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Lawrence Radiation Laboratory
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ZEEMAN EFFECT AS A PROTOTYPE FOR INTRA-ATOMIC INTERACTIONS

B. R. Judd

August 1965
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 $(nl)^{N+1} (n'l')^{T}$. 

ZEEMAN EFFECT AS A PROTOTYPE FOR INTRA-ATOMIC INTERACTIONS

B. R. Judd

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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, Racah$^1$ introduced the operators $e_0, e_1, e_2, e_3$, each corresponding to a pair of representations $\mathbf{WU}$ 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 $\mathbf{w}^{(\kappa k)}$ for which

$$(n_{\|} | n_{\perp} ) = [\kappa]^{1/2} [k]^{1/2} ,$$

where $[y] = 2y + 1$. The tensors $\mathbf{w}^{(\kappa k)}$ for $\kappa$ fixed and $k$ odd form the components of a generalized tensor corresponding to the representation $W = (110 \ldots 0)$ of $R_{2l+1}$; those for $\kappa$ fixed and $k$ even (and non-zero) form the components of a tensor corresponding to $W = (20 \ldots 0)$.

A further generalization is useful: The tensors $\mathbf{w}^{(\kappa k)}$ for $\kappa + k$ odd form the components of a tensor corresponding to the representation $(\sigma) = (20 \ldots 0)$ of the symplectic group $Sp_{4l+2}$; those for which $\kappa + k$ is even correspond to $(\sigma) = (110 \ldots 0)$. These statements remain valid if the tensors $\mathbf{w}^{(\kappa k)}$ are replaced by $\mathbf{w}^{(\kappa k)} = \Sigma_i (\mathbf{w}^{(\kappa k)})_i$, where the sum runs over the electrons. The notation $\mathbf{w}^{(\kappa k)K}$ indicates that $\kappa$ and $k$ are coupled to a resultant, $K$.

A detailed group-theoretical classification of the states of all $l^N$ for $l < 4$ is already available from the work of Racah and Jahn. The Wigner-Eckart theorem can thus be immediately applied in the calculation of the matrix elements of the $\mathbf{w}^{(\kappa k)}$. [A state of seniority $v$ corresponds to $(\sigma) = (1110 \ldots 0)$, in which $v$ ones and $2l + 1 - v$ zeros appear.] 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 zero. For the group $R_j$, we find $\Delta(D_jD_kD_j) \leq 1$, 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 $(Jk\ell')$ for their upper row, multiplied by certain phase factors.

Examples have been given elsewhere of the application of the Wigner-Eckart theorem to the calculation of the matrix elements of the spin-orbit interaction [proportional to $\mathcal{M}(\ell\ell\ell')$], the hyperfine interaction [involving $\mathcal{M}(\ell\ell'\ell')$ and $\mathcal{M}(\ell\ell'\ell')$, and the interaction of an atom with a crystalline electric field [involving $\mathcal{M}(\ell\ell\ell')$]. Our present interest lies in more complex cases, where the interaction cannot be immediately assigned representations $W$ and $(\sigma)$. 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 $N$, the contribution to the Hamiltonian arising from magnetic spin-spin interaction can be taken to be

$$H_{SS} = -2 \sum \sum [(x+1)(x+2)(2x+3)]^{1/2} M^k(\ell||c(k)||\ell)$$

$$\times (\ell||c(k)||\ell)(\mathcal{M}_k(1k)(1 k+2) (22) 0) ,$$

where $M^k$ is the radial integral defined by Marvin. Values of $M^k$ for a number of paramagnetic ions have recently been calculated by Watson and Elume from Hartree-Fock eigenfunctions. The tensors $c(k)$ are related to the
spherical harmonics $Y_{kq}$ by the equation $C^{(k)}_q = \left[ \frac{4\pi}{2k+1} \right]^{1/2} Y_{kq}$. The reduced matrix elements of $C^{(k)}_q$ vanish unless $k$ is even. Hence the curly bracket of Eq. (1) represents a coupled product of quantities that transform like $(\sigma)\mathcal{W} = (20...0)(20...0)$. For d electrons, $(\sigma)\mathcal{W} = (20000)(20)$. In this case, we find by the usual techniques 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 $\mathcal{Y}^{(kk)}$ with $\kappa + k$ odd. The branching rules for the reduction $Sp_{10} \to SU_2 \times R_5$, 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 $R_5 \to R_3$ given by Jahn\(^3\), 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 $(1...10...0)$ of $Sp_{10}$, for which

\[c((1...10...0)(40000)(1...10...0)) = 0.\]
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 $(20000)(20)^5D_0$ (for $h_1$) and $(20000)(22)^5D_0$ (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 Trees$^7$ and separate out the $J$ dependence by writing

$$\langle \gamma S L J | H_{ss} | \gamma' S' L' J \rangle = (-1)^{S'+L+J} \{S' L' J \} \langle \gamma S L | T^{(22)} | \gamma' S' L' \rangle.$$ 

The symbols $\gamma$ and $\gamma'$ 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 literature$^5$.$^7$.

It is convenient to introduce reduced matrix elements $\langle \psi | z_1 | \psi' \rangle$ for each $h_1$ by writing

$$\langle \psi | T^{(22)} | \psi' \rangle = a_1 \langle \psi | z_1 | \psi' \rangle + a_2 \langle \psi | z_2 | \psi' \rangle .$$  

(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 $a_1$. 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

$$\langle d^2 \ 3L | z_1 | d^2 \ 3L' \rangle = A \langle d^2 \ 3L | W^{(02)} | d^2 \ 3L' \rangle ,$$
where $A$ is independent of $L$ and $L'$. Reduced matrix elements of $\tilde{M}^{(02)}$ are proportional to those of the unit tensor $\tilde{W}^{(2)}$, which have been tabulated by Nielson and Koster $^8$. Since we have yet to calculate the $a_i$, the normalization of the matrix elements $(\psi|z_i|\psi')$ is at our disposal. A convenient choice is made and the results entered in Table II.

For $z_2$, we use the relation

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

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

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

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 $c(W'(22)) = 0$, for example, the matrix elements of $z_2$ taken between states corresponding to

\[\text{\ldots}\]
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 known\(^9\). For $f^N$, four operators $h_i$ are required: they all belong to $(2200000)$ of $Sp_{14}$, and their $WU^{2x+1}K$ 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 $(1\ldots10\ldots0)$ 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 $(\sigma)$. 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 elsewhere\(^11\).

4. Spin-other-orbit interaction. The magnetic interaction $H_{s0o}$ 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

$$H_{s0o} = \sum_i \sum_j \sum_k [(k+1)(2l+k+2)(2l-k)]^{1/2}$$

$$\times \left[ \begin{array}{c} (0\ k+1) \\ (1k) \end{array} \right] \left[ \begin{array}{c} (1l) \\ (0\ l) \end{array} \right] \left[ \begin{array}{c} (k+1) \\ (0\ k) \end{array} \right] \left[ \begin{array}{c} (0\ l) \\ (1k) \end{array} \right]$$

$$\times \left( M^{k-1} (2l||C(k+1)||l)^2 + 2M^{k} (l||C(k)||l)^2 \right)$$

$$+ \left( M^{k-1} (2l||C(k+1)||l)^2 + 2M^{k} (l||C(k)||l)^2 \right).$$
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 $H_{so0}$ 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 components. 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 $H_{so0}$ is not equivalent to Horie's separation, since his effective spin-orbit coupling parameter $\xi'$ depends on $N$. Our results are conveniently summarized by the equations

$$(\gamma_{SLJ}|H_{so0}|\gamma'S'L'J) = (-1)^{S' + L + J} \left\{ S' \begin{array}{c} L' \ J \\ L \ S \ 1 \end{array} \right\} (\gamma_{SL}|T^{(11)}|\gamma'S'L'),$$

where, for $d^2$,

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

in which the sum runs over $i = 3, 4, \ldots, 9$. 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 $(\psi|T^{(1)}|\psi')$ 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 rank $l$. In this way we may verify Horie's matrix elements of $H_{soo}$ for states of $d^4$ corresponding to $\nu = 2$ 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 $c((11)(31)(2l)) = 1$, we have

$$(\gamma(11)F||z_3||\gamma'(20)D):(\gamma(11)F||z_3||\gamma'(20)D)=(\gamma(11)F||z_3||\gamma'(20)G)$$

$$:3(14)^{1/2};3:5(3)^{1/2}.$$ 

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 $(nl)^{N+1} (n'l')^{1} \rightarrow (nl)^{N}$. 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

$$V(kk'k'') = 2\sqrt{2} \sum_{h \neq i \neq j} \sum_{q,q',q''} \left( \begin{array}{ccc} k & k' & k'' \\ q & q' & q'' \end{array} \right) \left( \begin{array}{c} \psi_{0q}^{(0k)} \\ \psi_{0q'}^{(0k')} \\ \psi_{0q''}^{(0k'')} \end{array} \right)_{i} \left( \begin{array}{c} \psi_{0q}^{(0k)} \\ \psi_{0q'}^{(0k')} \\ \psi_{0q''}^{(0k'')} \end{array} \right)_{j},$$

as well as the usual scalar two-particle operators characteristic of the linear theory of configuration interaction. 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 $t_{1}, t_{2}, \ldots, t_{9}$ for which $W^{2k+1}k = (000)(00)^{1}S, (220)(22)^{1}S, (222)(00)^{1}S, (222)(40)^{1}S, (400)(40)^{1}S, (420)(22)^{1}S,$ $(420)(42)^{1}S, (600)(60)^{1}S$, 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 $W = (210)$, for which $c((210)(400)(210)) = 1$. Hence $t_{5}$ can be taken up into $e_{2}$ provided the associated parameter $E_{2}^{2}$ 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 observation that more than five three-particle parameters for 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 $t_1$ and their properties with respect to symplectic symmetry and quasi-spin are described elsewhere. For d electrons, only two additional parameters are required for the three-particle operators.

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15) Feneuille, S., private communication.
Table I

Branching rules for the reduction $\text{Sp}_{10} \rightarrow SU_2 \times R_5$

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<thead>
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<th>$(\sigma)$</th>
<th>$2S+1_W$</th>
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<td>$^1(00)$</td>
</tr>
<tr>
<td>(11000)</td>
<td>$^1(20)\ 3(11)$</td>
</tr>
<tr>
<td>(20000)</td>
<td>$^1(11)\ 3(00)(20)$</td>
</tr>
<tr>
<td>(11110)</td>
<td>$^1(22)\ 3(21)\ 5(10)$</td>
</tr>
<tr>
<td>(22000)</td>
<td>$^1(00)(10)(20)(22)(40)\ 3(11)(20)(21)(31)\ 5(00)(20)(22)$</td>
</tr>
<tr>
<td>(40000)</td>
<td>$^1(00)(20)(22)\ 3(11)(20)(31)\ 5(00)(20)(40)$</td>
</tr>
</tbody>
</table>
Table II
Decomposition of matrix elements of spin-spin interactions for $d^2$

| $\psi$ | $\psi'$ | $(\psi||T^{(22)}||\psi')$ | $(\psi||z_1||\psi')$ | $(\psi||z_2||\psi')$ |
|-------|--------|--------------------------|----------------------|----------------------|
| $3_p$ | $3_p$  | $-84(M_0 + 12M_2)$       | -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 \( R_{20} \rightarrow SU_2 \times Sp_{10} \)

<table>
<thead>
<tr>
<th>(w)</th>
<th>( ^1(00000) )</th>
<th>( ^2(00000)(11000) )</th>
<th>( ^1(00000)(11000)(22000) )</th>
<th>( ^3(11000)(20000)(21100) )</th>
<th>( ^5(00000)(11000)(11110) )</th>
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<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>((110\ldots0))</td>
<td>( ^1(20000) )</td>
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<td></td>
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</tr>
<tr>
<td>((11110\ldots0))</td>
<td>( ^3(11000)(20000)(21100) )</td>
<td>( ^5(00000)(11000)(11110) )</td>
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### Table IV

Operators and parameters for spin-other-orbit interaction

<table>
<thead>
<tr>
<th>$z_1$</th>
<th>$2K+1(\sigma)\phi^{2K+1}k$</th>
<th>$a_1$</th>
</tr>
</thead>
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<tr>
<td>$z_3$</td>
<td>$^1(22000)(31)^3P$</td>
<td>$3(M_0-3M_2)$</td>
</tr>
<tr>
<td>$z_4$</td>
<td>$^5(11110)(21)^3P$</td>
<td>$4(M_0+37M_2)/3$</td>
</tr>
<tr>
<td>$z_5$</td>
<td>$^1(22000)(21)^3P$</td>
<td>$7(M_0+37M_2)/3$</td>
</tr>
<tr>
<td>$z_6$</td>
<td>$^1(22000)(11)^3P$</td>
<td>$-(107M_0-46M_2)/6$</td>
</tr>
<tr>
<td>$z_7$</td>
<td>$^1(11000)(11)^3P$</td>
<td>$35(M_0-2M_2)/6$</td>
</tr>
<tr>
<td>$z_8$</td>
<td>$^3(11000)(11)^3P$</td>
<td>$-21(M_0-6M_2)$</td>
</tr>
<tr>
<td>$z_9$</td>
<td>$^5(11000)(11)^3P$</td>
<td>$28(2M_0-M_2)/3$</td>
</tr>
</tbody>
</table>
Table V

Decomposition of matrix elements of spin-other-orbit interaction for d²

| ψ   | ψ'  | \( \langle \psi | T^{(11)} | \psi' \rangle \) | \( \| z_3 \| \) | \( \| z_4 \| \) | \( \| z_5 \| \) | \( \| z_6 \| \) | \( \| z_7 \| \) | \( \| z_8 \| \) | \( \| z_9 \| \) |
|-----|-----|----------------|--------|--------|--------|--------|--------|--------|--------|
| \( ^3p \) | \( ^3p \) | -252(\( M_0+12M_2 \)) | 0      | -14    | -28    | 7      | \( 6-1 \) | 1      | 2(3-1) |
| \( ^3p \) | \( ^3F \) | 18(14)\( \frac{1}{2} \)(-9M_0+17M_2) | 0      | \( 14 \frac{1}{2} \) | \( 2(14) \frac{1}{2} \) | \( 7(14) \frac{1}{2} \) | \( 14 \frac{1}{2} \)(6-1) | \( 14 \frac{1}{2} \) | \( 2(14) \frac{1}{2} \) \( 3-1 \) |
| \( ^1S \) | \( ^3p \) | 21(2)\( \frac{1}{2} \)(\( M_0+2M_2 \)) | 0      | 0      | 0      | 0      | \( 2 \frac{1}{2} \)(6-6) | \( 2 \frac{1}{2} \) | \( 3(2) \frac{1}{2} \)(2+1) |
| \( ^3p \) | \( ^1D \) | -15(14)\( \frac{1}{2} \)(\( M_0+4M_2 \)) | \( 3(14) \frac{1}{2} \) | \( 14 \frac{1}{2} \) | \( -14 \frac{1}{2} \) | \( 5(7/2) \frac{1}{2} \) | \( -7/2 \frac{1}{2} \)(6-1) | \( -7/2 \frac{1}{2} \) | \( -14 \frac{1}{2} \) \( 3-1 \) |
| \( ^1D \) | \( ^3F \) | 90(\( M_0-5M_2 \)) | 3      | 11     | -11    | -10    | \( 2(6-1) \) | 2      | \( 4(3-1) \) |
| \( ^3F \) | \( ^1G \) | -66(3)\( \frac{1}{2} \)(\( M_0+2M_2 \)) | \( -5(3) \frac{1}{2} \) | \( 5(3) \frac{1}{2} \) | \( -5(3) \frac{1}{2} \) | \( 5(3) \frac{1}{2} \) | \( -3 \frac{1}{2} \)(6-1) | \( -3 \frac{1}{2} \) | \( -2(3) \frac{1}{2} \) \( 3-1 \) |
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