.3.27)):

$$\sum_W (-1)^{x(W)}\begin{Bmatrix} w_q & w_l & W \\ w_l & w_l & W(m_1) \end{Bmatrix}\begin{Bmatrix} w_l & w_l & W \\ w_l & w_l & W(m_2) \end{Bmatrix}\begin{Bmatrix} w_l & w_l & W \\ w_l & w_q & W(m_3) \end{Bmatrix}$$

$$= \begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_l & w_l \end{Bmatrix}\begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_q & w_l \end{Bmatrix} \tag{21}$$

where W is necessarily of the type $W(m)$, and where

$$\begin{aligned}(-1)^{x(W(m))} &= \varepsilon_q^2\{W(m_1)\}\{w_l\}\{W(m_1)w_lw_l\}\{W(m_2)w_lw_l\}\{W(m_3)w_lw_l\} \\ &\quad\times\{W(m)w_qw_l\}\{W(m)w_lw_l\}\{W(m)w_lw_l\} \\ &= (-1)^{(m+m_1+m_2+m_3)/2+\tau}.\end{aligned} \tag{22}$$

This phase agrees with that of Edmonds (1957, equation (6.2.12)) when the substitutions of equations (9) are made. With the aid of equations (18) and (13), the sum becomes

$$\sum_m [8/\mathrm{Dim}(W(m))]^{1/2} d^{q+1/2}_{m+1/2,m_1+1/2}(\tfrac{1}{2}\pi)\, d^{l+1/2}_{m+1/2,m_2+1/2}(\tfrac{1}{2}\pi)\, d^{q+1/2}_{m+1/2,m_3+1/2}(\tfrac{1}{2}\pi)$$

$$= [\mathrm{Dim}(W(m_1))\,\mathrm{Dim}(W(m_2))\,\mathrm{Dim}(W(m_3))]^{1/2} \times \begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_l & w_l \end{Bmatrix} \begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_q & w_l \end{Bmatrix}. \quad (23)$$

We first perform this sum over m for $q = l$. The techniques for doing this are described in appendix 1 for the general case where q is not necessarily equal to l. Both 6-j symbols on the right-hand side of equation (23) become equal to each other, so we can extract either the positive or negative root from the sum (which turns out to be invariably a positive quantity). We write

$$\begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_l & w_l \end{Bmatrix} = \varepsilon_{123}[\mathrm{Dim}(W(m_1))\,\mathrm{Dim}(W(m_2))\,\mathrm{Dim}(W(m_3))\Delta^2(m_1m_2m_3)2^l]^{-1/2} \quad (24)$$

where

$$\Delta(m_1m_2m_3) = \begin{cases} [S_1^{23}!\,S_2^{31}!\,S_3^{12}!\,T_{123}!/(2l+1)!]^{1/2} & (l \text{ even}) \\ [S^1_{23}!\,S^2_{31}!\,S^3_{12}!\,T^{123}!/(2l+1)!]^{1/2} & (l \text{ odd}) \end{cases} \quad (25)$$

in which

$$S_k^{ij} = \tfrac{1}{2}(l - m_i - m_j + m_k) \qquad T_{123} = \tfrac{1}{2}(l + m_1 + m_2 + m_3 + 2),$$
$$S_{ij}^k = \tfrac{1}{2}(l + m_i + m_j - m_k + 1) \qquad T^{123} = \tfrac{1}{2}(l - m_1 - m_2 - m_3 - 1).$$

The phase ε_{123} in equation (24) should be chosen to reduce to Butler's phase $(-1)^{m_i/2}$ when $W(m_j) = (\dot{0})$ $(i \neq j)$. It should also be symmetric with respect to m_1, m_2 and m_3 and preferably real. One function that possesses the required properties is

$$\varepsilon_{123} = (-1)^{(m_2m_3 + m_3m_1 + m_1m_2)/4}. \quad (26)$$

However, we shall often retain the epsilon as a convenient abbreviation and to indicate how this particular phase choice percolates through the calculations.

8. Repetition for arbitrary q

We now repeat the sum of equation (23) without the limitation $q = l$. Details are given in appendix 1. The right-hand side of equation (23) gives two 6-j symbols, one of which we already know. We get

$$\begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_q & w_l \end{Bmatrix} = -\varepsilon_{123}\left[\frac{2q+2}{\mathrm{Dim}(W(m_2))\,\mathrm{Dim}(w_q)}\right]^{1/2} \begin{pmatrix} q+\tfrac{1}{2} & \tfrac{1}{2}(l-m_3) & \tfrac{1}{2}(l+m_3+1) \\ m_1+\tfrac{1}{2} & m_a & m_b \end{pmatrix} \quad (27)$$

where

$$\begin{aligned} m_a &= \tfrac{1}{2}(m_2 - m_1) & m_b &= -\tfrac{1}{2}(m_1 + m_2 + 1) & (l \text{ even}) \\ m_a &= -\tfrac{1}{2}(m_1 + m_2 + 1) & m_b &= \tfrac{1}{2}(m_2 - m_1) & (l \text{ odd}). \end{aligned} \quad (28)$$

The surprising appearance of an SO(3) 3-j symbol becomes even more striking if it is converted to a Clebsch-Gordan (CG) coefficient and if the SO($2l+1$) 6-j symbol is replaced by a U coefficient:

$$U\begin{pmatrix} W(m_1) & W(m_3) & W(m_2) \\ w_l & w_l & w_q \end{pmatrix}$$
$$= \varepsilon_{123}(\tfrac{1}{2}(l-m_3),\, m_a\,;\, \tfrac{1}{2}(l+m_3+1),\, m_b\,|\, q+\tfrac{1}{2},\, -m_1-\tfrac{1}{2}). \qquad (29)$$

We see that the unitary matrix formed by the U coefficients with respect to w_q and $W(m_2)$ is identical (apart from a possible phase) to the matrix formed by the CG coefficients, the rows being labelled by q and the columns by the pair $(m_a,\, m_b)$ for which the sum is equal to $-m_1-\frac{1}{2}$.

9. Regge's magic square

Before exploring the reason for equation (29), we note that neither the CG coefficient nor the 3-j symbol of equation (27) explicitly exhibits the symmetry with respect to m_1 and m_3 that the U coefficient does. The restructuring of the arguments of the 3-j symbol into a magic square, as described by Regge (1958), corrects this defect. We get, for l odd, the Regge symbol

$$\begin{bmatrix} l-q & q+m_1+1 & q-m_1 \\ q+m_3+1 & T^{123} & S^3_{12} \\ q-m_3 & S^1_{23} & S^2_{13} \end{bmatrix}$$

in which the $(m_1,\, m_3)$ symmetry appears as a reflection in the diagonal. A similar pattern emerges for l even.

The $(m_1,\, m_3)$ symmetry is also exposed by the representation of our 3-j symbol in terms of a quadruply stretched 9-j symbol, a possibility apparent from the formula of Lindner (1984, p 62):

$$\begin{pmatrix} q+\frac{1}{2} & \frac{1}{2}(l-m_3) & \frac{1}{2}(l+m_3+1) \\ m_1+\frac{1}{2} & \frac{1}{2}(m_2-m_1) & -\frac{1}{2}(m_1+m_2+1) \end{pmatrix}$$
$$= -\left[\frac{\mathrm{Dim}(w_q)(l-m_1+1)!(l+m_1+2)!(l-m_3+1)!(l+m_3+2)!}{2^l(2q+2)\Delta(m_1m_2m_3)(2l+1)!(2l+1)!}\right]^{1/2}$$
$$\times\begin{Bmatrix} \frac{1}{2}S^{13}_2 & \frac{1}{2}S^{12}_3 & \frac{1}{2}(l-m_1) \\ \frac{1}{2}S^{23}_1 & \frac{1}{2}T_{123} & \frac{1}{2}(l+m_1+1) \\ \frac{1}{2}(l-m_3) & \frac{1}{2}(l+m_3+1) & q+\frac{1}{2} \end{Bmatrix} \qquad (l\ \text{even}). \qquad (30)$$

This formula is of use later.

10. Vanishing symbols

It is usually a simple matter to understand why a particular 3-j symbol for SO(3) is zero. For example,

$$\begin{pmatrix} \frac{5}{2} & \frac{5}{2} & 1 \\ -\frac{3}{2} & -\frac{1}{2} & 2 \end{pmatrix} = 0$$

because $2>1$. When this 3-j symbol is converted to a 6-j symbol of SO(7) by means of equation (27), we get

$$\begin{Bmatrix} (110) & (100) & (110) \\ (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) & (\tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2}) & (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) \end{Bmatrix} \tag{31}$$

which obviously vanishes because $(100)\times(110)$ does not contain (110) in its reduction (see Wybourne 1970, table D-4).

Parallel statements are often not so easy to make for the class of SO($2l+1$) 6-j symbols deriving from the 3-j symbols

$$\begin{pmatrix} j & j & j' \\ m & m & -2m \end{pmatrix} \qquad (2j+j' \text{ odd})$$

which are all zero. For example, if we pick $j=\frac{5}{2}$, $j'=2$, $m=\frac{1}{2}$, we can deduce

$$\begin{Bmatrix} (1111) & (1110) & (1111) \\ (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) & (\tfrac{3}{2}\tfrac{3}{2}\tfrac{1}{2}\tfrac{1}{2}) & (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) \end{Bmatrix} = 0 \tag{32}$$

for SO(9). From the perspective of this group there is no obvious reason why equation (32) should hold. An opportunity to give an explanation in terms of the properties of SO($2l+1$) occurs when $W(m_2)=(110\ldots0)$, since we can construct Casimir's operator G from tensors of that type. For example, the choice of parameters given by $j=\frac{3}{2}$, $j'=2$, and $m=\frac{1}{2}$ leads to the SO(7) 6-j symbol

$$\begin{Bmatrix} (111) & (110) & (111) \\ (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) & (\tfrac{3}{2}\tfrac{3}{2}\tfrac{1}{2}) & (\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2}) \end{Bmatrix}. \tag{33}$$

In analogy to the well known result

$$\begin{Bmatrix} b & 1 & b \\ c & a & c \end{Bmatrix} \sim a(a+1)-b(b+1)-c(c+1)$$

for an SO(3) 6-j symbol, we find the SO(7) symbol (33) is proportional to

$$\langle G(\tfrac{3}{2}\tfrac{3}{2}\tfrac{1}{2})\rangle - \langle G(\tfrac{1}{2}\tfrac{1}{2}\tfrac{1}{2})\rangle - \langle G(111)\rangle$$

which evaluates to $(69-21-48)/40=0$. This kind of analysis only works for a few cases: it does not account for equation (32). Of course, we shall be able to understand such surprises as soon as we can give an explanation for equation (29). To that end, we turn to atomic quasiparticles.

11. Complementarity

The quasiparticle factorisation of an atomic l shell is described in appendix 2. The crucial point for us here is that there are two ways of representing an atomic state: we can couple a variety of irreps of SO($2l+1$), as indicated by the ket (A5), or we can use angular momentum quantum numbers like Q, M_Q, S, and M_S. The two schemes are complementary in the sense of Moshinsky and Quesne (1970). As we shall see immediately, a recoupling of the irreps leads to the U coefficient of equation (29), while a recoupling of the angular momenta provides the CG coefficient of that same equation. In setting things out, there is little point in introducing a new phase system, particularly since it would depend on the far from trivial choices entailed in defining the various quasiparticle vacua. We thus introduce the symbol $\simeq$, which is to be interpreted as meaning 'equals, to within a phase'.

The recoupling coefficient that enters when the state (A5) is expanded as a linear combination of the states

$$|\{(w_{l\lambda}w_{l\mu})_{p_A}W(m_A),\, w_{l\nu}\}w_q,\, w_{l\xi},\, W\alpha LM_L\rangle \tag{34}$$

is

$$\langle\{W(m_A)w_l\}w_q,\, w_l,\, W|\, W(m_A),\, (w_lw_l)W(m_B),\, W\rangle = U\begin{pmatrix} W(m_A) & W & W(m_B) \\ w_l & w_l & w_q \end{pmatrix}. \tag{35}$$

We have already seen from appendix 2 that T for the ket (34) is $q+\frac{1}{2}$, while M_T, from equation (A11), is $\pm(m_A+\frac{1}{2})$. As for the ket (A5), we can calculate values of Q, M_Q, S and M_S from the various irreps and parities listed therein, so the expansion of (34) in terms of the kets (A5) is equivalent to a mere change of quantisation. The assignments of quantum numbers can be worked out with the aid of table I of Racah (1949), the results of appendix 2, and the final two columns of table 1. We find that the CG coefficient of equation (29) can be identified with

$$(S\ M_S,\ Q\ M_Q\ |\ T\ M_T) \tag{36}$$

for l odd, $p_Ap_B \equiv$ ug, and for l even, $p_Ap_B \equiv$ gg; with

$$(S\ {-M_S},\ Q\ {-M_Q}\ |\ T\ {-M_T}) \tag{37}$$

for l odd, $p_Ap_B \equiv$ gu, and for l even, $p_Ap_B \equiv$ uu; with

$$(Q\ M_Q,\ S\ M_S\ |\ T\ M_T) \tag{38}$$

for l odd, $p_Ap_B \equiv$ uu, and for l even, $p_Ap_B \equiv$ gu; and with

$$(Q\ {-M_Q},\ S\ {-M_S}\ |\ T\ {-M_T}) \tag{39}$$

for l odd, $p_Ap_B \equiv$ gg, and for l even, $p_Ap_B \equiv$ ug. The four CG coefficients (36)-(39) are equal (to within a phase). Thus the structure of equation (29) is directly accounted for, and the vanishing of such SO($2l+1$) 6-j symbols as (32) and (33) receives a simple explanation.

12. Racah back-coupling

We can now extend our knowledge of 6-j symbols for SO($2l+1$) by using Racah's back-coupling formula (Edmonds 1957, equation (6.2.11)), as generalised by Butler (1981, equation (3.3.23)):

$$\begin{aligned}\begin{Bmatrix} w_l & w_s & W(m_3) \\ w_l & w_q & W(m_1)\end{Bmatrix} &= \sum_{W(m_2)} \mathrm{Dim}(W(m_2))\{W(m_1)w_qw_l\}\{w_lw_sW(m_1)\}\{w_lw_lW(m_2)\} \\ &\quad\times\begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_q & w_l\end{Bmatrix}\begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ w_l & w_s & w_l\end{Bmatrix}.\end{aligned} \tag{40}$$

With the aid of equations (1) and (29), we get

$$\begin{aligned}U\begin{pmatrix} w_l & W(m_3) & w_s \\ w_l & W(m_1) & w_q\end{pmatrix} &= \sum_{m_2\ \mathrm{even}} (-1)^{m_2/2}(\tfrac{1}{2}(l-m_3),\, m_a;\, \tfrac{1}{2}(l+m_3+1),\, m_b\,|\,q+\tfrac{1}{2},\, -m_1-\tfrac{1}{2}) \\ &\quad\times(\tfrac{1}{2}(l-m_3),\, m_a;\, \tfrac{1}{2}(l+m_3+1),\, m_b\,|\,s+\tfrac{1}{2},\, -m_1-\tfrac{1}{2})\end{aligned} \tag{41}$$

where m_a and m_b are defined in equations (28). By setting $s=l$ and explicitly performing the sum over m_2, we recover equations (13) and (18), with ε_q given by equation (19). For arbitrary s and q, the sum over m_2 in equation (41) does not appear amenable to simplification. However, it can be identified as a rotation in four-dimensional space by referring to the lecture notes of Wigner, as assembled by Talman (1968), with the angle of rotation (ϕ in Talman's equation (10.8)) set equal to $\pi/2$.

13. Rotations

We can take advantage of our quasiparticle scheme to give another explanation for equation (41). The vectors $\boldsymbol{Q}$ and $\boldsymbol{S}$ commute with each other and are a natural choice for the generators of SO(4), the rotation group in four dimensions. By evaluating

$$\exp[\tfrac{1}{2}\mathrm{i}\pi(Q_z-S_z)]\boldsymbol{\theta}^\dagger\exp[\tfrac{1}{2}\mathrm{i}\pi(S_z-Q_z)] \tag{42}$$

for our various quasiparticle operators $\boldsymbol{\theta}^\dagger$, we find that the transformation (42) produces the changes

$$\boldsymbol{\lambda}\to\boldsymbol{\lambda} \qquad \boldsymbol{\mu}\to\boldsymbol{\mu} \qquad \boldsymbol{\nu}\to\mathrm{i}\boldsymbol{\xi} \qquad \boldsymbol{\xi}\to\mathrm{i}\boldsymbol{\nu}. \tag{43}$$

So, on the one hand,

$$\begin{aligned}\exp[\tfrac{1}{2}\mathrm{i}\pi(Q_z-S_z)]&|(W(m_1),w_{l\nu})w_q,w_{l\xi},W\rangle\\ &\simeq|(W(m_1),w_{l\xi})w_q,w_{l\nu},W\rangle\\ &\simeq\sum_{w_s}U\begin{pmatrix}w_l & W & w_q\\ w_l & W(m_1) & w_s\end{pmatrix}|(W(m_1),w_{l\nu})w_s,w_{l\xi},W\rangle\end{aligned} \tag{44}$$

while, on the other hand,

$$\begin{aligned}\exp[\tfrac{1}{2}\mathrm{i}\pi(Q_z-S_z)]&|(QS)TM_T\rangle\\ &=\sum_{M_QM_S}(QM_Q,SM_S|TM_T)\exp[\tfrac{1}{2}\mathrm{i}\pi(M_Q-M_S)]|QM_Q,SM_S\rangle\\ &=\sum_{M_QM_ST'}\mathrm{i}^{M_Q-M_S}(QM_Q,SM_S|TM_T)(QM_Q,SM_S|T'M_T)|T'M_T\rangle.\end{aligned} \tag{45}$$

We see that $\mathrm{i}^{M_Q-M_S}=\mathrm{i}^{2M_Q-M_T}\simeq(-1)^{M_Q}\simeq(-1)^{m_2/2}$, so the U coefficient matches the sum over a product of two CG coefficients, weighted by $(-1)^{m_2/2}$, as previously derived in equation (41).

14. 9-*j* symbols

We use equation (3.3.37) of Butler (1981) to give

$$\begin{aligned}&\begin{Bmatrix}w_l & w_l & W(m_1)\\ w_l & w_l & W(m_2)\\ W(m_3) & W(m_4) & W(m)\end{Bmatrix}\\ &\qquad=\sum_{w_q}\mathrm{Dim}(w_q)\{w_q\}\begin{Bmatrix}w_l & w_l & W(m_3)\\ W(m_4) & W(m) & w_q\end{Bmatrix}\begin{Bmatrix}w_l & w_l & W(m_4)\\ w_l & w_q & W(m_2)\end{Bmatrix}\\ &\qquad\quad\times\begin{Bmatrix}W(m_1) & W(m_2) & W(m)\\ w_q & w_l & w_l\end{Bmatrix}.\end{aligned} \tag{46}$$

For us, $\{w_q\}=(-1)^\tau$, agreeing with the phase factor $(-1)^{2\varphi(w_q)}$ in equation (6.4.3) of Edmonds (1957) once the second substitution of the pair (9) is made. When we use our knowledge of the 6-j symbols in equation (46), we are confronted by a sum over a product of two 3-j symbols and a d function. It can be carried out by using equation (8.27) of Talman (1968), which, in a more suggestive notation, runs

$$\sum_T (2T+1)\begin{pmatrix} S & Q & T \\ M_S & M_Q & -M_T \end{pmatrix}\begin{pmatrix} S & Q & T \\ M'_S & M'_Q & -M'_T \end{pmatrix} d^T_{-M_T,-M'_T}(\tfrac{1}{2}\pi)$$
$$= d^S_{M_S,M'_S}(\tfrac{1}{2}\pi)\, d^Q_{M_Q,M'_Q}(\tfrac{1}{2}\pi). \tag{47}$$

Expressed in terms of the U coefficient of equation (2), the result is

$$U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_l & w_l & W(m_2) \\ W(m_3) & W(m_4) & W(m) \end{pmatrix}$$
$$= \varepsilon_{12m}\varepsilon_{34m}(-1)^{(m_2+m_4)/2}2^{1/2} d^{(l-m)/2}_{MN}(\tfrac{1}{2}\pi)\, d^{(l+m+1)/2}_{M'N'}(\tfrac{1}{2}\pi) \tag{48}$$

where

$$\begin{aligned} [M, N] &\equiv [\tfrac{1}{2}(m_3-m_4), \tfrac{1}{2}(m_1-m_2)] \\ [M', N'] &\equiv [-\tfrac{1}{2}(m_3+m_4+1), -\tfrac{1}{2}(m_1+m_2+1)] \end{aligned} \tag{49}$$

for l even, and the opposite for l odd. With the aid of equation (3.3.36) of Butler (1981), we recover our previous results on setting $W(m)=(\dot{0})$ or $W(m_4)=(\dot{0})$. In fact, the original argument for explaining the form of equation (13) depended on the recoupling corresponding to $W=(\dot{0})$ (Judd 1987).

The interpretation of equation (48) by rotations makes use of the operator $\exp(\tfrac{1}{2}\mathrm{i}\pi T_y)$, for which

$$\boldsymbol{\lambda}\to-\boldsymbol{\nu} \qquad \boldsymbol{\mu}\to\boldsymbol{\mu} \qquad \boldsymbol{\nu}\to\boldsymbol{\lambda} \qquad \boldsymbol{\xi}\to\boldsymbol{\xi}. \tag{50}$$

Thus, on the one hand,

$$\exp(\tfrac{1}{2}\mathrm{i}\pi T_y)|(w_{l\lambda}w_{l\mu})_{p_A}W(m_1), (w_{l\nu}w_{l\xi})_{p_B}W(m_2), W\rangle$$
$$\simeq |(w_{l\nu}w_{l\mu})_{p_A}W(m_1), (w_{l\lambda}w_{l\xi})_{p_B}W(m_2), W\rangle$$
$$\simeq \sum a(p_Ap_B, p'_Ap'_B)\, U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_l & w_l & W(m_2) \\ W(m_3) & W(m_4) & W(m) \end{pmatrix}$$
$$\times |(w_{l\lambda}w_{l\mu})_{p'_A}W(m_3), (w_{l\nu}w_{l\xi})_{p'_B}W(m_4), W\rangle \tag{51}$$

where the sum runs over p'_A, p'_B, $W(m_3)$ and $W(m_4)$; and on the other hand,

$$\exp(\tfrac{1}{2}\mathrm{i}\pi T_y)|QM_Q, SM_S\rangle = \sum_{M'_Q,M'_S} d^Q_{M_QM'_Q}(\tfrac{1}{2}\pi)\, d^S_{M_SM'_S}(\tfrac{1}{2}\pi)|QM'_Q, SM'_S\rangle. \tag{52}$$

The set of quantum numbers (QM_Q, SM_S) is enough to fix p_A and p_B; and it can be shown that the substitution $(M_Q, M_S)\to(-M_Q, -M_S)$ changes p_Ap_B according to the rules gg↔uu and gu↔ug. Thus every term (M'_Q, M'_S) in the sum of equation (52) has a companion of equal magnitude but associated with a different parity pair. It follows that

$$|a(p_Ap_B, p'_Ap'_B)| = 2^{-1/2} \tag{53}$$

Table 2. Values of $U\begin{pmatrix} (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & W(m_1) \\ (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & W(m_2) \\ W(m_3) & W(m_4) & (111) \end{pmatrix}$.

$W(m_3)\,W(m_4)$	$W(m_1)\,W(m_2)$					
	(000)(111)	(100)(110)	(100)(111)	(110)(110)	(110)(111)	(111)(111)
(000)(111)	1/8	$(3/64)^{1/2}$	−1/4	$(3/32)^{1/2}$	$-(3/16)^{1/2}$	$(9/32)^{1/2}$
(100)(110)	$(3/64)^{1/2}$	−1/8	$(3/16)^{1/2}$	$(9/32)^{1/2}$	−1/4	$-(3/32)^{1/2}$
(100)(111)	−1/4	$(3/16)^{1/2}$	−1/4	0	$(3/16)^{1/2}$	0
(110)(110)	$(3/32)^{1/2}$	$(9/32)^{1/2}$	0	−1/4	0	$-(3/16)^{1/2}$
(110)(111)	$-(3/16)^{1/2}$	−1/4	$(3/16)^{1/2}$	0	1/4	0
(111)(111)	$(9/32)^{1/2}$	$-(3/32)^{1/2}$	0	$-(3/16)^{1/2}$	0	1/4

provided the combined parities are the same. (They are zero otherwise because T_y preserves total parity.) In this way we can account for the structure of equation (48).

As an illustration of an actual calculation, we give in table 2 some 9-j symbols (in the form of U coefficients) for $W(m)=(111)$. The phases of equation (26) have been used in conjunction with equation (48). The zeros in the table correspond to identical 9-j symbols that can be related by an interchange of two rows or two columns, or by a transposition, and for which the sum of the nine φ functions, as given by equations (9), is an odd integer.

15. Extensions to W beyond $W(m)$

If $W=(2^x 1^{l-m'-x} 0^{m'})$, we can convert the 9-$j$ symbol of equation (46) to a stretched recoupling coefficient. The arguments of section 6 can now be repeated, with the result that we can write

$$U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_l & w_l & W(m_2) \\ W(m_3) & W(m_4) & W \end{pmatrix} = \varepsilon'_x U\begin{pmatrix} w_l & w_l & W(m_1) \\ w_l & w_l & W(m_2) \\ W(m_3) & W(m_4) & W(m) \end{pmatrix}$$

where the U coefficient on the right refers to $SO(2l-2x+1)$. The phase ε'_x is analogous to the ε_q of equation (18). For example,

$$\begin{Bmatrix} (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (100) \\ (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}\frac{1}{2}) & (100) \\ (110) & (110) & (200) \end{Bmatrix}$$

$$= \varepsilon'_1(5/147)\begin{Bmatrix} (\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}) & (00) \\ (\frac{1}{2}\frac{1}{2}) & (\frac{1}{2}\frac{1}{2}) & (00) \\ (10) & (10) & (00) \end{Bmatrix}$$

$$= \varepsilon'_1(2)^{1/2}(147)^{-1} d^0_{00}(\tfrac{1}{2}\pi) d^{5/2}_{3/2,-5/2}(\tfrac{1}{2}\pi) = \varepsilon'_1(5)^{1/2}/588. \qquad (54)$$

The quasiparticle approach provides a check. The irrep (200) in the 9-j symbol is involved in the two couplings $|((110)(110))(200)\rangle$ and $|((100)(100))(200)\rangle$. The first occurs in the atomic configuration f^4 (or f^{10}) in which two (or five) electrons have their spins up and the same number with their spins down. In this case $S=M_S=0$,

$Q=\frac{5}{2}$, $M_Q=-\frac{3}{2}$ (or $+\frac{3}{2}$). The second coupling requires one (or six) electrons with each spin orientation, and we now have $S=M'_S=0$, $Q=\frac{5}{2}$, $M'_Q=-\frac{5}{2}$ (or $+\frac{5}{2}$). From equation (47) we see that that the same two d functions are produced as appear in equation (54).

16. General 6-j symbol with six irreps of the type $W(m)$

We now propose to use the generalisation of the Biedenharn–Elliott identity in the form

$$\sum_W \mathrm{Dim}(W)(-1)^x \begin{Bmatrix} W(m_1) & w_l & W \\ w_l & W(m_3) & W(m_2) \end{Bmatrix} \begin{Bmatrix} W(m_3) & w_l & W \\ w_l & W(m_5) & W(m_4) \end{Bmatrix}$$

$$\times \begin{Bmatrix} W(m_5) & w_l & W \\ w_l & W(m_1) & W(m_6) \end{Bmatrix}$$

$$= \begin{Bmatrix} W(m_2) & W(m_4) & W(m_6) \\ w_l & w_l & w_l \end{Bmatrix} \begin{Bmatrix} W(m_2) & W(m_4) & W(m_6) \\ W(m_5) & W(m_1) & W(m_3) \end{Bmatrix} \quad (55)$$

where, from equation (3.3.27) of Butler (1981), we find $x=\Sigma_i m_i$. Our aim is to calculate the 6-j symbol on the far right in equation (55). Each 6-j symbol on the left-hand side of that equation can be converted to a 3-j symbol by means of equation (27); however, the appearance of $[\mathrm{Dim}(W)]^{-1/2}$ makes it difficult to carry out the sum over W. Instead, one of the 3-j symbols (say the first) is expressed in terms of the stretched 9-j symbol of equation (30). We now use the following formula for n-j symbols of SO(3), as given by Lindner (1984, p. 55):

$$\sum_{jm} (2j+1) \begin{pmatrix} c & f & j \\ r & u & m \end{pmatrix} \begin{pmatrix} g & h & j \\ v & w & m \end{pmatrix} \begin{Bmatrix} a & b & c \\ d & e & f \\ g & h & j \end{Bmatrix}$$

$$= \sum_{pqst} \begin{pmatrix} a & b & c \\ p & q & r \end{pmatrix} \begin{pmatrix} d & e & f \\ s & t & u \end{pmatrix} \begin{pmatrix} a & d & g \\ p & s & v \end{pmatrix} \begin{pmatrix} b & e & h \\ q & t & w \end{pmatrix}. \quad (56)$$

The arguments are assigned (for even l) as follows:

$a=\frac{1}{2}S_2^{13}$ $\quad b=\frac{1}{2}S_3^{12}$ $\quad c=\frac{1}{2}(l-m_1)$ $\quad d=\frac{1}{2}S_1^{23}$

$e=\frac{1}{2}T_{123}$ $\quad f=\frac{1}{2}(l+m_1+1)$ $\quad g=\frac{1}{2}(l-m_3)$ $\quad h=\frac{1}{2}(l+m_3+1)$

$j=q+\frac{1}{2}$ $\quad m=m_5+\frac{1}{2}$ $\quad r=\frac{1}{2}(m_6-m_5)$ $\quad u=-\frac{1}{2}(m_5+m_6+1)$

$v=\frac{1}{2}(m_4-m_5)$ $\quad w=-\frac{1}{2}(m_4+m_5+1)$.

All four 3-j symbols on the right-hand side of equation (56) possess a stretched upper row and thus reduce to a single term. Moreover, the sum over p, q, s and t does not include the third magnetic quantum number in each of the four 3-j symbols, so the sum is effectively over a single index. To expose the symmetry in the best possible way, we introduce y as our running index, where

$$y=p+\tfrac{1}{4}(l+m_1+m_2+m_3+2m_4+2m_6). \quad (57)$$

Putting all the parts together, we arrive finally at the result

$$\begin{Bmatrix} W(m_1) & W(m_2) & W(m_3) \\ W(m_4) & W(m_5) & W(m_6) \end{Bmatrix}$$
$$= \varepsilon_{123}\varepsilon_{156}\varepsilon_{246}\varepsilon_{345}(-1)^{(m_1+m_2+m_3+m_4+m_5+m_6)/2}(2l+1)!$$
$$\times \Delta(m_1m_2m_3)\Delta(m_1m_5m_6)\Delta(m_2m_4m_6)\Delta(m_3m_4m_5)\sum_y [f(y)]^{-1} \tag{58}$$

where

$$f(y)=(y+1)![\tfrac{1}{2}(l+m_1+m_2+m_3)-y]![\tfrac{1}{2}(l+m_1+m_5+m_6)-y]!$$
$$\times[\tfrac{1}{2}(l+m_2+m_4+m_6)-y]![\tfrac{1}{2}(l+m_3+m_4+m_5)-y]!$$
$$\times[y-\tfrac{1}{2}(m_1+m_3+m_4+m_6)]![y-\tfrac{1}{2}(m_1+m_2+m_4+m_5)]!$$
$$\times[y-\tfrac{1}{2}(m_2+m_3+m_5+m_6)]! \tag{59}$$

for l even. A repetition of the analysis for l odd yields equation (58) again, but this time $f(y)$ is given by

$$f(y)=(y-1)![\tfrac{1}{2}(l-m_1-m_2-m_3+1)-y]![\tfrac{1}{2}(l-m_1-m_5-m_6+1)-y]!$$
$$\times[\tfrac{1}{2}(l-m_2-m_4-m_6+1)-y]![\tfrac{1}{2}(l-m_3-m_4-m_5+1)-y]!$$
$$\times[y+\tfrac{1}{2}(m_1+m_3+m_4+m_6)]![y+\tfrac{1}{2}(m_1+m_2+m_4+m_5)]!$$
$$\times[y+\tfrac{1}{2}(m_2+m_3+m_4+m_6)]!. \tag{60}$$

As an example, the SO(7) 6-j symbol

$$\begin{Bmatrix} (110) & (110) & (110) \\ (110) & (110) & (110) \end{Bmatrix}$$

requires two terms in the sum (corresponding to $y=4$ and 5), and evaluates to 1/42, in agreement with the calculations of Li (1989). It is straightforward to confirm that the 6-j symbol of equation (58) reduces to

$$(-1)^{(m_1+m_2+m_3)/2+\tau}\delta(m_1,m_5)\delta(m_2,m_4)[\mathrm{Dim}(W(m_1))\,\mathrm{Dim}(W(m_2))]^{-1/2} \tag{61}$$

(as it should) when we set $W(m_6)=(\dot{0})$.

17. Negative dimensionality

The formula (58), augmented by equations (59) and (60), bears a striking resemblance to the classic expression for an SO(3) 6-j symbol (Edmonds 1957, equation (6.3.7)) as well as to the slightly more general formula for an Sp($2n$) 6-j symbol whose six irreps are all of the type $\langle\sigma_i 0\ldots 0\rangle$ (Judd and Lister 1987, equation (36)). There is a sum over a single running index; this index appears in eight factorial functions; four of these eight involve the four triads in the symbol, three of them involve the four entries in a pair of columns of the 6-j symbol, and one of them involves the running index by itself. However, this last factorial appears in the numerator in the SO(3) and Sp($2n$) formulae, but in the denominator in the SO($2l+1$) formula.

Dunne (1989) has recently revived interest in the connection between the groups SO(n) and Sp($-n$), a subject explored by Cvitanović and Kennedy (1982). In this scheme the antisymmetric irreps $(1^{\sigma}0^{l-\sigma})$ of SO($2l+1$) are related to the symmetric irreps $\langle\sigma 0\ldots 0\rangle$ of Sp($-2l-1$), and a formal correspondence should exist between the respective 6-j symbols. An expression of the form

$$(-1)^{z}(z+2n-1)!/(2n-1)! \tag{62}$$

occurs in the formula for an Sp($2n$) 6-j symbol, where z is the running index, and the substitution $2n\to -2l-1$ can be handled by writing (62) as

$$(-1)^{z}(z+2n-1)(z+2n-2)\ldots(2n)$$

which becomes

$$(-1)^{z}(z-2l-2)(z-2l-3)\ldots(-2l-1)=(2l+1)!/(2l+1-z)! \tag{63}$$

This accounts for the numerator-to-denominator switch mentioned above and also for the factor $(2l+1)!$ in equation (58). The relation $\langle\sigma 0\ldots 0\rangle\to(1^{\sigma}0^{l-\sigma})$ indicates that we should take $\sigma\to l-m'$, that is

$$\sigma\to l+\tfrac{1}{2}-(-1)^{m'}(m+\tfrac{1}{2}). \tag{64}$$

In other words,

$$\sigma\to l-m \qquad (l \text{ and } \sigma \text{ both even or both odd})$$

$$\sigma\to l+m+1 \qquad (l \text{ and } \sigma \text{ with opposite parities}).$$

A detailed analysis reveals that these various substitutions convert the Sp($2n$) formula into our expression (58), the only difference coming from a phase factor arising when the substitution $2n\to -2l-1$ is made in the Sp($2n$) Δ functions. Our analyses are thus consistent with the general statements made by Cvitanović and Kennedy (1982).

18. Concluding remarks

Our success in obtaining explicit algebraic expressions for several kinds of 6-j symbols for SO($2l+1$) should be tempered by the knowledge that they are all of a class that requires no additional labels to resolve multiplicity ambiguities. Extending them into that realm is a much more difficult task for which only very limited success has so far been achieved (see, for example, Cerkaski 1987). A crucial reason why our analysis has worked is the existence of a complementary group whose generators are the spin and quasispin associated with electrons in the atomic l shell. It is this connection that forces the rotation matrices d^{j}_{mn} to appear. Complementary groups have proved useful in other contexts, for example, in calculating 6-j symbols for the symmetric irreps $(n0\ldots0)$ of SO($2l+1$), as described by Ališauskas (1987). Just as in his case, our complementary group introduces quantities associated with SO(3). Without this connection it is difficult to see how any explanation could be offered for the vanishing matrix elements of the type exemplified by equation (32).

Extensions of our work to other irreps could clearly be made. However, we hesitate to embark upon further analysis without some underlying rationale. The existence of isotopic spin for nucleons indicates that nuclear quasiparticles would involve irreps beyond those needed in the atomic case, but whether such a development would be useful is not clear.

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Appendix 1. Combinatorics

The sum of equation (23) can be worked out by making use of the properties of binomial coefficients. The relevant formulas can be found in the books of Edmonds (1957, appendix 1), Jucys and Bandzaitis (1977, p 74), or Lindner (1984, appendix 1). Because of the elementary nature of the analysis, we give here only such detail as is necessary for an interested reader to be able to reconstruct our working.

When the d functions of equation (23) are expanded, we are confronted with the quadruple sum

$$\sum_{mtuv} (-1)^{t+u+v}[1+(-1)^m](q+m+1)!(q-m)!(l+m+1)!(l-m)!$$
$$\times\{(q+m+1-t)!(q-m_1-t)!t!(t+m_1-m)!(l+m+1-v)!$$
$$\times(l-m_2-v)!v!(v+m_2-m)!(q+m+1-u)!(q-m_3-u)!\,u!$$
$$\times(u+m_3-m)!\}^{-1}. \quad \text{(A1)}$$

The factor in square brackets is introduced to limit m to even values. The general strategy that we follow is similar to that used by Racah (1942, Appendix B) to find an expression for an SO(3) 6-j symbol: the occurrence of the index m is reduced until the sum over the factorials in which it appears can be carried out. This is done in a way that increases the number of factorial functions as little as possible. We make the following substitutions:

$$(q+m+1)!/t!u!(m-t+q+1)!(m-u+q+1)!$$
$$=\sum_s \{s!\,(t-s)!\,(u-s)!\,(q+1+m-t-u+s)!\}^{-1}$$

$$(q-m)!/(q-t-m_1)!\,(q-u-m_3)!\,(m_1+t-m)!(u+m_3-m)!$$
$$=\sum_x \{x!(q-t-m_1-x)!(q-u-m_3-x)!$$
$$\times(t+u+m_1+m_3-q-m+x)!\}^{-1}$$

$$(l-m)!/(l-v-m_2)!(l+1-v+m)!(v+m_2-m)!$$
$$=\sum_r (-1)^r(2l+1-v-r)![r!(l-v-m_2-r)!$$
$$\times(l+1-v+m-r)!(l+1+m_2)!]^{-1}.$$

The expression (A1) now involves just four factorials containing m, and the part multiplying $(-1)^m$ can be summed. For the other part, which we select to illustrate our methods, a further expansion is required:

$$(l+m+1)!/(q+1+m-t-u+s)!(l+1+m-v-r)!$$
$$=\sum_w (t+u-s+l-q)!(v+r)![w!(t+u-s+l-q-w)!(v+r-w)!$$
$$\times(q+1+m-t-u+s-v-r+w)!]^{-1}.$$

The sum over m can now be performed by using

$$\sum_m \{(q+1-t-u+s-v-r+w+m)!(t+u+m_1+m_3-q+x-m)!\}^{-1}$$
$$=2^{m_1+m_3+x+w+s-v-r}\{(m_1+m_3+x+w+s-v-r+1)!\}^{-1}. \tag{A2}$$

We set $r=k-v$ and perform the sums over v, t and u. A quadruple sum over w, s, x and k remains. We write $s=y-x$ and simplify the power of 2 in equation (A2) by first taking

$$(l-q+y-x)!/(y-x)!x!$$
$$=\sum_f (-1)^f(l-q)!(l-q+y-f)!/y!f!(l-q-f)!(x-f)!$$

and then summing over x, w and k. The sum over f now has as its essence the expression

$$\sum_f (-2)^{-f}(l-q+f)!/f!(l-q-f)!(f-2y+q-m_1-m_3+m_2)!.$$

By differentiating both sides of the identity

$$\sum_f z^{l-q+f}(-\tfrac{1}{2})^f(l-q)!/f!(l-q-f)!=[\tfrac{1}{2}-\tfrac{1}{2}(1-z^2)]^{l-q}$$

h times with respect to z, and then setting $z=1$, we find

$$\sum_f (-2)^{-f}(l-q+f)!/f!(l-q-f)!(l-q+f-h)!$$
$$=\begin{cases}0 & (h \text{ odd})\\ (-1)^{h/2}(l-q)!h!/(\tfrac{1}{2}h)!(l-q-\tfrac{1}{2}h)!2^{l-q} & (h \text{ even}).\end{cases}$$

To apply this result to our expression, we must take $h=l-2q+2y+m_1+m_3-m_2$. Since q and y are integers, while all m_i are even, our sum is non-vanishing only if l is even.

The sum over y remains. the total phase and the relevant factorials amount to

$$\sum_y (-1)^{y-q+(l+m_1-m_2+m_3)/2}\{(q-m_1-y)!(q-m_3-y)!y!(y+m_1+m_3+1)!$$
$$\times[y-q+\tfrac{1}{2}(l+m_1-m_2+m_3)]![l-y-\tfrac{1}{2}(l+m_1-m_2+m_3)]!\}^{-1}$$

for l even. On making the replacement $y=z+q-\frac{1}{2}(l+m_1-m_2+m_3)$, we can identify the sum over y, together with its associated phase, with what is required to produce the SO(3) 3-j symbol

$$-\begin{pmatrix}\tfrac{1}{2}(l-m_3) & \tfrac{1}{2}(l+m_3+1) & q+\tfrac{1}{2}\\ \tfrac{1}{2}(m_2-m_1) & -\tfrac{1}{2}(m_1+m_2+1) & m_1+\tfrac{1}{2}\end{pmatrix}$$

in agreement with equation (24). When the sum involving $(-1)^m$ of the expression (A1) is considered, we are led to the result appropriate for l odd.

Appendix 2. Atomic quasiparticles

The states of an atomic l shell comprise a collection of configurations l^N $(0 \leq N \leq 4l+2)$ corresponding to N equivalent electrons, each with angular momentum specified by the azimuthal quantum number l. The entire set forms a basis for the irrep $(\frac{1}{2}^{4l+2})$ of SO(8l+5) (Judd 1968). If the linear combinations

$$\begin{aligned}\lambda_m^\dagger &= 2^{-1/2}[a_{1/2,m}^\dagger + (-1)^{l-m} a_{1/2,-m}]\\ \mu_m^\dagger &= 2^{-1/2}[a_{1/2,m}^\dagger - (-1)^{l-m} a_{1/2,-m}]\\ \nu_m^\dagger &= 2^{-1/2}[a_{-1/2,m}^\dagger + (-1)^{l-m} a_{-1/2,-m}]\\ \xi_m^\dagger &= 2^{-1/2}[a_{-1/2,m}^\dagger - (-1)^{l-m} a_{-1/2,-m}]\end{aligned} \tag{A3}$$

are taken of the annihilation (a_i) and creation $(a_i^\dagger)$ operators for an electron in state i $(\equiv m_s, m_l)$, the four sets of coupled tensors $(\boldsymbol{\theta}^\dagger\boldsymbol{\theta})^{(k)}$ (k odd, $\theta = \lambda, \mu, \nu, \xi$) form the generators of the direct product

$$\mathrm{SO}_\lambda(2l+1) \times \mathrm{SO}_\mu(2l+1) \times \mathrm{SO}_\nu(2l+1) \times \mathrm{SO}_\xi(2l+1). \tag{A4}$$

The spinor $(\frac{1}{2}^{4l+2})$ breaks up into the direct sum

$$(\tfrac{1}{2}^l)^4_{gg} + (\tfrac{1}{2}^l)^4_{gu} + (\tfrac{1}{2}^l)^4_{ug} + (\tfrac{1}{2}^l)^4_{uu}$$

where the parity labels g and u specify the evenness or oddness of the numbers of electrons (N_A and N_B) in the spin-up $(m_s = \frac{1}{2})$ and spin-down $(m_s = -\frac{1}{2})$ spaces (Armstrong and Judd 1970a, b). In general, we write p_A and p_B for these labels. By selectively adding the generators of the four groups appearing in the direct product (A4), new SO(2l+1) groups can be formed, with the result that atomic states can be written in the coupled form

$$|\{(w_{l\lambda}w_{l\mu})_{p_A} W(m_A), (w_{l\nu}w_{l\xi})_{p_B} W(m_B)\} W\alpha L M_L\rangle. \tag{A5}$$

In this expression the classificatory symbol α has been included to distinguish angular momenta L that occur more than once in the irrep W of SO(2l+1), the group which coincides with that of Racah (1949) and whose generators are given by

$$(\boldsymbol{\lambda}^\dagger\boldsymbol{\lambda})^{(k)} + (\boldsymbol{\mu}^\dagger\boldsymbol{\mu})^{(k)} + (\boldsymbol{\nu}^\dagger\boldsymbol{\nu})^{(k)} + (\boldsymbol{\xi}^\dagger\boldsymbol{\xi})^{(k)} \tag{A6}$$

It is sometimes useful to consider the group SO(8l+4), which can be inserted as an intermediary between SO(8l+5) and the direct product (A4). It separates configurations with even N (of types gg and uu) from those with odd N (gu and ug).

The operators $a_i^\dagger$ and a_i (for a given i) can be thought of as the two components (corresponding to $m_q = \frac{1}{2}$ and $-\frac{1}{2}$) of a tensor of quasispin rank q equal to $\frac{1}{2}$ (Judd 1967). Thus the collection of operators for various i form the components of a triple tensor $\boldsymbol{a}^{(qsl)}$. The ranks specify the behaviour under commutation with respect to $\boldsymbol{Q}$ (the quasispin), $\boldsymbol{S}$ (the total spin), and $\boldsymbol{L}$ (the total orbital angular momentum). In order to study the coupling of the quasispin and spin spaces, we define $\boldsymbol{T} = \boldsymbol{Q} + \boldsymbol{S}$. Writing $\boldsymbol{a}^{((qs)tl)}$ more succinctly as $\boldsymbol{a}^{(tl)}$, we note, first, that t is limited to the two possibilities 0 and 1. It is straightforward to show that $\boldsymbol{a}^{(0l)}$ is proportional to $\boldsymbol{\xi}^\dagger$, and that $\boldsymbol{a}^{(1l)}$ is formed from $\boldsymbol{\lambda}^\dagger$, $\boldsymbol{\mu}^\dagger$ and $\boldsymbol{\nu}^\dagger$ (Judd *et al* 1986b). Thus $\boldsymbol{T}$, which is proportional to $(\boldsymbol{a}^{(1l)}\boldsymbol{a}^{(1l)})^{(10)}$, does not involve $\boldsymbol{\xi}^\dagger$. This has an interesting consequence. The sum (A6) is proportional to the orbital tensor $\boldsymbol{V}^{(k)}$, which commutes with both $\boldsymbol{Q}$ and $\boldsymbol{S}$, and hence with $\boldsymbol{T}$; thus the generators

$$(\boldsymbol{\lambda}^\dagger\boldsymbol{\lambda})^{(k)} + (\boldsymbol{\mu}^\dagger\boldsymbol{\mu})^{(k)} + (\boldsymbol{\nu}^\dagger\boldsymbol{\nu})^{(k)} \tag{A7}$$

of the group $SO_\eta(2l+1)$ also commute with $\boldsymbol{T}$ (though not necessarily with $\boldsymbol{Q}$ and $\boldsymbol{S}$ separately). Denoting by $SO_T(3)$ the group whose generators are the components of $\boldsymbol{T}$, we can use the reduction

$$SO(8l+4) \to SO_T(3) \times SO_\eta(2l+1)$$

to obtain the decomposition

$$(\tfrac{1}{2}^{4l+1} \pm \tfrac{1}{2}) \to \sum_q \mathscr{D}_{q+1/2} \times w_q. \tag{A8}$$

That is, for N even or N odd, a particular irrep w_q is associated with a unique T. Its value is given by $T = q + \frac{1}{2}$ (Judd *et al* 1986b, equation (8)).

The eigenvalues of Q_z, S_z, and T_z can be found by using the equations

$$Q_z = -\tfrac{1}{2}(2l+1) + \tfrac{1}{2}\sum_i a_i^\dagger a_i$$

$$S_z = \tfrac{1}{2}\sum_m (a_{1/2,m}^\dagger a_{1/2,m} - a_{-1/2,m}^\dagger a_{-1/2,m})$$

$$T_z = -\tfrac{1}{2}(2l+1) + \sum_m a_{1/2,m}^\dagger a_{1/2,m}$$

from which we get

$$M_Q = -\tfrac{1}{2}(2l+1-N) \tag{A9}$$

$$M_S = \tfrac{1}{2}(N_\mathrm{A} - N_\mathrm{B}) \tag{A10}$$

$$M_T = N_\mathrm{A} - \tfrac{1}{2}(2l+1) = \pm(m'_\mathrm{A} + \tfrac{1}{2}) \qquad (N_\mathrm{A} \gtreqless \tfrac{1}{2}(2l+1))$$

$$= \begin{cases} m_\mathrm{A} + \frac{1}{2} & (l \text{ even}, p_\mathrm{A} = \mathrm{u}; \text{ or } l \text{ odd}, p_\mathrm{A} = \mathrm{g}) \\ -(m_\mathrm{A} + \frac{1}{2}) & (l \text{ even}, p_\mathrm{A} = \mathrm{g}; \text{ or } l \text{ odd}, p_\mathrm{A} = \mathrm{u}). \end{cases} \tag{A11}$$

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