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Algebraic expressions for some generalised 6-j symbols for SO(n) and G_2

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Abstract. A class of generalised 6-j symbols, which enter naturally when a second pair of modes $\varepsilon + \tau_2$ is added to the octahedral Jahn-Teller system $\Gamma_8 \times (\varepsilon + \tau_2)$, has been evaluated for the group SO(5). The method involves the fictitious boson configurations $d^w d'$, and can be readily generalised to $l^w l'$. The resulting 6-j symbols for SO($2l+1$) can be used to produce others by means of generalisations of the equations satisfied by the ordinary 6-j symbols for SO(3). Extensions to SO($2l+2$) and G_2 are described, as well as the weight-space symmetries of Jucys. The relation between 6-j symbols and isoscalar factors is illustrated for SO(7) $\supset G_2$.

1. Introduction

It is now commonplace to find the groups SO(n), U(n) and Sp(n), as well as the occasional exceptional group, put to use in such disparate fields as atomic spectroscopy, nuclear structure and particle physics. The application of the Wigner-Eckart theorem has made it essential to extend much of the algebra of angular momentum theory, for which the underlying group is SO(3). In particular, attention has been paid to the generalisation of the 3-j and 6-j symbols. Because this work is so widespread, it is not practicable to give a comprehensive list of references here; however, an impression of what has been done can be gained from the articles of Hecht (1965, 1967, 1970), Draayer and Akiyama (1973), Butler and Wybourne (1976), Bickerstaff and Wybourne (1981) and Haase and Butler (1985). We should also mention that an extensive tabulation of the 3-j and 6-j symbols for point groups has been made by Butler (1981).

The chief difficulty in extending the theory for SO(3) to another Lie group G lies in the fact that a given irreducible representation (irrep) Γ of G may occur more than once in the decomposition of the Kronecker product $\Gamma' \times \Gamma''$. The coupling represented by $(\Gamma'\Gamma'')\Gamma$ may therefore require an additional label r to separate multiply occurring representations Γ. The situation is further complicated for 3-j symbols if the irreps γ of a subgroup H of G are taken to define the lower row of the 3-j symbol. Unlike the case for SO(3), where an irrep of SO(2) (defined by a single number M) occurs once or not at all in the irrep $\mathscr{D}_J$ of SO(3), it can happen that additional multiplicity labels are required when a given γ occurs more than once in the decompostion of a particular Γ.

2. The Jahn–Teller effect

The need for multiplicity labels such as r effectively prevents explicit expressions being found for the general 3-j or 6-j symbol. However, in our own work on the Jahn–Teller effect we have found that a large class of multiplicity-free 6-j symbols for SO(5) enter naturally in the calculations. This particular Lie group arises when an electronic state is coupled equally to a fivefold degenerate set of vibrations represented by the direct sum $\varepsilon+\tau_2$ of irreps of the double octahedral group O. A particular example for the electronic state is the fourfold degenerate irrep Γ_8 of O. As Pooler and O'Brien (1977) have shown, Γ_8 and $\varepsilon+\tau_2$ fit into the respective irreps $(\frac{1}{2}\frac{1}{2})$ and (10) of SO(5). (Throughout the present article we define an irrep of SO($2l+1$) by its highest weight.) A state of n phonons corresponds to the symmetric representation $[n]$ of U(5), which decomposes into the irreps $(w0)$ of SO(5), where $w=n, n-2, \ldots, 1$ or 0. A state of the total system can thus be written as

$$|[n](w0), (\tfrac{1}{2}\tfrac{1}{2}), (w\pm\tfrac{1}{2}, \tfrac{1}{2})\rangle \tag{1}$$

where the final representation $(w\pm\frac{1}{2}, \frac{1}{2})$ results from the two options possible from a coupling of the phonon representation $(w0)$ to the electronic state $(\frac{1}{2}\frac{1}{2})$.

To better approximate an actual cubic crystal, the effect of adding a second mode of the type $\varepsilon+\tau_2$ has been studied (Lister 1983). The state (1) generalises to

$$|([n_1](w_10), [n_2](w_20))(w_1'w_2'), (\tfrac{1}{2}\tfrac{1}{2}), (w_1'\pm\tfrac{1}{2}, w_2'\pm\tfrac{1}{2})\rangle \tag{2}$$

in which (w_10) and (w_20) are first coupled to $(w_1'w_2')$ before the coupling to the electronic state takes place. The Jahn–Teller Hamiltonian H_{JT} is an SO(5) scalar and can be written as

$$H_{\mathrm{JT}} = \hbar\omega_1(\boldsymbol{a}_1^\dagger\cdot\boldsymbol{a}_1+\tfrac{5}{2}) + \hbar\omega_2(\boldsymbol{a}_2^\dagger\cdot\boldsymbol{a}_2+\tfrac{5}{2}) + [c_1(\boldsymbol{a}_1^\dagger+\boldsymbol{a}_1)+c_2(\boldsymbol{a}_2^\dagger+\boldsymbol{a}_2)]\cdot\boldsymbol{T}^{(10)} \tag{3}$$

where $\boldsymbol{a}_i^\dagger$ and $\boldsymbol{a}_i$ create and annihilate the five phonon states of mode i, and $\boldsymbol{T}^{(10)}$ is a tensor acting in the electronic space for which we can conveniently choose the normalisation

$$((\tfrac{1}{2}\tfrac{1}{2})\|T^{(10)}\|(\tfrac{1}{2}\tfrac{1}{2}))=1.$$

The terms in H_{JT} involving ω_1 and ω_2 are diagonal with respect to the states (2) and present no computational problem. An interaction term such as $\boldsymbol{a}_1^\dagger\cdot\boldsymbol{T}^{(10)}$, when sandwiched between a bra and a ket of type (2), yields the SO(5) 6-j symbol

$$\begin{Bmatrix} (w_1'w_2') & (\tfrac{1}{2}\tfrac{1}{2}) & (w_1'\pm\tfrac{1}{2}, w_2'\pm\tfrac{1}{2}) \\ (\tfrac{1}{2}\tfrac{1}{2}) & (w_1''w_2'') & (10) \end{Bmatrix} \tag{4}$$

together with a reduced matrix element of $\boldsymbol{a}^\dagger$. For the latter not to vanish, it must take the form

$$(([n_1+1](w_1\pm1, 0), [n_2](w_20))(w_1''w_2'')\|a_1^\dagger\|([n_1](w_10), [n_2](w_20))(w_1'w_2')) \tag{5}$$

which can be expressed in terms of the SO(5) 6-j symbol

$$\begin{Bmatrix} (w_1''w_2'') & (10) & (w_1'w_2') \\ (w_10) & (w_20) & (w_1\pm1, 0) \end{Bmatrix} \tag{6}$$

and the reduced matrix element

$$([n_1+1](w_1\pm1, 0)\|a_1^\dagger\|[n_1](w_10)). \tag{7}$$

In considering the energy matrices it is natural to start with the most elementary and work up. Our attention so far has been limited to the two choices given by

$$(w_1'\pm\tfrac{1}{2},\, w_2'\pm\tfrac{1}{2})\equiv(\tfrac{1}{2}\tfrac{1}{2}) \text{ and } (\tfrac{3}{2}\tfrac{1}{2}) \tag{8}$$

for the overall symmetry of the system. Thus $w_1'=0$, 1 or 2, and $w_2'=0$ or 1. Similar ranges apply to w_1'' and w_2''. Under these conditions the generalised 6-j symbols (4) and (6) are multiplicity-free.

3. General method of evaluation

The limitation (8) means that only a few special cases of the 6-j symbol (4) are required. They can all be obtained from the work of Hecht (1967). No bounds, however, are placed on the weights w_1 and w_2 appearing in the generalised symbol (6) other than a constraint on their difference $|w_1-w_2|$. It is to 6-j symbols of the type (6) that we therefore turn our attention.

The obvious way to proceed is to follow the familiar analysis for SO(3). This entails first constructing Clebsch-Gordan (CG) coefficients using the recursion relations that parallel those of angular momentum theory. Two relations involving 6-j symbols are then used: one involves a sum over quadruple products of CG coefficients (Edmonds 1957, equation (6.1.5)), while the other involves a sum over triple products (Judd 1963, equations (3)-(6)). This is a tedious procedure, and for groups other than SO(3) it is by no means apparent which group-subgroup chain is the most convenient to define our states. For SO(5), Hecht (1967) uses the group-subgroup chain SO(5) $\supset$ U(1) $\times$ SU(2). This scheme affords a complete classification for the irreducible representations $(w0)$ and (11), but an additional classificatory symbol is required for the representations $(w1)$ when $w>1$. In spite of this complication, preliminary calculations were carried out to evaluate the CG coefficients and their factored parts, the so-called isoscalar factors, for the SO(5) couplings $(\Gamma'\Gamma'')\Gamma$ given by

$$((w0)(20))(w\pm 2,0) \qquad ((w0)(20))(w0) \qquad ((w0)(21))(w\pm 1,0).$$

The isoscalar factors, taken with those of Hecht (1967), enabled the numerical evaluation of all the required 6-j symbols of the type (6) to be carried out (Lister 1983). On examining these results, it was found that they could be fitted to rather simple algebraic formulae. This motivated us to search for an alternative approach to the problem, one that would avoid having to make a specific choice of a group-subgroup chain, with all the complexities which that entails.

It occurred to us to turn to the work of Racah (1942), where he introduced for the first time his celebrated W function, that is, an unsymmetrised 6-j symbol. The role of the W function in Racah's work was to express the matrix elements of operators of the type $\boldsymbol{C}_A^{(k)}\cdot\boldsymbol{C}_B^{(k)}$, i.e. operators that are formed by taking the scalar product of tensors transforming according to $\mathscr{D}_k$ of SO(3) and acting separately on the two parts A and B of a coupled system. If we could invent an operator $\boldsymbol{T}_A^{(W)}\cdot\boldsymbol{T}_B^{(W)}$, scalar in SO(5), whose two parts transform like the irrep W of SO(5), and if, in addition, we could construct a system (possibly fictitious) whose bras and kets take the forms $\langle(W_AW_B)W'|$ and $|(W_A'W_B')W'\rangle$, then the matrix elements of the operator would exhibit a dependence on W' specified (to within an arbitrary phase factor) by the SO(5) 6-j

symbol

$$\begin{Bmatrix} W'_A & W'_B & W' \\ W_B & W_A & W \end{Bmatrix}. \tag{9}$$

Merely to say that our matrix elements are proportional to (9) would be useless; we have also to be able to work them out reasonably easily by some other method. We might not have to repeat this calculation for every 6-*j* symbol, since the experience of Butler and Wybourne (1976) suggests that various equations that the 6-*j* symbols must satisfy can be put to use to generate other 6-*j* symbols.

Of course, the argument used above to introduce (9) is implicit in the derivation of (4), but the representations appearing there are not suitable for the purposes that we now have in mind. Instead, we consider the boson configuration $d^w d'$, where d and d' represent two inequivalent spin-free bosons for which $l=2$. We introduce single-particle tensors $\boldsymbol{v}_A^{(k)}$ and $\boldsymbol{v}_B^{(k)}$ whose amplitudes are specified by

$$(d\|v_A^{(k)}\|d) = (d'\|v_B^{(k)}\|d') = (2k+1)^{1/2}.$$

The abbreviation

$$\boldsymbol{V}_A^{(k)} = \sum_{i=1}^{w} (\boldsymbol{v}_A^{(k)})_i$$

is made for the individual bosons i comprising d^w. The two tensors $\boldsymbol{v}_B^{(2)}$ and $\boldsymbol{v}_B^{(4)}$ together form a single tensor transforming like the irrep (20) of SO(5), as do $\boldsymbol{V}_A^{(2)}$ and $\boldsymbol{V}_A^{(4)}$. The coupling that selects the SO(5) scalar (00) from the Kronecker product $(20)\times(20)$ corresponds to the linear combination

$$S = \boldsymbol{T}_A^{(20)} \cdot \boldsymbol{T}_B^{(20)} = \boldsymbol{V}_A^{(2)} \cdot \boldsymbol{v}_B^{(2)} + \boldsymbol{V}_A^{(4)} \cdot \boldsymbol{v}_B^{(4)} \tag{10}$$

whose matrix elements are straightforward to work out. The results of these calculations are assembled in a similar way to the diagonal sum method used by Slater (1929) to calculate the Coulomb energies of the *SL* terms of an atomic configuration.

4. The method exemplified

We begin with the stretched state

$$|d^w(w0), (10), (w+1, 0)LM_L\rangle \tag{11}$$

for which L and M_L are set equal to their (common) maximum value, $2w+2$. We can also write (11) in a form in which the individual m_l values of each boson are specified, namely $\{22\ldots 2, 2'\}_s$. The subscripted curly bracket indicates a state that is symmetrised and normalised. There are w numbers, all equal to 2, preceding the comma. The prime on the last 2 makes it clear that it corresponds to the d' boson. Now, on the one hand

$$\int \{22\ldots 2, 2'\}_s^* S \{22\ldots 2, 2'\}_s \, \mathrm{d}\tau = 5w\begin{pmatrix} 2 & 2 & 2 \\ -2 & 0 & 2 \end{pmatrix}^2 + 9w\begin{pmatrix} 2 & 4 & 2 \\ -2 & 0 & 2 \end{pmatrix}^2 = 3w/10 \tag{12}$$

while, on the other hand,

$$\langle d^w(w0), (10), (w+1, 0)LM_L|S|d^w(w0), (10), (w+1, 0)LM_L\rangle$$

$$= (-1)^x \begin{Bmatrix} (w0) & (10) & (w+1, 0) \\ (10) & (w0) & (20) \end{Bmatrix} \Xi \tag{13}$$

where $(-1)^x$ is a possible phase factor, and where Ξ is given by $\Xi = (d^w(w0)\| T_A^{(20)} \| d^w(w0))((10)\| T_B^{(20)} \|(10))$. Although we cannot easily proceed further to find Ξ, it turns out that we do not need to.

We now lower M_L and L one step at a time. For $M_L = 2w+1$, there are two possibilities for L, namely $L = 2w+2$ and $L = 2w+1$. To determine how these are distributed among the irreps W', we note that

$$(w0) \times (10) = (w+1, 0) + (w, 1) + (w-1, 0). \tag{14}$$

The relevant branching rules for $SO(5) \to SO(3)$ are

$$\begin{aligned} &(w+1, 0) \to \mathscr{D}_{2w+2} + \mathscr{D}_{2w} + \mathscr{D}_{2w-1} + \mathscr{D}_{2w-2} + \mathscr{D}_{2w-3} + 2\mathscr{D}_{2w-4} + \dots \\ &(w, 1) \to \mathscr{D}_{2w+1} + \mathscr{D}_{2w} + 2\mathscr{D}_{2w-1} + 2\mathscr{D}_{2w-2} + 3\mathscr{D}_{2w-3} + 3D_{2w-4} + \dots \\ &(w-1, 0) \to \mathscr{D}_{2w-2} + \mathscr{D}_{2w-4} + \dots \end{aligned} \tag{15}$$

as may be confirmed from table C-16 of Wybourne (1970). A general method for deriving equation (14) and the decompositions (15) is provided by the analysis of Williams and Pursey (1968). Both (14) and (15) need to be modified for small values of w; however, it is convenient to work with the general forms and make allowance later for special cases. It can be seen from (15) that the state for which $L = 2w+2$ occurs only in $(w+1, 0)$, while the state for which $L = 2w+1$ occurs only in $(w, 1)$. These two states are some pair of mutually orthogonal combinations of the boson states

$$\{22 \dots 21, 2'\}_s, \{22 \dots 2, 1'\}_s. \tag{16}$$

Although it is easy enough to determine the mixtures in question, all we need is the sum of the two diagonal elements of S, which, following the method that has led to (12), evaluates to $(w-5)/10$. We already know from (12) that the state for which $L = 2w+2$ contributes $3w/10$, and so the other (that is, the state for which $L = 2w+1$) must contribute $-(2w+5)/10$. A similar equation to (13) allows us to conclude that

$$\begin{Bmatrix} (w0) & (10) & (w+1, 0) \\ (10) & (w0) & (20) \end{Bmatrix} \left(\begin{Bmatrix} (w0) & (10) & (w1) \\ (10) & (w0) & (20) \end{Bmatrix} \right)^{-1} = \pm \frac{3w}{(2w+5)}. \tag{17}$$

The method can be continued to yield further relations. It can be seen from the reductions (15) that M_L has to be reduced three more steps to $2w-2$ before a 6-j symbol involving $(w-1, 0)$ enters the working. The two intermediate steps merely provide checks on equation (17). However, the configuration d^w provides not only the representation $(w0)$ appearing in (13) but also $(w-2, 0)$, which, when coupled to (10), can also produce $(w-1, 0)$. It is not difficult to project out the unwanted state in order to relate the 6-j symbol

$$\begin{Bmatrix} (w0) & (10) & (w-1, 0) \\ (10) & (w0) & (20) \end{Bmatrix} \tag{18}$$

to those appearing in (17). It is easier, however, to determine (18) from the orthonormality condition

$$\sum_{W'} D(W')\begin{Bmatrix}(w0) & (10) & W'\\ (10) & (w0) & W\end{Bmatrix}\begin{Bmatrix}(w0) & (10) & W'\\ (10) & (w0) & W''\end{Bmatrix}=\frac{\delta(W,W'')}{D(W)} \qquad (19)$$

where $D(W')$ is the dimension of W' (see, for example, Judd 1963, equation (5-64)). We can evaluate the second 6-j symbol in (19) when $W''\equiv(00)$ by relating it to a stretched recoupling coefficient (whose absolute value is necessarily 1):

$$\begin{Bmatrix}(w0) & (10) & W'\\ (10) & (w0) & (00)\end{Bmatrix}$$

$$=\pm[D(10)D(w0)]^{-1/2}(((10)(00))(10),(w0),W'|(10),((00)(w0))(w0),W')$$

$$=\pm[D(10)D(w0)]^{-1/2}=\pm[6/(w+1)(w+2)(2w+3)]^{1/2}.$$

Thus (19) can be used to relate the three 6-j symbols

$$\begin{Bmatrix}(w0) & (10) & W'\\ (10) & (w0) & (20)\end{Bmatrix} \qquad (W'\equiv(w+1,0),(w1),(w-1,0))$$

to one another and also to normalise them. They are determined to within a phase factor.

5. Generalisations

It is straightforward to repeat the analysis above for arbitrary l rather than for $l=2$. In this way we can find a number of 6-j symbols for SO($2l+1$). This generalisation gives us a method for fixing our immediate phases: we simply demand that our 6-j symbols for SO($2l+1$) reduce to those for SO(3) when we set $l=1$. The SO(3) analogue of equation (14) is

$$\mathscr{D}_w\times\mathscr{D}_1=\mathscr{D}_{w+1}+\mathscr{D}_w+\mathscr{D}_{w-1}$$

which indicates that, for SO($2l+1$), the irreps $(w0\ldots0)$ and $(w10\ldots0)$ both convert to $\mathscr{D}_w$ when the specialisation $l=1$ is made. The dimension formulae

$$D(w0\ldots0)=(2w+2l-1)(w+2l-2)!/w!(2l-1)!$$
$$D(w10\ldots0)=w(w+2l-1)(2w+2l-1)(w+2l-3)!/(w+1)!(2l-2)! \qquad (20)$$

become $D(\mathscr{D}_w)=2w+1$, as they should. Our insistence on recovering the SO(3) 6-j symbols when $l=1$ means that our phases are not necessarily coincident with those of Hecht (1967), but at least we have a self-consistent scheme that has an easily understood rationale.

To avoid factorial functions of the type occurring in equations (20), we replace the generalised 6-j symbol by a U function U_l for SO($2l+1$):

$$U_l\begin{pmatrix}W_1 & W_2 & W_3\\ W_4 & W_5 & W_6\end{pmatrix}=[D(W_3)D(W_6)]^{1/2}\begin{Bmatrix}W_1 & W_2 & W_3\\ W_4 & W_5 & W_6\end{Bmatrix}. \qquad (21)$$

This is an extension (to within a phase factor) of the U coefficient of Jahn (1951). The loss of symmetry between the third column of the U function and the other two is more than offset by the ease of tabulation.

Table 1. Equations giving generalised 6-*j* symbols, expressed as U functions, for SO$(2l+1)$. The connection between w and u is $u=2w+2l-1$. Additional formulae for the U functions can be found by making the simultaneous substitutions (25) in a U function and $u\to -u$ in the corresponding algebraic expression. An asterisk indicates that the algebraic expression must be multiplied by the overall factor of -1 when this procedure is carried out.

$$U_l\begin{pmatrix} w & 1 & w+1 \\ 1 & w & 0 \end{pmatrix} = \left(\frac{(u+2)(u+2l-1)}{(2l+1)u(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 1 & w,1 \\ 1 & w & 0 \end{pmatrix} = -\left(\frac{(2l-1)(u-2l+1)(u+2l-1)}{(2l+1)(u-2l+3)(u+2l-3)}\right)^{1/2}$$

$$U_l^*\begin{pmatrix} w & 1 & w+1 \\ 1 & w & 1,1 \end{pmatrix} = \left(\frac{(u+2)(u-2l+1)}{2u(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 1 & w,1 \\ 1 & w & 1,1 \end{pmatrix} = \left(\frac{2(2l-1)}{(u-2l+3)(u+2l-3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 1 & w+1 \\ 1 & w & 2 \end{pmatrix} = \left(\frac{(2l-1)(u-2)(u-2l+1)}{2(2l+1)u(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 1 & w,1 \\ 1 & w & 2 \end{pmatrix} = \left(\frac{2(u^2-4)}{(2l+1)(u+2l-3)(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} 1 & w & w+1 \\ 1 & w & w+1 \end{pmatrix} = \frac{2(2l-1)}{u(u-2l+3)}$$

$$U_l^*\begin{pmatrix} 1 & w & w+1 \\ 1 & w & w,1 \end{pmatrix} = \left(\frac{4(2l-1)(u+2)(u-2l+1)}{u(u+2l-3)(u-2l+3)^2}\right)^{1/2}$$

$$U_l\begin{pmatrix} 1 & w & w+1 \\ 1 & w & w-1 \end{pmatrix} = \left(\frac{(u^2-4)[u^2-(2l-1)^2]}{u^2[u^2-(2l-3)^2]}\right)^{1/2}$$

$$U_l\begin{pmatrix} 1 & w & w,1 \\ 1 & w & w,1 \end{pmatrix} = \frac{u^2-(2l-1)^2-4}{u^2-(2l-3)^2}$$

$$U_l\begin{pmatrix} 1 & w,1 & w-1,1 \\ 1 & w-1 & w \end{pmatrix} = -\left(\frac{[(u-2l+1)^2-4]}{(u-2l+1)^2}\right)^{1/2}$$

$$U_l\begin{pmatrix} 1 & w-1,1 & w,1 \\ 1 & w & w,1 \end{pmatrix} = -\frac{2}{u+2l-3}$$

$$U_l^*\begin{pmatrix} w+1,1 & 1 & w+1 \\ 1 & w & 1,1 \end{pmatrix} = -\left(\frac{(u-2l+5)}{2(u-2l+3)}\right)^{1/2}$$

$$U_l^*\begin{pmatrix} w+1,1 & 1 & w,1 \\ 1 & w & 1,1 \end{pmatrix} = \left(\frac{(u-2l+1)}{2(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w+1,1 & 1 & w+1 \\ 1 & w & 2 \end{pmatrix} = -\left(\frac{(u-2l+1)}{2(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w+1,1 & 1 & w,1 \\ 1 & w & 2 \end{pmatrix} = -\left(\frac{(u-2l+5)}{2(u-2l+3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 1,1 & w \\ 1 & w+1 & 2,1 \end{pmatrix} = -\left(\frac{(2l-1)(u+2l+1)}{2l(u+2l-1)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 1,1 & w+1,1 \\ 1 & w+1 & 2,1 \end{pmatrix} = -\left(\frac{(u-2l+1)}{2l(u+2l-1)}\right)^{1/2}$$

$$U_l^*\begin{pmatrix} w & 2 & w \\ 1 & w+1 & 2,1 \end{pmatrix} = -\left(\frac{(2l+1)(u-2)(u+2l+1)}{6l(u+2l-1)(u+2)}\right)^{1/2}$$

Table 1. (continued)

$$U_l\begin{pmatrix} w & 2 & w+1,1 \\ 1 & w+1 & 2,1 \end{pmatrix} = \frac{u+6l+1}{[6l(u-2l+5)(u+2l-1)]^{1/2}}$$

$$U_l^*\begin{pmatrix} w & 2 & w+2 \\ 1 & w+1 & 2,1 \end{pmatrix} = \left(\frac{(2l-1)(u+4)(u-2l+1)}{3l(u+2)(u-2l+5)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 2 & w+2 \\ 1 & w+1 & 3 \end{pmatrix} = \left(\frac{(2l-1)(u-2)(u-2l+1)}{3(2l+3)(u+2)(u-2l+5)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 2 & w+1,1 \\ 1 & w+1 & 3 \end{pmatrix} = \left(\frac{8(u-2)(u+4)}{3(2l+3)(u+2l-1)(u-2l+5)}\right)^{1/2}$$

$$U_l\begin{pmatrix} w & 2 & w \\ 1 & w+1 & 3 \end{pmatrix} = \left(\frac{2(2l+1)(u+4)(u+2l+1)}{3(2l+3)(u+2)(u+2l-1)}\right)^{1/2}$$

$$U_l\begin{pmatrix} 2 & w+1 & w+1 \\ 1 & w & w \end{pmatrix} = \left(\frac{(u-2)(u+4)(u-2l+1)(u+2l+1)}{u(u+2)(u-2l+3)(u+2l-1)}\right)^{1/2}$$

$$U_l^*\begin{pmatrix} 2 & w+1 & w,1 \\ 1 & w & w \end{pmatrix} = -\left(\frac{4(2l+1)(u-2)(u+2l+1)}{(u+2)(u-2l+3)(u+2l-1)(u+2l-3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} 2 & w+1 & w-1 \\ 1 & w & w \end{pmatrix} = \left(\frac{8(2l-1)(2l+1)}{u(u+2)(u+2l-1)(u+2l-3)}\right)^{1/2}$$

$$U_l^*\begin{pmatrix} 2 & w+1 & w+1 \\ 1 & w & w+1,1 \end{pmatrix} = \left(\frac{4(2l+1)(u+4)(u-2l+1)}{u(u-2l+3)(u-2l+5)(u+2l-1)}\right)^{1/2}$$

$$U_l\begin{pmatrix} 2 & w+1 & w,1 \\ 1 & w & w+1,1 \end{pmatrix} = \frac{(u+1)^2-4l^2-8}{[(u-2l+3)(u-2l+5)(u+2l-1)(u+2l-3)]^{1/2}}$$

$$U_l^*\begin{pmatrix} 2 & w+1 & w-1 \\ 1 & w & w+1,1 \end{pmatrix} = -\left(\frac{8(2l-1)(u-2)(u+2l+1)}{u(u+2l-1)(u+2l-3)(u-2l+5)}\right)^{1/2}$$

$$U_l\begin{pmatrix} 2 & w+1 & w+1 \\ 1 & w & w+2 \end{pmatrix} = \left(\frac{8(2l-1)(2l+1)}{u(u+2)(u-2l+3)(u-2l+5)}\right)^{1/2}$$

$$U_l^*\begin{pmatrix} 2 & w+1 & w,1 \\ 1 & w & w+2 \end{pmatrix} = \left(\frac{8(2l-1)(u+4)(u-2l+1)}{(u+2)(u-2l+3)(u-2l+5)(u+2l-3)}\right)^{1/2}$$

$$U_l\begin{pmatrix} 2 & w+1 & w-1 \\ 1 & w & w+2 \end{pmatrix} = \left(\frac{(u-2)(u+4)(u-2l+1)(u+2l+1)}{u(u+2)(u-2l+5)(u+2l-3)}\right)^{1/2}$$

The SO($2l+1$) 6-j symbols obtained as in § 4 can be rapidly augmented by using (a) the orthonormality relation (19), suitably generalised, (b) the so-called Racah back-coupling relation (Butler and Wybourne 1976) and (c) the Biedenharn-Elliott identity. Our results are assembled in table 1. For the reason described in § 8, it is convenient to use u, defined by

$$u = 2w + 2l - 1 \qquad (22)$$

rather than w when setting up the algebraic formulae. The abbreviations

$$(w0\ldots0) \to w \qquad (w10\ldots0) \to w, 1$$

for the irreps of SO($2l+1$) are made in table 1. It is to be noted that the numerical value of w cannot be reduced to a point where either the triangular conditions are no longer satisfied or the irreps do not specify the highest weight.

6. Half-integral l

The analysis has so far been limited to groups SO(n) for which n is odd. But just as Elliott (1958) showed how SO(6) could be used for the six orbital states of a d nucleon and an s nucleon, so may we introduce an s boson to increase the dimension provided by an l boson from $2l+1$ to $2l+2$. The result is that the formulae of table 1 remain valid provided all representations $(w0\ldots0)$ and $(w10\ldots0)$ of SO$(2l+2)$ end with a zero. Complications arise only for SO(4) and SO(2). For SO(4), equation (14) is replaced by

$$(w0)\times(10)=(w+1,0)+(w,1)+(w,-1)+(w-1,0) \tag{23}$$

in which the two representations $(w,1)$ and $(w,-1)$ put in an appearance. The representation $(w1)$ of SO(4) occurring in a 6-j symbol listed in table 1 must thus be regarded as a superposition of $(w,1)$ and $(w,-1)$. Properly speaking, we do not have a well defined U function at all; however we can interpret it as a linear combination of recoupling coefficients in which the bras and the kets correctly represent the required superposition.

Since SO(4) is locally isomorphic to SO(3) × SO(3), it should be possible to relate the 6-j symbols for these groups. To do this, we note that (w_1w_2) of SO(4) corresponds to $\mathscr{D}_{(1/2)(w_1+w_2)}\times\mathscr{D}_{(1/2)|w_1-w_2|}$ of SO(3) × SO(3). To illustrate the correspondence, we choose an example where the representations $(w1)$ and (21) have to be regarded as the superpositions of $(w,\pm1)$ and $(2,\pm1)$ respectively. We obtain

$$\begin{aligned}U_{3/2}\begin{pmatrix}w+1 & 2 & w,1\\ 1 & w & 2,1\end{pmatrix}&=U_1\begin{pmatrix}\frac{1}{2}(w+1) & 1 & \frac{1}{2}(w+1)\\ \frac{1}{2} & \frac{1}{2}w & \frac{3}{2}\end{pmatrix}U_1\begin{pmatrix}\frac{1}{2}(w+1) & 1 & \frac{1}{2}(w-1)\\ \frac{1}{2} & \frac{1}{2}w & \frac{1}{2}\end{pmatrix}\\ &\quad+U_1\begin{pmatrix}\frac{1}{2}(w+1) & 1 & \frac{1}{2}(w+1)\\ \frac{1}{2} & \frac{1}{2}w & \frac{1}{2}\end{pmatrix}U_1\begin{pmatrix}\frac{1}{2}(w+1) & 1 & \frac{1}{2}(w-1)\\ \frac{1}{2} & \frac{1}{2}w & \frac{3}{2}\end{pmatrix}\end{aligned}$$

which, from table 1 and the formulae of Edmonds (1957), corresponds to

$$-\frac{w-3}{3(w+1)}=-\frac{2w}{3(w+1)}+\frac{w+3}{3(w+1)}.$$

SO(2) is too trivial a group to require special attention, but it is worth noting that the U functions of table 1 involving only representations of the type $(w0\ldots0)$—the only ones to have an SO(2) analogue—frequently reduce to 1 or $1/\sqrt{2}$ when we set $l=\frac{1}{2}$. This property can be understood in terms of the superposition principle just described for SO(4).

7. The group G_2

Our interest in the Jahn-Teller effect makes the 6-j symbols of the groups SO(n) of prime concern to us. However, our general method is not limited to such groups. We can easily extend the analysis of § 4 to the group G_2 by considering f bosons. The G_2

scalars given by

$$S_1 = \boldsymbol{V}_A^{(3)} \cdot \boldsymbol{v}_B^{(3)}$$

$$S_2 = \boldsymbol{V}_A^{(1)} \cdot \boldsymbol{v}_B^{(1)} + \boldsymbol{V}_A^{(5)} \cdot \boldsymbol{v}_B^{(5)}$$

$$S_3 = \boldsymbol{V}_A^{(2)} \cdot \boldsymbol{v}_B^{(2)} + \boldsymbol{V}_A^{(4)} \cdot \boldsymbol{v}_B^{(4)} + \boldsymbol{V}_A^{(6)} \cdot \boldsymbol{v}_B^{(6)}$$

are operators of the type $\boldsymbol{T}_A^{(U)} \cdot \boldsymbol{T}_B^{(U)}$, where the G_2 representations U are (10), (11) and (20) respectively. They can be used in the same way as the operator S of equation (10). The resulting 6-j symbols for G_2 are set out in table 2. The chief interest here is that (20) occurs twice in the reduction of the Kronecker square $(w0)^2$ when $w \geq 2$. There are therefore two columns headed (20); the one obtained with S_3 is labelled $(20)_a$, while the other, which had to be determined from the orthonormality conditions, is labelled $(20)_b$. In analogy to equation (22), we have replaced $2w+5$ by u in the actual tabulation.

Unlike the situation for SO(n), we cannot appeal to the signs of the SO(3) coefficients to fix our G_2 phases. However, if we set $w = 1$ in table 2, several pairs of U coefficients are produced that are equivalent under the standard symmetry operations of a 6-j symbol. The limited arbitrariness in our phases is reduced by insisting that such U coefficients possess the same sign. The row for which $U' \equiv (w-1, 1)$ cannot be checked in this way because (01) is not acceptable as a highest weight. Accordingly, we have included the phase factor $\mathscr{E}$ in all the entries for that row. It turns out that Racah's phases correspond to $\mathscr{E} = 1$ but that subsequent calculations for other G_2 6-j symbols require $\mathscr{E} = -1$ if their invariance under the symmetry operations is to be preserved.

Preliminary work on the symplectic groups Sp($2j+1$) indicates that there is no special difficulty in extending our method in that direction (Suskin 1985). The well known isomorphism Sp(4) $\equiv$ SO(5) allows us to relate representations $\langle\sigma_1\sigma_2\rangle$ of Sp(4) to $(\frac{1}{2}\sigma_1 + \frac{1}{2}\sigma_2, \frac{1}{2}\sigma_1 - \frac{1}{2}\sigma_2)$ of SO(5), thereby providing a means of finding 6-j symbols of SO(5) in which the spinor representations (involving half-integral weights) appear. A few special cases of these have been found by Payne and Stedman (1983, table A3). We are also making an effort to tackle the unitary groups, where the fact that many irreps are not self-adjoint produces some complications. As for the other exceptional groups (F_4, E_6, E_7 and E_8), the absence of a pattern as simple as (14) and the far from obvious choice of angular momenta for the bosons make their study a formidable proposition.

8. Jucys symmetries

The symmetry of angular momentum theory under the substitution $l \to -l-1$ is well known, thanks to the extensive work of the Lithuanian school at Vilnius. Their results are summarised by Jucys and Savukynas (1973), who also describe the extensions from SO(3) to other Lie groups. An application to O(2, 1) and the associated quasispin $\boldsymbol{P}$ has been made by Judd (1981). For the irrep $(w_1 w_2 \ldots w_l)$ of SO($2l+1$), any number of the independent substitutions

$$w_i \to -w_i - 2l - 1 + 2i$$

are allowed. If we pick $i = 1$, we can write

$$(w0 \ldots 0) \to (-w-2l+1, 0 \ldots 0)$$

$$(w+1, 0 \ldots 0) \to (-(w+1) - 2l + 1, 0 \ldots 0) = (-w-2l, 0 \ldots 0) \qquad (24)$$

$$(w10 \ldots 0) \to (-w-2l+1, 10 \ldots 0)$$

Table 2. The functions $U\begin{pmatrix}(w0) & (10) & U' \\ (10) & (w0) & U''\end{pmatrix}$ for G_2†.

U'	U'': (00)	(10)	(11)	$(20)_a$	$(20)_b$
$(w+1,0)$	$\left(\frac{(u+2)(u+5)}{7u(u-3)}\right)^{1/2}$	$\left(\frac{(u+2)(u-5)}{6u(u-3)}\right)^{1/2}$	$\left(\frac{(u+2)(u-5)}{3u(u-3)}\right)^{1/2}$	$\left(\frac{5(u-2)(u-5)}{14u(u-3)}\right)^{1/2}$	0
$(w1)$	$-\left(\frac{2(u-5)(u+7)}{7u(u-3)}\right)^{1/2}$	$\left(\frac{(u-1)^2(u+7)}{3u(u-3)(u+5)}\right)^{1/2}$	$-\left(\frac{(u-7)^2(u+7)}{6u(u-3)(u+5)}\right)^{1/2}$	$\left(\frac{4(u+7)(u^2-4)}{35u(u-3)(u+5)}\right)^{1/2}$	$-\left(\frac{(u-7)(u-3)}{10u(u+5)}\right)^{1/2}$
$(w0)$	$-\left(\frac{1}{7}\right)^{1/2}$	$-\left(\frac{6}{(u^2-25)}\right)^{1/2}$	$\left(\frac{12}{(u^2-25)}\right)^{1/2}$	$\left(\frac{2(u^2-4)}{35(u^2-25)}\right)^{1/2}$	$\left(\frac{4(u^2-49)}{5(u^2-25)}\right)^{1/2}$
$(w-1,1)$	$-\mathscr{C}\left(\frac{2(u+5)(u-7)}{7u(u+3)}\right)^{1/2}$	$-\mathscr{C}\left(\frac{(u+1)^2(u-7)}{3u(u+3)(u-5)}\right)^{1/2}$	$\mathscr{C}\left(\frac{(u+7)^2(u-7)}{6u(u+3)(u-5)}\right)^{1/2}$	$\mathscr{C}\left(\frac{4(u-7)(u^2-4)}{35u(u+3)(u-5)}\right)^{1/2}$	$-\mathscr{C}\left(\frac{(u+7)(u+3)}{10u(u-5)}\right)^{1/2}$
$(w-1,0)$	$\left(\frac{(u-2)(u-5)}{7u(u+3)}\right)^{1/2}$	$-\left(\frac{(u-2)(u+5)}{6u(u+3)}\right)^{1/2}$	$-\left(\frac{(u-2)(u+5)}{3u(u+3)}\right)^{1/2}$	$\left(\frac{5(u+2)(u+5)}{14u(u+3)}\right)^{1/2}$	0

† To find the corresponding 6-j symbols, divide each entry in the table by $[D(U')D(U'')]^{1/2}$, where $D(u_1u_2)=(u_1+u_2+3)(u_1+2)(2u_1+u_2+5)(u_1+2u_2+4)(u_1-u_2+1)(u_2+1)/120$.

and so on. Such substitutions, made in a formula for a specified U function, merely change the appearance of the irreps occurring in the U function, but leave the algebraic expression for it untouched. However, we can now make the formal replacement $w \to -w-2l+1$ everywhere, i.e. in both the U function and in the algebraic expression for it. When combined with the changes of the type (24), the irreps of the U function are transformed as follows:

$$
\begin{array}{ll}
(w0\ldots0)\to(w0\ldots0) & (w+1,0\ldots0)\to(w-1,0\ldots0) \\
(w10\ldots0)\to(w10\ldots0) & (w-1,0\ldots0)\to(w+1,0\ldots0) \\
(w+2,0\ldots0)\to(w-2,0\ldots0) & (w-2,0\ldots0)\to(w+2,0\ldots0) \\
(w+1,10\ldots0)\to(w-1,10\ldots0) & (w-1,10\ldots0)\to(w+1,10\ldots0).
\end{array}
\tag{25}
$$

Owing to equation (22), the appropriate replacement for u in an algebraic expression is $u\to -u$. For example,

$$(u-2)(u+4)\to(u+2)(u-4).$$

Although we have not used this kind of symmetry to evaluate our U functions, its existence enables us to almost halve the size of table 1. It does not, however, fix relative phases. When a sign reversal is called for the U function is asterisked in table 1.

The situation is slightly different for G_2 because of the oblique coordinate system used to define the highest weights. The algebraic expressions for the 6-j symbol in table 2 again exhibit a symmetry under the interchange $u\leftrightarrow -u$, but the substitutions (25) are replaced by

$$
\begin{array}{ll}
(w0)\to(w0) & (w\pm1,0)\to(w\mp1,0) \\
(w-1,1)\to(w1) & (w1)\to(w-1,1).
\end{array}
\tag{26}
$$

9. Isoscalar factors

If the U function of a group G is thought of as a recoupling coefficient, it is clear that it can be expressed as a linear combination of the U functions of a subgroup of G. The coefficients are quadruple products of isoscalar factors in which irreps of G and H appear. Take, for example, $G\equiv SO(7)$ and $H\equiv G_2$. Picking a particular U function of SO(7), we get

$$
\begin{aligned}
&U_3\begin{pmatrix}(100) & (w00) & (w10)\\ (w00) & (100) & (110)\end{pmatrix}\\
&\quad=(((w00)(100))(w10),(100),(w00)|(w00),((100)(100))(110),(w00))\\
&\quad=\sum_{U',U''}U\begin{pmatrix}(10) & (w0) & U'\\ (w0) & (10) & U''\end{pmatrix}((w00)(w0)+(100)(10)|(w10)\,U')\\
&\qquad\times((w10)\,U'+(100)(10)|(w00)(w0))((100)(10)+(100)(10)|(110)\,U'')\\
&\qquad\times((w00)(w0)+(110)\,U''|(w00)(w0)).
\end{aligned}
\tag{27}
$$

Following the work of Racah (1949), we can show that the four isoscalar factors in equation (27) are

$$1 \qquad [D(U')/D(w10)]^{1/2} \qquad 1 \qquad [D(U'')/D(110)]^{1/2}$$

respectively. Their product is thus known to within a phase factor. When the appropriate U functions are selected from tables 1 and 2 and inserted into equation (27), it is found that complete consistency is obtained provided the phase factor in question is taken to be $+1$. This result confirms the assertion made at the beginning of this section. It also makes it clear that the choice of phases for the U functions of G and H imposes phase conditions on the isoscalar factors involving irreps of G and H. These may or may not conflict with choices already made in the literature. We have been anxious not to burden the reader (or ourselves, for that matter) with a formal analysis of phase conventions. The book of Butler (1981) shows how complex the situation can become just for finite groups. Particular problems demand particular solutions, and it seems to us that it would not be profitable to embark on a detailed discussion of phases at this time.

10. Concluding remarks

Among sources that provide checks on our analysis, we should mention the tabulation of 6-j symbols for certain elementary irreps of U(n) given by Haase and Butler (1985). The isomorphism $U(4) \equiv SO(6)$ implies the equivalence of the generalised 6-j symbols for U(4) and SO(6), and it is straightforward to verify that setting $n = 4$ in table III of Haase and Butler (1985) produces 6-j symbols that coincide (to within a phase) with those determined from the functions $U_{5/2}$ of our table 1 for certain special values of w.

Although we have not considered in detail how to handle the multiplicity problems mentioned in § 1, our method can be used to set up equations that the 6-j symbols requiring multiplicity labels r must satisfy. For each triad $(\Gamma'\Gamma''\Gamma)_r$ an arbitrary separation must be made and carried forward in the synthesis of other 6-j symbols. How best to do this will depend to some extent at least on the physical problem in hand. For the triad $((w0)(w0)(20))_r$ of G_2, the separation corresponding to $r = a$, b of table 2 worked out well, the algebraic expressions of columns $(20)_a$ and $(20)_b$ being no more complex than others in the table. We cannot expect this happy state of affairs to be often repeated.

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