Three-Particle Operators for Equivalent Electrons

B. R. JUDD
Lawrence Radiation Laboratory, University of California, Berkeley, California
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Interaction between the electronic configurations $(nl)^N$ and $(nl)^{N\pm1}(n'l')^{\mp1}$ can be represented for $(nl)^N$ by the addition of effective three-particle operators to the Hamiltonian, the effective two-particle parts being absorbed by operators already present in the elementary linear theory of configuration interaction. For f electrons, the three-particle operators are decomposed into nine operators t_i that are labeled by irreducible representations of R_7 and G_2. The effects of three of them can be reproduced by two-particle operators; hence, only six additional parameters are required to describe the interaction. Tables of matrix elements are given, and the properties of the operators t_i with respect to symplectic symmetry and quasispin are examined.

I. INTRODUCTION

The use of effective operators is a common feature of atomic spectroscopy. For example, the spin-orbit interaction for a many-electron system is $\sum_i \xi(r_i) \times \mathbf{s}_i\cdot \mathbf{l}_i$; but within a given Russell-Saunders multiplet it can be replaced by the effective operator $\lambda\mathbf{S}\cdot\mathbf{L}$, where $\mathbf{S}$ and $\mathbf{L}$ are the vector sums of the spins $\mathbf{s}_i$ and orbital angular momenta $\mathbf{l}_i$ of all the electrons i. The parameter λ depends on the detailed character of $\xi(r)$, but for the purpose of fitting the levels of a multiplet, it is often convenient to regard it as an adjustable parameter.

This principle can be extended to allow for the term displacements produced by configuration interaction. The effective operator $\alpha\mathbf{L}^2$, which possesses eigenvalues $\alpha L(L+1)$, significantly improves the energy-level structure of configurations of d electrons.[1] This is ascribed to its ability to represent the perturbing effect of those configurations that involve two-electron excitations.[2] Formally, another operator βQ should also be included to make the substitution rigorous to second order in perturbation theory. Although more difficult to detect, its existence is now beyond dispute.[3] For f electrons, a third operator is necessary to take into account two-electron excitations; it has been introduced by Trees[4] in his analysis of Pr III $4f^3$. A convenient general form for these operators is

$$y_k=\sum_{i\neq j}(\mathbf{v}_i^{(k)}\cdot\mathbf{v}_j^{(k)}),$$

where the tensor operator $\mathbf{v}^{(k)}$ is related to the unit operator $\mathbf{u}^{(k)}$ by the equation[5] $\mathbf{v}^{(k)}=\mathbf{u}^{(k)}[k]^{1/2}$. The operator $\alpha\mathbf{L}^2$, for example, is simply related to y_1; the remaining effective operators involve other scalar products y_k for which k is odd. Since the ordinary Coulomb interaction within a configuration $(nl)^N$ can be expanded in terms of the y_k for which k is even, the total electrostatic Hamiltonian, including both real and effective parts, can be expressed as a linear combination of the $y(k)$ for which $0\leq k\leq 2l$.

The question how to represent the single-particle excitations has been recently attacked by Rajnak and Wybourne.[6] They found that effective operators can again be constructed to absorb such interactions; but unlike those so far considered, these operators have necessarily to include three-electron components of the type

$$V(kk'k'')=\sum_{h\neq i\neq j}\sum_{q,q',q''}\begin{pmatrix}k & k' & k''\\ q & q' & q''\end{pmatrix}\times(v_q^{(k)})_h(v_{q'}^{(k')})_i(v_{q''}^{(k'')})_j.$$

The reason for the occurrence of three-electron operators can be most easily seen if the method of second quantization is used.[7]

The number of parameters that are needed to preface the various operators $V(kk'k'')$ is not as large as might at first appear. If either k, k', or k'' is zero, $V(kk'k'')$ reduces to an operator of the type y_k. It also turns out that k, k', and k'' must all be even, and that an interchange of any two of them leaves $V(kk'k'')$ invariant. Their upper bound is set at $2l$ by the triangular conditions. For f electrons, these considerations limit the triad $(kk'k'')$ to the ten possibilities (222), (224), (244), (246), (444), (446), (266), (466), (666), and (226). This accounts for the statement that ten parameters are needed to completely describe the three-electron operators.[6,8] A partial parametrization has recently been made by Rajnak,[8] who greatly improved the fit with the observed levels of Pr III $4f^3$. In order to probe the nature of the perturbing configurations, she took as operators the linear combinations

$$X(kk',l')=\sum[k'']^{1/2}[k]^{-1/2}[k']^{-1/2}\times\begin{Bmatrix}k & k' & k''\\ l & l & l'\end{Bmatrix}V(kk'k''),$$

[1] R. E. Trees, Phys. Rev. **83**, 756 (1951); 84, 1089 (1951).
[2] G. Racah, Phys. Rev. **85**, 381 (1952).
[3] Y. Shadmi, Phys. Rev. **139**, A43 (1965).
[4] R. E. Trees, J. Opt. Soc. Am. **54**, 651 (1964).
[5] Here and elsewhere the traditional abbreviation $[x]=2x+1$ is made for a single symbol (possibly subscripted) within square brackets. Actual numbers (or λ) within square brackets will as usual stand for representations of a unitary group, however.
[6] K. Rajnak and B. G. Wybourne, Phys. Rev. **132**, 280 (1963).
[7] B. R. Judd, University of California Lawrence Radiation Laboratory Report UCRL-16098, 1965 (unpublished).
[8] K. Rajnak, J. Opt. Soc. Am. **55**, 126 (1965).

where the sum runs over even values of k'', excluding $k''=0$. The various $X(kk',l')$ for a given l' are sufficient to represent the three-particle part of the effect of $(nl)^{N\pm1}(n'l')^{\mp1}$ on $(nl)^N$. The assumption that excitations of the type $f\rightarrow h$ can be neglected limits l' to 1 and 3, for which there are nine operators $X(kk',l')$ in all. However, Rajnak found that five of these operators are sufficient to obtain a good fit with experiment, and that the inclusion of more operators leads to little improvement.

There is little doubt that analyses of free-ion configurations such as f^4, f^5, or f^6 will be attempted soon. The usefulness of the three-particle effective operators will then be tested much more critically than has been possible for f^3. It is the purpose of this paper to present a detailed analysis of these operators, thereby giving a theoretical basis to the method of parametrization. From a practical standpoint, the principal result is that for f electrons the number of additional parameters that are needed to represent the three-particle operators are not ten, as appears from the argument above, but only six. To arrive at this result, a study is made of the symmetry properties of the operators. These properties are of considerable interest in themselves, and strikingly illustrate the great value of the theory of continuous groups in atomic spectroscopy.

II. TWO-PARTICLE OPERATORS

In his analysis of the Coulomb interaction within configurations of equivalent f electrons, Racah[9] constructed the following linear combinations of the operators y_k:

$$e_0=7y_0/2\,,$$
$$e_1=9y_0/2+y_2+y_4+y_6\,,$$
$$e_2=143y_2-130y_4+35y_6\,,$$
$$e_3=11y_2+4y_4-7y_6\,.$$

In terms of the irreducible representations W and U of the groups R_7 and G_2, respectively, these linear combinations correspond to $WU=(000)(00)$, $(000)(00)$, $(400)(40)$, and $(220)(22)$. By using W and U to label the eigenfunctions as well, Racah was able to relate matrix elements of each e_i to others with similar $WUSL$ descriptions. This technique exposes the properties of the Coulomb interaction in a striking and profound manner. It also suggests an approach to the parametrization of the three-particle operators. For suppose linear combinations t_i of the $V(kk'k'')$ are constructed that correspond to definite representations WU. If we find a WU designation that has already arisen in the treatment of the e_i, then there is a possibility that the effect of the corresponding operator t_i can be taken up merely by changing the parameters of the Coulomb interaction.

[9] G. Racah, Phys. Rev. **76**, 1352 (1949).

Since operators y_k for odd k have also been included in the Hamiltonian, the number of irreducible operators available for absorbing the effects of the operators t_i is even larger than might at first appear. The possible WU designations that arise from this source are easily found. The operators $\mathbf{v}^{(1)}$, $\mathbf{v}^{(3)}$, and $\mathbf{v}^{(5)}$ transform like the representation (110) of R_7 (see Racah[9]); the scalar products y_k must therefore correspond to the S states that occur in the Kronecker product $(110)\times(110)$. Including the appropriate representations U of G_2, we find that the operators y_k for odd k can be assembled into three linear combinations e_4, e_5, and e_6, for which $WU=(000)(00)$, $(111)(00)$, and $(220)(22)$, respectively. A detailed construction (with arbitrary normalization) gives

$$e_4=y_1+y_3+y_5\,,$$
$$e_5=y_1-2y_3+y_5\,,$$
$$e_6=11y_1-3y_5\,.$$

The operator e_6 is identical to Ω of Racah.[9] The eigenvalues of e_4, e_5, and e_6, unlike those for e_2 and e_3, can be easily expressed in terms of Casimir's operators G for G_2 and R_7. In order, they are $5G(R_7)-3N$ (for e_4), $12G(G_2)-10G(R_7)$ (for e_5), and $\frac{1}{2}L(L+1)-12G(G_2)$ (for e_6). The parameters E_i associated with the operators e_i $(i\geq4)$ are related to the parameters α, β, and γ of Rajnak and Wybourne[6] through the identity

$$E^4[5G(R_7)-3N]+E^5[12G(G_2)-10G(R_7)]+E^6[\tfrac{1}{2}L(L+1)-12G(G_2)]\equiv\alpha L(L+1)+\beta G(G_2)+\gamma G(R_7)+\delta\,.$$

This corresponds to using

$$\sum_{i=0}^{6} e_iE^i$$

as the total two-particle part of the effective electrostatic Hamiltonian for the configuration f^N.

III. COUPLED TENSORS

The tensors $\mathbf{v}^{(2)}$, $\mathbf{v}^{(4)}$, and $\mathbf{v}^{(6)}$ are the basic operators for the construction of the linear combinations t_i of the $V(kk'k'')$. They comprise 27 components in all, and transform according to the representations $WU=(200)(20)$. Since the t_i must be totally symmetric under the interchange of any two electrons, they must all correspond to the representation [3] of the unitary group U_{27}. The branching rules for the reduction of several representations $[\lambda]$ of U_{27} to representations W of R_7 are given in Table I. They can be unambiguously determined by dimensional considerations and the knowledge that [2] must contain the representations associated with the completely symmetric operators e_i $(0\leq i\leq3)$. The dimensions $D[\lambda]$ are included in the table.

TABLE I. Branching rules for the reduction $U_{27} \to R_7$.

$D[\lambda]$	$[\lambda]$	W
27	[1]	(200)
378	[2]	(000) (200) (220) (400)
351	[11]	(110) (310)
3654	[3]	$(000)\,(200)^2(220)\,(222)\,(310)\,(400)\,(420)\,(600)$
6552	[21]	$(110)\,(200)^2(211)\,(220)\,(310)^2(321)\,(400)\,(420)\,(510)$
2925	[111]	(110) (211) (310) (330) (411)

To find the group-theoretical descriptions of the operators t_i, we have only to pick out the representations W that occur in [3] and that at the same time contain a representation D_K of R_3 for which $K=0$. Nine such representations exist; they are listed with the accompanying representations U of G_2 in Table II. Each t_i is a linear combination of the $V(kk'k'')$. Since we have given ten possible triads $(kk'k'')$ in Sec. I, it might appear that Table II is incomplete. However, $V(226)$ is identically zero, since the triangular condition on k, k', and k'' is not satisfied. This fact, which reduces the number of three-particle parameters to at most nine, seems to have been overlooked in previous work.

The actual construction of the operators t_i involves coupling coefficients in which representations of U_{27}, R_7, G_2, R_3, and R_2 appear. For some representations U, a given representation of R_3 occasionally occurs more than once; the additional symbol τ is then required to make the designation unambiguous. The operator

$$
\begin{aligned}
t(WU)=\sum\big([1](200)(20)kq;\,[1](200)(20)k'q'\,|\\
[2]W'U'\tau'k'',\,-q''\big)\,\big([2]W'U'\tau'k'',\,-q'';\\
[1](200)(20)k''q''\,|\,[3]WU00\big)\\
\times(v_q{}^{(k)})_h(v_{q'}{}^{(k')})_i(v_{q''}{}^{(k'')})_i,
\end{aligned}
$$

where the sum runs over $W'U'\tau'kk'k''qq'q''$, is the scalar component of a generalized tensor transforming as WU. On factoring out the vector-coupling (VC) coefficients and summing over $h\neq i\neq j$, it becomes

$$t(WU)=\sum(kk'k''\,|\,WU)V(kk'k''), \qquad (1)$$

where the sum runs over even nonzero values of k, k', and k'', and where

$$
\begin{aligned}
(kk'k''\,|\,WU)
&=\sum_{W'U'\tau'}\big([1](200)(20)k\\
&\quad+[1](200)(20)k'\,|\,[2]W'U'\tau'k''\big)\\
&\quad\times\big([2]W'U'\tau'k''+[1](200)(20)k''\,|\,[3]WU0\big). \qquad (2)
\end{aligned}
$$

TABLE II. Description of operators.

t_i	WUK
t_1	(000) (00)0
t_2	(220) (22)0
t_3	(222) (00)0
t_4	(222) (40)0
t_5	(400) (40)0
t_6	(420) (22)0
t_7	(420) (40)0
t_8	(420) (42)0
t_9	(600) (60)0

The operators t_i are identified with the $t(WU)$ according to the listing in Table II. Thus $t_7\equiv t((420)(40))$.

To find the coefficients $(kk'k''\,|\,WU)$, the two coupling coefficients of Eq. (2) must be calculated. It is convenient to use a theorem of Racah[9] to make the factorization

$$
\begin{aligned}
&\big([2]W'U'\tau'k''+[1](200)(20)k''\,|\,[3]WU0\big)\\
&\qquad=\big([2]W'+[1](200)\,|\,[3]W\big)\\
&\qquad\quad\times\big(W'U'\tau'k''+(200)(20)k''\,|\,WU0\big).
\end{aligned}
$$

The factor $([1](200)+[1](200)\,|\,[2]W')$, which arises when an analogous decomposition is carried out for the other coupling coefficient, can be taken equal to $+1$.

TABLE III. The coefficients $(W'U'k''+(200)(20)k''\,|\,WU0)$ for $W'\neq(400)$.

		k''		
$W'U'$	WU	2	4	6
(200) (20)	(000) (00)	$(5/27)^{1/2}$	$(1/3)^{1/2}$	$(13/27)^{1/2}$
	(220) (22)	$-(55/126)^{1/2}$	$-(8/77)^{1/2}$	$(91/198)^{1/2}$
	(400) (40)	$(143/378)^{1/2}$	$-(130/231)^{1/2}$	$(35/594)^{1/2}$
(220) (20)	(220) (22)	$(5/2016)^{1/2}$	$(1/1694)^{1/2}$	$-(91/34848)^{1/2}$
	(222) (00)	$-(5/27)^{1/2}$	$-(1/3)^{1/2}$	$-(13/27)^{1/2}$
	(222) (40)	$(715/21168)^{1/2}$	$-(325/6468)^{1/2}$	$(25/4752)^{1/2}$
	(420) (22)	$(325/784)^{1/2}$	$(585/5929)^{1/2}$	$-(845/1936)^{1/2}$
	(420) (40)	$-(143/784)^{1/2}$	$(585/2156)^{1/2}$	$-(5/176)^{1/2}$
(220) (21)	(220) (22)	$(100/693)^{1/2}$	$(325/1386)^{1/2}$	0
	(222) (40)	$(26/147)^{1/2}$	$-(16/147)^{1/2}$	0
	(420) (22)	$-(416/24255)^{1/2}$	$-(676/24255)^{1/2}$	0
	(420) (40)	$(130/441)^{1/2}$	$-(80/441)^{1/2}$	0
(220) (22)	(220) (22)	$(325/1056)^{1/2}$	$(325/2178)^{1/2}$	$(5525/34848)^{1/2}$
	(222) (40)	$-(1/112)^{1/2}$	$(361/924)^{1/2}$	$-(119/528)^{1/2}$
	(420) (22)	$(7/2640)^{1/2}$	$(7/5445)^{1/2}$	$(119/87120)^{1/2}$
	(420) (40)	$(1/1680)^{1/2}$	$-(361/13860)^{1/2}$	$(119/7920)^{1/2}$
	(420) (42)	$(17/35)^{1/2}$	$-(51/385)^{1/2}$	$-(21/55)^{1/2}$

The part that remains can be easily calculated in this case by means of the Wigner-Eckart theorem. In this way we get, for k, k' and k'' even,

$$
\begin{aligned}
&\big((200)(20)k+(200)(20)k'\,|\,(200)(20)k''\big)\\
&\quad=(7/55[k''])^{1/2}\big(f^2(200)(20)^1k\|V^{(k')}\|f^2(200)(20)^1k''\big),\\
&\big((200)(20)k+(200)(20)k'\,|\,(220)Uk''\big)\\
&\quad=(5/12[k''])^{1/2}\big(f^4(200)(20)^1k\|V^{(k')}\|f^4(220)U^1k''\big),\\
&\big((200)(20)k+(200)(20)k'\,|\,(400)(40)\tau'k''\big)\\
&\quad=(7/5[k''])^{1/2}\big(f^6(220)(20)^1k\|V^{(k')}\|f^6(222)(40)\tau'^1k''\big).
\end{aligned}
$$

The reduced matrix elements of $\mathbf{V}^{(k')}$ can be readily obtained by using the relation $\mathbf{V}^{(k')}=[k']^{1/2}\mathbf{U}^{(k')}$ and referring to the tables of Nielson and Koster.[10] The

[10] C. W. Nielson and G. F. Koster, *Spectroscopic Coefficients for the p^n, d^n, and f^n Configurations* (MIT Press, Cambridge, Massachusetts, 1963).

TABLE IV. The coefficients $((400)(40)\tau k''+(200)(20)k''|WU0)$.

WU	$\tau k''$ 2	$A4$	$B4$	$A6$	$B6$
(400)(40)	$(11/225)^{1/2}$	$(1/75)^{1/2}$	$-(238/825)^{1/2}$	$(76/279)^{1/2}$	$-(3213/8525)^{1/2}$
(420)(22)	$(11/63)^{1/2}$	$-(16/189)^{1/2}$	$(34/297)^{1/2}$	$(133/279)^{1/2}$	$(51/341)^{1/2}$
(420)(40)	$-(1849/6300)^{1/2}$	$(16384/51975)^{1/2}$	$(136/675)^{1/2}$	$(532/3069)^{1/2}$	$-(51/3100)^{1/2}$
(420)(42)	$-(51/700)^{1/2}$	$-(748/1575)^{1/2}$	$(32/225)^{1/2}$	0	$-(31/100)^{1/2}$
(600)(60)	$(646/1575)^{1/2}$	$(646/5775)^{1/2}$	$(57/225)^{1/2}$	$-(238/3069)^{1/2}$	$-(114/775)^{1/2}$

numerical constants in the above equations are determined by insisting that the coefficients be normalized according to

$$\sum (WU\tau K|W_1U_1\tau_1K_1+W_2U_2\tau_2K_2)\times(W_1U_1\tau_1K_1+W_2U_2\tau_2K_2|W'U'\tau'K)=\delta(W,W')\delta(U,U')\delta(\tau,\tau'),$$

where the sum runs over $U_1U_2\tau_1\tau_2K_1K_2$.

The coefficients $(W'U'\tau'k''+(200)(20)k''|WU0)$ are rather more difficult to evaluate, since some of them involve representations W and U that do not occur in the classification of the states of f^n. To deal with them, we adapt the projection method used by Nutter and Nielson for fractional parentage coefficients.[11] Taking the labels a and b to refer to the two parts $W'U'\tau'k''$ and $(200)(20)k''$ of a coupled system, we write

$$|WU0)=\sum_{U',\tau',k''}(W'U'\tau'k''+(200)(20)k''|WU0)\times|W'U'\tau'k'',\,(200)(20)k'',\,0)$$

and solve for the coefficients by operating first with

$$5G(W)-5G(W')-5G(200)-4G(U)+4G(U')+4G(20) \quad (3)$$

and then with the equivalent operator $2(\mathbf{V}_a^{(3)}\cdot\mathbf{V}_b^{(3)})$. On equating the two results, a system of simultaneous linear equations is obtained from which the coefficients can be calculated. This is the immediate extension to the group R_7 of the method of Stevens for calculating VC coefficients.[12]

A difficulty arises in using $(\mathbf{V}_a^{(3)}\cdot\mathbf{V}_b^{(3)})$. Its matrix elements are given by

$$(W'U'\tau'k'',\,(200)(20)k'',\,0|(\mathbf{V}_a^{(3)}\cdot\mathbf{V}_b^{(3)})|W'U''\tau''k',\,(200)(20)k',\,0)=-\{[k'][k'']\}^{-1/2}(W'U'\tau'k''\|V^{(3)}\|W'U''\tau''k')\times((200)(20)k''\|V^{(3)}\|(200)(20)k'),$$

but the reduced matrix elements for $W'=(400)$ do not appear in the tables of Nielson and Koster.[10] Fortunately, $c((40)(10)(40))$, the number of times the identity representation occurs in the triple Kronecker product $(40)\times(10)\times(40)$, is unity. Moreover, (400) contains the sole representation (40) of G_2. Hence, we can write

$$((400)U'\tau'k''\|V^{(3)}\|(400)U''\tau''k')=A((222)(40)\tau'k''\|V^{(3)}\|(222)(40)\tau''k').$$

The constant A is immediately found to be -2 by picking out the states of highest weight and using the fact that in terms of Weyl's operators H_i for R_7, we have $V_0^{(3)}=(H_1-H_2-H_3)6^{-1/2}$.[13]

An accidental degeneracy occurs for $W'=(400)$. For both pairs (420)(40) and (600)(60) of WU, the expression (3) is 8/3. To separate the coefficients, we extend the projection method to G_2. As equivalent operators, we use $(\mathbf{V}_a^{(5)}\cdot\mathbf{V}_b^{(5)})$ and

$$2G(U)-2G(U')-2G(20)+k''(k''+1)/28.$$

By these techniques, the required coupling coefficients $(W'U'\tau'k''+(200)(20)k''|WU0)$ can be found. They are assembled in Tables III and IV.

The factor $([3]W|[2]W'+[1](200))$ remains. It can be calculated for the W' of interest by demanding that $(kk'k''|WU)$ be symmetric with respect to the interchange of any two of the triad $kk'k''$. The results are set out in Table V. The $(kk'k''|WU)$ themselves are given in Table VI. This table completely defines the operators t_i. The rows are orthonormal in the sense that

$$\sum n(kk'k'')(kk'k''|WU)(kk'k''|W'U')=\delta(WW')\delta(UU'),$$

where the sum runs over the nine distinct triads

TABLE V. The coefficients $([3]W|[2]W'+[1](200))$.

W	W' (000)	(200)	(220)	(400)
(000)	0	1	0	0
(220)	0	$(1/5)^{1/2}$	$(4/5)^{1/2}$	0
(222)	0	0	1	0
(400)	0	$(5/11)^{1/2}$	0	$(6/11)^{1/2}$
(420)	0	0	$(5/9)^{1/2}$	2/3
(600)	0	0	0	1

[11] P. Nutter and C. Nielson, Raytheon Technical Memorandum, T-331, 1963 (unpublished).
[12] K. W. H. Stevens, Proc. Phys. Soc. (London) **A65**, 209 (1952).
[13] B. R. Judd, *Operator Techniques in Atomic Spectroscopy* (McGraw-Hill Book Company, Inc., New York, 1963).

TABLE VI. The coefficients $(kk'k''|WU)$.

WU	$\{222\}$	$\{224\}$	$\{244\}$	$\{246\}$
(000) (00)	$-(11/1134)^{1/2}$	$(4/189)^{1/2}$	$(1/847)^{1/2}$	$(26/3267)^{1/2}$
(220) (22)	$(605/5292)^{1/2}$	$-(6760/43659)^{1/2}$	$-(1805/391314)^{1/2}$	$-(4160/754677)^{1/2}$
(222) (00)	$(32761/889056)^{1/2}$	$(33/1372)^{1/2}$	$-(4/33957)^{1/2}$	$-(13/264)^{1/2}$
(222) (40)	$(3575/889056)^{1/2}$	$-(325/37044)^{1/2}$	$-(54925/373527)^{1/2}$	$(625/26136)^{1/2}$
(400) (40)	$-(17303/396900)^{1/2}$	$(416/33075)^{1/2}$	$-(117/296450)^{1/2}$	$(256/571725)^{1/2}$
(420) (22)	$-(1573/8232)^{1/2}$	$-(15028/305613)^{1/2}$	$(4693/12326391)^{1/2}$	$(1568/107811)^{1/2}$
(420) (40)	$(264407/823200)^{1/2}$	$(28717/2778300)^{1/2}$	$-(1273597/28014525)^{1/2}$	$(841/1960200)^{1/2}$
(420) (42)	$(21879/274400)^{1/2}$	$-(37349/926100)^{1/2}$	$(849524/9338175)^{1/2}$	$-(17/653400)^{1/2}$
(600) (60)	$-(46189/231525)^{1/2}$	$-(8398/694575)^{1/2}$	$-(134368/3112725)^{1/2}$	$-(15827/245025)^{1/2}$

WU	$\{444\}$	$\{446\}$	$\{266\}$	$\{466\}$	$\{666\}$
(000) (00)	$-(6877/139755)^{1/2}$	$(117/1331)^{1/2}$	$(2275/19602)^{1/2}$	$(12376/179685)^{1/2}$	$(4199/539055)^{1/2}$
(220) (22)	$(55016/717409)^{1/2}$	$-(195/204974)^{1/2}$	$(1625/143748)^{1/2}$	$(88400/1185921)^{1/2}$	$(29393/790614)^{1/2}$
(222) (00)	$(49972/622545)^{1/2}$	$(52/1089)^{1/2}$	$(325/199584)^{1/2}$	$-(442/12705)^{1/2}$	$(205751/784080)^{1/2}$
(222) (40)	$(92480/1369599)^{1/2}$	$(529/11979)^{1/2}$	$(6889/2195424)^{1/2}$	$-(10880/251559)^{1/2}$	$-(79135/1724976)^{1/2}$
(400) (40)	$(178802/978285)^{1/2}$	$-(2025/18634)^{1/2}$	$71/198$	$-(1088/179685)^{1/2}$	$(2261/1078110)^{1/2}$
(420) (22)	$-(297680/5021863)^{1/2}$	$-(49/395307)^{1/2}$	$-(1/223608)^{1/2}$	$-(174080/8301447)^{1/2}$	$(79135/175692)^{1/2}$
(420) (40)	$-(719104/2282665)^{1/2}$	$-(1369/35937)^{1/2}$	$(625/81312)^{1/2}$	$-(8704/3773385)^{1/2}$	$(15827/319440)^{1/2}$
(420) (42)	$-(73644/2282665)^{1/2}$	$(68/11979)^{1/2}$	$(1377/27104)^{1/2}$	$-(103058/1257795)^{1/2}$	$-(8379/106480)^{1/2}$
(600) (60)	$-(2584/18865)^{1/2}$	0	$(323/22869)^{1/2}$	$-(19/31185)^{1/2}$	$-(98/1485)^{1/2}$

$(kk'k'')$, each with associated degeneracy $n(kk'k'')$. For convenience, $n(kk'k'')$ is listed in Table VII.

It is interesting to note that

$$(kk'k''|(000)(00))$$
$$=\{28[k][k'][k'']/1485\}^{1/2}\begin{Bmatrix} k & k' & k'' \\ 3 & 3 & 3 \end{Bmatrix}.$$

It follows that for the complete scalar t_1,

$$t_1=(28/1485)^{1/2}\sum[k][k']X(kk',3),$$

where the sum runs over even nonzero values of k and k'.

TABLE VII. The numbers $n(kk'k'')$.

$\{kk'k''\}$	$n(kk'k'')$
{222}	1
{224}	3
{244}	3
{246}	6
{444}	1
{446}	3
{266}	3
{466}	3
{666}	1

IV. MATRIX ELEMENTS

By means of Eq. (1) and Table VI, the matrix elements of the operators t_i can be rapidly expressed in terms of those for $V(kk'k'')$. The latter were very kindly supplied by Dr. K. Rajnak, who had already calculated them as an intermediate step to finding the matrix elements of $X(kk',l')$.[8] The results for the t_i are given in Table VIII; the numbers F are multiplicative constants common to all members of a column. The abbreviated notation of Nielson and Koster[10] is used to label the states ψ and ψ' of f^3; for example, $4S$ stands for $(111)(00)^4S$, and $2D1$ for $(210)(20)^2D$.

Table VIII is extremely rich in examples of a group-theoretical nature. Every zero corresponds to the absence of an identity representation in a triple Kronecker product, that is, to the vanishing of $c(WW'W'')$ or $c(UU'U'')$. For example, the equation $c((11)(22)(21))=0$ implies $(2H1|t_6|2H2)=0$, since $2H1$, t_6, and $2H2$ correspond to the representations (11), (22), and (21) of G_2. When an identity representation occurs once in a triple Kronecker product, the Wigner-Eckart theorem can often be applied to relate the matrix elements of different operators. For example, the equations

$$154(26)^{1/2}(f^3(210)(11)^2L|t_2|f^3(210)(11)^2L)$$
$$=22(35)^{1/2}(f^3(210)(11)^2L|t_6|f^3(210)(11)^2L)$$
$$=5(13)^{1/2}(f^3(210)(11)^2L|e_3|f^3(210)(11)^2L)$$

hold for both values of L (1 or 5) because t_2, t_6, and e_3 all correspond to the representation (22), for which $c((11)(22)(11))=1$.

Sometimes the numbers $c(WW'W'')$ and $c(UU'U'')$ exceed unity. Instead of being simply proportional the matrix elements of operators belonging to the same representation are now related by linear equations. For example, $c((21)(40)(21))=2$. For the operator e_2 [which corresponds to $U=(40)$], Racah[9] introduced the quantities $((21)|\chi_1(L)|(21))$ and $((21)|\chi_2(L)|(21))$, in terms of which the matrix elements of e_2 can be ex-

TABLE VIII. The matrix elements $(\psi|t_i|\psi')$.

ψ	ψ'	t_i / F	t_1 $(33/6860)^{1/2}$	t_2 $(2)^{1/2}/2156$	t_3 $(6720)^{-1/2}$	t_4 $1/56(15015)^{1/2}$	t_5 $3/49(17160)^{1/2}$	t_6 $1/924(455)^{1/2}$	t_7 $1/168(5005)^{1/2}$	t_8 $(16336320)^{-1/2}$	t_9 1
$4S$	$4S$		6	0	288	0	0	0	0	0	0
$4D$	$4D$		6	1694	8	−8008	0	0	0	0	0
$4F$	$4F$		6	0	−72	0	0	0	0	0	0
$4G$	$4G$		6	616	8	7280	0	0	0	0	0
$4I$	$4I$		6	−1078	8	−1960	0	0	0	0	0
$2P$	$2P$		−1	−385	−48	0	0	−30030	0	0	0
$2D1$	$2D1$		−1	−319	32	−1144	286	12870	10296	0	0
	$2D2$		0	$36(33)^{1/2}$	0	$468(33)^{1/2}$	$156(33)^{1/2}$	$-624(33)^{1/2}$	$156(33)^{1/2}$	0	0
$2D2$	$2D2$		−1	−423	−3	3237	−377	−1677	−1833	4641	0
$2F1$	$2F1$		−15	0	0	0	0	0	0	0	0
	$2F2$		0	$231(22)^{1/2}$	0	0	0	0	0	0	0
$2F2$	$2F2$		−1	−21	−3	1365	−455	1365	−1365	−3315	0
$2G1$	$2G1$		−1	−116	32	1040	−260	4680	−9360	0	0
	$2G2$		0	$3(4290)^{1/2}$	0	$-24(4290)^{1/2}$	$-8(4290)^{1/2}$	$-52(4290)^{1/2}$	$-8(4290)^{1/2}$	0	0
$2G2$	$2G2$		−1	11	−3	−2475	561	1221	1947	1309	0
$2H1$	$2H1$		−1	105	−48	0	0	8190	0	0	0
	$2H2$		0	0	0	$84(455)^{1/2}$	$-28(455)^{1/2}$	0	$252(455)^{1/2}$	0	0
$2H2$	$2H2$		−1	−399	−3	−1995	−49	−2709	567	−1071	0
$2I$	$2I$		−1	203	32	−280	70	−8190	2520	0	0
$2K$	$2K$		−1	56	−3	1827	315	−252	21	−1071	0
$2L$	$2L$		−1	336	−3	−525	−245	1260	−315	945	0

pressed for any representation (21) in the f shell. These quantities can equally well serve as suitable basic sets for the operators t_4, t_5, and t_7, all of which correspond to (40). Thus we find

$$112(f^3(210)(21)^2L|t_4|f^3(210)(21)^2L) = (15/1001)^{1/2}((21)|\chi_1(L)|(21)) + 3(21/715)^{1/2}((21)|\chi_2(L)|(21))$$

and

$$112(5005)^{1/2}(f^3(210)(21)^2L|t_7|f^3(210)(21)^2L) = -3((21)|\chi_1(L)|(21)) - 7((21)|\chi_2(L)|(21))$$

for all L.

V. PARAMETERS

The methods of the previous section can be extended to solve the parametrization problem raised in Sec. II. To begin with, we note that $c(WW'(600))=0$ for all representations W and W' that occur in the classification of the f-electron states. It follows that the matrix elements of t_9 are always null, and hence this operator can be dropped from the effective Hamiltonian. Secondly, $c(WW'(400))$ is zero for all pairs W and W' that occur in f^3 except one, namely that defined by $W=W'=(210)$. In this case it is unity. Hence the matrix elements of t_5 [which corresponds to (400)] are proportional to those of e_2. From Table VIII, the exact relationship is found to be

$$14(4290)^{1/2}(f^3\psi|t_5|f^3\psi') = -(f^3\psi|e_2|f^3\psi').$$

Since t_5 is a three-particle operator while e_2 is a two-particle operator, the generalization to f^N runs

$$14(4290)^{1/2}(f^N\Psi|t_5|f^N\Psi') = -(N-2)(f^N\Psi|e_2|f^N\Psi').$$

It is clear that the effect of t_5 in the effective Hamiltonian is completely absorbed by the parameter E^2 associated with the operator e_2.

The matrix elements of the complete scalar t_1 are diagonal with respect to all quantum numbers. For f^3, they take on just three values, corresponding to $W=(111)$, (100), and (210). However, the two-particle effective Hamiltonian already contains three independent completely scalar operators, namely e_0, e_1, and e_4. It follows that the effect of t_1 can be absorbed by the parameters E^0, E^1, and E^4. (In actual fact, E^0 and E^1 suffice.) Thus t_1, like t_5, can be dropped from the effective Hamiltonian.

Although this is as far as we can go on strictly general grounds, there remains the possibility that other operators are dispensable. This would be the case if the matrix elements of t_2 were reproducible by some combination of those of e_3 and e_6 (which correspond to the same WU as t_2) for all the states of f^3, or if the matrix elements of t_3 could be constructed from those of e_0, e_1, e_4, and e_5 [which, like t_3, correspond to $U=(00)$] for all the states of f^3. Detailed analyses show that fortuitous simplifications such as these do not occur. Nor does any linear relationship exist for all the states of f^3 between matrix elements of t_4, t_7, and e_2, although the operators all correspond to $U=(40)$. The actual numerical values of the matrix elements of the operators t_i do not permit us to go beyond what is allowed on general group-theoretical principles. We conclude that the effect of the three-particle operators can be adequately represented by the addition of

$$t_2T^2+t_3T^3+t_4T^4+t_6T^6+t_7T^7+t_8T^8$$

to the two-particle Hamiltonian, provided the parameters E^i and T^i are regarded as freely adjustable. Thus only six, and not ten, additional parameters are required to describe the effect of the three-particle operators.

It is extremely likely that this is the reason why Rajnak found that more than five additional parameters led to little improvement in the fit between theory and experiment for Pr III. The objection that she reached the limit with five rather than six parameters largely disappears when it is noticed that the upper ^2F multiplet has not been observed experimentally. Being essentially of a lower seniority than all the others, it is quite likely that its future inclusion in the analysis will demand a sixth additional parameter. However, too much weight should not be put on arguments of this kind, since the residual discrepancies between experiment and theory are of the same order of magnitude as neglected interactions, such as spin-spin and spin-orbit; and what constitutes a meaningful improvement in the fit is not altogether clear.

To express the strengths of the operators $X(kk',l')$, Rajnak introduced the parameters $Y(kk',l')$. For $l'=1$ and 3, there are nine of them in all. Unfortunately, they cannot be unambiguously related to the parameters T^i. This is because the operators $X(kk',l')$, on close examination, turn out to be related through the equation

$$11X(22,1)+24X(22,3)+3(22)^{1/2}X(42,1)=66X(42,3).$$

They are therefore not linearly independent, and a set of T_i values cannot imply a unique set of $Y(kk',l')$. But we can, of course, represent any set of $Y(kk',l')$ by means of the T_i, since the operators t_i must accommodate all special cases. For the final column of Table II of Rajnak,[8] we obtain (in cm^{-1}) $T_2=391$, $T_3=35$, $T_4=86$, $T_6=-262$, $T_7=320$, and $T_8=316$. These numbers should be useful as starting values for more elaborate calculations.

VI. SENIORITY

The treatment so far has been confined to the configuration f^3. The straightforward way to find the matrix elements of the operators t_i for any configuration f^N is to set up a chain calculation with f^3 as its starting point. The matrix elements for f^N are related to those of f^{N-1} by means of the formula

$$(f^N\Psi|t_i|f^N\Psi')=[N/(N-3)]\sum(\Psi\{|\bar{\Psi})(\Psi'\{|\bar{\Psi}')\times(f^{N-1}\bar{\Psi}|t_i|f^{N-1}\bar{\Psi}'),\quad(4)$$

where the sum runs over $\bar{\Psi}$ and $\bar{\Psi}'$. The fractional parentage coefficients $(\Psi\{|\bar{\Psi})$ and $(\Psi'\{|\bar{\Psi}')$ have been tabulated by Nielson and Koster.[10] Equation (4) is the extension to three-particle operators of Eq. (1) of Racah.[9]

Although Eq. (4) completely solves the problem of finding the matrix elements of the operators t_i, it is of great interest to investigate the implications of group theory. Many of the numbers $c(UU'U'')$ and $c(WW'W'')$ that are required have already been given by Racah in his analysis of the operators e_i; those that remain are set out in Tables IX, X, and XI. The

TABLE IX. The numbers $c(WW'(222))$.

W	W' (000)	(100)	(110)	(200)	(111)	(210)	(211)	(220)	(221)	(222)
(000)	0	0	0	0	0	0	0	0	0	1
(100)	0	0	0	0	0	0	0	0	1	1
(110)	0	0	0	0	0	0	1	0	1	1
(200)	0	0	0	0	0	0	0	1	1	1
(111)	0	0	0	0	1	0	1	0	1	1
(210)	0	0	0	0	0	1	1	1	2	1
(211)	0	0	1	0	1	1	2	1	2	1
(220)	0	0	0	1	0	1	1	1	1	1
(221)	0	1	1	1	1	2	2	1	2	1
(222)	1	1	1	1	1	1	1	1	1	1

Kronecker products listed by Nutter[14] were extremely useful in constructing these tables. Their function is to allow us to extend the arguments used in Sec. IV to relate the matrix elements in different configurations.

TABLE X. The numbers $c(WW'(420))$.

W	W' (000)	(100)	(110)	(200)	(111)	(210)	(211)	(220)	(221)	(222)
(000)	0	0	0	0	0	0	0	0	0	0
(100)	0	0	0	0	0	0	0	0	0	0
(110)	0	0	0	0	0	0	0	0	0	0
(200)	0	0	0	0	0	0	0	1	0	0
(111)	0	0	0	0	0	0	0	0	0	0
(210)	0	0	0	0	0	1	0	0	1	0
(211)	0	0	0	0	0	0	1	1	1	0
(220)	0	0	0	1	0	0	1	1	0	1
(221)	0	0	0	0	0	1	1	0	2	1
(222)	0	0	0	0	0	0	0	1	1	1

For example, the fact that $c((21)(21)(42))=1$ implies that the number A in the equation

$$(f^NW(21)SL|t_8|f^NW'(21)SL)=A(f^3(210)(21)SL|t_8|f^3(210)(21)SL)$$

is independent of L. A detailed description of such methods is given elsewhere.[13]

No use has yet been made of the idea of seniority or of its group-theoretical counterpart, symplectic symmetry. It might seem scarcely worthwhile to pursue the subject, since the basic operators $\mathbf{v}^{(2)}$, $\mathbf{v}^{(4)}$, and

TABLE XI. The numbers $c(UU'(42))$.

U	U' (00)	(10)	(11)	(20)	(21)	(30)	(22)	(31)	(40)
(00)	0	0	0	0	0	0	0	0	0
(10)	0	0	0	0	0	0	0	0	0
(11)	0	0	0	0	0	0	0	1	0
(20)	0	0	0	0	0	0	1	1	1
(21)	0	0	0	0	1	1	1	2	2
(30)	0	0	0	0	1	1	1	3	2
(22)	0	0	0	1	1	1	1	2	2
(31)	0	0	1	1	2	3	2	5	4
(40)	0	0	0	1	2	2	2	4	4

[14] P. B. Nutter, Raytheon Technical Memorandum T-544, 1964 (unpublished).

$\mathbf{v}^{(6)}$ from which the t_i are constructed do not span a complete representation of the symplectic group Sp_{14}. Hence it appears that we cannot assign irreducible representations (σ) of Sp_{14} to our operators. However, it is only necessary that the matrix elements for a given t_i within f^3 be proportional to those of an operator of well-defined symplectic symmetry for us to enjoy the advantages of this symmetry throughout the entire f shell. Even if a direct proportionality of this kind is unobtainable, there is always the possibility that two or more operators of well-defined symplectic symmetry can be found to reproduce the matrix elements of the given operator t_i.

To this end, we introduce the three-particle operators

$$W(\kappa\kappa'\kappa'', kk'k'')=\sum\begin{pmatrix}\kappa & \kappa' & \kappa'' \\ \pi & \pi' & \pi''\end{pmatrix}\begin{pmatrix}k & k' & k'' \\ q & q' & q''\end{pmatrix} \times (w_{\pi q}{}^{(\kappa k)})_h (w_{\pi' q'}{}^{(\kappa' k')})_i (w_{\pi'' q''}{}^{(\kappa'' k'')})_j,$$

where the sum runs over $\pi\pi'\pi''qq'q''$ and $h\neq i\neq j$. The amplitude of the double tensors $\mathbf{w}^{(\kappa k)}$ is defined by

$$(sl\|w^{(\kappa k)}\|sl)=[\kappa]^{1/2}[k]^{1/2}.$$

The tensors $\mathbf{w}^{(\kappa k)}$ for $\kappa+k$ even transform according to the representation (1100000) of Sp_{14}.[13] Just as we found the permissible representations W and U to which the linear combinations t_i of the $V(kk'k'')$ belong, we may find the representations (σ) of Sp_{14} to which the linear combinations u_i of the $W(\kappa\kappa'\kappa'',kk'k'')$ belong. We impose the condition that $\kappa+k$, $\kappa'+k'$, and $\kappa''+k''$ be even. The branching rules $U_{27}\rightarrow R_7$ are replaced by $U_{90}\rightarrow Sp_{14}$. The complete tensorial character of the u_i may be found by studying the reduction $Sp_{14}\rightarrow SU_2\times R_7$, which separates out the spin and orbital structure. Representations of SU_2 are written D_κ. The descriptions of the operators u_i are given in Table XII. There are 30 of them; this number coincides with the number of possible operators $W(\kappa\kappa'\kappa'',kk'k'')$ that can be constructed from the $\mathbf{w}^{(\kappa k)}$ (with $\kappa+k$ even) without violating any triangular conditions.

TABLE XII. Description of operators.

u_i	$(\sigma)WU\kappa$K
u_1	(0000000) (000) (00)00
u_2	(1111000) (220) (22)00
u_3	(2200000) (000) (00)00
u_4	(2200000) (111) (00)00
u_5	(2200000) (220) (22)00
u_6	(2200000) (400) (40)00
u_7	(1111110) (222) (00)00
u_8	(1111110) (222) (40)00
u_9	(2211000) (111) (00)00
u_{10}	(2211000) (220) (22)00
u_{11}	(2211000) (222) (00)00
u_{12}	(2211000) (222) (40)00
u_{13}	(2211000) (311) (22)00
u_{14}	(2211000) (311) (40)00
u_{15}	(2211000) (321) (22)00
u_{16}	(2211000) (321) (40)00
u_{17}	(2211000) (420) (22)00
u_{18}	(2211000) (420) (40)00
u_{19}	(2211000) (420) (42)00
u_{20}	(3300000) (000) (00)00
u_{21}	(3300000) (220) (22)00
u_{22}	(3300000) (222) (00)00
u_{23}	(3300000) (222) (40)00
u_{24}	(3300000) (311) (22)00
u_{25}	(3300000) (311) (40)00
u_{26}	(3300000) (400) (40)00
u_{27}	(3300000) (420) (22)00
u_{28}	(3300000) (420) (40)00
u_{29}	(3300000) (420) (42)00
u_{30}	(3300000) (600) (60)00

TABLE XIII. The numbers $c((v)(v')(2211000))$.

	v							
v'	0	1	2	3	4	5	6	7
0	0	0	0	0	0	0	0	0
1	0	0	0	0	0	0	0	0
2	0	0	0	0	1	0	0	0
3	0	0	0	1	0	1	0	0
4	0	0	1	0	1	0	1	0
5	0	0	0	1	0	1	0	1
6	0	0	0	0	1	0	1	0
7	0	0	0	0	0	1	0	0

At first sight, Table XII appears discouraging, since every WU used in labeling the t_i ($i=2$, 3, 4, 6, 7, 8) occurs against at least two different operators u_i. This seems to imply that every t_i has first to be expressed as a linear combination of the u_i before useful applications can be made. However, the irreducible representations (σ) used to describe the states of f^N are all of the type $(11\cdots10\cdots0)$, in which v symbols 1 and $7-v$ symbols 0 appear. [Such a representation is conveniently abbreviated to (v).] It turns out that $c((v)(v')(3300000))=0$ for all v and v'. Hence the 11 operators $u_i(20\leq i\leq 30)$ all have zero matrix elements, and can be ignored. Thus the matrix elements of t_6, t_7, and t_8 are proportional to those of u_{17}, u_{18}, and u_{19}, since these are the only three u_i remaining that correspond to $W=(420)$. For calculating their matrix elements, the operators t_6, t_7, and t_8 can therefore be regarded as belonging to the representation (2211000) of Sp_{14}. The numbers $c((v)(v')(2211000))$ are given in Table XIII.

The representation (222), corresponding to the operators t_3 and t_4, occurs in the decomposition of both (1111110) and (2211000). The situation for t_2 is worse, since (220) occurs in the decomposition of three representations (σ). In these cases, the operators

TABLE XIV. The numbers $c((v)(v')(1111110))$.

	v							
v'	0	1	2	3	4	5	6	7
0	0	0	0	0	0	0	1	0
1	0	0	0	0	0	1	0	1
2	0	0	0	0	1	0	1	0
3	0	0	0	1	0	1	0	0
4	0	0	1	0	1	0	0	0
5	0	1	0	1	0	0	0	0
6	1	0	1	0	0	0	0	0
7	0	1	0	0	0	0	0	0

themselves must be broken down to determine how their matrix elements stand with respect to seniority. In doing this, it is convenient to introduce the concept of quasispin, this being the most natural way to study the dependence of the matrix elements on N. For completeness, $c((v)(v')(1111110))$ is given at this point in Table XIV.

VII. QUASISPIN

The theory of quasispin can be based on the triple tensor operators $\mathbf{a}^{(qsl)}$, which are related to the usual creation and annihilation operators by the equations

$$a_{\frac{1}{2}m_sm_l}{}^{(qsl)}=a_{m_sm_l}{}^{\dagger},$$
$$a_{-\frac{1}{2}-m_s-m_l}{}^{(qsl)}=(-1)^{s+l+m_s+m_l}a_{m_sm_l}.$$

The coupled tensors $\mathbf{X}^{(K\kappa k)}=(\mathbf{a}^{(qsl)}\mathbf{a}^{(qsl)})^{(K\kappa k)}$ contain as special cases the second-quantized forms for the double tensors $\sum_i(\mathbf{w}^{(\kappa k)})_i$. For example, $\mathbf{S}=-\frac{1}{2}[l]^{1/2}\times\mathbf{X}^{(010)}$. The quantity $-\frac{1}{2}[l]^{1/2}\mathbf{X}^{(100)}$ is defined as the quasispin $\mathbf{Q}$. Its quantum numbers (Q,M_Q) can be used to label eigenfunctions, and it turns out that for the states of l^N with seniority v,

$$Q=(2l+1-v)/2,\quad M_Q=-(2l+1-N)/2.$$

If we know that one of our operators t_i behaves as a tensor of rank K with respect to quasispin, then the dependence on N of its matrix elements between states of fixed quasispin Q and Q' is contained in the expression

$$(-1)^{Q-M_Q}\begin{pmatrix} Q & K & Q' \\ -M_Q & 0 & M_Q \end{pmatrix}. \tag{5}$$

This result follows from an application of the Wigner-Eckart theorem to quasispin; a detailed account is given in Ref. 7. It may happen, of course, that a given t_i does not correspond to a unique rank K. In this case, it must be decomposed into component operators with well-defined K values.

To begin the program of assigning ranks K to the operators t_i, we use the fact that for f electrons the $\mathbf{X}^{(K\kappa k)}$ with $K+\kappa+k$ odd can be regarded as the infinitesimal operators of the group R_{28}. Furthermore, the states of f^N with even N form the basis for the irreducible representation $(\frac{1}{2},\frac{1}{2}\cdots\frac{1}{2},\frac{1}{2})$; those with odd N span $(\frac{1}{2},\frac{1}{2}\cdots\frac{1}{2},-\frac{1}{2})$. These results are proved elsewhere.[7] It can also be shown that

$$(\tfrac{1}{2},\tfrac{1}{2}\cdots\tfrac{1}{2},\pm\tfrac{1}{2})\times(\tfrac{1}{2},\tfrac{1}{2}\cdots\tfrac{1}{2},\pm\tfrac{1}{2}) =(0\cdots0)+(110\cdots0)+(11110\cdots0)+\cdots +(11\cdots1\pm1), \tag{6}$$

in which either the upper or the lower sign is taken throughout. If we construct operators that transform according to irreducible representations (w) of R_{28}, only those corresponding to the representations on the right-hand side of Eq. (6) have nonzero matrix elements. Now $\mathbf{X}^{(100)}$ and $\mathbf{X}^{(0\kappa k)}$ (with $\kappa+k$ odd) form the operators of the subgroup $SU_2\times Sp_{14}$ of R_{28}. Hence we have only to find the decomposition of those representations of R_{28} on the right in Eq. (6) into representations of $SU_2\times Sp_{14}$ to obtain the association between quasispin and symplectic symmetry. In the quasispin formalism, an r-particle operator is expressed as sums over $2r$-fold products of the operators $\mathbf{a}^{(qsl)}$. The 28 components of $\mathbf{a}^{(qsl)}$ transform like $(10\cdots0)$ of R_{28}, so it is clear that for three-particle operators we may restrict our attention to representations $(11\cdots10\cdots0)$ which contain no more than six symbols 1. The branching rules for the relevant representations of R_{28} are given in Table XV. The quasispin multiplicity is represented by a superscript to the representations (σ) of Sp_{14}.

TABLE XV. Branching rules for the reduction $R_{28}\rightarrow SU_2\times Sp_{14}$.

(w)	${}^{2K+1}(\sigma)$
$(0\cdots0)$	${}^1(0000000)$
$(110\cdots0)$	${}^1(2000000)$
	${}^3(0000000)(1100000)$
$(11110\cdots0)$	${}^1(0000000)(1100000)(2200000)$
	${}^3(1100000)(2000000)(2110000)$
	${}^5(0000000)(1100000)(1111000)$
$(1111110\cdots0)$	${}^1(2000000)(2110000)(2220000)$
	${}^3(0000000)(2200000)(1100000)^2$
	${}^3(1111000)(2110000)(2211000)$
	${}^5(1100000)(2000000)(2110000)$
	${}^5(1111000)(2111100)$
	${}^7(0000000)(1100000)(1111000)(1111110)$

VIII. OPERATORS

It can be seen from Table XV that the representation (2211000) of Sp_{14} occurs once only, and with a quasispin rank K of 1. It follows that the dependence of t_6, t_7, and t_8 on N is contained in the expression (5) if we put $K=1$. Thus, we obtain

$$(f^Nv\Psi|t_i|f^Nv\Psi')=[(7-N)/(7-v)](f^vv\Psi|t_i|f^vv\Psi'),$$
$$(f^Nv\Psi|t_i|f^Nv-2\Psi')=[(16-v-N)\times(N+2-v)/4(8-v)]^{1/2}(f^vv\Psi|t_i|f^vv-2\Psi'), \tag{7}$$

where, in both equations, $i=6$, 7, or 8. These equations completely solve the problem of the N dependence of the matrix elements of t_6, t_7, and t_8 taken between states of given seniority. The coefficients in the above equations are characteristic of $K=1$ tensors and are identical to those in Eqs. (69b) and (67) of Racah,[15] which correspond to the component ${}^3(1100000)$ in the reduction of $(110\cdots0)$ of R_{28}.

The operators t_3 and t_4 correspond to $W=(222)$, and, as mentioned in Sec. VI, they share the characteristics of (2211000) and (1111110). For f^3, their only nonzero

[15] G. Racah, Phys. Rev. 63, 367 (1943).

TABLE XVI. The matrix elements $(\psi|t_i'|\psi')$ and $(\psi|t_i''|\psi')$. The singly primed operators correspond to quasispin $K=3$; the doubly primed to $K=1$. Matrix elements for t_2' and t_2'' are broken up into contributions from the two-particle part and the three-particle part, given in that order.

ψ	ψ'	$(\psi\|t_3'\|\psi')$	$(\psi\|t_3''\|\psi')$	$(\psi\|t_4'\|\psi')$	$(\psi\|t_4''\|\psi')$	$(\psi\|t_2'\|\psi')$	$(\psi\|t_2''\|\psi')$
4S	4S	72	−288	0	0	0+0	0+0
4D	4D	2	−8	−2002	8008	−231+77	−616−308
4F	4F	−18	72	0	0	0+0	0+0
4G	4G	2	−8	1820	−7280	−84+28	−224−112
4I	4I	2	−8	−490	1960	147−49	392+196
2P	2P	−48	−48	0	0	231−77	616−112
2D1	2D1	32	32	−1144	−1144	165−55	440−40
	2D2	0	0	$468(33)^{1/2}$	$468(33)^{1/2}$	$(-36+12)(33)^{1/2}$	$(-96+432/11)(33)^{1/2}$
2D2	2D2	−3	−3	3237	3237	171−57	456+468/11
2F1	2F1	0	0	0	0	0+0	0+0
	2F2	0	0	0	0	$(63+21)(22)^{1/2}$	$(168-84)(22)^{1/2}$
2F2	2F2	−3	−3	1365	1365	−189+63	−504+4368/11
2G1	2G1	32	32	1040	1040	60−20	160−160/11
	2G2	0	0	$-24(4290)^{1/2}$	$-24(4290)^{1/2}$	$(-3+1)(4290)^{1/2}$	$(-8+36/11)(4290)^{1/2}$
2G2	2G2	−3	−3	−2475	−2475	−165+55	−440+320
2H1	2H1	−48	−48	0	0	−63+21	−168+336/11
	2H2	0	0	$84(455)^{1/2}$	$84(455)^{1/2}$	0+0	0+0
2H2	2H2	−3	−3	−1995	−1995	315−105	840−2940/11
2I	2I	32	32	−280	−280	−105+35	−280+280/11
2K	2K	−3	−3	1827	1827	42−14	112−1484/11
2L	2L	−3	−3	−525	−525	−126+42	−336−588/11

matrix elements are diagonal with respect to (111) and (210). Moreover

$$c((111)(111)(222))=c((210)(210)(222))=1.$$

So, in constructing other sets of matrix elements corresponding to (222), we have only one useful parameter—the magnitude of the matrix elements of the quartets relative to those of the doublets. A particular value of this parameter will give the matrix elements of u_7, corresponding to (1111110)(222)(00). Now the grandparents of ^2O of f^5 are ^4I, ^2I, ^2K, ^2L, and the two ^2H terms of f^3. But ^2O has a seniority of 5, for which $c((5)(5)(1111110))=0$; hence, the matrix element $(^2O|u_7|^2O)$ must be zero. This condition can be used to fix the parameter in question and thus determine the matrix elements of u_7 for f^3. They are tabulated with a convenient normalization under the heading $(\psi|t_3'|\psi')$ in Table XVI. The matrix elements of u_{11}, corresponding to (2211000)(222)(00), are easily obtained (apart from an arbitrary normalization) by interpreting the orthogonality of functions corresponding to (2211000) and (1111110) in terms of matrix elements. They are entered in Table XVI under the heading $(\psi|t_3''|\psi')$. A precisely similar analysis can be performed for t_4; the entries in Table XVI under t_4' and t_4'' correspond to $(\sigma)=(1111110)$ and (2211000), respectively. The equations

$$40(105)^{1/2}t_3=8t_3'-3t_3'',$$
$$280(15015)^{1/2}t_4=8t_4'-3t_4'', \tag{8}$$

decompose t_3 and t_4 into parts that correspond to (1111110) and (2211000). From Table XV, we see that (1111110) is associated with the unique quasispin $K=3$; and we have already found that (2211000) corresponds to $K=1$. The dependences on N of the matrix elements of the component parts of t_3 and t_4, taken between states of given seniority, are thus completely determined. For our purposes, the primed and doubly primed operators are closely enough defined by the entries of Table XVI and the knowledge that they behave like three-particle operators. Equation (4) can be used to construct their matrix elements for states for which $v>3$.

There only remains t_2, for which $W=(220)$. This operator is more complicated to treat than t_3 or t_4, but the general approach is similar. The only new feature is that the representations (1111000) and (2200000) [which both contain (220)] occur in the reduction of $(11110\cdots0)$ of R_{28} as well as $(1111110\cdots0)$. This means that operators of well-defined K may comprise both three-particle and two-particle parts. The final result may be written in several different ways. The most convenient appears to be

$$1400t_2\sqrt{2}=8t_2'-3t_2''+20t_2'''. \tag{9}$$

In this equation, the operator t_2' possesses a quasispin of 3 and corresponds to $(\sigma)=(1111000)$; the operator t_2'' possesses a quasispin of 1 and corresponds to a mixture of (1111000) and (2211000). The matrix elements of t_2' and t_2'' for f^3 are given in Table XVI; each column has been broken down into contributions from the two-particle part (listed first) and the three-particle part (listed after a plus or minus sign). To construct the matrix elements of t_2' and t_2'' for states of f^N for which $v>3$, we must use Eq. (4) for the three-particle part and Eq. (1) of Racah[9] for the two-particle part. At each stage of the chain calculation, the two-particle parts cancel when the sum $8t_2'-3t_2''$ of Eq. (9) is performed; but it is essential to preserve them in order to generate sets of matrix elements corresponding to unique values of the quasispin K. The operator t_2''' is a three-particle operator whose matrix elements for f^3 are identical to those of e_3; hence,

$$(f^N\Psi|t_2'''|f^N\Psi')=(N-2)(f^N\Psi|e_3|f^N\Psi'). \quad (10)$$

The quasispin of t_2''' is ill defined, but since we may use the tables of Nielson and Koster[10] to evaluate the right-hand side of Eq. (10), this disadvantage is of no practical importance. Moreover, if the T^i and E^i are treated as freely adjustable parameters, the effect of t_2''' can be absorbed into e_3. There is thus no need to evaluate the matrix elements of t_2''' at all.

We conclude this section with an example of the use of Eqs. (8) and (9). Suppose the diagonal matrix element of t_3 is required for the term ^4I $(v=3)$ of f^5. We put $Q=Q'=2$ in expression (5), corresponding to $v=3$. The ratio

$$-\begin{pmatrix}2 & K & 2\\ 1 & 0 & -1\end{pmatrix}\Big/\begin{pmatrix}2 & K & 2\\ 2 & 0 & -2\end{pmatrix}$$

is -2 for $K=3$ and $\frac{1}{2}$ for $K=1$. From Eqs. (8) and Table XVI, we find

$$(f^5\ {}_3{}^4I|t_3|f^5\ {}_3{}^4I)=[8(-2)(2)-3(1/2)(-8)]/40(105)^{1/2}=-(420)^{-1/2}.$$

IX. CONCLUSION

The main result is this: When configuration interaction is extended from two-particle excitations to include the interaction between f^N and excited configurations of the type $f^{N\pm1}(n'l')^{\mp1}$ the effect on the levels of f^N can be adequately represented by the addition to the Hamiltonian of the six terms t_iT^i $(i=2, 3, 4, 6, 7, 8)$. The T^i are parameters, and the t_i are three-particle operators whose matrix elements for f^3 are given in Table VIII. The dependence on N of matrix elements involving states of given seniorities can be found from Eqs. (7), (8), (9), and Table XVI. Equations (8) and (9) can be regarded as the analogs of Racah's decomposition

$$e_3=(e_3+\Omega)-\Omega,$$

which breaks e_3 up into operators corresponding to quasispins $K=2$ and $K=0$, respectively. [The operator e_2 is a pure $K=0$ operator, which accounts for the simplicity of Eq. (73) of Racah.[9]]

All parts of the operators t_i that are not absorbed by the e_i possess odd quasispin. For a half-filled shell, $M_Q=0$, and the 3-j symbol of (5) vanishes if $Q+Q'$ is even. The Coulomb interaction within the half-filled shell leads to states ϕ which are mixtures either of Q odd or of Q even.[7] It follows that all matrix elements of the t_i not absorbed by the e_i are zero if diagonal with respect to ϕ. In other words, there is no need to consider any three-particle operators at all for f^7, provided the configuration is close to Russell-Saunders coupling and that their effect is sufficiently small that matrix elements off-diagonal in ϕ can be neglected.

The methods described above can be extended to other configurations of the type l^N. An analysis by Feneuille[16] indicates that for d^N, four three-particle operators t_i can be constructed, corresponding to the representations (00), (22), (42), and (60) of R_5. The first can be absorbed into coexisting two-particle operators, and the last ignored because its matrix elements are all null. Only two parameters are thus required to describe the three-particle operators in d^N.

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[16] S. Feneuille (private communication).