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Effective operators in the quark model of the atomic f shell

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Abstract. The use of the quark configuration $(s+f)^4$ to represent the states of the atomic f shell calls for a simultaneous transformation of operators. Operator equivalences are developed for z_0 , a two-electron operator associated with spin-spin interactions, and t_{11} , a scalar three-electron operator appearing in third order in perturbation theory. Both belong to the irreducible representation (1R) (111) of Racah's group $SO(7)$, and can be represented by combinations of the single-quark operators of the types $(f_\theta^\dagger f_\theta)^{(2)}$ and $(f_\theta^\dagger f_\theta)^{(0)} - 7^{1/2} s_\theta^\dagger s_\theta$, where θ distinguishes the four quarks. The group $SO(7)'$ (which plays the same role for the f quarks as $SO(7)$ does for the f electrons) is used to establish relations between matrix elements of z_0 and those of other electronic operators such as $U^{(2)}$ and $W^{(12)}$, thereby accounting for various unexpected connections and proportionalities that go beyond what would be expected from straightforward applications of the Wigner-Eckart theorem.

1. Introduction

The concept of effective operators is often used in atomic shell theory. A very familiar example is the equivalence

$$H_{SO} = \zeta \sum_i s_i \cdot l_i \equiv \lambda S \cdot L \quad (1)$$

for the electronic spin-orbit interaction H_{SO} . The operator on the left can be evaluated in a basis provided by Slater determinants, while that on the right is suitable for Russell-Saunders states of the type $^{2S+1}L_J$. Energies of the levels of an SL multiplet can now be very easily reproduced in terms of the single parameter λ , which varies with S and L . In a similar way, the equivalences that we establish in the present paper are valid for particular sets of spectroscopic terms only. However, they are useful to expose special properties of the electron operators, just as the use of λ above avoids the need to expand every J level in Slater determinants when finding its energy.

The present paper aims to account for some of the otherwise unsuspected properties of electronic operators by representing them by effective operators that act on a basis built from fictitious particles that we have called quarks (Judd and Lister 1991, 1992a, b, 1993). For f electrons, this amounts to replacing the 15 configurations f^N ($0 \leq N \leq 14$) by the states q^4 , where each one of the four quarks q belongs to the irreducible representation (1R) $(\frac{1}{2} \frac{1}{2} \frac{1}{2})$ of the group $SO(7)$ of Racah (1949). Individual quarks are distinguished by the four subscripts λ, μ, ν, ξ (and indicated generically by θ). The use of

the name 'quark' is intended to draw out the parallel with the quarks of high-energy physics: both kinds cannot be observed singly, and both are described by the $\mathbf{1R}$ of a Lie group. No radial character is assigned to the quarks: their role is purely to represent the angular properties of the f electrons. To completely define the angular part of an electronic state in the quark basis, two parity labels are also required: they denote the oddness or evenness of the numbers of electrons with spins up and spins down. Our quarks q are statistically independent (that is, unlike electrons, they do not have to satisfy a Pauli principle), and they each possess the angular-momentum structure $s+f$. When working at the $\text{SO}(3)$ level, it is convenient to take advantage of the decomposition $q \rightarrow s+f$ by referring to the s and f components as quarks in their own right. In what follows we distinguish f quarks from f electrons by using italics for the former. The quark model preserves the orbital angular momenta L of the electronic states, but the total spin S and the electron number N are often mixed.

Much of our previous work on the quark model has been aimed at explaining certain properties of the three-electron operators t_i (Judd and Lister 1991, 1993). The t_i enter when configuration interaction via the Coulomb interaction is being studied (Judd 1966), and the unexpected results of detailed computations for these operators are particularly hard to understand in a simple way by traditional methods. One of the advantages of the quark model is that we can use the automorphisms of $\text{SO}(8)$ (Georgi 1982). In this approach the $\mathbf{1R}$ (1000) of $\text{SO}(8)$, which encompasses the eight-dimensional $\mathbf{1R}$ ($\frac{1}{2} \frac{1}{2} \frac{1}{2}$) of $\text{SO}(7)$, can also be thought of as spanning the two $\mathbf{1Rs}$ (100)' and (000)' of a second $\text{SO}(7)$ group, which we refer to as $\text{SO}(7)'$. An f quark now belongs to (100)' and an s quark to (000)'. A third $\text{SO}(7)$ group, distinguished by a double prime, can also be introduced by reversing the relative phases of the s and f quarks appearing in the generators of $\text{SO}(7)$. However, its relevance to the subject of effective operators is not readily apparent, and it will be considered no further.

2. Effective quark operators

In the present paper we focus on operators whose quark realizations involve operators that act on only one quark at a time. This is the simplest situation of all. The coupled products $(q^\dagger q)^W$ necessarily introduce only those $\mathbf{1Rs}$ W of $\text{SO}(7)$ that appear in the reduction of the Kronecker product of ($\frac{1}{2} \frac{1}{2} \frac{1}{2}$) (corresponding to $q^\dagger$) with ($\frac{1}{2} \frac{1}{2} \frac{1}{2}$) (corresponding to q). By standard techniques (as described, for example, by Wybourne 1970) we get

$$(\frac{1}{2} \frac{1}{2} \frac{1}{2})^2 = (000) + (100) + (110) + (111). \quad (2)$$

The $\mathbf{1R}$ (111) appearing here is of special interest because it cannot be produced by single-electron operators, for which

$$(100)^2 = (000) + (110) + (200). \quad (3)$$

Thus electron operators that belong to (111), and that necessarily act on more than a single electron at a time, might be susceptible to a representation by sums of single-quark operators. Perhaps the most obvious example is one of the generalized Trees (1952) operators that allows for some of the effects of two-electron excitations on a configuration f^N . The one belonging to (111) has been denoted by e'_β (Judd and Suskin 1984). However, its eigenvalues can be expressed in terms of Casimir's operators for $\text{SO}(7)$ and its subgroup G_2 , as Rajnak and Wybourne (1963) have made clear, so there

Table 1. Matrix elements in f^2 , reduced with respect to both S and L , of the operator z_0 (Crosswhite *et al* 1968). All matrix elements involving the singlets of f^2 vanish.

ψ	ψ'	$(f^2 \psi z_0 f^2 \psi')$
3P	3P	9
3P	3F	$(27)^{1/2}$
3F	3F	$-2(14)^{1/2}$
3F	3H	$(22)^{1/2}$
3H	3H	$-(143)^{1/2}$

is little incentive for finding a quark representation for it. Among other operators belonging to (111) of $SO(7)$ is the non-scalar two-electron operator $g_{11}^{(k)}$, which has been used in crystal-field theory (Judd 1977). This operator also does not have a high priority for our attention because it is not required in the delta-function version of the theory (Lo and Reid 1993).

For the purposes of the present paper we fix our attention on two other operators belonging to (111). The first is the two-electron operator z_0 , which completes the set of five orthogonal operators whose other members z_i ($1 \leq i \leq 4$) represent the magnetic interactions between the spins of the *f* electrons (Crosswhite *et al* 1968). It behaves as a double tensor of rank 2 with respect to both S and L . The ranks can be made explicit by writing $(z_0)^{(22)}$. It belongs to the $1R$ $\langle 1111000 \rangle$ of $Sp(14)$ (Armstrong and Taylor 1969) and this can be used to show that, as a two-electron operator, it possesses a rank 2 with respect to the quasispin Q (Judd 1966, table XV). It is completely defined by specifying its matrix elements in f^2 , and this is done in table 1. Armstrong and Taylor (1969) have given the reduced matrix elements of the five z_i for the electronic configuration f^4 , but spot checks indicate that the entries in their table I need to be corrected by multiplication by 4. (The general formula for their entries, as given in their equation (4), is nevertheless correct.)

The second operator belonging to (111) is the three-electron operator t_{11} , which enters when electrostatic interactions are taken to third order in perturbation theory (Judd and Suskin 1984). It is scalar with respect to S and L and belongs to the $1R$ (00) of G_2 . It is thus diagonal with respect to the $1R_s$ U of G_2 . It is convenient to make it orthogonal to the Trees operator e'_β , in which case it possesses a pure quasispin rank of 1. It is completely defined through its matrix elements for f^3 , and they are set out in table 2.

Table 2. Diagonal matrix elements of the scalar three-electron operator t_{11} in f^3 (Judd and Suskin 1984, table 1). All off-diagonal matrix elements vanish. Spectroscopic terms with the same S and L are distinguished by adding the labels 1 or 2 following the scheme of Nielson and Koster (1963). The corresponding $1R_s$ W and U of $SO(7)$ and G_2 are included for reference.

WU	ψ	$(660/7)^{1/2} (f^3 \psi t_{11} f^3 \psi)$
(111)(00)	4S	18
(111)(20)	$^4D, ^4G, ^4I$	-3
(111)(10)	4F	9
(100)(10)	2F1	0
(210)(11)	$^2P, ^2H1$	-6
(210)(20)	$^2D1, ^2G1, ^2I$	-4
(210)(21)	$^2D2, ^2F2, ^2G2, ^2H2, ^2K, ^2L$	3

3. Operator equivalences

Rather than use the quark operators $(q^\dagger q)^W$, in which the coupling of $q^\dagger$ with q is performed at the SO(7) level, it is usually more convenient to use the f and s components of the quarks and work at the SO(3) level of angular-momentum theory, as has been already indicated in section 1. The quark operators now become

$$(s^\dagger s)^{(0)} \quad (f^\dagger s)^{(3)} \quad (s^\dagger f)^{(3)} \quad (f^\dagger f)^{(k)} \quad (0 \leq k \leq 6). \quad (4)$$

Each of the quark operators in these expressions can be subscripted with one of the four possibilities for θ , corresponding to the four quarks at our disposal. We have now to ask how our operators z_0 and t_{11} can be represented by the quark operators. The orbital rank of z_0 is 2, and this can only be produced by single-quark operators of the type $(f^\dagger f)^{(2)}$. We are thus led to examine under what circumstances we can make replacements of the type

$$z_0 \rightarrow \sum_{\theta} A_{\theta} (f_{\theta}^{\dagger} f_{\theta})^{(2)} \quad (5)$$

where the A_{θ} are numerical coefficients. In the case of t_{11} , however, its zero orbital rank can be produced by both $(f^\dagger f)^{(0)}$ and $(s^\dagger s)^{(0)}$. These two possibilities correspond to the existence of an SO(3) scalar in both (000) and (111) appearing on the right-hand side of equation (2) (Wybourne 1970, table C-17). In order to produce an operator labelled by (111), we need the isoscalar factors

$$((\frac{1}{2} \frac{1}{2} \frac{1}{2}) 3 + (\frac{1}{2} \frac{1}{2} \frac{1}{2}) 3 | (111) 0) = (\frac{1}{8})^{1/2} \quad (6)$$

$$((\frac{1}{2} \frac{1}{2} \frac{1}{2}) 0 + (\frac{1}{2} \frac{1}{2} \frac{1}{2}) 0 | (111) 0) = -(\frac{7}{8})^{1/2} \quad (7)$$

that have been obtained elsewhere (Judd and Lister 1992a, equation (26)). The analogue of equation (5) is thus

$$t_{11} \equiv \sum_{\theta} B_{\theta} [7^{1/2} (f_{\theta}^{\dagger} f_{\theta})^{(0)} - 7 (s_{\theta}^{\dagger} s_{\theta})^{(0)}] \quad (8)$$

$$= \sum_{\theta} B_{\theta} \left[\sum_m f_{\theta m}^{\dagger} f_{\theta m} - 7 s_{\theta}^{\dagger} s_{\theta} \right]. \quad (9)$$

In both equations (5) and (9) we have four independent quark operators corresponding to $\theta = \lambda, \mu, \nu$ and ξ . However, their matrix elements, taken between quark states labelled by the IRs W and W' of SO(7), might not be independent. The Wigner-Eckart theorem plays a crucial role here. The maximum number of independent sets of matrix elements is equal to the number of times that (111) occurs in the reduction of the Kronecker product $W \times W'$. Racah (1949) denotes this number by $c(WW'(111))$. When $c(WW'(111)) = 1$, we can choose the sums of equations (5) and (9) to run over any subset of the θ s that we wish, provided the associated quark operator specified by (5) and (9) does not give vanishing matrix elements. In the case of equation (5), an obvious choice to make (whenever possible) is to set all of the A_{θ} equal to each other, for in that case the replacement operator appearing in (5) is the generator of the unitary group U(7)' that contains the group SO(7)' of section 1, just as the electron operator $(f^\dagger f)^{(02)}$ is a generator of Racah's U(7) that contains SO(7). A simplification also occurs if we can set all the B_{θ} of equation (9) equal to each other, since now the operator just counts the number of f quarks and subtracts seven times the number of s quarks.

Of all the pairs (W, W') occurring in the atomic f shell, four satisfy $c(WW'(111)) = 2$. They are

$$WW' = (210)(211), \quad (211)(211), \quad (211)(221), \quad (221)(221). \quad (10)$$

No cases occur for which $c(WW'(111)) > 2$. The four possibilities given in (10) are of special interest to us because we would expect to find it necessary to choose coefficients A_θ and B_θ that vary with θ .

4. Automorphisms of $SO(8)$

As a first example of the usefulness of effective operators, consider the matrix elements of z_0 within the states of maximum spin in f^4 , all of which belong to the $1\mathbf{R}$ (111) of $SO(7)$ (Racah 1949). If we select those for which $S = M_S = 2$, we can work entirely in the electronic spin-up space, where only the two quarks q_λ and q_μ are needed. To establish an operator equivalence, we compare the result of using the (corrected) matrix element for $^5\mathbf{I}$ given by Armstrong and Taylor (1969, table I) with the corresponding matrix element in the quark scheme. The former provides the following equation (for $M_S = 2$):

$$\langle f^4(111)^5\mathbf{I}, M_L = 6 | (z_0)_{00}^{(22)} | f^4(111)^5\mathbf{I}, M_L = 6 \rangle = -1. \quad (11)$$

The latter requires the f components of the two quarks q_λ and q_μ , for which

$$\begin{aligned} & \left\langle f^2(111)\mathbf{I}, M_L = 6 \left| A \sum_{\theta} (f_{\theta}^{\dagger} f_{\theta})_0^{(2)} \right| f^2(111)\mathbf{I}, M_L = 6 \right\rangle \\ &= \left\langle [3_{\lambda} 3_{\mu}] \left| A \sum_{\theta} (f_{\theta}^{\dagger} f_{\theta})_0^{(2)} \right| [3_{\lambda} 3_{\mu}] \right\rangle = 5A(21)^{-1/2} \end{aligned} \quad (12)$$

where 3_{θ} denotes the m_{θ} quantum number of the quark q_{θ} , which is necessarily of type f . Since the bra label (111) occurs just once in the reduction of the Kronecker product $(111) \times (111)$ coming from the operator and the ket (as may be verified, for example, by referring to table D-4 of Wybourne (1970)), we have established the operator equivalence

$$(z_0)_0^{(22)} \equiv -\left(\frac{21}{25}\right)^{1/2} \sum_{\theta} (f_{\theta}^{\dagger} f_{\theta})^{(2)} \quad (13)$$

for all the states of f^4 for which $S = M_S = 2$. The single zero placed beneath the ranks (22) indicates reduction with respect to S only. That is, $(z_0)_0^{(22)}$ is diagonal with respect to M_S , but remains a tensor of rank 2 with respect to L .

We can turn the equivalence (13) to our advantage by introducing the automorphisms of $SO(8)$ via the group $SO(7)'$. The $1\mathbf{R}$ (111) appearing in the bra and ket of equation (12) corresponds to the symmetric two-quark $1\mathbf{R}$ (2000) of $SO(8)$ (Judd and Lister 1992a, table 1). Now (2000) contains the angular momenta $S + D + F + G + I$ (the terms of maximum multiplicity of f^4) just as (111) does; but the distribution is different for $SO(7)'$. In fact, we have

$$(2000) \rightarrow (000)' + (100)' + (200)' \quad (14)$$

$$(000)' \rightarrow S \quad (100)' \rightarrow F \quad (200)' \rightarrow D + G + I. \quad (15)$$

Furthermore, each quark operator $(f_\theta^\dagger f_\theta)^{(2)}$ must belong to $(200)'$ of $SO(7)'$, since $(200)'$ is the only ir occurring in $(100)' \times (100)'$ that contains a tensor of rank 2. However, the mathematical manipulations in evaluating a quark reduced matrix element such as

$$\left(f^2(200)'L \left\| \sum_\theta (f_\theta^\dagger f_\theta)^{(2)} \right\| f^2(200)'L' \right) \quad (16)$$

must be identical to those used to evaluate the electron matrix element

$$\left(f^2(200)L \left\| \sum_i v_i^{(2)} \right\| f^2(200)L' \right). \quad (17)$$

The results will be numerically identical provided $v_i^{(2)}$ (for electron i) possesses the same single-particle reduced matrix element as $(f_\theta^\dagger f_\theta)^{(2)}$. That is, we require

$$(f \| (f_\theta^\dagger f_\theta)^{(2)} \| f) = (f \| v^{(2)} \| f) = 5^{1/2}. \quad (18)$$

We can deduce that, for L and L' equal to 2, 4 or 6,

$$(f^4 {}^5L, M_S=2 \| (z_0)^{(22)} \| f^4 {}^5L', M_S=2) = -(\frac{21}{25})^{1/2} (f^2 {}^1L \| V^{(2)} \| f^2 {}^1L') \quad (19)$$

where, in general, $V^{(k)} = \sum_i v_i^{(k)}$. On reducing the matrix element on the left with respect to S and setting $V^{(2)} = 5^{1/2} U^{(2)}$, we get, for L and L' even (and non-zero),

$$(f^4 {}^5L \| z_0 \| f^4 {}^5L') = -7(\frac{3}{2})^{1/2} (f^2 {}^1L \| U^{(2)} \| f^2 {}^1L') \quad (20)$$

a result that can be easily confirmed by referring to the tables of Nielson and Koster (1963). The intervention of the quarks has thus enabled two purely electronic matrix elements to be related.

It should be mentioned that the proportionality represented by equation (20) has already been established by a different argument in which one of the possible $SO(8)$ labels for z_0 (namely the ir $(111-1)$) is shown to be ineffective (Judd 1992). However, the use of equivalent operators has enabled us to go much further and find the constant of proportionality itself.

5. States involving s quarks

The analysis of the previous section has been limited to the 5D , 5G and 5I terms of f^4 . The relevant quark states have been thereby restricted to those that only involve f quarks. However, the two other quintets of f^4 , namely 5S and 5F , both require some components from s quarks. The expansions for the ir (2000) of $SO(8)$ run as follows (Judd and Lister 1992a, table 3):

$$|f^4 {}^5S, M_S=2\rangle = |(2000)(111)S\rangle = (\frac{1}{3})^{1/2} |f^2 {}^3S\rangle - (\frac{2}{3})^{1/2} |s^2 S\rangle \quad (21)$$

$$|f^4 {}^5F, M_S=2\rangle = |(2000)(111)F\rangle = (\frac{1}{2})^{1/2} |(s_\lambda f_\mu)F\rangle + (\frac{1}{2})^{1/2} |(f_\lambda s_\mu)F\rangle. \quad (22)$$

The equivalence (13) can again be applied to the components for which $M_S=2$ because the S and F states belong to the same ir (111) as before. The only non-zero value is given by

$$(f^4 {}^5S \| z_0 \| f^4 {}^5D) = -7(\frac{3}{16})^{1/2} (f^2 {}^1S \| U^{(2)} \| f^2 {}^1D) \quad (23)$$

the additional factor of $(\frac{1}{8})^{1/2}$ (compared to the coefficient in equation (20)) coming from the first coefficient on the right in equation (21). The s quarks appearing in the ket $|s^2 S\rangle$ are irrelevant because the operator $(f_\theta^\dagger f_\theta)^{(2)}$ cannot connect them to the configuration f^2 needed to describe the D term.

An operator equivalence similar to (13) can be established for t_{11} by considering the I term of f^4 with $S=M_S=2$. We compare the value of the quark operator (9) (taking all B_θ equal to B) with the result of a direct calculation for a three-electron operator (Judd 1966, equation 4). The first is $2B$, since there are just two f quarks (namely f_λ and f_μ) in $|(2000)(111)I\rangle$. The direct calculation yields $-(\frac{21}{55})^{1/2}$, whence we get

$$t_{11} \equiv -(\frac{21}{220})^{1/2} \sum_{\theta, m} [f_{\theta m}^\dagger f_{\theta m} - 7s_\theta^\dagger s_\theta] \quad (24)$$

for the terms of f^4 for which $S=M_S=2$. For the 5S and 5F terms of f^4 , which are given (for $M_S=2$) by equations (21) and (22), the eigenvalues of the operator on the right-hand side of the equivalence (24) are

$$-(\frac{21}{220})^{1/2} [(\frac{1}{8})2 - 7(\frac{7}{8})2] = 12(\frac{21}{220})^{1/2} \quad (25)$$

$$-(\frac{21}{220})^{1/2} [(\frac{1}{2})(1-7) + (\frac{1}{2})(1-7)] = 6(\frac{21}{220})^{1/2} \quad (26)$$

respectively, in agreement with the result of a direct calculation. A further check is provided by the ratios $-2:12:6$ for the I, S and F terms, which must be proportional to the entries $-3:18:9$ of table 2, since the terms of maximum multiplicity of f^3 , like those of f^4 , belong to (111) , and the Kronecker product $(111)^2$ contains (111) just once.

6. The group G_2

In the above analysis, no mention has been made of Racah's group G_2 , which contains $SO(3)$ and is a subgroup of both $SO(7)$ and $SO(7)'$. Since the terms 3D , 3G and 5I of f^4 span the $1R$ (20) of G_2 (Wybourne 1965, table 2-1), and since both z_0 and $U^{(2)}$ also belong to the $1R$ (20), it might be thought that the proportionality represented by equation (20) could be understood by applying the Wigner-Eckart theorem for G_2 to the matrix elements appearing there. However, since $c((20)(20)(20))=2$ (Wybourne 1970, table E-4), this argument does not apply, and we would expect the right-hand side of equation (20) to comprise a linear combination of two independent sets of matrix elements. The quark model has thus provided an explanation of what would otherwise appear to be an unexpected simplification.

As we proceed to more complicated cases, the role of G_2 becomes crucial. Its $1Rs$ U serve to distinguish to a large extent the repeated L values occurring in a given $1R$ W of $SO(7)$, as Racah (1949) discovered. At the same time, G_2 is the source of most of the puzzling simplifications that have proliferated in the atomic f shell over the years. Racah himself found that matrix elements of the Coulomb interaction are related to one another in a way that is much simpler than what would be expected on the basis of a straightforward application of the Wigner-Eckart theorem. Similar results hold for the scalar three-electron operators used in studies of configuration interaction (Bentley *et al* 1992). We have already gained some understanding of these properties with the help of the quark model, and much of the motivation for the present work comes from a desire to make further progress in that direction.

7. Effective operators for which $c(WW'(111)) = 2$

When the $1\mathbf{R}$ (111) occurs twice in the reduction of the Kronecker product $W \times W'$, we can expect to have to choose coefficients A_θ or B_θ in the operator equivalences that vary with θ . All the possible pairs WW' listed in the sequences (10) correspond to $1\mathbf{R}$ s W and W' for which the associated spins S are not their highest for a given configuration. Thus electrons occur with spins both up and down, which implies that all four quarks have now to be brought into play. Our options for choosing the coefficients A_θ and B_θ are more limited than might appear at first sight because it frequently happens that the operators multiplying the various A_θ and B_θ possess matrix elements that are not independent of one another. A form that is often useful for z_0 has $A_\lambda = A_\mu$ and $A_\nu = A_\xi$. To take advantage of the anticipated rational nature of A_λ/A_ν , it is convenient to write

$$(z_0)_0^{(22)} \equiv A[(f_\lambda^\dagger f_\lambda)^{(2)} + (f_\mu^\dagger f_\mu)^{(2)} + \tau(f_\nu^\dagger f_\nu)^{(2)} + \tau(f_\xi^\dagger f_\xi)^{(2)}]. \quad (27)$$

The coefficients A and τ can be obtained for states labelled by a particular W and W' once their quark expansions are known. Examples of such expansions are discussed in

Table 3. Values of A and τ in the equivalence (27) when set between states ψ and ψ' . The numbers in the braces specify values of M_S where appropriate. In two cases the quark operators cannot adequately represent z_0 , and the undetermined parameters are indicated by footnotes. The significance of the subscript c is explained in section 8.

ψ	ψ'	A	τ
$(2110)_c(211)$	$(2110)_c(210)$	$-(9/20)(21)^{1/2}$	1
$(2110)_c(211)$	$(2110)_c(211)$	$(1/20)(21)^{1/2}$	-3
$(2110)_c(211)$	$(3100)_c(221)$	†	†
$f^8(211)\{-1\}$	$f^8(211)\{-1\}$	$(3/5)(21)^{1/2}$	-2
$f^8(211)\{-1\}$	$f^8(221)\{-1\}$	$-(3/5)(21)^{1/2}$	1
$f^4(211)\{1\}$	$f^4(211)\{1\}$	‡	‡

† The states ψ and ψ' involve the respective $1\mathbf{R}$ s $[211]$ and $[31]$ of $U(8)$, between which the effective operator (27) with $\tau = 1$, being a generator of $U(8)$, must vanish; and hence the spin-up and spin-down parts of an operator for which $\tau \neq 1$ do not provide two independent parts.

‡ The states of f^4 for $M_S = 1$ correspond to a single electron in the spin-down space belonging to (100) of $SO(7)$. Any operator with the label (111) vanishes when taken between two (100) states, and so the effective operator (27) does not possess two independent parts.

appendix 1. Some values for A and τ are set out in table 3 for systems for which the numbers of electrons with spins up (N_+) and spins down (N_-) are both odd.

Similar analyses can be made for t_{11} . As a single example, which holds for the triplet states of f^8 belonging to (221) of $SO(7)$ and for which $M_S = -1$, we cite

$$t_{11} \equiv -(\frac{7}{5940})^{1/2}[7(Z_\lambda + Z_\mu) - 13(Z_\nu + Z_\xi)] \quad (28)$$

where

$$Z_\theta = \sum_m f_{\theta m}^\dagger f_{\theta m} - 7s_\theta^\dagger s_\theta. \quad (29)$$

The matrix elements of each Z_θ are very simple to calculate once the quark expansions of the states are known. Examples of such expansions are given in the appendix.

8. Spins both up and down

The presence of both orientations of electron spin and the consequent need to use all four quarks makes it somewhat more difficult to bring $SO(8)$ and its subgroup $SO(7)'$ into play. Symbols (such as the ir W and the electron number N) are subscripted $+$ or $-$ when referring to spins up or spins down. The two quarks in either of these categories can be described by either the symmetric ir [2] or the antisymmetric ir [11] of $U(8)$. The former provides the irs (2000) and (0000) of $SO(8)$, the latter just (1100) (Wybourne 1970, table C-6). A particular ir of $SO(8)$ for the full four-quark system such as (2110) can be formed by taking one of three possibilities $(1100)_+ \times (1100)_-$, $(1100)_+ \times (2000)_-$ or $(2000)_+ \times (1100)_-$. We indicate this choice by the subscripts a, b or c to (2110) (Judd and Lister 1992b). In some cases a state defined by an ir of $SO(8)$ can be represented by a single electronic state, as in section 4. For example, we find (Judd and Lister 1992b, table 7)

$$|(2110)_c(210)\rangle = |f^8(210), M_S = -1\rangle \quad (30)$$

$$|(2110)_c(221)\rangle = |f^8(221), M_S = -1\rangle. \quad (31)$$

However, other cases require the superposition of several electronic states, and this complicates matters. For example,

$$|(2110)_c(211)\rangle = \frac{1}{2}|f^4(211), M_S = 1\rangle - \left(\frac{3}{4}\right)^{1/2}|f^8(211), M_S = -1\rangle. \quad (32)$$

We can find the possible irs W_+ and W_- of $SO(7)$ or W'_+ and W'_- of $SO(7)'$ implied by a subscript a, b or c by using the decompositions $SO(8) \rightarrow SO(7)$ or $SO(8) \rightarrow SO(7)'$. In the example above, the states of the configuration f^8 for which $M_S = -1$ correspond to $N_+ = 3$ and $N_- = 5$; for f^4 and $M_S = 1$ we have $N_+ = 3$ and $N_- = 1$. The ir (2000) $_+$ yields the single ir (111) of $SO(7)$, while the ir (1100) $_-$ yields (110) and (100) (Judd and Lister 1992a, table 1). Now (110) can appear only for $N_- = 5$ or 2, and (100) only for $N_- = 1$ or 6 (Racah 1949, table I). Thus we know that the two kets on the right-hand side of equation (32) correspond to $(111)_+ \times (100)_-$ and $(111)_+ \times (110)_-$ respectively.

It is often more difficult to determine the irs of $SO(7)'$. The problem frequently occurs in the form in which a given ir U of G_2 appearing in the decomposition of a specified V of $SO(8)$ may involve various irs W' of $SO(7)'$ as intermediaries. An account of how to calculate the overlaps $(VWU|VW'U)$ has recently been made (Judd *et al* 1993), and the methods described there can be called upon when necessary.

9. An example

Of the two operators z_0 and t_{11} , the former exhibits a greater richness in its properties because it is not a G_2 scalar. Of the many matrix elements we might pick to exemplify our techniques, we select the collection

$$(f^6(210)U^5L\|z_0\|f^6(211)(30)^3L') \quad (U = (20) \text{ or } (21); \text{ all } L, L') \quad (33)$$

where the double uprights indicate reduction with respect to both S and L . We begin by replacing f^6 by its conjugate f^8 , selecting $M_S = -1$, and using equations (30) and (32) to convert (33) to

$$\left(\frac{40}{3}\right)^{1/2}((2110)_c(210)UL\|(z_0)_0^{(22)}\|(2110)_c(211)(30)L') \quad (34)$$

where now the matrix element is reduced only with respect to L . We next introduce $SO(7)'$ and the equivalence (27) with $\tau=1$ from table 3. The expression (34) becomes

$$-9\left(\frac{7}{10}\right)^{1/2} \sum_{W'} ((2110)(210)U|(2110)W'U) \\ \times \left((2110)_c W' UL \left\| \sum_{\theta} (f_{\theta}^{\dagger} f_{\theta})^{(2)} \right\| (2110)_c (211)'(30)L' \right). \quad (35)$$

The next step is to limit the sum over W' to the one possibility $(211)'$. To do this, we note first that the eight states of a quark q_{θ} , which belong to the $1\mathbf{R}$ (1000) of $SO(8)$, can also be thought of as spanning the $1\mathbf{R}$ [1] of $U(8)$. When four quarks are considered, the only component of $[1]^4$ that contains the $1\mathbf{R}$ (2110) of $SO(8)$ is $[211]$ of $U(8)$. If we now reduce $U(8)$ to $SO(7)'$ via the $U(7)'$ group mentioned in section 3 (rather than via $SO(8)$), the $1\mathbf{R}$ $(211)'$ appearing in the matrix element of the sum (35) must belong to $[211]'$ of $U(7)'$. The operator $\sum_{\theta} (f_{\theta}^{\dagger} f_{\theta})^{(2)}$ is a generator of $U(7)'$, and is therefore diagonal with respect to $[211]'$. This means that the only W' of interest are those contained in $[211]'$, namely $(211)'$ and $(110)'$ (Wybourne 1970, table C-5). If $U=(21)$ or (20) , the only possible W' is $(211)'$; and this limits the sum over W' in (35) to a single term.

The relevant overlaps in (35) are calculated to be

$$((2110)(210)(21)|(2110)(211)'(21)) = -\left(\frac{3}{2}\right)^{1/2} \quad (36)$$

$$((2110)(210)(20)|(2110)(211)'(20)) = \left(\frac{1}{6}\right)^{1/2}. \quad (37)$$

For $U=(21)$ and (20) , the matrix element in (35) must be equal to the electron matrix element

$$\left(211UL \left\| \sum_i v_i^{(2)} \right\| 211(30)L' \right) \quad (38)$$

since we can pass from f quarks to f electrons just as easily here as in the previous analysis that involved going from (16) to (17). As in section 4, statistics are again irrelevant, this time because the orbital symmetries are the same, namely, $[211]$ for electrons and $[211]'$ for quarks. Just as $[211]'$ is a collection of four-quark states, so $[211]$ is a collection of four-electron states, namely the states of f^4 for which $S=1$ (Racah 1949, section 4.1). Bringing all the parts together, and using equation (18), we arrive at the result

$$(f^6(210)U^5L \| z_0 \| f^6(211)(30)^3L') \\ = A(f^4(211)U^3L \| U^{(2)} \| f^4(211)(30)^3L') \quad (\text{all } L \text{ and } L') \quad (39)$$

where $A=9\left(\frac{21}{8}\right)^{1/2}$ for $U=(21)$ and $-3\left(\frac{21}{4}\right)^{1/2}$ for $U=(20)$. These results can be confirmed with the help of the tables of Nielson and Koster (1963). The matrix element of z_0 in equation (39) is reduced with respect to both S and L , while that of $U^{(2)}$ is reduced solely with respect to L . The proportionalities represented in equation (39) would not be expected for $U=(21)$ because (21) occurs twice in the reduction of $(20) \times (30)$ (Wybourne 1970, table E-4).

There remains the case of $U=(11)$ in equation (39). This possibility has been excluded from the analysis because the sum over W' can no longer be reduced to a single term, and the treatment necessarily becomes more complex. Very surprisingly,

the terms in the sum cancel and the final answer is zero. A direct calculation using quark fractional parentage confirms this result. Some other mechanism is apparently at work. We simply note here two suggestive features. As has already been observed, the relevant equivalent operator is a generator of $U(7)'$, and, as such, is also a generator of $U(8)$ that possesses $SO(8)$ as a subgroup. Secondly, the $1\mathbf{R}$ (2110) that appears in equation (35) possesses what has been called null triality (Wybourne 1992). This imposes additional symmetries on the $1\mathbf{R}$ s of $SO(7)$, $SO(7)'$ and $SO(7)''$. However, an exploration of these matters would take us too far afield and is best left for a future article.

10. Further applications

The previous example illustrates the power of the quark method. Equation (39) exposes an unexpected connection between the matrix elements of different operators taken between states whose bras differ with respect to S and W . Many other relations of an equally striking kind can be established with a little ingenuity. The details require descriptions of a similar type and length to those that lead up to equation (39), and, in the interests of keeping the present paper within reasonable bounds, we restrict ourselves to very brief introductions to the final results.

Both (210) and (220) can be embedded in the $1\mathbf{R}$ (2200) of $SO(8)$. If the quasispin rank of z_0 (namely, 2) is brought into play to connect configurations that differ with respect to the number of electrons, this embedding can be used to show that

$$\begin{aligned} & (f^6(210)(21)^3 L \| z_0 \| f^6(220)(21)^1 L') \\ &= \left(\frac{2}{3}\right)^{1/2} [f^3(210)(21)^2 L \| U^{(2)} \| f^3(210)(21)^2 L'] \\ & \quad - (f^4(220)(21)^1 L \| U^{(2)} \| f^4(220)(21)^1 L')]. \end{aligned} \quad (40)$$

This result is remarkable in that it converts the matrix element for one operator that is off-diagonal with respect to W into the difference between two matrix elements of another operator that are diagonal with respect to W .

Perhaps an even more striking result is the following:

$$\begin{aligned} & (f^4(211)(30)^3 L \| z_0 \| f^4(211) U^3 L') \\ &= B(U) \left(\frac{42}{5}\right)^{1/2} (f^4(211)(30)^3 L \| W^{(12)} \| f^4(211) U^3 L') \end{aligned} \quad (41)$$

where $W^{(1k)}$, familiar in hyperfine-structure studies (see, for example, Woodgate 1966), is a sum of single-electron double tensors $w^{(1k)}$ each of whose reduced matrix elements is $[3(2k+1)]^{1/2}$. The overlaps $B(U)$ between $SO(7)$ and $SO(7)'$ are given by

$$\begin{aligned} B(U) &= ((2110)(211)(30) | (2110)(211)' U) \\ &= 1, \quad -\frac{1}{2}, \quad -\frac{1}{2}, \quad \frac{2}{3}, \quad \frac{1}{10} \end{aligned} \quad (42)$$

for $U=(30)$, (21) , (20) , (11) and (10) , respectively. Equation (41) can be confirmed by using the (corrected) table of Armstrong and Taylor (1969) for z_0 and the tables for $V^{(k1)} (= [2(2k+1)]^{-1/2} W^{(1k)})$ given by Karazija *et al* (1967). Both z_0 and $W^{(12)}$ belong to the same $1\mathbf{R}$ (namely (20)) of G_2 , but the proportionality represented by equation (42) would not be expected for $U=(30)$ or (21) because $(20) \times (30)$ and $(20) \times (21)$ contain (30) twice.

The appearance of the overlaps $B(U)$ suggests a strategy for proving the validity of equation (42). Both the bra and the ket of the first matrix element of equation (41) are expressed in terms of the $1\mathbf{R}$ (2110) of $\text{SO}(8)$, and then the new states are expanded in terms of the $1\mathbf{R}$ s of $\text{SO}(7)'$. Some manipulation is required to show that the operator $W^{(12)}$ suffices in the second matrix element, rather than a superposition of $W^{(12)}$ and $U^{(2)}$. Of course, the explicit appearance of $B(U)$ as a proportionality factor demonstrates the relevance of $\text{SO}(8)$ and thereby the basic role played by the eight-dimensional quarks. Although fictional, they make themselves felt in purely electronic matters.

11. Concluding remarks

The preceding analysis has shown how the quark model of the atomic f shell can be used to establish relations between the matrix elements of electronic operators. Equations (20), (39), (40) and (41) are obtained by traditional means only as a result of detailed numerical calculations. The group $\text{SO}(7)'$ plays a central role in augmenting Racah's $\text{SO}(7)$, and this feature derives from the automorphisms of $\text{SO}(8)$, a property that can be exploited only for the f shell. The absence of analogous automorphisms in the d shell is perhaps the reason for the lack of comparable puzzles and unexpected simplifications there. A quark analysis for the d shell is thus limited to setting the traditional analysis in a new perspective, though the necessary equivalence between the two approaches leads to some interesting relations between various $6-j$ symbols (Godefroid *et al* 1994).

In the present article we have focused on electronic operators that can be represented by sums of single-quark operators. This simplification is exceptional. The success already achieved for other operators such as the three-electron scalars t_2 , t_4 , t_6 , t_7 and t_8 has depended on either relating them to two-quark operators or else taking advantage of the detailed nature of their $\text{SO}(7)$ labels (Judd and Lister 1991, 1992a, 1993). However, much remains to be done. For example, we have so far been unable to give an explanation for the frequent proportionality between the matrix elements of the three-electron operators t_4 and t_7 (Bentley *et al* 1992, table 2). Similar unexpected proportionalities hold for the operators z_6 and z_8 , which, with eight others, make up the spin-other-orbit interaction (Lister and Judd 1992, Judd 1994). The quark model has a long way to go yet.

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Appendix. Quark states

It is often useful to know how Racah's f -electron states appear in the quark basis. Godefroid *et al* (1994) have described the analogues for the d shell. A straightforward approach is to express a state in Racah's formalism as a sum of coupled spin-up and spin-down states, and then replace each of the two parts by their quark counterparts using expressions that have been worked out already (see Judd and Lister 1992a,

Table A1. Expansion coefficients for various states of the *f* shell for which $M_L=9$. Those for f^8 correspond to $M_S=-1$; that for f^4 to $M_S=1$. The subscript *c* refers to the coupling $(2000)_1 \times (1100)_1$, as described in section 8.

Coeff.	$f^4(211)(30)^3M$	$f^8(221)(30)^3M$	$f^8(211)(30)^3M$	$f^8(221)(31)^3M$	$f^8(221)(31)^3N$	$f^8(221)(31)^3O$	$(2110)_c(211)(30)M$
<i>a</i>	-1/2	$-(2/3)^{1/2}$	$-(1/12)^{1/2}$	0	0	0	0
<i>b</i>	1/2	$-(1/6)^{1/2}$	$(1/12)^{1/2}$	$-(3/70)^{1/2}$	$(18/55)^{1/2}$	$-(10/77)^{1/2}$	0
<i>c</i>	$-(1/2)^{1/2}$	$(1/12)^{1/2}$	$(1/6)^{1/2}$	$-(3/140)^{1/2}$	$(9/55)^{1/2}$	$-(5/77)^{1/2}$	$-(1/2)^{1/2}$
<i>d</i>	0	$(1/24)^{1/2}$	$-(1/3)^{1/2}$	$(27/280)^{1/2}$	$(1/110)^{1/2}$	$-(40/77)^{1/2}$	1/2
<i>e</i>	0	$-(1/24)^{1/2}$	$(1/3)^{1/2}$	$(15/56)^{1/2}$	$-(5/22)^{1/2}$	$-(10/77)^{1/2}$	-1/2
<i>f</i>	0	0	0	$-(4/7)^{1/2}$	$-(3/11)^{1/2}$	$-(12/77)^{1/2}$	0

Table A2. Expansion coefficients for various states of the f shell for which $M_L=8$. Those for f^8 correspond to $M_S=-1$; those for f^4 to $M_S=1$. The subscript c to (2110) has the same significance as in table A1.

Coeff.	$f^4(211)(21)^3L$	$f^4(211)(30)^3M$	$f^8(210)(21)^3L$	$f^8(211)(21)^3L$	$f^8(221)(21)^3L$
g	0	0	$-1/4$	$1/2$	$-(11/16)^{1/2}$
h	$(1/12)^{1/2}$	$-(1/6)^{1/2}$	$1/4$	$-1/3$	$-(11/144)^{1/2}$
i	$-(1/6)^{1/2}$	$-(1/12)^{1/2}$	$-(1/8)^{1/2}$	$(2/9)^{1/2}$	$(11/72)^{1/2}$
j	$(1/3)^{1/2}$	$(1/6)^{1/2}$	0	$1/3$	$(4/99)^{1/2}$
k	$-(1/12)^{1/2}$	$(1/6)^{1/2}$	$-1/4$	$-1/3$	$-(25/1584)^{1/2}$
m	$-(1/6)^{1/2}$	$-(1/12)^{1/2}$	$(1/8)^{1/2}$	0	$-(1/88)^{1/2}$
n	$(1/6)^{1/2}$	$-(1/3)^{1/2}$	$-(1/8)^{1/2}$	0	$(1/88)^{1/2}$
p	0	0	$-(1/8)^{1/2}$	$-(1/18)^{1/2}$	$-(1/792)^{1/2}$
q	0	0	$1/4$	$1/6$	$(1/1584)^{1/2}$
r	0	0	$1/2$	$1/3$	$(1/396)^{1/2}$
s	0	0	0	0	0
Coeff.	$f^8(211)(30)^3M$	$f^8(221)(30)^3M$	$f^8(221)(31)^3L$	$f^8(221)(31)^3M$	$f^8(221)(31)^3N$
g	0	0	0	0	0
h	$-(1/18)^{1/2}$	$-2/3$	0	0	0
i	$-1/6$	$-(2/9)^{1/2}$	0	0	0
j	$(1/18)^{1/2}$	$-1/3$	$(5/209)^{1/2}$	$-(1/35)^{1/2}$	$(108/1045)^{1/2}$
k	$-(1/18)^{1/2}$	$-1/6$	$-(20/209)^{1/2}$	$(1/140)^{1/2}$	$(147/1045)^{1/2}$
m	$1/2$	0	$(10/209)^{1/2}$	$-(2/35)^{1/2}$	$(216/1045)^{1/2}$
n	0	$(1/8)^{1/2}$	$-(10/209)^{1/2}$	$(1/280)^{1/2}$	$(147/2090)^{1/2}$
p	$1/3$	$-(1/72)^{1/2}$	$(10/1881)^{1/2}$	$-(125/504)^{1/2}$	$-(135/418)^{1/2}$
q	$(2/9)^{1/2}$	$-1/6$	$-(80/209)^{1/2}$	$(5/28)^{1/2}$	$-(15/209)^{1/2}$
r	$-(2/9)^{1/2}$	$1/6$	$-(20/1881)^{1/2}$	$-(121/1260)^{1/2}$	$-(48/1045)^{1/2}$
s	0	0	$(22/57)^{1/2}$	$(8/21)^{1/2}$	$-(8/209)^{1/2}$
Coeff.	$f^8(221)(31)^3O$	$(2110)_c(211)(30)M$	$(2110)_c(211)(21)L$		
g	0	0	$-(3/16)^{1/2}$		
h	0	0	$(3/16)^{1/2}$		
i	0	0	$-(3/8)^{1/2}$		
j	$-(2/77)^{1/2}$	0	0		
k	$-(18/77)^{1/2}$	$(1/6)^{1/2}$	$(1/48)^{1/2}$		
m	$-(4/77)^{1/2}$	$-(1/3)^{1/2}$	$-(1/24)^{1/2}$		
n	$-(9/77)^{1/2}$	$-(1/12)^{1/2}$	$(1/24)^{1/2}$		
p	$-(9/77)^{1/2}$	$-(1/12)^{1/2}$	$(1/24)^{1/2}$		
q	$-(2/77)^{1/2}$	$-(1/6)^{1/2}$	$-(1/48)^{1/2}$		
r	$-(18/77)^{1/2}$	$(1/6)^{1/2}$	$-(1/12)^{1/2}$		
s	$-(15/77)^{1/2}$	0	0		

table 3). In what follows we choose $M_S=+1$ in f^4 and $M_S=-1$ in f^8 , for which the odd number of electrons in the spin-up space span (111) , while the odd number of electrons in the spin-down space span (100) (for f^4) or (110) (for f^8). The $1R$ (111) belongs to the symmetric $1R$ $[2]$ of $U(8)$, while the other two belong to the antisymmetric $1R$ $[11]$ of $U(8)$ (Judd and Lister 1992b, table 7). This means that quark states of the type $[abcd]$, where each entry denotes m_θ and l_θ of q_θ , appear in the combination

$$\langle abcd \rangle = \frac{1}{2}([abcd] - [abdc] + [bacd] - [badc]) \tag{A1}$$

for $a=b$ and $c=d$, or in the combination

$$\langle aacd \rangle = (\frac{1}{2})^{1/2}([aacd] - [aadc]) \tag{A2}$$

if the first two quark states are identical.

Two kinds of states are of interest to us: those for which $M_L=9$ and $M_L=8$. The label I_θ can be dropped provided we add a prime to the m_θ value of an s quark, which is necessarily 0; all unprimed m_θ values correspond to an f quark. We write

$$|M_L=9\rangle = a\langle 3330'\rangle + b\langle 3330\rangle + c\langle 3321\rangle + d\langle 3231\rangle + e\langle 3132\rangle + f\langle 2232\rangle \quad (\text{A3})$$

and

$$|M_L=8\rangle = g\langle 30'32\rangle + h\langle 3230'\rangle + i\langle 3320'\rangle + j\langle 333-1\rangle + k\langle 3230\rangle + m\langle 3320\rangle \\ + n\langle 3221\rangle + p\langle 2132\rangle + q\langle 3032\rangle + r\langle 2231\rangle + s\langle 3131\rangle. \quad (\text{A4})$$

The coefficients in these expansions are given in table A1 and A2 for various Ψ . The (211) states of f^4 for which $M_S=1$ can be combined with the corresponding (211) states of f^8 for which $M_S=-1$ to produce states belonging to the 1R (2110) of SO(8) (Judd and Lister 1992b, table 7); some of these are also included in tables A1 and A2.

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