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A complete set of f-electron scalar operators

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Abstract. A complete set of scalar effective operators acting within the configurations f^N has been found. Through the use of Lie groups this set is resolved into orthogonal operators which act on N electrons simultaneously. A direct group theoretic correspondence is established between N-body electron operators and N-body nuclear states. This connection is utilised to expedite the electron classification scheme. Unlike the case of the d shell, little simplification occurs as N increases. In addition to the 21 previously established operators with $N \leqslant 3$, we have 65 four-body, 107 five-body, 182 six-body and 50 seven-body operators. Also, it is shown how the Hermiticity of each operator can be established by examining its transformation properties under the Lie group Sp(14).

1. Introduction

In atomic shell theory it is convenient to replace operators of direct physical significance by linear combinations H_i that are orthogonal to one another in the following sense:

$$\sum \langle \phi | H_i | \phi' \rangle \langle \phi' | H_j | \phi \rangle = A(H_i) \delta(i, j).$$

The sum runs over all states ϕ and ϕ' of a given configuration. The relative strengths of the operators can be found by performing a least squares fit of the predicted and observed energy levels of the configuration. The advantage of using orthogonal operators lies in the fact that their associated parameters are independent of one another, as long as the energies are linear functions of the parameters. This is approximately true in most cases, thus allowing one to unambiguously determine the strength of each operator individually.

If the states of the configuration form the basis for a representation of a Lie group G, then as long as the product H_iH_j does not contain the identity representation of G, the operators will be orthogonal (Judd 1984). If one chooses operators that transform themselves as irreducible representations Γ_i and Γ_j, then this condition is assured as long as Γ_i and Γ_j are distinct and G is self-adjoint.

Complete sets of orthogonal scalar operators have been found and classified for the configurations pd, p^2d, pd^2 and p^3d by Dothe *et al* (1985) and for the configurations d^N by Judd and Leavitt (1986). Furthermore, Judd and Suskin (1984) have determined all scalar operators in the f shell up to the configuration f^3. Hansen *et al* (1985) have found it necessary to use four-body operators for the configuration p^3d due to the inadequacies of the second-order perturbative expansion. In fact, any progression past second order for configurations larger than l^3 will necessitate the use of effective operators that act upon four or more electrons simultaneously. The purpose of this paper is to complete the analysis for the configurations f^N. Upon performing the group theoretical analysis a direct correspondence is found between the well established group structure of N-body nuclear states (Jahn 1950, Flowers 1952) and our N-body electron operators. This connection can be utilised to greatly facilitate the actual classification of the orthogonal operators.

2. Quasispin and isospin

An effective operator is represented in second-quantised form by a string of N creation and N annihilation operators,

$$a_\alpha^\dagger a_\beta^\dagger \ldots a_\mu^\dagger a_\nu \ldots a_\sigma a_\tau$$

which act upon N electrons simultaneously. Each subscript represents the four quantum numbers n, l, m_s, m_l. The group structure of this operator is determined by the coupling of the spin and orbit of the individual creation and annihilation operators. The $4l+2$ components of $\boldsymbol{a}^\dagger$ transform as the representation $[10^{4l+1}]$ of $\mathrm{U}(4l+2)$ whose irreducibility is preserved through the following reduction:

$$\mathrm{U}(4l+2) \rightarrow \mathrm{Sp}(4l+2) \rightarrow \mathrm{SO}_S(3) \times \mathrm{SO}(2l+1) \rightarrow \mathrm{SO}_S(3) \times \mathrm{SO}_L(3).$$

Therefore we can choose linear combinations of operators which transform as irreducible representations of groups in this chain. The last labels give the total spin S and total angular momentum L of the operator. These results are given by Judd (1968). As suggested by Judd (1967) we can extend the method by considering creation and annihilation operators as two components of a spin-$\frac{1}{2}$ vector labelled quasispin. If we have $\boldsymbol{a}^\dagger$ and $\boldsymbol{a}$ as creation and annihilation operators with tensorial ranks s and l, then let $\bar{\boldsymbol{a}}$ represent the single operator with ranks q, s and l. The two components of this tensor are given by

$$\bar{a}_{1/2\beta\gamma} = a_{\beta\gamma} \qquad \bar{a}_{-1/2\beta\gamma} = a_{-\beta-\gamma}(-1)^{s+l-\beta-\gamma}$$

where now β and γ represent m_s and m_l. The generators for $\mathrm{SO}_Q(3)$ are given by

$$\boldsymbol{Q} = -\tfrac{1}{2}(2l+1)^{1/2}(\bar{\boldsymbol{a}}\bar{\boldsymbol{a}})^{(100)}.$$

The $8l+4$ components of $\bar{\boldsymbol{a}}$ form the basis (10^{4l+1}) of $\mathrm{SO}(8l+4)$ and allow the group chain to be extended to

$$\mathrm{SO}(8l+4) \rightarrow \mathrm{SO}_Q(3) \times \mathrm{Sp}(4l+2).$$

Because our N-body operators conserve electron number and hence correspond to the $M_Q = 0$ projection, they do not span the complete representations of $\mathrm{SO}_Q(3)$. Distinctions at this level do not therefore guarantee the orthogonality of two operators, but the quasispin is nonetheless a useful label (Judd and Leavitt 1986).

Furthermore, the uses of quasispin are expanded by establishing the connection between its role in atomic physics and that played by isospin in the nuclear case. In the shell theory of nucleons a physical state can be separated into isospin, spin and orbital spaces. Nuclear states are formed by the successive application of creation operators with ranks of isospin $= \frac{1}{2}$, spin $= \frac{1}{2}$ and orbit $= l$. We can represent these operators as $\boldsymbol{b}^\dagger$. The tensorial properties of $\boldsymbol{b}^\dagger$ are identical to those of the tensors $\bar{\boldsymbol{a}}$. When considering nuclear states one generally treats the spin and isospin spaces separately from the orbital space. This allows a classification of states according to the transformation properties of the supermultiplet group $\mathrm{U}(4)$ and the standard orbital group SO$(2l+1)$ (Flowers 1952). However, this classification is evidently more general than what is available for the N-body operators since U(4) $\times$ SO$(2l+1)$ is not a subgroup of SO$(8l+4)$. This is easily witnessed by observing the generators for U(4), which, by ordering the ranks in sequence isospin, spin and orbit, appear as

$$(\boldsymbol{b}^{\dagger}\boldsymbol{b})^{(000)},\ (\boldsymbol{b}^{\dagger}\boldsymbol{b})^{(100)},\ (\boldsymbol{b}^{\dagger}\boldsymbol{b})^{(010)},\ (\boldsymbol{b}^{\dagger}\boldsymbol{b})^{(110)}.$$

These types of operators are not available in the electronic quasispin scheme since the distinction between the creation and annihilation operators constitutes the addition of an implicit fourth label.

3. Generators and group structure

In nuclear theory, quasispin does not appear to be as useful as it is in atomic theory. We can consider the two vectors $\boldsymbol{b}^{\dagger}$ and $\boldsymbol{b}$ as two components of a spin-$\frac{1}{2}$ vector, but the analogous quasispin generators cannot be formed. We have

$$(\bar{\boldsymbol{b}}\bar{\boldsymbol{b}})^{(1000)}=0$$

where now the ranks run q, t, s and l. For that matter, if we treat quasispin, isospin and spin on an equal footing, we cannot form a vector in any one space while leaving the other ranks zero. This results from the fact that

$$(\bar{\boldsymbol{b}}\bar{\boldsymbol{b}})^{(QTSL)}=0$$

if $Q+T+S+L$ is odd. This puzzle is cleared up by observing again the generators for U(4). In this notation they become

$$(\bar{\boldsymbol{b}}\bar{\boldsymbol{b}})^{(0000)},\ (\bar{\boldsymbol{b}}\bar{\boldsymbol{b}})^{(1100)},\ (\bar{\boldsymbol{b}}\bar{\boldsymbol{b}})^{(1010)},\ (\bar{\boldsymbol{b}}\bar{\boldsymbol{b}})^{(0110)}$$

with the total quasispin projection M_Q set equal to zero. Evidently the second and third operators represent the isospin and spin generators that produce the $\mathrm{SO}_T(3)\times \mathrm{SO}_S(3)$ subgroup of U(4). These generators act as vectors in the spin and isospin spaces alone only if they operate on states built up entirely from quasispin projections of $+\frac{1}{2}$ (or $-\frac{1}{2}$), otherwise the tensor properties are disturbed by the non-zero quasispin rank. Since nuclear states are constructed from a number of creation operators alone, these labels (spin and isospin) are perfectly legitimate.

Now we are in a position to construct a direct analogy between nuclear states and atomic operators. If we carry along all four labels in both cases, we find that the roles of isospin and quasispin are merely reversed between the two. Whereas isospin, spin and orbit are useful labels for states of maximum quasispin projection, we now find that quasispin, spin and orbit are valid for operators of maximum isospin projection. Isospin then enters into atomic physics as an additional label that is used to construct our generators, and is then projected out by considering only the $m_t=\frac{1}{2}$ states. Of course, this additional label need not be called isospin, as its accrued meaning does not apply to electrons. However, its initial sense of like spin is still relevant.

The $16l+8$ elements $\bar{\boldsymbol{b}}$ transform as the vector representation of the group SO$(16l+8)$. We can branch immediately to U$(8l+4)$ which is the parent group of both the SO$(8l+4)$ group containing all electron operators, and the U(4) $\times$ SO$(2l+1)$ product which represents all nuclear states. U(4) $\times$ SO$(2l+1)$ can also be considered a label for electron operators where now U(4) is a supermultiplet of spin and quasispin. The two alternative branchings are

$$\mathrm{SO}(16l+8)\rightarrow \mathrm{SO}(8l+4)\rightarrow \mathrm{SO}_Q(3)\times \mathrm{Sp}(4l+2)\rightarrow \mathrm{SO}_Q(3)\times \mathrm{SO}_S(3)\times \mathrm{SO}(2l+1)$$

$$\mathrm{SO}(16l+8)\rightarrow \mathrm{U}(8l+4)\rightarrow \mathrm{U}(4)\times \mathrm{SO}(2l+1)\rightarrow \mathrm{SO}_Q(3)\times \mathrm{SO}_S(3)\times \mathrm{SO}(2l+1).$$

Now we are in a position to resolve an interesting puzzle discussed by Judd and Leavitt (1986). An N-body operator transforms as $(1^{2N}0^{4l+2-2N})$ under operations of the group SO$(8l+4)$. When performing the reduction to $\mathrm{SO}_Q(3)\times \mathrm{Sp}(4l+2)$ it is sufficient to consider the reduction of the same representation of U$(8l+4)$ to $\mathrm{SO}_Q(3)\times \mathrm{U}(4l+2)$, and then continue the reduction to Sp$(4l+2)$. This result was somewhat surprising as the generators of U$(4l+2)$ and U$(8l+4)$ could not be formed from the standard operators $\bar{\boldsymbol{a}}$. However, with the introduction of the additional isospin label, the group generators are well defined and the groups exist as an alternative reduction of U$(8l+4)$:

$$\mathrm{U}(8l+4)\rightarrow \mathrm{SO}_Q(3)\times \mathrm{U}_\zeta(4l+2)\rightarrow \mathrm{SO}_Q(3)\times \mathrm{Sp}(4l+2).$$

The $\mathrm{U}_\zeta(4l+2)$ group is labelled by the subscript ζ to distinguish it from the U$(4l+2)$ whose vector representation is spanned by the operators $\boldsymbol{a}^\dagger$. This second group, call it $\mathrm{U}_\eta(4l+2)$, discussed by Judd (1968), serves to distinguish N and N' bodied operators for $N\neq N'$, and has generators which do not commute with the quasispin generators. Table 1 contains a complete list of the relevant generators.

Table 1. The groups and their generators.

Group	Generators	Number of generators
SO$(16l+8)$	$(\bar{b}\bar{b})^{(QTSL)}_{\alpha\beta\gamma\delta}$	$(8l+4)(16l+7)$
U$(8l+4)$	$(\bar{b}\bar{b})^{(QTSL)}_{\alpha 0\gamma\delta}$	$(8l+3)(8l+5)$
SO$(8l+4)$	$(\bar{b}\bar{b})^{(Q1SL)}_{\alpha 0\gamma\delta}$	$(4l+2)(8l+3)$
$\mathrm{U}_\zeta(4l+2)$	$(\bar{b}\bar{b})^{(0TSL)}_{00\gamma\delta}$	$(4l+1)(4l+3)$
$\mathrm{U}_\eta(4l+2)$	$(\bar{b}\bar{b})^{(Q1SL)}_{00\gamma\delta}$	$(4l+1)(4l+3)$
Sp$(4l+2)$	$(\bar{b}\bar{b})^{(01SL)}_{00\gamma\delta}$	$(2l+1)(4l+3)$
SO$(2l+1)$	$(\bar{b}\bar{b})^{(010l)}_{000\delta}$	$l(2l+1)$
$\mathrm{U}_{QS}(4)$	$(\bar{b}\bar{b})^{(QTS0)}_{\alpha 0\gamma 0}$	15
$\mathrm{U}_{TS}(4)$	$(\bar{b}\bar{b})^{(QTS0)}_{0\beta\gamma 0}$	15
$\mathrm{SO}_Q(3)$	$(\bar{b}\bar{b})^{(1100)}_{\alpha 000}$	3
$\mathrm{SO}_S(3)$	$(\bar{b}\bar{b})^{(0110)}_{00\gamma 0}$	3

$Q+T+S+L$ must be even.

4. Operator labels

While it is clear that a relationship exists between nuclear states and electron effective operators, it remains to be seen how this connection can be put to use. As explained by Flowers (1952), the following chain of labels $[\lambda]TM_TSM_SWLM_L$ can be used to represent the states of l^N nucleons. $[\lambda]$ stands for a representation of U(4) and W for one of SO$(2l+1)$. In the case of $l=\mathrm{f}$ an additional label for the exceptional group G_2 can be inserted between SO(7) and $\mathrm{SO}_L(3)$. We can of course attach these same labels to our N-body operators acting within the configurations l^N by substituting Q

and M_Q for T and M_T. However, since the electron conserving operators $(M_Q=0)$ do not span the representations for U(4) and $SO_Q(3)$, distinctions at these levels do not guarantee the orthogonality of different operators. Similarly we can define operators according to the group chain

$$SO(8l+4) \to SO_Q(3) \times Sp(4l+2) \to SO_Q(3) \times SO_S(3) \times SO(2l+1).$$

In this case $SO(8l+4)$ and $SO_Q(3)$ are not spanned by the operators either. However, quasispin is useful in determining relationships between the operator matrix elements within different configurations (Judd and Leavitt 1986).

The best classification scheme starts with the $U_\eta(4l+2)$ subgroup of $SO(8l+4)$. Operators with $M_Q=0$ completely span representations of $U(4l+2)$ of the type $[1^N 0^{4l+2-2N} -1^N]$. Thus of all the operators contained in $(1^{2N}0^{4l+2-2N})$ of $SO(8l+4)$ only those contained in the subrepresentation $[1^N 0^{4l+2-2N} -1^N]$ are orthogonal to the fewer-body operators established from the smaller representations of $SO(8l+4)$ (Judd 1968).

The connection to nuclear states does not prove useful in the classification of atomic operators, but does serve as an efficient computational tool when one works out the conventional classification. To demonstrate the following technique, we choose l to be 3, and work out the complete set of operators for the configurations f^N. The method is valid for any l.

To generate a complete set of N-body operators one can begin with the representation $(1^{2N}0^{14-2N})$ of SO(28), perform the branching to $SO_Q(3) \times Sp(14)$ and then continue the reduction of Sp(14) to $SO_S(3) \times SO(7)$. The first reduction is easily accomplished by the aforementioned method of considering $U(28) \to SO_Q(3) \times U_\zeta(14)$. In this case we have

$$[1^{2N}0^{28-2N}] \to {}^1[2^N 0^{14-N}] + {}^3[2^{N-1}1^2 0^{13-N}] + \ldots + {}^{2N+1}[1^{2N}0^{14-2N}].$$

The superscripts preceding the representations on the right stand for $2Q+1$. The branching from U(14) to Sp(14) can be read off directly from table C-15 of Wybourne (1970). Since $[1^{2N}0^{14-2N}]$ is still irreducible upon branching to SO(28) the reduction is complete. Table 2 contains the results.

The reduction of Sp(14) to $SO_S(3) \times SO(7)$ proves more involved. The branchings can be found using the techniques described by Wybourne (1970), but the method becomes excessively cumbersome and complicated for large values of N. Fortunately, reference to the nuclear classifications greatly simplifies the problem. The branching

$$U(28) \to U(4) \times SO(7) \to SO_Q(3) \times SO_S(3) \times SO(7)$$

is much easier to obtain. In fact, the complete branching is given by Flowers (1952). The final representations will be identical to those established by the alternative group chain. Furthermore we have already established the reduction to $SO_Q(3) \times Sp(14)$. Consider the reduction from $[1^{2N}0^{28-2N}]$ of U(28). The product $SO_Q(3) \times U(14)$ contains only a single U(14) representation for each value of quasispin. Therefore upon reducing to Sp(14) there will be only one symplectic label of order $2N$ for each quasispin value. All other representations are of order $2N-2$ or less. Assume that the branchings from Sp(14) have already been found for these lesser representations. This procedure allows one to work progressively up from $N=0$. One can now subtract off the reductions of these lesser representations from the $SO_Q(3) \times SO_S(3) \times SO(7)$ labels given by Flowers (1952). The remaining representations can be uniquely determined as coming from the single symplectic label of order $2N$ associated with each value of quasispin.

Table 2. Branching rules for $SO(28) \rightarrow SO_Q(3) \times Sp(14)$.

(1^N0^{14-N})	Q	$\langle\sigma\rangle$
(0^{14})	0	$\langle 0^7\rangle$
(1^20^{12})	0	$\langle 20^6\rangle$
	1	$\langle 0^7\rangle\langle 1^20^5\rangle$
(1^40^{10})	0	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 2^20^5\rangle$
	1	$\langle 1^20^5\rangle\langle 20^6\rangle\langle 21^20^4\rangle$
	2	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle$
(1^60^8)	0	$\langle 20^6\rangle\langle 21^20^4\rangle\langle 2^30^4\rangle$
	1	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle\langle 21^20^4\rangle\langle 2^20^5\rangle\langle 2^21^10^3\rangle$
	2	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 20^6\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle$
	3	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$
(1^80^6)	0	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle\langle 2^40^3\rangle$
	1	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 20^6\rangle\langle 21^20^4\rangle^2\langle 21^40^2\rangle\langle 2^21^20^3\rangle\langle 2^30^4\rangle\langle 2^31^20^2\rangle$
	2	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^2\langle 1^60\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle$
	3	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle\langle 20^6\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle$
	4	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$
$(1^{10}0^4)$	0	$\langle 20^6\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 2^30^4\rangle\langle 2^31^20^2\rangle\langle 2^50^2\rangle$
	1	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^2\langle 1^60\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle^2\langle 2^21^40\rangle\langle 2^31^20^2\rangle\langle 2^40^3\rangle\langle 2^41^20\rangle$
	2	$\langle 1^20^5\rangle\langle 1^40^3\rangle^2\langle 1^60\rangle\langle 20^6\rangle\langle 21^20^4\rangle^2\langle 21^40^2\rangle^2\langle 21^6\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^30^4\rangle\langle 2^31^20^2\rangle\langle 2^31^4\rangle$
	3	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^2\langle 1^60\rangle^2\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle$
	4	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle\langle 20^6\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle$
	5	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle$
$(1^{12}0^2)$	0	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^40^3\rangle\langle 2^41^20\rangle\langle 2^60\rangle$
	1	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle\langle 20^6\rangle\langle 21^20^4\rangle^2\langle 21^40^2\rangle^2\langle 21^6\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^30^4\rangle$ $\langle 2^31^20^2\rangle^2\langle 2^31^4\rangle\langle 2^41^20\rangle\langle 2^50^2\rangle\langle 2^51^2\rangle$
	2	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^3\langle 1^60\rangle^2\langle 21^20^4\rangle\langle 21^40^2\rangle^2\langle 21^6\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle^2\langle 2^21^40\rangle^2\langle 2^31^20^2\rangle\langle 2^40^3\rangle\langle 2^31^4\rangle\langle 2^41^20\rangle$
	3	$\langle 1^20^5\rangle\langle 1^40^3\rangle^2\langle 1^60\rangle^2\langle 20^6\rangle\langle 21^20^4\rangle^2\langle 21^40^2\rangle^2\langle 21^6\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^30^4\rangle\langle 2^31^20^2\rangle$
	4	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^2\langle 1^60\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle$
	5	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 20^6\rangle\langle 21^20^4\rangle$
	6	$\langle 0^7\rangle\langle 1^20^5\rangle$
(1^{14})	0	$\langle 20^6\rangle\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle\langle 2^30^4\rangle\langle 2^31^20^2\rangle\langle 2^31^4\rangle\langle 2^50^2\rangle\langle 2^51^2\rangle\langle 2^7\rangle$
	1	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^2\langle 1^60\rangle^2\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle^2\langle 2^21^40\rangle^2\langle 2^31^20^2\rangle$ $\langle 2^31^4\rangle\langle 2^40^3\rangle\langle 2^41^20\rangle^2\langle 2^51^2\rangle\langle 2^60\rangle$
	2	$\langle 1^20^5\rangle\langle 1^40^3\rangle^2\langle 1^60\rangle^2\langle 20^6\rangle\langle 21^20^4\rangle^2\langle 21^40^2\rangle^3\langle 21^6\rangle\langle 2^21^20^3\rangle\langle 2^21^40\rangle^2\langle 2^30^4\rangle\langle 2^31^20^2\rangle^2\langle 2^31^4\rangle\langle 2^41^20\rangle\langle 2^50^2\rangle$
	3	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle^3\langle 1^60\rangle^2\langle 21^20^4\rangle\langle 21^40^2\rangle^2\langle 21^6\rangle\langle 2^20^5\rangle\langle 2^21^20^3\rangle^2\langle 2^21^40\rangle\langle 2^31^20^2\rangle\langle 2^40^3\rangle$
	4	$\langle 1^20^5\rangle\langle 1^40^3\rangle^2\langle 1^60\rangle\langle 20^6\rangle\langle 21^20^4\rangle^2\langle 21^40^2\rangle\langle 2^21^20^3\rangle\langle 2^30^4\rangle$
	5	$\langle 0^7\rangle\langle 1^20^5\rangle^2\langle 1^40^3\rangle\langle 21^20^4\rangle\langle 2^20^5\rangle$
	6	$\langle 1^20^5\rangle\langle 20^6\rangle$
	7	$\langle 0^7\rangle$

The remaining reduction to total S and total L give the tensor properties of the effective operators. These can be written as $T^{(SL)J}$ where S and L are the spin and orbital ranks and J is the total angular momentum. $T^{(00)0}$ represents operators that are scalar in both S and L and thus reproduce the effects of the Coulomb interaction taken to arbitrary orders of perturbation. $T^{(11)0}$ give the spin-orbit and spin-other-orbit type interactions. Restricting oneself to a specific type of operator further simplifies the procedure. Considering a total spin of rank k allows one to deal only with the $S = k$ parts of the products from $SO_Q(3) \times SO_S(3) \times SO(7)$, allowing one to ascertain this part of the branching without examining the other irrelevant pieces. As an example the spin-scalar part of the reduction of $Sp(14)$ to $SO_S(3) \times SO(7)$ is given in table 3.

Table 3. Branching rules for $Sp(14) \rightarrow SO_S(3) \times SO(7)$. Spin = 0 part only.

$\langle\sigma\rangle$	$(w_1 w_2 w_3)$
$\langle 0^7 \rangle$	(000)
$\langle 1^2 0^5 \rangle$	(200)
$\langle 1^4 0^3 \rangle$	(220)
$\langle 1^6 0 \rangle$	(222)
$\langle 2 0^6 \rangle$	(110)
$\langle 2 1^2 0^4 \rangle$	(110)(211)(310)
$\langle 2 1^4 0^2 \rangle$	(211)(221)(321)
$\langle 2 1^6 \rangle$	(221)(322)
$\langle 2^2 0^5 \rangle$	(000)(111)(200)(220)(400)
$\langle 2^2 1^2 0^3 \rangle$	(111)(200)(210)(211)(220)(222)(310)(311)(321)(420)
$\langle 2^2 1^4 0 \rangle$	(111)(210)(220)(221)(222)(311)(320)(321)(322)(331)(422)
$\langle 2^3 0^4 \rangle$	(100)(110)(211)(221)(310)(330)(411)
$\langle 2^3 1^2 0^2 \rangle$	(100)(110)(210)(211)^2(221)^2(300)(310)(311)(320) (321)^2(322)(330)(332)(411)(421)(431)
$\langle 2^3 1^4 \rangle$	(210)(211)(221)(311)(320)(321)(322)(331)(332)(421)(432)
$\langle 2^4 0^3 \rangle$	(000)(111)(200)(210)(220)^2(222)(311)(321)(331)(400)(410)(420)(422)(440)
$\langle 2^4 1^2 0 \rangle$	(111)(200)(210)(211)(220)(221)(222)(310)(311)^2(320)(321)^2(322)(331)^2(332)(333)(410) (420)(421)(422)(430)(431)(432)(442)
$\langle 2^5 0^2 \rangle$	(110)(211)(221)(300)(310)(320)(321)(322)(330)(332)(411)(421)(431)(433)(441)
$\langle 2^5 1^2 \rangle$	(110)(211)(221)(310)(320)(321)(322)(330)(331)(332)(411)(421)(431)(432)(433)(441)(443)
$\langle 2^6 0 \rangle$	(000)(200)(220)(222)(311)(321)(331)(333)(400)(420)(422)(430)(432)(440)(442)(444)
$\langle 2^7 \rangle$	(310)(322)(431)(443)

5. Hermiticity

There is one additional constraint on the operators. Only Hermitian operators are of physical interest. The Hermiticity can be established on the symplectic level by the following scheme. The presentation that is given here generalises the analysis given for f^3 (Judd and Suskin 1984, § 5) and corrects a garbled argument (Judd and Leavitt 1986, § 4) which, nevertheless, led to no subsequent error. To examine N-body orthogonal operators we want only to consider those contained in the representation $[1^N 0^{14-2N} - 1^N]$ of $U_\eta(14)$. All operators of this form can be found by taking the product of $[1^N 0^{14-N}]$ and $[0^{14-N} - 1^N]$ and subtracting out the terms such as $[1^M 0^{14-2M} - 1^M]$ with $M < N$. On the symplectic level this corresponds to taking the product $\langle 1^N 0^{14-N} \rangle \times \langle 1^N 0^{14-N} \rangle$. The Hermitian and antiHermitian operators are related to the symmetric and antisymmetric parts of this product.

Consider operators of the type $a^\dagger_{\alpha\beta} a_{\gamma\delta}$ belonging to $[10^{4l} - 1]$ of $U(4l+2)$. (These are just the standard s and l creation and annihilation operators.) To be Hermitian $a^\dagger_{\alpha\beta} a_{\gamma\delta}$ must occur with the same sign as its adjoint, $a^\dagger_{\gamma\delta} a_{\alpha\beta}$. In the more extended vector notation these two terms become

$$\bar{a}_{1/2\alpha\beta} \bar{a}_{-1/2-\gamma-\delta} (-1)^{s+l-\gamma-\delta} + \bar{a}_{1/2\gamma\delta} \bar{a}_{-1/2-\alpha-\beta} (-1)^{s+l-\alpha-\beta}.$$

Alone, these terms correspond to neither the symmetric nor antisymmetric part of the product $\langle 10^{2l} \rangle \times \langle 10^{2l} \rangle$. However, one typically considers operators coupled to some final ranks in S and L, or in J. Consider the operator

$$A = (\boldsymbol{a}^\dagger \boldsymbol{a})^{(SL)J}_M .$$

By uncoupling, taking the adjoint and recoupling, one finds

$$A^\dagger = (-1)^{S+L+J-M} (\boldsymbol{a}^\dagger \boldsymbol{a})^{(SL)J}_{-M} .$$

Table 4. Branching rules for U(14) → Sp(14) ($(\langle 1^N0^{7-N}\rangle \times \langle 1^N0^{7-N}\rangle)$) and Hermiticity for operators $\boldsymbol{T}^{(kk)0}(\langle\sigma\rangle)$.

$[1^N0^{14-2N}-1^N]$	$\langle 1^N0^{7-N}\rangle \times \langle 1^N0^{7-N}\rangle_{\text{symmetric}}$	$\langle 1^N0^{7-N}\rangle \times \langle 1^N0^{7-N}\rangle_{\text{antisymmetric}}$	$\langle\sigma\rangle_{\text{Hermitian}}$	$\langle\sigma\rangle_{\text{antiHermitian}}$
$[0^{14}]$	$\langle 0^7\rangle$		$\langle 0^7\rangle$	
$[10^{12}-1]$	$\langle 20^6\rangle$	$\langle 1^20^5\rangle$	$\langle 1^20^5\rangle$	$\langle 20^6\rangle$
$[1^20^{10}-1^2]$	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 2^20^5\rangle$	$\langle 1^20^5\rangle\langle 21^20^4\rangle$	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 2^20^5\rangle$	$\langle 1^20^5\rangle\langle 21^20^4\rangle$
$[1^30^8-1^3]$	$\langle 1^40^3\rangle\langle 20^6\rangle\langle 21^20^4\rangle$	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$	$\langle 1^40^3\rangle\langle 20^6\rangle\langle 21^20^4\rangle$
	$\langle 21^40^2\rangle\langle 2^30^4\rangle$	$\langle 21^20^4\rangle\langle 2^21^20^3\rangle$	$\langle 21^20^4\rangle\langle 2^21^20^3\rangle$	$\langle 21^40^2\rangle\langle 2^30^4\rangle$
$[1^40^6-1^4]$	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle^2$	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle^2$	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$
	$\langle 1^60\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle$	$\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle$	$\langle 1^60\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle$	$\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle$
	$\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^40^3\rangle$	$\langle 2^21^20^3\rangle\langle 2^41^20\rangle$	$\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^40^3\rangle$	$\langle 2^21^20^3\rangle\langle 2^41^20\rangle$
$[1^50^4-1^5]$	$\langle 1^40^3\rangle\langle 1^60\rangle\langle 20^6\rangle$	$\langle 0^7\rangle\langle 1^40^3\rangle\langle 1^60\rangle$	$\langle 0^7\rangle\langle 1^40^3\rangle\langle 1^60\rangle$	$\langle 1^40^3\rangle\langle 1^60\rangle\langle 20^6\rangle$
	$\langle 21^20^4\rangle\langle 21^40^2\rangle^2\langle 2^21^40\rangle$	$\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle$	$\langle 21^20^4\rangle\langle 21^40^2\rangle\langle 21^6\rangle$	$\langle 21^20^4\rangle\langle 21^40^2\rangle^2\langle 2^21^40\rangle$
	$\langle 2^30^4\rangle\langle 2^31^20^2\rangle\langle 2^31^4\rangle$	$\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^31^20^2\rangle$	$\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^31^20^2\rangle$	$\langle 2^30^4\rangle\langle 2^31^20^2\rangle\langle 2^31^4\rangle$
	$\langle 2^50^2\rangle$	$\langle 2^41^20\rangle$	$\langle 2^41^20\rangle$	$\langle 2^50^2\rangle$
$[1^60^2-1^6]$	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle$	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$	$\langle 0^7\rangle\langle 1^20^5\rangle\langle 1^40^3\rangle$	$\langle 1^20^5\rangle\langle 1^40^3\rangle\langle 1^60\rangle$
	$\langle 1^60\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle$	$\langle 21^20^4\rangle\langle 21^6\rangle\langle 2^21^20^3\rangle$	$\langle 1^60\rangle\langle 21^40^2\rangle\langle 2^20^5\rangle$	$\langle 21^20^4\rangle\langle 21^6\rangle\langle 2^21^20^3\rangle$
	$\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^31^4\rangle$	$\langle 2^21^40\rangle\langle 2^31^20^2\rangle\langle 2^41^20\rangle$	$\langle 2^21^20^3\rangle\langle 2^21^40\rangle\langle 2^31^4\rangle$	$\langle 2^21^40\rangle\langle 2^31^20^2\rangle\langle 2^41^20\rangle$
	$\langle 2^40^3\rangle\langle 2^41^20\rangle\langle 2^60\rangle$	$\langle 2^51^2\rangle$	$\langle 2^40^3\rangle\langle 2^41^20\rangle\langle 2^60\rangle$	$\langle 2^51^2\rangle$
$[1^7-1^7]$	$\langle 20^6\rangle\langle 21^40^2\rangle\langle 2^30^4\rangle$	$\langle 21^20^4\rangle\langle 21^6\rangle\langle 2^31^20^2\rangle$	$\langle 21^20^4\rangle\langle 21^6\rangle\langle 2^31^20^2\rangle$	$\langle 20^6\rangle\langle 21^40^2\rangle\langle 2^30^4\rangle$
	$\langle 2^31^4\rangle\langle 2^50^2\rangle\langle 2^7\rangle$	$\langle 2^51^2\rangle$	$\langle 2^51^2\rangle$	$\langle 2^31^4\rangle\langle 2^50^2\rangle\langle 2^7\rangle$

Contained within A are the two terms $\bar{a}_{1/2\alpha\beta}\bar{a}_{-1/2\gamma\delta}$ and $\bar{a}_{1/2\gamma\delta}\bar{a}_{-1/2\alpha\beta}$ with identical coupling coefficients except for a phase difference of $(-1)^{1+S+L}$. If $S+L$ is even, this implies an antisymmetric product, while $S+L$ odd gives a symmetric product. In the event that M is 0, the constraint of Hermiticity forces $S+L+J$ to be even. Therefore if J is even, the Hermitian operators fall into the antisymmetric products. If J is odd, the Hermitian operators are contained in the symmetric products. The situation is reversed for antiHermitian operators. If M is not zero the symmetry of the product no longer specifies the Hermiticity. This analysis is easily generalised to include N-body operators coupled to a final rank J. In this case, if $N+J$ is even the Hermitian operators fall into the symmetric part of the product $\langle 1^N 0^{2l+1-N}\rangle \times \langle 1^N 0^{2L+1-N}\rangle$. If $N+J$ is odd the Hermitian operators are found in the antisymmetric part. Table 4 yields the decomposition of $[1^N 0^{14-2N} - 1^N]$ into the symmetric and antisymmetric pieces of Sp(14) and the Hermitian and antiHermitian parts for operators of the form $T^{(kk)0}$. As previously noted by Judd and Leavitt (1986) N-body operators for $N > 2l+1$ need not be considered.

6. f-electron scalar operators

We are now in a position to classify all scalar operators available within the f shell. This gives a scheme for reproducing the effects of the Coulomb operator to an arbitrary order of perturbation theory. Since the group $U_\eta(14)$ used to classify the operators does not commute with quasispin, the quasispin ranks are not necessarily well defined. By examining the branching $SO(28) \rightarrow SO_Q(3) \times Sp(14)$ one can determine the available quasispin ranks for each symplectic label. Furthermore, use can be made of the theorem established by Judd and Leavitt (1986) that for a Hermitian N-body orthogonal operator the quasispin must have the same parity as N. This further restricts the available quasispin values for each operator. Table 5 presents a complete list of N-body scalar operators for N less than five. The operator nomenclature is similar to that used by Judd and Leavitt (1986). Although the zero-, two- and three-body operators given are the same as those presented by Judd and Suskin (1984), one should note that the operator names are slightly different. Judd and Suskin (1984) also give the connection between these operators and those appearing earlier in the literature. If needed, the five-, six- or seven-body operators can be easily read off from tables 3 and 4.

There are several interesting points. One is that for N greater than three the group chain is not sufficient to uniquely specify each operator. For example, when $N=4$ two separate pairs of operators occur with identical labels. In practice this causes little problem as the operators can be algebraically orthogonalised before being put to use. In no case were there more than two operators with the same labels. It was hoped that a general group theoretic scheme could be uniformly applied to eliminate these multiplicities. However, the duplications occur at almost all levels for the many-body operators. (They occur at the Sp(14), SO(7), G_2 and $SO_L(3)$ levels.) Therefore a simple method of resolving these multiplicities appears unlikely.

Since these operators represent all possible scalar interactions within each configuration, the total number of operators acting between states of a given configuration must be equal to the number of available matrix elements. The number of matrix elements can be easily counted from the list of states provided by Nielson and Koster (1963), providing an independent check of the classification scheme. Table 6 presents the total number of Hermitian scalar f-electron operators and the number of multiplicities that occur at each level.

Table 5. N-electron $T^{(00)0}$ operators in the f shell.

Name	N	Sp(14)	SO(7)	G_2	$SO_Q(3)$
e_0	0	$\langle 0^7\rangle$	(000)	(00)	0
e_1	2	$\langle 0^7\rangle$	(000)	(00)	0, 2
e_2	2	$\langle 1^4 0^3\rangle$	(220)	(22)	2
e_3	2	$\langle 2^2 0^5\rangle$	(000)	(00)	2
e_4	2	$\langle 2^2 0^5\rangle$	(111)	(00)	2
e_5	2	$\langle 2^2 0^5\rangle$	(220)	(22)	2
e_6	2	$\langle 2^2 0^5\rangle$	(400)	(40)	2
t_1	3	$\langle 1^4 0^3\rangle$	(220)	(22)	1, 3
t_2	3	$\langle 1^6 0\rangle$	(222)	(00)	3
t_3	3	$\langle 1^6 0\rangle$	(222)	(40)	3
t_4	3	$\langle 2^2 1^2 0^3\rangle$	(111)	(00)	1
t_5	3	$\langle 2^2 1^2 0^3\rangle$	(220)	(22)	1
t_6	3	$\langle 2^2 1^2 0^3\rangle$	(222)	(00)	1
t_7	3	$\langle 2^2 1^2 0^3\rangle$	(222)	(40)	1
t_8	3	$\langle 2^2 1^2 0^3\rangle$	(311)	(22)	1
t_9	3	$\langle 2^2 1^2 0^3\rangle$	(311)	(40)	1
t_{10}	3	$\langle 2^2 1^2 0^3\rangle$	(321)	(22)	1
t_{11}	3	$\langle 2^2 1^2 0^3\rangle$	(321)	(40)	1
t_{12}	3	$\langle 2^2 1^2 0^3\rangle$	(420)	(22)	1
t_{13}	3	$\langle 2^2 1^2 0^3\rangle$	(420)	(40)	1
t_{14}	3	$\langle 2^2 1^2 0^3\rangle$	(420)	(42)	1
f_1	4	$\langle 0^7\rangle$	(000)	(00)	0, 2, 4
f_2	4	$\langle 1^4 0^3\rangle_A$	(220)	(22)	0, 2, 4
f_3	4	$\langle 1^4 0^3\rangle_B$	(220)	(22)	0, 2, 4
f_4	4	$\langle 1^6 0\rangle$	(222)	(00)	2, 4
f_5	4	$\langle 1^6 0\rangle$	(222)	(40)	2, 4
f_6	4	$\langle 2 1^4 0^2\rangle$	(321)	(22)	2, 4
f_7	4	$\langle 2 1^4 0^2\rangle$	(321)	(40)	2, 4
f_8	4	$\langle 2^2 0^5\rangle$	(000)	(00)	0, 2
f_9	4	$\langle 2^2 0^5\rangle$	(111)	(00)	0, 2
f_{10}	4	$\langle 2^2 0^5\rangle$	(220)	(22)	0, 2
f_{11}	4	$\langle 2^2 0^5\rangle$	(400)	(40)	0, 2
f_{12}	4	$\langle 2^2 1^2 0^3\rangle$	(111)	(00)	0, 2
f_{13}	4	$\langle 2^2 1^2 0^3\rangle$	(220)	(22)	0, 2
f_{14}	4	$\langle 2^2 1^2 0^3\rangle$	(222)	(00)	0, 2
f_{15}	4	$\langle 2^2 1^2 0^3\rangle$	(222)	(40)	0, 2
f_{16}	4	$\langle 2^2 1^2 0^3\rangle$	(311)	(22)	0, 2
f_{17}	4	$\langle 2^2 1^2 0^3\rangle$	(311)	(40)	0, 2
f_{18}	4	$\langle 2^2 1^2 0^3\rangle$	(321)	(22)	0, 2
f_{19}	4	$\langle 2^2 1^2 0^3\rangle$	(321)	(40)	0, 2
f_{20}	4	$\langle 2^2 1^2 0^3\rangle$	(420)	(22)	0, 2
f_{21}	4	$\langle 2^2 1^2 0^3\rangle$	(420)	(40)	0, 2
f_{22}	4	$\langle 2^2 1^2 0^3\rangle$	(420)	(42)	0, 2
f_{23}	4	$\langle 2^2 1^4 0\rangle$	(111)	(00)	2
f_{24}	4	$\langle 2^2 1^4 0\rangle$	(220)	(22)	2
f_{25}	4	$\langle 2^2 1^4 0\rangle$	(222)	(00)	2
f_{26}	4	$\langle 2^2 1^4 0\rangle$	(222)	(40)	2
f_{27}	4	$\langle 2^2 1^4 0\rangle$	(311)	(22)	2
f_{28}	4	$\langle 2^2 1^4 0\rangle$	(311)	(40)	2
f_{29}	4	$\langle 2^2 1^4 0\rangle$	(320)	(22)	2
f_{30}	4	$\langle 2^2 1^4 0\rangle$	(321)	(22)	2
f_{31}	4	$\langle 2^2 1^4 0\rangle$	(321)	(40)	2
f_{32}	4	$\langle 2^2 1^4 0\rangle$	(322)	(40)	2
f_{33}	4	$\langle 2^2 1^4 0\rangle$	(331)	(22)	2

Table 5. (continued)

Name	N	Sp(14)	SO(7)	G_2	$SO_Q(3)$
f_{34}	4	$\langle 2^2 1^4 0\rangle$	(331)	(40)	2
f_{35}	4	$\langle 2^2 1^4 0\rangle$	(331)	(42)	2
f_{36}	4	$\langle 2^2 1^4 0\rangle$	(422)	(22)	2
f_{37}	4	$\langle 2^2 1^4 0\rangle$	(422)	(40)	2
f_{38}	4	$\langle 2^2 1^4 0\rangle$	(422)	(42)	2
f_{39}	4	$\langle 2^2 1^4 0\rangle$	(422)	(60)	2
f_{40}	4	$\langle 2^4 0^3\rangle$	(000)	(00)	0
f_{41}	4	$\langle 2^4 0^3\rangle$	(111)	(00)	0
f_{42}	4	$\langle 2^4 0^3\rangle$	$(220)_A$	(22)	0
f_{43}	4	$\langle 2^4 0^3\rangle$	$(220)_B$	(22)	0
f_{44}	4	$\langle 2^4 0^3\rangle$	(222)	(00)	0
f_{45}	4	$\langle 2^4 0^3\rangle$	(222)	(40)	0
f_{46}	4	$\langle 2^4 0^3\rangle$	(311)	(22)	0
f_{47}	4	$\langle 2^4 0^3\rangle$	(311)	(40)	0
f_{48}	4	$\langle 2^4 0^3\rangle$	(321)	(22)	0
f_{49}	4	$\langle 2^4 0^3\rangle$	(321)	(40)	0
f_{50}	4	$\langle 2^4 0^3\rangle$	(331)	(22)	0
f_{51}	4	$\langle 2^4 0^3\rangle$	(331)	(40)	0
f_{52}	4	$\langle 2^4 0^3\rangle$	(331)	(42)	0
f_{53}	4	$\langle 2^4 0^3\rangle$	(400)	(40)	0
f_{54}	4	$\langle 2^4 0^3\rangle$	(410)	(40)	0
f_{55}	4	$\langle 2^4 0^3\rangle$	(420)	(22)	0
f_{56}	4	$\langle 2^4 0^3\rangle$	(420)	(40)	0
f_{57}	4	$\langle 2^4 0^3\rangle$	(420)	(42)	0
f_{58}	4	$\langle 2^4 0^3\rangle$	(422)	(22)	0
f_{59}	4	$\langle 2^4 0^3\rangle$	(422)	(40)	0
f_{60}	4	$\langle 2^4 0^3\rangle$	(422)	(42)	0
f_{61}	4	$\langle 2^4 0^3\rangle$	(422)	(60)	0
f_{62}	4	$\langle 2^4 0^3\rangle$	(440)	(40)	0
f_{63}	4	$\langle 2^4 0^3\rangle$	(440)	(42)	0
f_{64}	4	$\langle 2^4 0^3\rangle$	(440)	(43)	0
f_{65}	4	$\langle 2^4 0^3\rangle$	(440)	(44)	0

Table 6. The number of N-body scalar operators.

N	Number of operators	Multiplicities
0	1	0
1	0	0
2	6	0
3	14	0
4	65	2
5	107	12
6	182	7
7	50	3

It is important to note that one can just as easily classify non-scalar effective operators, such as those that reproduce any crystal-field effects. These operators would appear as $T^{(0k)}_{0q}$ where the spin rank is zero and k and q give the orbital rank and orientation. These operators would be useful for considering the crystal-field interactions as combined with other scalar perturbations. However, the efficacy of this approach is limited by serious multiplicity problems as well as by the difficulty of dealing with a quite large set of operators. For example, in the f shell there are 11 two-body, 106 three-body and 333 four-body operators with the rank $T^{(04)}_{0q}$. The sheer number of available operators would make this approach impractical when considering effects smaller than second order.

7. Conclusions

Before using these operators, it is necessary to evaluate their matrix elements within the configurations f^N. Judd and Suskin (1984) have given the matrix elements up to f^3. It is straightforward but tedious to evaluate the matrix elements for higher N. A matrix element of any operator can be expressed as a product of generalised Clebsch-Gordan coefficients or isoscalar factors times a reduced matrix element at the U(14) level. Judd (1963) presents a method for evaluating these coefficients. Judd and Leavitt (1986), however, describe a simpler technique. Given the matrix elements of all operators in f^{n-1}, one can evaluate the matrix elements of all operators acting on $n-1$ or fewer electrons within the configuration f^n by using the equation

$$\langle l^n\psi|H_i|l^n\psi'\rangle = [n/(n-N)] \sum_{\phi,\phi'} (\psi\{|\phi)\langle l^{n-1}\phi|H_i|l^{n-1}\phi'\rangle(\phi'|\}\psi')$$

where H_i is an N-body operator and the coefficients of fractional parentage $(\psi\{|\phi)$ are given by Nielson and Koster (1963). The matrix elements of the n-body operators can be found by requiring orthogonality with the fewer-body operators. This method is facilitated by using known proportionalities between operators with some (but not all) identical labels. In this manner one could extend the results of Judd and Suskin (1984) in a stepwise fashion to higher N.

While the four-body operators should prove useful in configurations larger than f^3, the effects of the higher-order operators will most likely be small compared to those given by the spin-orbit, spin-other-orbit, and spin-spin interactions. It would then be necessary to classify and examine operators of the type $T^{(11)0}$ and $T^{(22)0}$. In these cases the situation is more complicated due to the increased number of operators and group label multiplicities.

These orthogonal operators present a convenient scheme for reproducing the effects of physical interactions. Once a fit of the experimental data has been performed, one can extract explicit physical information from these operators. Linear combinations of orthogonal operators will be needed to give the effect of any one physical process, and in general not all operators will be needed at each level of perturbation. In third order only a subset of the four-body operators will contribute. One can perform the perturbation, relate the physical operators to the effective operators and thus extract the size of the associated radial contributions. The effective operator approach thus provides a coherent scheme for generating physical information from an experimental fit.

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