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Lawrence Radiation Laboratory
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B. R. Judd

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Synopsis

The existence of the familiar product gM_J that occurs in an analysis of the Zeeman effect can be regarded as an example of the Wigner-Eckart theorem for the rotation group R_3 . Correspondence is made with the treatment of intra-atomic interactions by means of higher groups, such as R_5 for d electrons. The spin-spin and spin-other-orbit interactions are examined in detail, and an outline is made of the decomposition of the scalar three-particle operators that are required to partially represent the effect on the configuration $(nl)^N$ of excited configurations of the type $(nl)^{N+1} (n'l')^{+1}$.

1. Introduction. When an atom is placed in a unit magnetic field, the energies of the components of a level J are given in units of the Bohr magneton by gM_J , where g is the Landé factor and M_J the quantum number of the projection J_z of J . That gM_J should be a simple product is a consequence of the Wigner-Eckart theorem, applied to the group R_3 of rotations in ordinary three-dimensional space. Since intra-atomic interactions are all scalars in R_3 , a similar application of the Wigner-Eckart theorem to these cases does not give useful results. However, if our eigenfunctions are described by the representations of higher groups, such as R_5 for d electrons or R_7 and G_2 for f electrons, the Wigner-Eckart theorem can again be applied when the interactions have been broken down into parts having well-defined symmetry properties with respect to these groups.

For the Coulomb interaction between equivalent f electrons, for example, Racah¹) introduced the operators e_0, e_1, e_2 , and e_3 , each corresponding to a pair of representations WU of R_7 and G_2 . His tables of $(U|x(L)|U')$ and $(U|\phi(L)|U')$ now appear as the analogues of M_J , and the tables of $x(W, UU')$ and $y(f^n, vSU, vSU')$ correspond to the Landé g factors. The fact that operators and eigenfunctions occurring in nature are mixtures of representations usually obscures the striking correspondence with the Zeeman effect, though a few special cases illustrate the mathematical substratum in a spectacular way. For example, the separation of the terms ${}^4D, {}^4G, {}^4S, {}^4F$, and 4I of f^3 are proportional to those of the terms ${}^5D, {}^5G, {}^5S, {}^5F$, and 5I of f^4 ; and the ratios of the separations are independent of the Slater integrals F_k .

It is the purpose of this note to point out that this approach can be extended to other terms in the Hamiltonian. The general method is illustrated in detail for spin-spin and spin-other-orbit interactions. For simplicity, we restrict our attention to configurations of equivalent electrons, particularly those of the type d^N .

2. Single-particle operators. It is convenient to represent the interactions of interest in terms of the single-particle tensors $\underline{w}^{(\kappa\kappa)}$ for which

$$(nl\|\underline{w}^{(\kappa\kappa)}\|nl) = [\kappa]^{1/2} [k]^{1/2},$$

where $[y] \equiv 2y + 1$. The tensors $\underline{w}^{(\kappa\kappa)}$ for κ fixed and k odd form the components of a generalized tensor corresponding to the representation $W = (110\dots 0)$ of $R_{2\ell+1}$; those for κ fixed and k even (and non-zero) form the components of a tensor corresponding to $W = (20\dots 0)^1$. A further generalization is useful: The tensors $\underline{w}^{(\kappa\kappa)}$ for $\kappa + k$ odd form the components of a tensor corresponding to the representation $(\sigma) = (20\dots 0)$ of the symplectic group $Sp_{4\ell+2}$; those for which $\kappa + k$ is even correspond to $(\sigma) = (110\dots 0)^2$. These statements remain valid if the tensors $\underline{w}^{(\kappa\kappa)}$ are replaced by $\underline{w}^{(\kappa\kappa)} = \sum_i (\underline{w}^{(\kappa\kappa)})_i$, where the sum runs over the electrons. The notation $\underline{w}^{(\kappa\kappa)K}$ indicates that κ and k are coupled to a resultant, K .

A detailed group-theoretical classification of the states of all ℓ^N for $\ell < 4$ is already available from the work of Racah¹⁾ and Jahn³⁾. The Wigner-Eckart theorem can thus be immediately applied in the calculation of the matrix elements of the $\underline{w}^{(\kappa\kappa)}$. [A state of seniority v corresponds to $(\sigma) = (11\dots 10\dots 0)$, in which v ones and $2\ell + 1 - v$ zeros appear²⁾.] Suppose that the bra, the operator, and the ket for a given matrix element correspond to the irreducible representations R_a , R_b , and R_c of a group G . Then $c(R_a R_b R_c)$, the number of times that the identity representation occurs in the triple Kronecker product $R_a \times R_b \times R_c$, plays a crucial role in the application of the Wigner-Eckart theorem. If $c(R_a R_b R_c) = x$, then at most x linearly independent sets of matrix elements associated with the labels R_a , R_b , and R_c can exist; and if $x = 0$,

all matrix elements are zero⁴). For the group R_3 , we find $c(D_J D_K D_J) \leq 1$, so all non-zero matrix elements are proportional to just one basic set—which can be conveniently taken to be the collection of 3-j symbols with (JkJ') for their upper row, multiplied by certain phase factors.

Examples have been given elsewhere²) of the application of the Wigner-Eckart theorem to the calculation of the matrix elements of the spin-orbit interaction [proportional to $\underline{W}^{(11)0}$], the hyperfine interaction [involving $\underline{W}^{(01)1}$ and $\underline{W}^{(12)1}$], and the interaction of an atom with a crystalline electric field [involving $\underline{W}^{(0k)k}$]. Our present interest lies in more complex cases, where the interaction cannot be immediately assigned representations W and (σ) . The problem of decomposing an interaction into parts having well-defined group-theoretical properties arises typically in the study of two-particle operators like the Coulomb interaction. The generalization of Racah's approach is probably best described by analyzing special cases. We turn first to the magnetic interaction between the spins of the electrons of an atom.

3. Spin-spin interaction. For a configuration ℓ^N , the contribution to the Hamiltonian arising from magnetic spin-spin interaction can be taken to be

$$H_{ss} = -2 \sum_{i \neq j} \sum_k [(k+1)(k+2)(2k+3)]^{1/2} M^k (\ell \| C^{(k)} \| \ell) \\ \times (\ell \| C^{(k+2)} \| \ell) \{ \underline{W}_i^{(1k)} \underline{W}_j^{(1 \ k+2)} \} (22)0, \quad (1)$$

where M^k is the radial integral defined by Marvin⁵). Values of M^k for a number of paramagnetic ions have recently been calculated by Watson and Blume from Hartree-Fock eigenfunctions⁶). The tensors $\underline{C}^{(k)}$ are related to the

spherical harmonics Y_{kq} by the equation $C_q^{(k)} = [4\pi/(2k+1)]^{1/2} Y_{kq}$. The reduced matrix elements of $C_q^{(k)}$ vanish unless k is even. Hence the curly bracket of Eq. (1) represents a coupled product of quantities that transform like $(\sigma)W \equiv (20\dots 0)(20\dots 0)$. For d electrons, $(\sigma)W \equiv (20000)(20)$. In this case, we find by the usual techniques²⁾ that

$$(20000) \times (20000) = (00000) + (11000) + (20000) + (22000) + (31000) + (40000)$$

and

$$(20) \times (20) = (00) + (11) + (20) + (22) + (31) + (40).$$

Since H_{ss} is symmetrical with respect to the electrons' co-ordinates, not all the representations contained in the Kronecker products are useful; in fact, we can restrict our attention to (00000) , (11000) , (22000) and (40000) of Sp_{10} , which comprise the symmetrical representation [2] of the unitary group U_{55} spanned by the 55 components of $\underline{w}^{(\kappa k)}$ with $\kappa+k$ odd. The branching rules for the reduction $Sp_{10} \rightarrow SU_2 \times R_5$, which separates the spin and orbital spaces, are given in Table I. They can be obtained by a chain calculation in the usual way.

The transformation properties of the spin and orbital parts of H_{ss} are identical to those of the state 5D_0 . With the aid of Table I and the table of branching rules for $R_5 \rightarrow R_3$ given by Jahn³⁾, we see that 5D arises in the decomposition of $(22000)({}^5(20))$, $(22000)({}^5(22))$, and also the representations belonging to (40000) . The last can be discarded, since all states arising in d^N transform like representations $(1\dots 10\dots 0)$ of Sp_{10} , for which

$$c((1\dots 10\dots 0)(40000)(1\dots 10\dots 0)) = 0.$$

Our conclusion is that for d electrons, H_{ss} can be expressed as the sum of two operators h_1 and h_2 , whose transformation properties are determined by the sequences of representations $(22000)(20)^5D_0$ (for h_1) and $(22000)(22)^5D_0$ (for h_2).

Since H_{ss} is a two-particle operator, h_1 and h_2 are adequately defined for the d shell when their matrix elements for d^2 are given. By omitting an explicit construction of these operators, we circumvent the awkward problem of finding coupling coefficients in which representations of Sp_{10} and $SU_2 \times R_5$ appear. To begin, we follow Trees⁷⁾ and separate out the J dependence by writing

$$(\gamma SLJ | H_{ss} | \gamma' S' L' J) = (-1)^{S'+L+J} \begin{Bmatrix} S' & L' & J \\ L & S & 2 \end{Bmatrix} (\gamma SL || T^{(22)} || \gamma' S' L').$$

The symbols γ and γ' are included to completely define the states. Values of the reduced matrix elements of $T^{(22)}$ are given in Table II for d^2 . They can be obtained from Eq. (1), and agree with the results in the literature⁵⁾⁷⁾. It is convenient to introduce reduced matrix elements $(\psi || z_i || \psi')$ for each h_i by writing

$$(\psi || T^{(22)} || \psi') = a_1 (\psi || z_1 || \psi') + a_2 (\psi || z_2 || \psi') \quad (2)$$

The dependence on M^k of each of the two terms on the right hand side of this equation is contained in the parameters a_i . Now the terms 3P and 3F of d^2 belong to the representation (11) of R_5 , for which $c((11)(20)(11)) = 1$; hence for the triplets of d^2 we can write

$$(d^2 {}^3L || z_1 || d^2 {}^3L') = A (d^2 {}^3L || W^{(02)} || d^2 {}^3L') ,$$

where A is independent of L and L' . Reduced matrix elements of $\underline{W}^{(02)}$ are proportional to those of the unit tensor $\underline{U}^{(2)}$, which have been tabulated by Nielson and Koster⁸). Since we have yet to calculate the a_1 , the normalization of the matrix elements $(\psi \| z_1 \| \psi')$ is at our disposal. A convenient choice is made and the results entered in Table II.

For z_2 , we use the relation

$$(d^2 \ 3_L \| z_2 \| d^2 \ 3_P) = B (d^4(11) \ 3_L \| W^{(11)} \| d^4(22) \ 1_D)$$

to give two of the three matrix elements of z_2 ; the third is obtained by using the orthogonality of functions transforming like (20) and (22). Interpreted in terms of matrix elements for d^2 this is

$$\sum_{L, L'} (3_L \| z_1 \| 3_{L'}) (3_{L'} \| z_2 \| 3_L) = 0.$$

The parameters a_1 and a_2 are now determined by insisting that Eq. (2) be satisfied. We find

$$a_1 = 12(M_0 - 8M_2) \quad , \quad a_2 = -120M_2,$$

where

$$M_0 = M_0/7 \quad \text{and} \quad M_2 = M^2/49.$$

Trees' chain calculation for finding the matrix elements of $T^{(22)}$ for other states of d^N can be repeated for z_1 and z_2 separately. The work can be simplified by taking advantage of the fact that t_1 and t_2 correspond to $(\sigma)W$ values of $(22000)(20)$ and $(22000)(22)$ respectively. When $c(WW'(22)) = 0$, for example, the matrix elements of z_2 taken between states corresponding to

W and W' is zero. Since Trees has given a complete tabulation for d^N , this analysis is little more than an exercise; but it points the way to a treatment of f^N , for which only the diagonal matrix elements of H_{ss} for terms of maximum multiplicity are known⁹). For f^N , four operators h_i are required: they all belong to (2200000) of Sp_{14} , and their WU^{2k+1}_k designations are $(200)(20)^5D$, $(220)(20)^5D$, $(220)(21)^5D$, and $(220)(22)^5D$.

The dependence on N of matrix elements involving states of given seniorities is most easily found by introducing the concept of quasi-spin. A method has been described for assigning quasi-spin quantum numbers K to the representations $(\sigma)^{10}$; for d electrons it involves finding the decompositions of representations of the type $(1...10...0)$ of R_{20} into representations of $SU_2 \times Sp_{10}$. Sufficient decompositions for the study of two-particle operators are given in Table III. The quasi-spin multiplicity $[K]$ appears as a prefix to (σ) . Since (22000) occurs only once in this table and with a quasi-spin of zero, we may immediately deduce that matrix elements of H_{ss} are diagonal with respect to seniority and, for a given seniority, independent of N . Details of this technique are given elsewhere¹¹).

4. Spin-other-orbit interaction. The magnetic interaction H_{soo} between the spin of one electron and the orbital motion of another is more complex to treat than spin-spin interaction. However, the general approach is similar, and it seems necessary only to summarize the results. For configurations of equivalent electrons we can write

$$H_{soo} = \sum_{i \neq j} \sum_k [(k+1)(2\ell+k+2)(2\ell-k)]^{1/2} \\ \times \left\{ \begin{Bmatrix} 0 & k+1 \\ \underline{w}_1 \end{Bmatrix} \begin{Bmatrix} 1k \\ \underline{w}_j \end{Bmatrix} (11)0 \left\{ M^{k-1} (\ell \| C^{(k+1)} \| \ell)^2 + 2M^k (\ell \| C^{(k)} \| \ell)^2 \right\} \right. \\ \left. + \begin{Bmatrix} 0k \\ \underline{w}_1 \end{Bmatrix} \begin{Bmatrix} 1 & k+1 \\ \underline{w}_j \end{Bmatrix} (11)0 \left\{ M^k (\ell \| C^{(k)} \| \ell)^2 + 2M^{k-1} (\ell \| C^{(k+1)} \| \ell)^2 \right\} \right\}.$$

As in the preceding section, we specialize to d electrons. A difference with H_{ss} at once appears: the rank k can now be odd as well as even. The additional decompositions $(11000) \times (11000) = (00000) + (11000) + (20000) + (11110) + (21100) + (22000)$ and $(11) \times (11) = (00) + (11) + (20) + (10) + (21) + (22)$ are required. The transformation properties of the spin and orbital parts of H_{soo} are identical to those of the state 3P_0 . Of the available $(\sigma)W$, the following contain 3P and are symmetrical with respect to the interchange of two electrons: $(11000)(11)$, $(11110)(21)$, $(22000)(11)$, $(22000)(21)$, and $(22000)(31)$. From Table III, the quasi-spins associated with (22000) and (11110) are seen to be 0 and 2 respectively; but (11000) is a mixture of $K = 0, 1$, and 2. A further complication is that (11000) occurs in the reduction of $(110...0)$ of R_{20} as well as $(11110...0)$, and this implies that operators of good quasi-spin for $(\sigma) = (11000)$ may contain single-particle as well as two-particle components¹⁰. The single-particle part corresponds to $(11000)(11){}^3P_0$ and possesses $K = 1$; physically it is absorbed by the ordinary spin-orbit interaction. This separation of an effective spin-orbit part from H_{soo} is not equivalent to Horie's separation, since his effective spin-orbit coupling parameter ξ' depends on N ¹².

Our results are conveniently summarized by the equations

$$(\gamma SLJ | H_{soo} | \gamma' S' L' J) = (-1)^{S'+L+J} \begin{Bmatrix} S' & L' & J \\ L & S & 1 \end{Bmatrix} (\gamma SL || T^{(11)} || \gamma' S' L'),$$

where, for d^2 ,

$$(\psi || T^{(11)} || \psi') = \sum a_i (\psi || z_i || \psi'),$$

in which the sum runs over $i = 3, 4, \dots, 9$. The parameters a_i and the group-theoretical description of the z_i are given in Table IV; the reduced matrix

elements of the t_i for d^2 are listed in Table V. For convenience, values of $(\psi||T^{(11)}||\psi')$ for d^2 are included in this table. In using Table V to calculate matrix elements for $N > 2$, it is to be noted that z_3, z_4, z_5 , and z_6 behave like two-particle operators; t_7 and t_9 are essentially mixtures of single-particle and two-particle operators (whose contributions are listed in sequence in Table V); and t_8 behaves as a sum of single-particle operators. Once the matrix elements have been calculated for states of given seniority, the dependence on N can be rapidly found from the quasi-spin rank¹¹). In this way we may verify Horie's matrix elements of H_{soo} for states of d^4 corresponding to $v = 2$ and 0.

Returning to our central theme, the matrix elements of the z_i are the analogues of the number M_J occurring in the Zeeman effect; and the a_i are the analogues of the Landé g factors. For example, since $c((11)(31)(21)) = 1$, we have

$$(\gamma(11)P||z_3||\gamma'(20)D):(\gamma(11)F||z_3||\gamma'(20)D):(\gamma(11)F||z_3||\gamma'(20)G) \\ :: 3(14)^{1/2}:3:-5(3)^{1/2}.$$

This is to be compared to the matrix elements of J_z for, say, a $J = 1$ state, which run as 1:0:-1 for $M_J = 1, 0, -1$. As far as the actual contribution to H_{soo} goes, the effect of z_3 is controlled by a_3 (given in Table IV), just as the Zeeman splitting of a level is determined by g .

5. Three-particle operators. The techniques described in the previous sections can be extended to deal with effective operators. One of the most interesting of these arises in the study of the perturbing effect of the configuration $(nl)^{N+1} (n'l')^{\mp 1}$ on $(nl)^N$. To second order in perturbation theory, we can exactly reproduce the displacements of the terms of $(nl)^N$ by including in the Hamiltonian a number of three-particle operators of the type

$$V(kk'k'') = 2\sqrt{2} \sum_{h \neq i \neq j} \sum_{q, q', q''} \begin{pmatrix} k & k' & k'' \\ q & q' & q'' \end{pmatrix} (w_{0q}^{(0k)})_h (w_{0q'}^{(0k')})_i (w_{0q''}^{(0k'')})_j,$$

as well as the usual scalar two-particle operators characteristic of the linear theory of configuration interaction¹³). It turns out that k , k' , and k'' must all be even, non-zero, at most $2l$, and consistent with the triangular condition. These restrictions allow four $V(kk'k'')$ for d^N and nine for f^N .

It has already been seen that the part z_0 of the spin-other-orbit interaction can be absorbed by the ordinary spin-orbit interaction. When the $V(kk'k'')$ are decomposed into parts having well-defined group-theoretical properties, the possibilities for absorption are much greater, since the Hamiltonian already contains several scalar operators. For f electrons, the $V(kk'k'')$ can be expressed in terms of the nine operators $t_1, t_2, \dots, t_9$ for which $WU^{2k+1}_k \equiv (000)(00)^1s, (220)(22)^1s, (222)(00)^1s, (222)(40)^1s, (400)(40)^1s, (420)(22)^1s, (420)(40)^1s, (420)(42)^1s$, and $(600)(60)^1s$, respectively. The matrix elements of the last (t_9) are always zero, since $c(WW'(600)) = 0$ for all W and W' occurring in f^N . The fifth (t_5) corresponds to the same WU as e_2 ; moreover its matrix elements vanish for all W of f^3 except $W \equiv (210)$, for which $c((210)(400)(210)) = 1$. Hence t_5 can be taken up into e_2 provided the associated parameter E^2 is regarded as freely variable. Similarly, the total scalar

t_1 can be absorbed into e_0 and e_1 . Hence, for f electrons, at most six new parameters are required to represent the effect of the $V(kk'k'')$. This appears to be the explanation for Rajnak's observation¹⁴⁾ that more than five three-particle parameters for $\text{PrIII } 4f^3$ effect little improvement in the fit between experiment and theory—particularly when it is noticed that a sixth parameter would in all probability be required to fit the as yet unobserved upper 2F multiplet. The matrix elements of the t_i and their properties with respect to symplectic symmetry and quasi-spin are described elsewhere¹⁰⁾. For d electrons, only two additional parameters are required for the three-particle operators¹⁵⁾.

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Table I

Branching rules for the reduction $Sp_{10} \rightarrow SU_2 \times R_5$

(σ)	$2S+1_{-W}$
(00000)	$1_{(00)}$
(11000)	$1_{(20)} \ 3_{(11)}$
(20000)	$1_{(11)} \ 3_{(00)(20)}$
(11110)	$1_{(22)} \ 3_{(21)} \ 5_{(10)}$
(22000)	$1_{(00)(10)(20)(22)(40)} \ 3_{(11)(20)(21)(31)} \ 5_{(00)(20)(22)}$
(40000)	$1_{(00)(20)(22)} \ 3_{(11)(20)(31)} \ 5_{(00)(20)(40)}$

Table II

Decomposition of matrix elements of spin-spin interactions for d^2

ψ	ψ'	$(\psi T^{(22)} \psi')$	$(\psi z_1 \psi')$	$(\psi z_2 \psi')$
3_P	3_P	$-84(M_0+12M_2)$	-7	14
3_P	3_F	$24(14)^{1/2}(M_0-13M_2)$	$2(14)^{1/2}$	$(14)^{1/2}$
3_F	3_F	$12(14)^{1/2}(M_0-38M_2)$	$(14)^{1/2}$	$3(14)^{1/2}$

Table III

Branching rules for the reduction $R_{20} \rightarrow SU_2 \times Sp_{10}$

(w)

(0...0)	$^1(00000)$
(110...0)	$^1(20000) \ ^3(00000)(11000)$
(11110...0)	$^1(00000)(11000)(22000)$
	$^3(11000)(20000)(21100)$
	$^5(00000)(11000)(11110)$

Table IV

Operators and parameters for spin-other-orbit interaction

z_i	$^{2K+1}(\sigma)W^{2K+1}_k$	a_i
z_3	$^1(22000)(31)^3P$	$3(M_0 - 3M_2)$
z_4	$^5(11110)(21)^3P$	$4(M_0 + 37M_2)/3$
z_5	$^1(22000)(21)^3P$	$7(M_0 + 37M_2)/3$
z_6	$^1(22000)(11)^3P$	$-(107M_0 - 46M_2)/6$
z_7	$^1(11000)(11)^3P$	$35(M_0 - 2M_2)/6$
z_8	$^3(11000)(11)^3P$	$-21(7M_0 - 6M_2)$
z_9	$^5(11000)(11)^3P$	$28(2M_0 - M_2)/3$

Table V

Decomposition of matrix elements of spin-other-orbit interaction for d^2

ψ	ψ'	$(\psi T^{(11)} \psi')$	(z_3)	(z_4)	(z_5)	(z_6)	(z_7)	(z_8)	(z_9)
3_P	3_P	$-252(M_0 + 12M_2)$	0	-14	-28	7	(6-1)	1	$2(3-1)$
3_F	3_F	$18(14)^{1/2}(-9M_0 + 17M_2)$	0	$(14)^{1/2}$	$2(14)^{1/2}$	$7(14)^{1/2}$	$(14)^{1/2}(6-1)$	$(14)^{1/2}$	$2(14)^{1/2}(3-1)$
1_S	3_P	$21(2)^{1/2}(M_0 + 2M_2)$	0	0	0	0	$(2)^{1/2}(6-6)$	$(2)^{1/2}$	$3(2)^{1/2}(2+1)$
3_P	1_D	$-15(14)^{1/2}(M_0 + 4M_2)$	$3(14)^{1/2}$	$(14)^{1/2}$	$-(14)^{1/2}$	$5(7/2)^{1/2}$	$-(7/2)^{1/2}(6-1)$	$-(7/2)^{1/2}$	$-(14)^{1/2}(3-1)$
1_D	3_F	$90(M_0 - 5M_2)$	3	11	-11	-10	$2(6-1)$	2	$4(3-1)$
3_F	1_G	$-66(3)^{1/2}(M_0 + 2M_2)$	$-5(3)^{1/2}$	$5(3)^{1/2}$	$-5(3)^{1/2}$	$5(3)^{1/2}$	$-(3)^{1/2}(6-1)$	$-(3)^{1/2}$	$-2(3)^{1/2}(3-1)$

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