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Overlaps between the irreducible representations of two SO(7) subgroups of SO(8) used in the quark model of the atomic f shell

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Abstract. In his studies of f electrons in atoms, Racah introduced the group SO(7) and its subgroup G_2, with irreducible representations (irreps) W and U. By using a quarklike basis, these groups can be conveniently embedded in SO(8). This larger group, with irreps V, possesses two other SO(7) groups as subgroups that themselves contain G_2 as a common subgroup. One of them, SO(7)′ (with irreps W'), has been used to derive new selection rules on operators of physical interest. We describe methods for calculating the overlaps $(VWU|VW'U)$, the ultimate aim being to facilitate the transformations between SO(7) and SO(7)′. A table of relevant 6-U symbols (the G_2 generalizations of 6-j symbols) is given. When V possesses null triality (that is, when the symbols labelling the open ends of the Dynkin diagram for SO(8) are equal), an undetermined phase in the overlaps can be used to generate matrix representations of S_3, the permutation group on three objects. A brief table of zero overlaps is given. A remarkable factorization of the overlaps $((4310)W(40)|(4310)W'(40))$ is noted, where (4310) is the irrep of SO(8) with dimension 25725.

1. Introduction

Within the last two years, the group SO(8) has been introduced into the theory of the atomic f shell, thereby leading to explanations for some unexpected properties of the matrix elements of certain three-electron operators t_i for such complex configurations as f^6 and f^7 (Judd and Lister 1991, 1992a–e, 1993a–d). A key feature of the analysis is the augmenting of the group sequence $SO(8) \supset SO(7) \supset G_2$, in which the standard groups SO(7) and G_2 of Racah (1949) appear, with the alternative route $SO(8) \supset SO(7)' \supset G_2$. This procedure takes advantage of the well known automorphisms of SO(8), as discussed, for example, by Georgi (1982). The group SO(7)′ provides alternative labels for our states and operators, in terms of which new selection rules and additional applications of the Wigner–Eckart theorem can be made.

Consider, for example, the state $|VWU\rangle$, where V, W and U are irreducible representations (irreps) of SO(8), SO(7), and G_2. Further labels may be necessary, of course, to completely define the state, but for present purposes they are irrelevant.

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When the reductions $SO(8) \to SO(7)'$ and $SO(7)' \to G_2$ are considered, the irrep V can be expected to break up into several irreps W' of $SO(7)'$, each of which contains U of G_2. We can write

$$|VWU\rangle = \sum_{W'} (VW'U|VWU)|VW'U\rangle. \tag{1}$$

Our attention in the present paper is directed to the overlaps $(VW'U|VWU)$. It is convenient to specify the irreps appearing in these coefficients by means of their highest weights, following the scheme of Racah (1949). For an irrep V of reasonably small dimension, the overlaps can be found by elementary methods, as we have indicated already (Judd and Lister 1992c). However, for irreps V that describe some of our three-electron operators, the dimensions of V can run quite high. In a recent study of the operators t_6 and t_7 in the half-filled f shell, it has been noticed that some selection rules could be accounted for if the overlaps

$$((4310)(420)(40)|(4310)(311)'(40)) \tag{2}$$

and

$$((4310)(420)(40)|(4310)(410)'(40)) \tag{3}$$

were both zero (Judd and Lister 1993d). The dimension of (4310) is 25725 and the elementary methods for finding the overlaps (2) and (3) can no longer be applied. Although this problem provided much of the motivation for the present analysis, a knowledge of non-zero overlaps is crucial to any numerical work involving transformations from SO(7) to SO(7)$'$. It is to the evaluation of such coefficients that we turn our attention here.

2. Group structure

Each generator for Racah's groups SO(7) and G_2 is a coupled product of a creation and an annihilation operator for an f electron. When extending the theory to SO(8), sextuple products of these operators are introduced. The ensuing complications can be avoided by using the creation and annihilation operators for quarklike objects rather than electrons, as was first noticed by Labarthe (1980). In this scheme, the 16384 states of the atomic f shell are formed by coupling four statistically independent elementary spinors $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$ of SO(7). Two parity labels are also required (Judd and Lister 1991). Each spinor possesses eight components; they span the irrep (1000) of SO(8). The angular-momentum structure of (1000) is $s+f$, thereby providing what we call an s quark and an f quark. The four different quarks can be distinguished by a subscript θ, which runs over the range λ, μ, ν, and ξ. It is convenient to make the definitions

$$V^{(k)} = \sum_{\theta} (f_\theta^\dagger f_\theta)^{(k)} \qquad Z^{(3)} = (\tfrac{1}{2})^{1/2} \sum_{\theta} [(s_\theta^\dagger f_\theta)^{(3)} - (f_\theta^\dagger s_\theta)^{(3)}] \tag{4}$$

in terms of which the generators of SO(8) are the 28 components of the tensors $V^{(1)}$, $V^{(3)}$, $V^{(5)}$ and $Z^{(3)}$ (Judd and Lister 1992c). The generators of the SO(7) subgroup used by Racah (1949) in his classic analysis now take the form

$$V^{(1)} \qquad V^{(5)} \qquad -\tfrac{1}{2}V^{(3)} + (\tfrac{3}{4})^{1/2} Z^{(3)} \tag{5}$$

while those of SO(7)′ are simply $V^{(1)}$, $V^{(3)}$ and $V^{(5)}$. If we had used the creation and annihilation operators of electrons rather than quarks in the definition of $V^{(k)}$, the three tensors for which $k=1$, 3 and 5 would have given the generators of SO(7) *instead of SO(7)′. This demonstrates a remarkable reciprocity between the f quark* and the f electron (it is convenient to continue to distinguish these two objects by using italic and roman characters, respectively).

By reversing the relative phase between each *s* quark and the corresponding *f* quark (that is, by making the replacements $s_\theta^\dagger \to -s_\theta^\dagger$ and $s_\theta \to -s_\theta$, or, alternatively, $f_\theta^\dagger \to -f_\theta^\dagger$ and $f_\theta \to -f_\theta$), a third SO(7) group can be formed, which we call SO(7)″ (Judd and Lister 1992a). Its generators are

$$V^{(1)} \qquad V^{(5)} \qquad -\tfrac{1}{2}V^{(3)} - (\tfrac{3}{4})^{1/2} Z^{(3)}. \tag{6}$$

All three groups SO(7), SO(7)′ and SO(7)″ possess a common subgroup in G_2, whose 14 generators are the components of $V^{(1)}$ and $V^{(5)}$.

3. Casimir's operators

An obvious way to calculate the overlap coefficients is to diagonalize Casimir's *operator G for SO(7) using the basis* $|VW'U\rangle$. *We find, following the usual prescrip*tion (see, for example, Wybourne 1974 p 139),

$$G(\mathrm{SO}(7)) = (V^{(1)})^2 + (V^{(5)})^2 + \tfrac{1}{4}(V^{(3)})^2 - (\tfrac{3}{4})^{1/2}(V^{(3)} \cdot Z^{(3)}) + \tfrac{3}{4}(Z^{(3)})^2. \tag{7}$$

We can take advantage of our knowledge of other Casimir operators, namely

$$G(\mathrm{SO}(8)) = (V^{(1)})^2 + (V^{(3)})^2 + (V^{(5)})^2 + (Z^{(3)})^2 \tag{8}$$

$$G(\mathrm{SO}(7)') = (V^{(1)})^2 + (V^{(3)})^2 + (V^{(5)})^2 \tag{9}$$

$$G(\mathrm{G}_2) = \tfrac{1}{4}[(V^{(1)})^2 + (V^{(5)})^2] \tag{10}$$

to cast equation (7) in the form

$$G(\mathrm{SO}(7)) = \tfrac{3}{4}G(\mathrm{SO}(8)) - \tfrac{1}{2}G(\mathrm{SO}(7)') + 3G(\mathrm{G}_2) - (\tfrac{3}{4})^{1/2}(V^{(3)} \cdot Z^{(3)}). \tag{11}$$

In terms of the highest weights $(v_1v_2v_3v_4)$ of V, $(w_1'w_2'w_3')$ of W' and (u_1u_2) of G_2, the eigenvalues $\langle G\rangle$ of the various Casimir operators are given by

$$\langle G(\mathrm{SO}(8))\rangle = \tfrac{1}{2}[v_1(v_1+6) + v_2(v_2+4) + v_3(v_3+2) + v_4^2] \tag{12}$$

$$\langle G(\mathrm{SO}(7)')\rangle = \tfrac{1}{2}[w_1'(w_1'+5) + w_2'(w_2'+3) + w_3'(w_3'+1)] \tag{13}$$

$$\langle G(\mathrm{G}_2)\rangle = \tfrac{1}{12}[u_1^2 + u_2^2 + u_1u_2 + 5u_1 + 4u_2]. \tag{14}$$

The only term in equation (11) that presents us with a problem is the last. The tensor $V^{(3)}$ belongs to (110)′ of SO(7)′, just as Racah's $U^{(3)}$ belongs to (110) of SO(7). As for $Z^{(3)}$, it is formed by coupling an *s* quark (belonging to (000)′ of SO(7)′) to an *f* quark (belonging to (100)′), and thus possesses the SO(7)′ label (100)′. The only SO(3) scalar in (110)′ × (100)′ is contained in (111)′ and consequently in (00) of G_2, which are therefore the appropriate labels for $V^{(3)} \cdot Z^{(3)}$. However, $V^{(3)}$ is a generator of SO(7)′ and therefore cannot connect different irreps of that group. Thus the selection rules for $V^{(3)} \cdot Z^{(3)}$ are those of an operator with the labels (100)′ of SO(7)′ and (00) of G_2.

4. Elementary methods

Even though the matrix elements of $V^{(3)} \cdot Z^{(3)}$ may be unknown, we can often use our knowledge of the eigenvalues of $G(\mathrm{SO}(7))$ to find the overlaps we seek. Consider, for example, the irrep (3100) of SO(8). It is of interest to us because it is the sole source for the irrep (221) that labels some states appearing in the atomic configurations f^6 and f^7 (Racah 1949, table 1). We have given the branching rules for the reductions SO(8)→SO(7) and SO(8)→SO(7)′ elsewhere (Judd and Lister 1992a, table 1); for the present case they run

$$(3100) \rightarrow (211) + (221) \tag{15}$$

$$(3100) \rightarrow (100)' + (110)' + (200)' + (210)' + (300)' + (310)'. \tag{16}$$

The irreps (10), (20) and (30) of G_2 each appear twice in (3100). More precisely, each appears just once in both (211) and (221) and, for a particular $(u0)$, just once in $(u00)'$ and $(u10)'$. We find $\langle G(\mathrm{SO}(8))\rangle$ is 16 for (3100); $\langle G(\mathrm{SO}(7)')\rangle$ is $\frac{1}{2}u(u+5)$ for $(u00)'$ and $\frac{1}{2}(u+1)\,(u+4)$ for $(u10)'$; and $3\langle G(\mathrm{G}_2)\rangle$ is $\frac{1}{4}u(u+5)$ for $(u0)$. Within the basis provided by $(u00)'\,(u0)$ and $(u10)'(u0)$, the matrix of $G(\mathrm{SO}(7))$, from equation (11), takes the form

$$\begin{pmatrix} 12 & x \\ x & 11 \end{pmatrix}. \tag{17}$$

The cancellation of all terms in u and u^2 appears to be quite remarkable, until it is recognized that $\langle G(\mathrm{SO}(7))\rangle$ is 10 for (211) and 13 for (221), and that these numbers, being the eigenvalues of the matrix (17), must add to give the diagonal sum of that matrix, namely 23. Diagonal sums of this kind provide very useful checks on the working. The term involving $V^{(3)} \cdot Z^{(3)}$ produces the off-diagonal entries x. No contribution is made to the diagonal because the Kronecker squares $(u10)'^2$ and $(u00)'^2$ do not contain (100)′ (see Wybourne 1970, table D-4, with extensions).

It only remains to diagonalize (17). The fact that the eigenvalues are 10 and 13 fixes the magnitude of x at $2^{1/2}$, and we get

$$\begin{aligned} |(3100)(211)(u0)\rangle &= (\tfrac{1}{3})^{1/2}|(3100)(u00)'(u0)\rangle + (\tfrac{2}{3})^{1/2}|(3100)(u10)'(u0)\rangle \\ |(3100)(221)(u0)\rangle &= (\tfrac{2}{3})^{1/2}|(3100)(u00)'(u0)\rangle - (\tfrac{1}{3})^{1/2}|(3100)(u10)'(u0)\rangle \end{aligned} \tag{18}$$

for $u=1$, 2, or 3. The coefficients in these equations give the required overlaps. All phases (consistent with orthonormality) are arbitrary at this point, though as contact is made with other analyses certain constraints may be imposed.

Once the phases have been fixed we can write down the expansions of the states $|(3100)(211)''(u0)\rangle$ and $|(3100)(221)''(u0)\rangle$, in which irreps of SO(7)″ appear, by simply reversing the relative phases of the s and f quarks in the expansions (18). Take, for example, $u=3$. A four-quark state produces the irreps of SO(7)′ appearing in $(s+f)^4$, that is, in

$$[(000)' + (100)']^4. \tag{19}$$

The irrep (300)′ can only derive from $(000)'(100)'^3$, while the source of (310)′ can only be $(100)'^4$. The first corresponds to sf^3, the second to f^4. Thus we can obtain the required expansions for (211)″ and (221)″ by reversing the signs preceding either both initial kets or both final kets in the expansions (18). Similar results hold for $u=1$ and $u=2$. Again, constraints on our options may come from phase choices made elsewhere. We return to this point later.

5. Null triality

The branching rules for SO(8)→SO(7) and SO(8)→SO(7)′ given for (3100) in the decompositions (15) and (16) are strikingly different. However, for many irreps of interest they are the same. As Wybourne (1992) has pointed out, this occurs for the irrep $(v_1v_2v_30)$ of SO(8) when $v_2+v_3=v_1$. In Dynkin's notation (as used, for example, by McKay and Patera 1981), this implies identical labels on the free ends of the three arms of the diagram (a triskelion) for SO(8). Wybourne (1992) refers to such an event as null triality. A simple example is the irrep (2200) of dimension 300, corresponding to Dynkin labels 0 at the ends of the arms and 2 at the centre. The irrep (20) of G_2 occurs three times in (2200) corresponding to $W=(200)$, (210) and (220). Because of null triality, we know that the W' labels must be the same, namely (200)′, (210)′ and (220)′. The method of the previous section gives the overlaps $((2200)W'\ (20)|$ $(2200)\,W(20))$, which can be presented in the form of a matrix $R(\alpha)$:

$$R(\alpha)=\begin{pmatrix} 3/10 & -(7/20)^{1/2} & -(14/25)^{1/2} \\ -\alpha(7/20)^{1/2} & \alpha/2 & -\alpha(2/5)^{1/2} \\ -(14/25)^{1/2} & -(2/5)^{1/2} & 1/5 \end{pmatrix}. \tag{20}$$

We have anticipated the use of $R(\alpha)$ in section 10, where Racah's phases eliminate most of the sign choices for the overlaps. However, an ambiguity in α remains, as is made explicit in equation (20).

We can regard the matrix $R(\alpha)$ as a coordinate transformation in ordinary three-dimensional space. It is easy to check that $[R(-1)]^3=1$ and $[R(1)]^2=1$. Moreover, $\det R(-1)=1$ and $\det R(1)=-1$. Thus $R(-1)$ can be thought of as a rotation through $2\pi/3$ and $R(1)$ as a reflection. We can in fact use various powers of $R(1)$ and $R(-1)$ to form a matrix representation of the crystallographic point group C_{3v}, which is isomorphic to the permutation group on three objects, S_3. These groups are manifestations of the six outer automorphisms of SO(8), which seem to have been first recognized as relevant to problems in particle theory by Flowers and Szpikowski (1964), who refer to the mathematics as 'a bewildering world [where] a physicist may prefer to be guided by his physics'.

Bewildering or not, we can apply the conditions on $R(\alpha)$ to greatly assist us in our determination of the overlaps for cases where matrices larger than 3×3 occur. Unfortunately we cannot go very far because quartic and quintic equations soon appear. The largest matrix we have successfully solved by using the null triality condition is 6×6, corresponding to the overlaps $((4220)\,W'(22)|(4220)\,W(22))$, where

$$W=(220),(320),(321),(420),(421),(422). \tag{21}$$

Before turning to the development of a more systematic procedure, we note that the ambiguity in α corresponds to the impossibility of distinguishing SO(7) from SO(7)″ without a knowledge of the signs of the matrix elements of $Z^{(3)}$, which lie outside the range of the analysis of Racah (1949). The middle row of the matrix (20) corresponds to $W'=(210)'$ of sf^3, and we see that the elements in this row, all of which involve α, reverse their signs in step with the sign change of s or f in going from SO(7) to SO(7)″.

6. Induced transformations

Since our model of the atomic f shell comprises four quarks, no physical operator involves more than four creation operators and four annihilation operators. Thus no representations of W' beyond those appearing in $[(000)'+(100)']^8$ are required. This limits the interesting irreps $(v_1v_2v_3v_4)$ of SO(8) to those for which the sum of the four weights v_i does not exceed 8. All of these can be formed by coupling pairs (V_1, V_2) of irreps for each of which the sum of the weights does not exceed four. A useful choice is $V_1=V_2=(2200)$, since $(2200)^2$ generates the irreps

$$\begin{gathered}(0000), (2000), (2200)\ \text{(twice)}, (111\pm1), (2220), (222\pm2), (311\pm1),\\ (3210), (331\pm1), (4000), (4200), (4220), (4400) \qquad (22)\end{gathered}$$

in its symmetric part and

$$(1100), (2110), (221\pm1), (3100), (3210), (322\pm1), (3300), (4110), (4310) \qquad (23)$$

in its antisymmetric part. Most of the irreps of interest to us are included in the sequences (22) and (23), and we can take advantage of the symmetry or antisymmetry of their origin when working out the coupling coefficients.

A transformation of the type $R(\alpha)$ leaves the G_2 label for the states invariant. This is also true, of course, for its inverse, which expands a state labelled by W' in terms of the W states. This means that we do not need to work out the complete Clebsch–Gordan coefficients involved in coupling V_1 and V_2 to V but only the part comprising the group labels U, W (or W'), and V. Coefficients of this type are usually referred to as isoscalar factors (Edmonds 1962). In the notation of Racah (1949), the isoscalars of interest to us for the problem at hand are

$$(((2200)\,(2200))VW'U|(2200)W'_1U_1+(2200)W'_2U_2). \qquad (24)$$

Once these coefficients are known we can make the substitutions for $(2200)W'_1U_1$ and $(2200)W'_2U_2$ with the aid of the inverses of matrices of the type (20) and then couple the parts $(2200)W_1U_1$ and $(2200)W_2U_2$ to obtain the states defined by VWU. By this device the transformations from W'_i to W_i in each of the component irreps (2200) induce the transformation from W' to W that gives the required overlaps.

7. Isoscalar factors

To calculate the isoscalars (24) we can appeal to well-established techniques, such as that of Nutter and Nielsen (1963). Adapting their approach, we first consider the two parts (a and b) of a system coupled at the SO(7)′ level. That is, we take the state $|(W'_1W'_2)W'U\rangle$ and require that the eigenvalues of $V_a^{(3)}\cdot V_b^{(3)}$, calculated in the basis $|W'_1U_1, W'_2U_2, U\rangle$ (for various U_1 and U_2) be equal to those of

$$\tfrac{1}{2}(V_a^{(3)}+V_b^{(3)})^2-\tfrac{1}{2}(V_a^{(3)})^2-\tfrac{1}{2}(V_b^{(3)})^2. \qquad (25)$$

The eigenfunctions are just the isoscalars $(W'U|W'_1U_1+W'_2U_2)$ we seek. The operator (25) can be evaluated by using equations (9) and (10) to convert the three parts to the differences between two Casimir operators, and then determining their eigenvalues from equations (13) and (14). When calculating the matrix elements of $V_a^{(3)}\cdot V_b^{(3)}$, we take advantage of the fact that our three-electron operators are scalar with respect to the orbital angular momentum L, so we can limit our analysis to irreps U of G_2 that contain the SO(3) scalar. We use equation (7.1.6) of Edmonds (1957), with recoupled bras and kets at the G_2 level, to give

$$\langle W_1'U_1, W_2'U_2, U0|V_a^{(3)}\cdot V_b^{(3)}|W_3'U_3, W_4'U_4, U0\rangle$$

$$= -\sum_{L_1, L_3} [(2L_1+1)(2L_3+1)]^{-1/2}(U0|U_1L_1+U_2L_1)(U_3L_3+U_4L_3|U0)$$

$$\times (W_1'U_1L_1\|V_a^{(3)}\|W_3'U_3L_3)(W_2'U_2L_1\|V_b^{(3)}\|W_4'U_4L_3). \tag{26}$$

To reduce mathematical clutter in equation (26), we have suppressed any multiplicity labels that might be necessary to define the states. The reduced matrix elements of $V^{(3)}$ in this expression can be read off from the tables of Nielson and Koster (1963) provided their entries for $U^{(3)}$ are multiplied by $7^{1/2}$. Some of the isoscalar factors involving L_1 and L_3 in equation (26) can be extracted from tables VIa and XIVa of Racah (1949); others need to be calculated. In a few cases U occurs twice in the reduction of $U_1\times U_2$. Our choice of multiplicity labels is described in the appendix.

It is convenient to choose phases so that

$$(U0|U_1L_1+U_2L_1) = (U0|U_2L_1+U_1L_1). \tag{27}$$

We have the freedom to make this choice when $U_1\neq U_2$ (see, for example, Butler 1981 p 50). When $U_1=U_2$, it might be thought that there was a possibility of conflict should U occur in the antisymmetric part of U_1^2. However, the SO(3) scalar always occurs in the symmetric part of $L_1\times L_1$, so the isoscalar factors necessarily vanish in that case.

8. 6-U symbols

To describe our results we generalize equation (7.1.6) of Edmonds (1957) from SO(3) to G_2. The tensor $V^{(3)}$ is rewritten as $V^{(10)}$ to indicate the G_2 irrep to which $V^{(3)}$ belongs. Equation (26) becomes

$$\langle W_1'U_1, W_2'U_2, U|V_a^{(10)}\cdot V_b^{(10)}|W_3'U_3, W_4'U_4, U\rangle$$

$$= \begin{Bmatrix} U_1 & U_2 & U \\ U_4 & U_3 & (10) \end{Bmatrix} (W_1'U_1\|\|V_a^{(10)}\|\|W_3'U_3)(W_2'U_2\|\|V_b^{(10)}\|\|W_4'U_4) \tag{28}$$

and we identify the right-hand side of equation (26) with the right-hand side of equation (28). The array of six irreps of G_2 is a generalization of a 6-j symbol; we call it a 6-U symbol. Objects of this kind have been widely discussed for various groups (see, for example, Griffith (1962), Butler (1981) and Judd (1986)). In fact, equation (28) can be regarded as a special case of equation (19.9) of Butler (1975). The triple uprights appearing in the matrix elements above indicate reduction with respect to G_2 rather than to SO(3). That is, the L dependence inherent in an SO(3) reduced matrix element has been removed by factoring out an isoscalar factor according to the scheme

$$(W_1'U_1\|\|V^{(10)}\|\|W_3'U_3)(U_3L_3+(10)3|U_1L_1)$$

$$= [\mathrm{Dim}(U_1)/(2L_1+1)]^{1/2}(W_1'U_1L_1\|V^{(3)}\|W_3'U_3L_3). \tag{29}$$

According to Nielson and Koster (1963), the interchange $W_1'U_1L_1 \leftrightarrow W_3'U_3L_3$ in the matrix element of $V^{(3)}$ introduces the phase $(-1)^{L_1-L_3}$. The reciprocity condition of

Table 1. Values of the reduced matrix elements $((2200)W_1'U_1\|T^{(10)}\|(2200)W_2'U_2)$ for $T^{(10)}=V^{(10)}$ and $Z^{(10)}$. The zero entries derive from the SO(7)′ labels for $V^{(10)}$ and $Z^{(10)}$ (namely (110)′ and (100)′, respectively) and the fact that $V^{(10)}$ is a generator SO(7)′ and must necessarily be diagonal with respect to W'.

$W_1'U_1$	$W_2'U_2$	$V^{(10)}$	$Z^{(10)}$
(200)′(20)	(200)′(20)	$3(7)^{1/2}$	0
	(210)′(11)	0	$-3(14/5)^{1/2}$
	(210)′(20)	0	$-9(3/5)^{1/2}$
	(210)′(21)	0	$-24/(5)^{1/2}$
(210)′(11)	(210)′(20)	$-3(6)^{1/2}$	0
	(210)′(21)	4	0
	(220)′(20)	0	$-12/(5)^{1/2}$
	(220)′(21)	0	4
(210)′(20)	(210)′(20)	$3(7)^{-1/2}$	0
	(210)′(21)	$12(3/7)^{1/2}$	0
	(220)′(20)	0	$12(6/35)^{1/2}$
	(220)′(21)	0	$-12(3/7)^{1/2}$
(210)′(21)	(210)′(21)	$4(22/7)^{1/2}$	0
	(220)′(20)	0	$-3(2/35)^{1/2}$
	(220)′(21)	0	$-4(22/7)^{1/2}$
	(220)′(22)	0	$-(154)^{1/2}$
(220)′(20)	(220)′(20)	$-24/(7)^{1/2}$	0
	(220)′(21)	$-9(10/7)^{1/2}$	0
(220)′(21)	(220)′(21)	$-4(22/7)^{1/2}$	0
	(220)′(22)	$(154)^{1/2}$	0

Racah (1949, equation (47)), when applied to the isoscalar appearing in equation (29), precisely cancels this phase so that the rule

$$(W_1'U_1\|V^{(10)}\|W_3'U_3)=(W_3'U_3\|V^{(10)}\|W_1'U_1) \tag{30}$$

is valid. Values of the triply reduced matrix elements relevant to the problems under study are set out in table 1. The condition (30), taken with equation (27) and the Hermiticity of the operator $V_a^{(3)}\cdot V_b^{(3)}$, leads to the very convenient symmetry conditions

$$\begin{Bmatrix} U_1 & U_2 & U \\ U_4 & U_3 & (10) \end{Bmatrix} = \begin{Bmatrix} U_2 & U_1 & U \\ U_3 & U_4 & (10) \end{Bmatrix} = \begin{Bmatrix} U_3 & U_4 & U \\ U_2 & U_1 & (10) \end{Bmatrix}$$
$$= \begin{Bmatrix} U_4 & U_3 & U \\ U_1 & U_2 & (10) \end{Bmatrix} \tag{31}$$

on the 6-U symbols. These relations are unaffected by the inclusion (when necessary) of multiplicty labels for the triads $[U_1, U_2, U]$ and $[U_3, U_4, U]$. A tabulation of values is given in table 2 for $U=(22)$, (40) and (42). These irreps are appropriate for analyses (to second-order in perturbation theory) of the non-trivial scalar operators in the atomic f shell.

9. Extensions to SO(8)

The tabulation of the 6-U symbols is a by-product of the calculation of the SO(7)′

isoscalar factors $(W'U|W_1'U_1+W_2'U_2)$, which, as stated at the beginning of section 7, is the first part of our project for calculating the isoscalars (24). However, the 6-U symbols are very useful when we move up from SO(7)′ to SO(8) because the analogous operator to $V_a^{(3)}\cdot V_b^{(3)}$, namely $Z_a^{(3)}\cdot Z_b^{(3)}$, is built from tensors of the type $Z^{(3)}$ that belong to the same irrep (10) of G_2 that the tensors of the type $V^{(3)}$ do. Thus the same 6-U symbols appear in the analogue of equation (28) as before. All the phase choices buried in the calculation of the entries of table 2, and depending, of course, on choices made by Racah (1949) and Nielson and Koster (1963), are automatically carried forward without the need for additional analysis.

The procedure for SO(8) follows that described in section 7 for SO(7)′. The matrix of $Z_a^{(3)}\cdot Z_b^{(3)}$ is calculated in the basis provided by the states

$$|(2200)\,W_1'U_1,\,(2200)\,W_2'U_2,\,U\rangle \tag{32}$$

for various W_1', W_2', U_1 and U_2. The replacements $V_i^{(10)}\to Z_i^{(10)}$ are made in equation (28) for $i=a$ and $i=b$. The new reduced matrix elements are given in table 1, and the 6-U symbols can be read off from table 2. The eigenvalues of the matrix are necessarily those of

$$\tfrac{1}{2}(Z_a^{(3)}+Z_b^{(3)})^2-\tfrac{1}{2}(Z_a^{(3)})^2-\tfrac{1}{2}(Z_b^{(3)})^2 \tag{33}$$

which can be expressed in terms of Casimir's operators for irreps of SO(8), SO(7)′, $SO_a(8)$, $SO_a(7)'$, $SO_b(8)$ and $SO_b(7)'$ (taken in that order) as

$$\tfrac{1}{2}[G(V)-G(W)-G(2200)+G(W_1')-G(2200)+G(W_2')] \tag{34}$$

with the help of equations (8) and (9). The eigenfunctions of the matrix give the required isoscalars (24).

This procedure can be simplified by taking advantage of the separation of $(2200)^2$ into symmetric and antisymmetric parts, as given by the sequences (22) and (23). For example, for $V=(4310)$ it is better to replace the basis (32) by the antisymmetric forms

$$(\tfrac{1}{2})^{1/2}|(2200)\,W_1'U_1,\,(2200)\,W_2'U_2,\,U\rangle-(\tfrac{1}{2})^{1/2}|(2200)\,W_2'U_2,\,(2200)\,W_1'U_1,\,U\rangle. \tag{35}$$

We also note that the matrix of $Z_a^{(10)}\cdot Z_b^{(10)}$, calculated in this basis, breaks up into two non-interacting blocks. This is because we can regard both $Z_a^{(10)}$ and $Z_b^{(10)}$ as changing the number of s quarks in each space (a and b) by 1, thereby preserving the evenness or oddness of the total number of s quarks in the coupled forms (35). This greatly simplifies the process of diagonalization.

10. Overlaps

We are now ready to follow the procedure outlined at the end of section 6 to calculate the overlaps. The expansions of $|(2200)WU\rangle$ in terms of $|(2200)\,W'U\rangle$, as found by the elementary methods of sections 4 and 5, contain many arbitrary phases. Severe limitations can now be imposed on these phases by insisting that the transformation from SO(7) to SO(7)′, followed by a recoupling of $(2200)\,W_1'U_1$ and $(2200)\,W_2'U_2$, produces states belonging to the original V and not to any others. In this way the phase choices of Racah (1949) and Nielson and Koster (1963) make themselves felt. However, the phase α is not constrained and is carried forward in the calculations.

As an example of our analyses we give in table 3 the overlaps $S(\alpha)$ for the irreps W and W' belonging to (4310) of SO(8) and containing (22) of G_2. Since (4310) possesses null triality, we expect $S(\alpha)$ to have similar properties to $R(\alpha)$. It is straightforward to confirm that the matrices $S(1)$, $S(-1)$, and their various products form a represen-

Table 2. Values of the 6-U symbols

$$\begin{Bmatrix} U_1 & U_2 & U \\ U_4 & U_3 & (10) \end{Bmatrix}$$

for $U=(22)$, (40) and (42). When required, multiplicity labels for the couplings $(U_1U_2)U$ or $(U_3U_4)U$ are indicated by the subscripts 1 and 2. When a coupling requires a multiplicity label for a particular U but not for a different U, the entry for the latter is listed just once opposite the subscripted coupling 1. All numbers following a solidus are in the denominator.

U_1 U_2	U_3 U_4	(22)	(40)	(42)
(11) (21)	(20) (20)	0	$-1/12(21)^{1/2}$	0
	(20) (21)	0	$1/8(231)^{1/2}$	0
	(20) (22)	0	$-5/28(165)^{1/2}$	0
	(21) (11)	0	$-1/64$	0
	(21) (20)	0	$3/64(21)^{1/2}$	0
	$[(21)\ (21)]_1$	0	$-5/32(385)^{1/2}$	0
	$[(21)\ (21)]_2$	0	$-3/16(231)^{1/2}$	0
	$[(21)\ (22)]_1$	0	$-11/896$	0
	$[(21)\ (22)]_2$	0	$15/128(1155)^{1/2}$	0
(11) (22)	(20) (21)	$-1/12(77)^{1/2}$	0	0
	$[(21)\ (21)]_1$	$-1/8(154)^{1/2}$	0	0
	$[(21)\ (21)]_2$	0	0	0
(20) (20)	(20) (20)	$-4/189$	$2/189$	0
	(20) (21)	$5/168(15)^{1/2}$	$1/42(2)^{1/2}$	0
	$[(21)\ (21)]_1$	$(15)^{1/2}/252$	$-5/168(15)^{1/2}$	0
	$[(21)\ (21)]_2$	$-(39)^{1/2}/672$	$1/112$	0
(20) (21)	(20) (21)	$29/504(22)^{1/2}$	$-1/126(22)^{1/2}$	0
	(20) (22)	$-(143)^{1/2}/792$	$-5/18(770)^{1/2}$	0
	(21) (20)	$-1/84$	$-13/1344$	0
	$[(21)\ (21)]_1$	$1/56(22)^{1/2}$	$-25/224(165)^{1/2}$	0
	$[(21)\ (21)]_2$	$(1430)^{1/2}/3696$	$-1/336(11)^{1/2}$	0
	$[(21)\ (22)]_1$	0	$3/128(21)^{1/2}$	0
	$[(21)\ (22)]_2$	0	$25/384(55)^{1/2}$	0
(20) (22)	$[(21)\ (21)]_1$	0	$-1/8(231)^{1/2}$	$-1/8(231)^{1/2}$
	$[(21)\ (21)]_2$	$(55)^{1/2}/1056$	$-5/48(385)^{1/2}$	0
$[(21)\ (21)]_1$	$[(21)\ (21)]_1$	$-5/448$	$3/4928$	$7/2112$
	$[(21)\ (21)]_2$	$-(65)^{1/2}/2464$	$(15)^{1/2}/1232$	0
	$[(21)\ (22)]_1$	0	$-5/64(385)^{1/2}$	$-13/132(182)^{1/2}$
	$[(21)\ (22)]_2$	0	$-(3)^{1/2}/704$	0
	$[(22)\ (22)]_1$	$-1/28(11)^{1/2}$	$-(15)^{1/2}/2156$	$5/132(70)^{1/2}$
	$[(22)\ (22)]_2$	0	0	0
$[(21)\ (21)]_2$	$[(21)\ (21)]_2$	$-27/4928$	$31/4928$	0
	$[(21)\ (22)]_1$	0	$-3/32(231)^{1/2}$	0
	$[(21)\ (22)]_2$	0	$(5)^{1/2}/352$	0
	$[(22)\ (22)]_1$	$-(715)^{1/2}/27104$	$5/1232$	0
	$[(22)\ (22)]_2$	$-9/176(33)^{1/2}$	0	0
$[(21)\ (22)]_1$	$[(22)\ (21)]_1$	0	$1/2816$	$-1/132$
	$[(22)\ (21)]_2$	0	$15/256(1155)^{1/2}$	0
$[(21)\ (22)]_2$	$[(22)\ (21)]_2$	0	$-13/2816$	0

Table 3. The overlaps $((4310)W'(22)|(4310)W(22))$. The entries below correspond to $S(1)$ of section 10. To find $S(-1)$, the last four rows should be multiplied by -1. These rows are labelled by irreps W' with highest weights $(w_1'w_2'w_3')$ whose sum $w_1'+w_2'+w_3'$ is odd, corresponding to an odd number of s quarks.

W'	W (321)	(431)	(420)	(311)
(321)′	27/50	$(286/625)^{1/2}$	$-(13/625)^{1/2}$	$(27/350)^{1/2}$
(431)′	$(286/625)^{1/2}$	$-3/50$	$-(11/1250)^{1/2}$	$-(143/525)^{1/2}$
(420)′	$-(13/625)^{1/2}$	$-(11/1250)^{1/2}$	$-12/25$	$-(104/525)^{1/2}$
(311)′	$(27/350)^{1/2}$	$-(143/525)^{1/2}$	$-(104/525)^{1/2}$	2/21
(320)′	$-(14/125)^{1/2}$	$(143/875)^{1/2}$	$-(234/875)^{1/2}$	$-(16/735)^{1/2}$
(331)′	$-(143/3500)^{1/2}$	$(72/875)^{1/2}$	$-(11/875)^{1/2}$	$-(143/1470)^{1/2}$
(421)′	0	$-(1/84)^{1/2}$	$-(11/42)^{1/2}$	$(143/441)^{1/2}$

	W (320)	(331)	(421)
(321)′	$-(14/125)^{1/2}$	$-(143/3500)^{1/2}$	0
(431)′	$(143/875)^{1/2}$	$(72/875)^{1/2}$	$-(1/84)^{1/2}$
(420)′	$-(234/875)^{1/2}$	$-(11/875)^{1/2}$	$-(11/42)^{1/2}$
(311)′	$-(16/735)^{1/2}$	$-(143/1470)^{1/2}$	$(143/441)^{1/2}$
(320)′	3/35	$(286/1225)^{1/2}$	$(143/735)^{1/2}$
(331)′	$(286/1225)^{1/2}$	$-51/70$	$(2/735)^{1/2}$
(421)′	$(143/735)^{1/2}$	$(2/735)^{1/2}$	$-19/42$

tation of the permutation group S_3, as before. That is, all matrix multiplications involving the various products of the $S(\alpha)$ are identical to those of the $R(\alpha)$ if we make the correspondences $S(1)\leftrightarrow R(1)$ and $S(-1)\leftrightarrow R(-1)$. In particular, $[S(1)]^2=1$ and $[S(-1)]^3=1$.

We have examined several sets of overlaps for which V and U correspond to operators of physical interest. Table 4 lists the null overlaps we have found. They are more numerous than might have been expected; however, the overlaps (2) and (3), whose possibly null values provided much of the motivation for our calculations, turn out to be $-(11/70)^{1/2}$ and $(9/70)^{1/2}$, neither of which is zero.

Table 4. Null overlaps $(VW'U|VWU)$. The entries in the columns W and W' can be interchanged, the prime remaining in the column W'. Irreps W or W' that occur more than once in a particular V are distinguished by subscripts.

V	W	W'	U
(3311)	none		(22), (40), (42)
(4220)	(320)	(421)′	(22)
(4220)	(322)	(421)′	(40)
(4220)	none		(42)
(4310)	(321)	(421)′	(22)
(4310)	(430)	(430)′	(33)
(4310)	none		(40)
(4310)	$(431)_1$	$(431)_2$	(42)
	(420)	$(431)_2$	
(4400)	(410)	(430)	(40)

Table 5. Irreps W occurring in $(4310)W(u0)$. They are arranged to emphasize an inherent triplet structure.

$(u0)$	W
(20)	(311)(321)(331)
(30)	(311)(321)(331), (310)(320)(330), (411)(421)(431)
(40)	(311)(321)(331), (410)(420)(430), (411)(421)(431)
(50)	(411)(421)(431)

11. The special case $(4310)W(u0)$

The irreps W containing $(u0)$ of G_2 occur in a remarkable triplet pattern in (4310). This is shown in table 5. The elementary methods of section 4 can be used to determine the overlaps for $u=2$ and $u=5$. Ordering the irreps W and W' in the sequence $(w11)$, $(w21)$ and $(w31)$, where $w=3$ and 4 for $u=2$ and 5 respectively, we obtain the same matrix $T(\alpha)$ for both values of u, namely

$$T(\alpha)=\begin{pmatrix} 2/7 & (5/14)^{1/2} & (55/98)^{1/2} \\ \alpha(5/14)^{1/2} & (\alpha/2) & -\alpha(11/28)^{1/2} \\ (55/98)^{1/2} & -(11/28)^{1/2} & 3/14 \end{pmatrix}. \tag{36}$$

We have also calculated the overlaps $((4310)W'(40)|(4310)W(40))$ by the methods of sections 7–10, getting a 9×9 matrix $P(\alpha)$. Very remarkably, every entry in $P(\alpha)$ can be written as a product of one entry of $T(\alpha)$ and one entry of $Q(\alpha)$, where

$$Q(\alpha)=\begin{pmatrix} -3\alpha/5 & \alpha(1/5)^{1/2} & \alpha(11/25)^{1/2} \\ (1/5)^{1/2} & -1/2 & (11/20)^{1/2} \\ \alpha(11/25)^{1/2} & -\alpha(11/20)^{1/2} & -\alpha/10 \end{pmatrix}. \tag{37}$$

The rule of composition is as follows. We write $T(\alpha)$ as $(w_2'|w_2)$, where the rows of $T(\alpha)$ are labelled by $w_2'=1, 2, 3$ and the columns by $w_2=1, 2, 3$. We write $Q(\alpha)$ as $(w_1'w_3'|w_1w_3)$, where the rows of $Q(\alpha)$ are labelled by $(w_1'w_3')=(40), (41), (31)$ and the columns by $(w_1w_3)=(40), (41), (31)$. Then

$$((4310)(w_1'w_2'w_3')(40)|(4310)(w_1w_2w_3)(40))=(w_2'|w_2)(w_1'w_3'|w_1w_3). \tag{38}$$

The matrices $T(\alpha)$ and $Q(\alpha)$, as well as the composites $P(\alpha)$, separately follow the same multiplication rules in S_3 as $R(\alpha)$ and $S(\alpha)$. A factorization of the kind represented by equation (38) is unique among the overlaps we have calculated.

In quantum mechanics, we are familiar with the principle that the eigenfunctions of independent systems multiply while their eigenvalues add. Since the overlaps are the eigenfunctions of $G(\mathrm{SO}(7))$, we anticipate being able to write

$$\begin{aligned}&\langle(4310)(w_1'w_2'w_3')(40)|G(\mathrm{SO}(7))|(4310)(w_1''w_2''w_3'')(40)\rangle\\ &\quad=\delta(w_1', w_1'')\delta(w_3', w_3'')\langle w_2'|A|w_2''\rangle+\delta(w_2', w_2'')\langle w_1'w_3'|B|w_1''w_3''\rangle\end{aligned} \tag{39}$$

where $(w_1'w_2'w_3')$ and $(w_1''w_2''w_3'')$ are two irreps of $\mathrm{SO}(7)'$. This indeed turns out to be so. Moreover, the eigenvalues of A (which, with an arbitrary additive constant C, are $C-4$, $C-1$ and $C+3$) can be combined in all nine ways with the eigenvalues of B (namely, $19-C$, $24-C$, $25-C$) to give the roots

$$15, 18, 22; 20, 23, 27; 21, 24, 28 \tag{40}$$

that we know must occur by evaluating $\langle G(\mathrm{SO}(7))\rangle$ for the nine irreps appearing opposite (40) in table 5. We can thus see in a transparent way how the factorization (38) guarantees that the correct roots are produced. However, it is not obvious that the requirement of correct roots forces the factorization to take place; indeed, for all other cases we have studied it does not. Our understanding is thus a limited one, and we are not in a position to specify other irreps V of SO(8) and U of G_2 where similar properties obtain.

12. Concluding remarks

The techniques described above allow us to calculate the overlaps $(VWU|VW'U)$ for all operators in the atomic f shell that are scalar with respect to L. Extensions to others, such as the spin–orbit interaction, call for a generalization of equation (26). Instead of being able to limit ourselves to the scalar component 0 of U, we would have to be prepared to cope with the appearance of other SO(3) ranks. The right-hand side of equation (26) would contain a 6-j symbol and the summations over running indices would become more lengthy. However, no new principle would have to be invoked.

The permutation group S_3 makes itself felt particularly strongly in cases of null triality, where the matrices of the type $R(-1)$, $S(-1)$, etc. can be interpreted as rotations through $2\pi/3$. This property had already appeared in simple cases where only two values of W and W' occur, such as (2200) W(21) (Judd and Lister 1992c). The overlaps here turn out to be $\frac{1}{2}$ and $(\frac{3}{4})^{1/2}$, clearly indicative of 120° rotations.

The reader may wonder whether explicit expressions might exist for the overlaps. In the course of our work we noticed that the matrix for (3210) W(22) was the same as a rotation matrix for SO(3). In detail

$$((3210)\,W(22)|(3210)\,W'(22)) = 2^{1/2} d^{7/2}_{MN}(\tfrac{1}{2}\pi) \tag{41}$$

where $M = -\frac{7}{2}, -\frac{3}{2}, \frac{1}{2}, \frac{5}{2}$ for $W = (220)$, (320), (321) and (311) (with analogous correspondences for N and W'). However, an analytic result of this type cannot be easily generalized, since multiplicity labels are sometimes required to separate identical irreps of SO(7) or SO(7)$'$. An example of this complication occurs in table 4. For the moment the unexpected results we have uncovered remain as suggestive examples for future analysis.

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Appendix. Isoscalars with multiplicity labels

In the course of our work we have had to separate pairs of resultants U coming from several couplings of the type $[U_1U_2]U$. For [(21)(21)](22) and [(22)(22)](22), we have used the result of Racah (1949, equation 78) to give

$$((22)_1 0|(21)L + (21)L) = A(2L+1)^{1/2}[\tfrac{1}{2}L(L+1) - 21] \tag{A1}$$

Table A1. Isoscalars $(U_i0|U_1L+U_2L)$ with multiplicity labels i. The two columns headed by a particular $[U_1U_2]U_i$ correspond to $i=1$ and $i=2$, respectively. All entries must be multiplied by $[(2L+1)/F]^{1/2}$, where the factor F is given at the foot of the column to which it applies.

	$[U_1U_2]U_i$							
L	$[(21)(21)](22)_i$		$[(22)(22)](22)_i$		$[(21)(21)](40)_i$		$[(21)(22)](40)_i$	
0	0	0	−30	−598	0	0	0	0
1	0	0	0	0	0	0	0	0
2	−18	39	−27	−316	104	13	$9(78)^{1/2}$	$63(78)^{1/2}$
3	−15	−78	0	0	65	−65	0	0
4	−11	−66	−20	496	−99	55	$-27(11)^{1/2}$	$7(11)^{1/2}$
5	−6	99	−15	−299	−44	−75	$-3(546)^{1/2}$	$-17(546)^{1/2}$
6	0	0	−9	−164	0	0	0	0
7	7	21	0	0	21	133	0	0
8	15	−27	6	366	5	−75	$5(665)^{1/2}$	$-9(665)^{1/2}$
9	0	0	0	0	0	0	0	0
10	0	0	25	−147	0	0	0	0
F	9240	216216	25410	7135128	200200	480480	440440	4204200

$$((22)_10|(22)L+(22)L)=B(2L+1)^{1/2}[\tfrac{1}{2}L(L+1)-30]. \qquad \text{(A2)}$$

To normalize the isoscalars, we take $A=(9240)^{-1/2}$ and $B=(216216)^{-1/2}$. The orthogonal sets of coefficients are denoted by the subscript 2 and are set out in table A1.

For [(21)(21)](40) the choice is not so obvious. The analogues of equations (A1) and (A2) can be found in table VIa of Racah (1949), but his entries $(21|\chi_i|21)$ for $i=1$ and 2 are not orthogonal. To avoid high prime numbers as far as possible we pick

$$((40)_10|(21)L+(21)L)=[(2L+1)/200200]^{1/2}[\tfrac{1}{4}(21|\chi_1|21)+\tfrac{3}{4}(21|\chi_2|21)] \qquad \text{(A3)}$$

$$((40)_20|(21)L+(21)L)=[(2L+1)/480480]^{1/2}(21|\chi_2|21). \qquad \text{(A4)}$$

For his work on the Coulomb interaction in the f shell, Racah only needed one set of coefficients coming from the coupling [(21)(22)](40) in spite of the fact that (40) occurs twice in $(21)\times(22)$. The pair we use are given in table A1. A linear combination of them is required to produce Racah's $(21|\chi|22)$.

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