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Calculation and Checking of Electrostatic Energy Matrices by Computer*

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A method is developed for calculating by computer the electrostatic energy matrices in the Racah–Slater method. The method considers three basic points: the simplicity of the programming, the reliability of the results and computer time optimization. A general description of the computer program which is based on this method is given.

I. INTRODUCTION

The calculation of the energy matrices of complex spectra by the "Slater–Racah method" is long and tedious and can be performed efficiently only with the aid of a computer. Several computer programs have already been written in this area [1–4]. The algorithms used for calculating the algebraic formulas of the electrostatic energy matrix elements $(\psi \mid \sum_{i<j} V_{ij} \mid \psi')$ are based upon reduction to the matrix element $(\psi_{12} \mid V_{12} \mid \psi'_{12})$. We wrote a computer program using the alternative approach where $(\psi \mid \sum_{i<j} V_{ij} \mid \psi')$ is decomposed in terms of one-particle–operator matrices. This approach has the following advantages:

a. The problem is reduced to the calculation of one-particle operator matrix elements which is by nature simpler than that of two-particle operators.

b. As shown previously [5], the decomposition mentioned above can be made in two different ways, thus providing an easy check of the calculation. This check has been found to be an essential tool in the construction of the matrices. The importance of such a check is fully discussed in Ref. [5].

c. In many cases, particularly simple expressions are obtained [5, 6].

d. Since magnetic and effective interactions can also be decomposed in terms of one particle-operators of the same type, it is possible to use the same routines to calculate these interactions as well.

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In this paper we describe the entire algorithm used in the program.

In Section II we review the decomposition of the electrostatic interaction operator into products of one-particle operators. In Section III we discuss the choice of a suitable coupling scheme. In Section IV we introduce the method for deriving the formula for a general matrix element of a one-particle operator.

The computer program based on this algorithm [7] calculates and checks formulas and numerical values of matrix elements of electrostatic and two-body electrostatic effective interactions. A brief review of the program, its possibilities and limitations is given in Section V.

II. DECOMPOSITION OF THE ELECTROSTATIC INTERACTION MATRIX INTO MATRICES OF ONE-PARTICLE OPERATORS [8]

The electrostatic interaction between the electrons in the "central field approximation" can be written in the following way:

$$\sum_{i<j} e^2/r_{ij} = e^2 \sum_{k} \sum_{n_a l_a n_b l_b n_a' l_a' n_b' l_b'} X^k(n_a l_a n_b l_b\,, n_a' l_a' n_b' l_b') \times \sum_{i<j} Z_i^{(k)}(n_a l_a\,, n_a' l_a') \cdot Z_j^{(k)}(n_b l_b\,, n_b' l_b'), \tag{1}$$

where $Z_i^{(k)}(nl, n'l')$ is a tensor operator of degree k operating on the i-th electron, with reduced matrix elements given by

$$(n''l'' \,\|\, Z_i^{(k)}(nl, n'l') \,\|\, n'''l''') = \delta(n'', n)\, \delta(l'', l)\, \delta(n''', n')\, \delta(l''', l')$$

and

$$X^k(n_a l_a n_b l_b\,, n_a' l_a' n_b' l_b') = (l_a \,\|\, C^{(k)} \,\|\, l_a')(l_b \,\|\, C^{(k)} \,\|\, l_b') \times R^{(k)}(n_a l_a n_b l_b\,, n_a' l_a' n_b' l_b'),$$

where R^k are the Slater integrals and $C^{(k)}$ are the spherical harmonices normalized by Eq. (5.19) of Ref. [9]. (This reference is referred to as F.R. in the sequel).

The coefficient of X^k can be rewritten as

$$\frac{1}{1 + \delta(n_a\,, n_b)\, \delta(l_a\,, l_b)\, \delta(n_a', n_b')\, \delta(l_a', l_b')} S^k(n_a l_a n_b l_b\,, n_a' l_a' n_b' l_b'), \tag{2}$$

where

$$S^k(n_a l_a n_b l_b\,, n_a' l_a' n_b' l_b') = \sum_{i \neq j} Z_i^{(k)}(n_a l_a\,, n_a' l_a') \cdot Z_j^{(k)}(n_b l_b\,, n_b' l_b').$$

In the "Racah–Slater method," X^k are considered as adjustable parameters and one has to calculate only the matrices of (2).

S^k can be further written in either of the following equivalent expressions

$$Z^{(k)}(n_a l_a\,, n_a' l_a') \cdot Z^{(k)}(n_b l_b\,, n_b' l_b') \\ - \delta(l_a\,, l_b')\,\delta(n_b\,, n_a')\,\delta(l_b\,, l_a')[l_a]^{-1/2}\,Z^{(0)}(n_a l_a\,, n_b' l_a), \tag{3a}$$

$$Z^{(k)}(n_b l_b\,, n_b' l_b') \cdot Z^{(k)}(n_a l_a\,, n_a' l_a') \\ - \delta(l_b\,, l_a')\,\delta(n_a\,, n_b')\,\delta(l_a\,, l_b')[l_b]^{-1/2}\,Z^{(0)}(n_b l_b\,, n_a' l_b), \tag{3b}$$

where $Z^{(k)} = \sum_i^{(k)}$.

For the matrix elements of (3) we get, by F.R. (15.16),

$$\sum_{\psi''} (-)^{J-J''-k}\,[J]^{-1}\,(\psi \,\|\, Z^{(k)}(n_a l_a\,, n_a' l_a') \,\|\, \psi'')(\psi'' \,\|\, Z^{(k)}(n_b l_b\,, n_b' l_b') \,\|\, \psi') \\ - \delta(l_a\,, l_b')\,\delta(n_b\,, n_a')\,\delta(l_b\,, l_a')[l_a\,, J]^{-1/2}\,(\psi \,\|\, Z^{(0)}(n_a l_a\,, n_b' l_a) \,\|\, \psi'), \tag{4a}$$

$$\sum_{\psi'''} (-)^{J-J'''-k}\,[J]^{-1}\,(\psi \,\|\, Z^{(k)}(n_b l_b\,, n_b' l_b') \,\|\, \psi''')(\psi''' \,\|\, Z^{(k)}(n_a l_a\,, n_a' l_a') \,\|\, \psi') \\ - \delta(l_b\,, l_a')\,\delta(n_a\,, n_b')\,\delta(l_a\,, l_b')[l_b\,, J]^{-1/2}\,(\psi \,\|\, Z^{(0)}(n_b l_b\,, n_a' l_b) \,\|\, \psi'), \tag{4b}$$

where J, J'' and J''' are the total angular momenta of the states ψ, ψ'' and ψ''', respectively. We use the traditional contractions $[x] = (2x + 1)$, $[x, y \cdots] = (2x + 1)(2y + 1) \cdots$.

Thus the calculation of the energy matrix (1) is reduced to that of the matrix elements of the one-particle operators $Z^{(k)}$.

Because of the special characteristics of the operators $Z^{(k)}$ the summations over ψ'' and ψ''' are reduced each to a single configuration Γ'' and Γ''', respectively where, in general, $\Gamma'' \neq \Gamma'''$. In such cases (4a) and (4b) lead to two basically different formulas resulting in the same numerical values and providing an element-by-element check of the matrices. There is a symmetry between (4a) and (4b) in the sense that one expression is obtained from the other by the index exchange $a \leftrightarrow b$ and therefore only one routine is needed to calculate both of them.

It should be mentioned here that for parameters of the type $X^k(nlnl, n'l'n'l')$, the configurations Γ'' and Γ''' in (4) are identical, and both (4a) and (4b) lead to the same expression and the check is trivial. On the other hand, for parameters of the type $X^k(nln'l', nln'l')$ with $nl \neq n'l'$, although $\Gamma'' \equiv \Gamma'''$ the commutativity of $Z^{(k)}(nl, nl)$ and $Z^k(n'l', n'l')$ still provides a check.

III. Coupling Schemes—The Standard Scheme

The calculation of various interactions in different coupling schemes might be algebraically interesting. However, a program capable of handling all types of coupling schemes is by nature rather complicated.

It was shown by Racah [10] that once one has the energy matrices in any arbitrary coupling scheme, it is always possible to obtain the components of the physical states in any other desired scheme by diagonalizing these energy matrices with fictitious values of the parameters. For practical purposes we therefore developed a calculation method for a "Standard Scheme" which is in most atomic problems close to the physical scheme. We now define this scheme.

The Standard Scheme

Let Γ be a general configuration of q-ordered shells: $\Gamma = l_1^{N_1} l_2^{N_2} \cdots l_q^{N_q}$ [11]. In the i-th shell there are N_i electrons whose individual quantum numbers are $n_i l_i$.

The Standard Scheme is an L–S coupling scheme where the angular momenta of each shell are coupled to the resultant angular momenta of all the shells on its left. Specifically, the states of Γ in the standard scheme will be

$$| \, l_1^{N_1}(\alpha_1 S_1 L_1), l_2^{N_2}(\alpha_2 S_2 L_2) \, \bar{S}_2 \bar{L}_2 , \ldots, l_q^{N_q}(\alpha_q S_q L_q) \, \bar{S}_q \bar{L}_q \rangle,$$

where $\alpha_i S_i L_i$ characterizes the states of the i-th shell in L–S coupling, and $\bar{S}_i \bar{L}_i$ are the resultant orbital and spin angular momenta, respectively, of all the shells from 1 to i.

In the sequel we refer only to states in the standard scheme.

In cases where no confusion might arise we denote a general state in the standard scheme by specifying the ordered shells alone omitting the additional quantum numbers, i.e.,

$$| \, l_1^{N_1} l_2^{N_2} \cdots l_q^{N_q} \rangle \equiv | \, l_1^{N_1}(\alpha_1 S_1 L_1), l_2^{N_2}(\alpha_2 S_2 L_2) \, \bar{S}_2 \bar{L}_2 , \ldots, l_q^{N_q}(\alpha_q S_q L_q) \, \bar{S}_q \bar{L}_q \rangle. \tag{5}$$

IV. THE METHOD OF CALCULATING THE MATRIX ELEMENT $(\psi \| Z^{(k)}(l, l') \| \psi')$[1]

Since we are interested in a method which is simple for programming, we deal with all possible cases in a similar way (even if it is roundabout in some of them), using simple elementary repeated steps.

The outline of the method is as follows: We change the order of the shells in the states ψ and ψ' to a new order defined below, still retaining the standard coupling scheme. In this new order we use a closed formula for the matrix elements of the corresponding operator $Z^{(k)}$. (This closed formula was calculated once and is given below.) The expression for $(\psi \| Z^{(k)}(l, l') \| \psi')$, which is obtained in this way is unnecessarily complicated and must then be contracted to the simplest possible form. The three main stages of the method are therefore:

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[1] ψ and ψ' are antisdmmetricai States in the Standard Scheme.

1. The transformation to the new shell order;
2. The use of the closed formula in the reordered standard scheme;
3. The contraction process.

These stages are discussed in detail below.

1. *The Reordering of the Shells*

In order to calculate the matrix element

$$(l_1^{N_1} l_2^{N_2} \cdots l_i^{N_i} \cdots l_j^{N_j} \cdots l_r^{N_r} l_{r+1}^{N_{r+1}} \cdots l_q^{N_q} \,\|\, Z^{(k)}(l, l') \,\|\, l_{k_1}^{N_{k_1}} l_{k_2}^{N_{k_2}} \cdots l_{k_r}^{N_{k_r}} l_{r+1}^{N_{r+1}} \cdots l_q^{N_q}), \tag{6}$$

where $l_i = l$ and $l_j = l' \neq l$, or vice versa, and where $k_1 \cdots k_r$ is a permutation of $1 \cdots r$ in which $k_r \neq r$, we remove the shells $l_{r+1}^{N_{r+1}} \cdots l_q^{N_q}$ by F.R. (15.7) and transform to the following shell order:

$$l_1 l_2 \cdots l_{i-1} l_{i+1} \cdots l_{j-1} l_{j+1} \cdots l_r l l'.$$

The matrix element (6) is thus expressed in terms of matrix elements in the reordered scheme:

$$(l_1^{N_1} l_2^{N_2} \cdots l_r^{N_r} l^N l'^{N'} \,\|\, Z^{(k)}(l, l') \,\|\, l_1^{N_1} l_2^{N_2} \cdots l_r^{N_r} l^{N-1} l'^{N'+1}). \tag{7}$$

In the case $l = l'$, the matrix element

$$(l_1^{N_1} l_2^{N_2} \cdots l_i^{N_i} \cdots l_r^{N_r} l_{r+1}^{N_{r+1}} \cdots l_q^{N_q} \,\|\, Z^{(k)}(l, l) \,\|\, l_{k_1}^{N_{k_1}} l_{k_2}^{N_{k_2}} \cdots l_{k_r}^{N_{k_r}} l_{r+1}^{N_{r+1}} \cdots l_q^{N_q}) \tag{6a}$$

is similarly expressed in terms of

$$(l_1^{N_1} \cdots l_r^{N_r} l^N \,\|\, Z^{(k)}(l, l) \,\|\, l_1^{N_1} \cdots l_r^{N_r} l^N). \tag{7a}$$

we denote the bra and ket in the reordered scheme by ψ_z and ψ_z', respectively.

Specifically, the transformation from (6) to (7) is done by two elementary repeated steps: First the shells l_q, l_{q-1},..., l_{r+1} are removed one by one by repeated use of F.R. (15.7). Each such step introduces $6j$ symbol and a multiplicative factor. For example, in the first step, removing the l_q shell, one has

$$\begin{aligned}
&(\bar{\alpha}_{q-1} \bar{S}_{q-1} \bar{L}_{q-1}\,,\, l_q^{N_q}(\alpha_q S_q L_q)\, \bar{S}_q \bar{L}_q \,\|\, Z^{(k)}(l, l') \,\|\, \bar{\alpha}'_{q-1} \bar{S}_{q-1} \bar{L}'_{q-1}\,,\, l_q^{N_q}(\alpha_q S_q L_q)\, \bar{S}_q \bar{L}_q{}')\\
&\quad = (\bar{\alpha}_{q-1} \bar{S}_{q-1} \bar{L}_{q-1} \,\|\, Z^{(k)}(l, l') \,\|\, \bar{\alpha}'_{q-1} \bar{S}_{q-1} \bar{L}'_{q-1})\\
&\qquad \times (-1)^{\bar{L}_q{}' + \bar{L}_{q-1} + L_q + k}\, [\bar{L}_q\,,\, \bar{L}_q{}']^{1/2} \begin{Bmatrix} \bar{L}_q & \bar{L}_q{}' & k \\ \bar{L}'_{q-1} & \bar{L}_{q-1} & L_q \end{Bmatrix},
\end{aligned} \tag{8}$$

where $\bar{\alpha}_{q-1}$ and $\bar{\alpha}'_{q-1}$ represent all other quantum numbers appearing in the bra and ket of (6), respectively.

Secondly, the remaining shells are reordered, by another repeated step in which two neighboring shells exchange places. This step will be called "exchange" in the sequel. Since in any stage the coupling remains in the standard form, such exchange introduces a summation, a recoupling coefficient and a phase factor which originates from the antisymmetrization of the states. Specifically,

$$\begin{aligned} &| \cdots \bar{S}_A\bar{L}_A\,,\, l_s^{N_s}(\alpha_s S_s L_s)\,\bar{S}_B\bar{L}_B\,,\, l_t^{N_t}(\alpha_t S_t L_t)\,\bar{S}_C\bar{L}_C \cdots\rangle \\ &= (-1)^{N_s\times N_t} \sum_{\bar{S}_B''\bar{L}_B''} (-1)^{L_s+S_s+L_t+S_t+\bar{L}_B+\bar{S}_B+\bar{L}_B''+\bar{S}_B''} \\ &\quad\times \begin{Bmatrix} \bar{L}_A & L_s & \bar{L}_B \\ \bar{L}_C & L_t & \bar{L}_B'' \end{Bmatrix} \begin{Bmatrix} \bar{S}_A & S_s & \bar{S}_B \\ \bar{S}_C & S_t & \bar{S}_B'' \end{Bmatrix} \\ &\quad\times | \cdots \bar{S}_A\bar{L}_A\,,\, l_t^{N_t}(\alpha_t S_t L_t)\,\bar{S}_B''\bar{L}_B''\,,\, l_s^{N_s}(\alpha_s S_s L_s)\,\bar{S}_C\bar{L}_C \cdots\rangle \end{aligned} \tag{9}$$

The phase factor $(-1)^{N_s\times N_t}$ enters since $N_s \times N_t$ electron transpositions have been made. The recoupling coefficient is an application of F.R. Eq. (11.10).

It was also found useful to use the following identity:

$$(\psi \,\|\, Z^{(k)}(l, l') \,\|\, \psi') = (-)^{L-L'-k}\,(\psi' \,\|\, Z^{(k)}(l', l) \,\|\, \psi), \tag{10}$$

where L and L' are the total orbital angular momenta of ψ and ψ', respectively.

We calculate that side of (10) which involves a smaller number of exchanges during the reordering process. This saves complications in the contraction stage (paragraph 3 below).

2. *The Formula for* $(\psi_Z \,\|\, Z^{(k)}(l, l') \,\|\, \psi_Z')$ [2]

As mentioned above, the calculation of the matrix element $(\psi_Z \,\|\, Z^{(k)}(l, l') \,\|\, \psi_Z')$ is made only once and is used throughout the program without further modifications. We present its derivation by the second quantization technique where it turns out to be extremely short compared to conventional methods.

As was shown by Judd [12], the second quantization form of $Z^{(k)}(l_1, l_2)$ is [13]

$$Z^{(k)}(l_1, l_2) = -\{a^+ b\}^{(0k)}\,(2/[k])^{1/2}, \tag{11}$$

where a^+ creates an $n_1 l_1$ electron and b destroys an $n_2 l_2$ electron.

Since a^+ and b are double tensors of rank $(1/2, l_1)$ and $(1/2, l_2)$, respectively, which operate each on a different system it is possible to use here directly Eq. (15.4) of F.R.

---

[2] ψ_Z and ψ_Z' are antisymmetrized states in the reordered scheme.

$$
\begin{aligned}
&(\psi_Z \,\|\, \{a^+b\}^{(0k)} \,\|\, \psi_Z{}') = \\
&(\bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_1^{N_1}(\alpha_1 S_1 L_1)\,\bar{S}_1\bar{L}_1\,,\, l_2^{N_2}(\alpha_2 S_2 L_2)\, SL \,\|\, \{a^+b\}^{(0k)} \,\|\, \bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_1^{N_1-1}(\alpha_1{}'S_1{}'L_1{}') \\
&\qquad\quad \bar{S}_1{}'\bar{L}_1{}' l_2^{N_2+1}(\alpha_2{}'S_2{}'L_2{}')\, SL') \\
&\quad = (\bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_1^{N_1}(\alpha_1 S_1 L_1)\,\bar{S}_1\bar{L}_1 \,\|\, a^+ \,\|\, \bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_1^{N_1-1}(\alpha_1{}'S_1{}'L_1{}')\,\bar{S}_1{}'\bar{L}_1{}') \\
&\quad\times (l_2^{N_2}\alpha_2 S_2 L_2 \,\|\, b \,\|\, l_2^{N_2+1}\alpha_2{}'S_2{}'L_2{}')[S, S, L, L', k]^{1/2} \\
&\quad\times \begin{Bmatrix} \bar{S}_1 & \bar{S}_1{}' & 1/2 \\ S_2 & S_2{}' & 1/2 \\ S & S & 0 \end{Bmatrix} \begin{Bmatrix} \bar{L}_1 & \bar{L}_1{}' & l_1 \\ L_2 & L_2{}' & l_2 \\ L & L' & k \end{Bmatrix}.
\end{aligned}
\tag{12}
$$

$\bar{S}_0$ and $\bar{L}_0$ are the spin and orbital total angular momenta of all other shells with nl different from both n_1l_1 and n_2l_2. α_0 denotes the additional quantum numbers needed to characterize the states.

We make use of the known identities:

1. F.R. Eq. (12.14)

$$
\begin{Bmatrix} \bar{S}_1 & \bar{S}_1{}' & 1/2 \\ S_2 & S_2{}' & 1/2 \\ S & S & 0 \end{Bmatrix} = \begin{Bmatrix} \bar{S}_1 & \bar{S}_1{}' & 1/2 \\ S_2{}' & S_2 & S \end{Bmatrix} [1/2, S]^{-1/2} (-1)^{\bar{S}_1{}'+1/2+S_2+S}.
$$

2. F.R. Eq. (15.7′)

$$
\begin{aligned}
&(\bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_1^{N_1}(\alpha_1 S_1 L_1)\,\bar{S}_1\bar{L}_1 \,\|\, a^+ \,\|\, \bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_1^{N_1-1}(\alpha_1{}'S_1{}'L_1{}')\,\bar{S}_1{}'\bar{L}_1{}') \\
&\quad = (-1)^{\bar{L}_1+l_1+L_1{}'+\bar{L}_0+\bar{S}_1+1/2+S_1{}'+\bar{S}_0} [\bar{L}_1\,,\, \bar{L}_1{}', \bar{S}_1\,,\, \bar{S}_1{}']^{1/2} \\
&\qquad \times \begin{Bmatrix} \bar{L}_1 & \bar{L}_1{}' & l_1 \\ L_1{}' & L_1 & \bar{L}_0 \end{Bmatrix} \begin{Bmatrix} \bar{S}_1 & \bar{S}_1{}' & 1/2 \\ S_1{}' & S_1 & \bar{S}_0 \end{Bmatrix} (l_1^{N_1}\alpha_1 S_1 L_1 \,\|\, a^+ \,\|\, l_1^{N_1-1}\alpha_1{}'S_1{}'L_1{}')
\end{aligned}
$$

3. Equations (31), (32) of Ref. [12]

$$
\begin{aligned}
&(l_1^{N_1}\alpha_1 S_1 L_1 \,\|\, a^+ \,\|\, l_1^{N_1-1}\alpha_1{}'S_1{}'L_1{}') \\
&\qquad = (-1)^{N_1} \sqrt{N_1}[S_1\,,\, L_1]^{1/2}\, (l_1^{N_1}\alpha_1 S_1 L_1 \,|\}\, l_1^{N_1-1}\alpha_1{}'S_1{}'L_1{}'), \\
&(l_2^{N_2}\alpha_2 S_2 L_2 \,\|\, b \,\|\, l_2^{N_2+1}\alpha_2{}'S_2{}'L_2{}') \\
&\qquad = (-1)^{N_2+1+S_2+L_2-1/2-l_2-S_2{}'-L_2{}'} \\
&\qquad\qquad \times \sqrt{N_2+1}[S_2{}', L_2{}']^{1/2}\, (l_2^{N_2}\alpha_2 S_2 L_2 \{|\, l_2^{N_2+1}\alpha_2{}'S_2{}'L_2{}').
\end{aligned}
$$

In addition, remembering that $(\psi_Z \,\|\, Z^{(k)}(l_1\,,\, l_2) \,\|\, \psi_Z{}')$ is a reduced matrix element only with respect to the orbital angular momentum while $(\psi_Z \,\|\, \{a^+b\}^{(0k)} \,\|\, \psi_Z{}')$ is reduced with respect to both spin and orbital angular momenta, we have by (11) and by F.R. (14.5),

$$
(\psi_Z \,\|\, Z^{(k)}(l_1\,,\, l_2) \,\|\, \psi_Z{}') = -[S, k]^{-1/2} \sqrt{2}(\psi_Z \,\|\, \{a^+b\}^{(0k)} \,\|\, \psi_Z{}').
$$

We finally get

$$
\begin{aligned}
&(\psi_Z \| Z^{(k)}(l_1, l_2) \| \psi_Z') \\
&\quad = \delta(S, S') \sqrt{N_1(N_2+1)}(-1)^{N_1+l_1+l_2+\bar{L}_0+\bar{L}_1+L_1'+L_2+L_2'+\bar{S}_0+\bar{S}_1+S_1'+\bar{S}_1'-S_2'+S+1/2} \\
&\qquad \times [L_2', L_1, \bar{L}_1, \bar{L}_1', L, L', S_2', S_1, \bar{S}_1, \bar{S}_1']^{1/2} \begin{Bmatrix} \bar{L}_1 & \bar{L}_1' & l_1 \\ L_1' & L_1 & \bar{L}_0 \end{Bmatrix} \\
&\qquad \times \begin{Bmatrix} \bar{S}_1 & \bar{S}_1' & 1/2 \\ S_2' & S_2 & S \end{Bmatrix} \begin{Bmatrix} \bar{S}_1 & \bar{S}_1' & 1/2 \\ S_1' & S_1 & \bar{S}_0 \end{Bmatrix} \begin{Bmatrix} \bar{L}_1 & \bar{L}_1' & l_1 \\ L_2 & L_2' & l_2 \\ L & L' & k \end{Bmatrix} \\
&\qquad \times (l_1^{N_1}\alpha_1 S_1 L_1 \,|\}\, l_1^{N_1-1}\alpha_1' S_1' L_1')(l_2^{N_2}\alpha_2 S_2 L_2 \,\{|\, l_2^{N_2+1}\alpha_2' S_2' L_2'). \qquad (13)
\end{aligned}
$$

The notations in (13) and (14) are as in (12).

For the case where $l_2 = l_1$ we get by Ref. [14] (see p. 187) and by F.R. Eq. (15.7′)

$$
\begin{aligned}
&(\bar{\alpha}_0 \bar{S}_0 \bar{L}_0, l_1^{N_1}(\alpha_1 S_1 L_1)\, SL \| Z^{(k)}(l_1, l_1) \| \bar{\alpha}_0 \bar{S}_0 \bar{L}_0, l_1^{N_1}(\alpha_1' S_1' L_1')\, SL') \\
&\quad = N_1(-1)^{\bar{L}_0+L_1'+L+l_1+L_1} [L, L', L_1, L_1']^{1/2} \begin{Bmatrix} L & L' & k \\ L_1' & L_1 & L_0 \end{Bmatrix} \delta(S_1, S_1') \\
&\qquad \times \sum_{l_1^{N_1-1}\alpha'' S'' L''} (-1)^{L''} \begin{Bmatrix} l_1 & L_1 & L'' \\ L_1' & l_1 & k \end{Bmatrix} (l_1^{N_1}\alpha_1 S_1 L_1 \,|\}\, l_1^{N_1-1}\alpha'' S'' L'') \\
&\qquad \times (l_1^{N_1-1}\alpha'' S'' L'' \,\{|\, l_1^{N_1-1}\alpha_1' S_1' L_1'). \qquad (14)
\end{aligned}
$$

3. *The Contraction of the Formulas*

As was mentioned above, the formula obtained as a result of stages 1 and 2 contains unnecessary summations. The purpose of the contraction process is to remove these summations using known identities. In our computer program, the five following identities are used:

1. $\sum_x [x] \begin{Bmatrix} a & b & x \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & x \\ a & b & q \end{Bmatrix} = \delta_{pq} \dfrac{\Delta(a, d, p)\, \Delta(c, b, p)}{[p]}$,

2. $\sum_x (-1)^{p+q+x} [x] \begin{Bmatrix} a & b & x \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & x \\ b & a & q \end{Bmatrix} = \begin{Bmatrix} c & a & q \\ d & b & p \end{Bmatrix}$,

3. $\sum_x (-1)^{a+b+c+d+e+f+p+q+r+x} [x] \begin{Bmatrix} a & b & x \\ c & d & p \end{Bmatrix} \begin{Bmatrix} c & d & x \\ e & f & q \end{Bmatrix} \begin{Bmatrix} e & f & x \\ b & a & r \end{Bmatrix}$

   $= \begin{Bmatrix} p & q & r \\ e & a & d \end{Bmatrix} \begin{Bmatrix} p & q & r \\ f & b & c \end{Bmatrix}$,

4. $\sum_x [x] \begin{Bmatrix} a & f & x \\ d & q & e \\ p & c & b \end{Bmatrix} \begin{Bmatrix} a & f & x \\ e & b & \lambda \end{Bmatrix} = (-1)^{2\lambda} \begin{Bmatrix} c & d & \lambda \\ e & f & q \end{Bmatrix} \begin{Bmatrix} a & b & \lambda \\ c & d & p \end{Bmatrix}$,

$$5.\quad \sum_{x,x'} (-1)^{c+e+e''+d''-b-b'-d'-x'} [x, x'] \begin{Bmatrix} e'' & e' & e \\ c'' & x' & x \end{Bmatrix} \begin{Bmatrix} b & d & e \\ c'' & x' & c' \end{Bmatrix} \begin{Bmatrix} b' & d' & e' \\ c'' & x & c \end{Bmatrix}$$

$$\times \begin{Bmatrix} b & b' & d'' \\ c' & c & d'' \\ x' & x & e'' \end{Bmatrix} = \begin{Bmatrix} d & d' & d'' \\ c & c' & c'' \end{Bmatrix} \begin{Bmatrix} b & b' & b'' \\ d & d' & d'' \\ e & e' & e'' \end{Bmatrix}.$$

In all applications made until now [15] these identities were sufficient to contract the formulas to the most simple form.

The outline of the contraction process is as follows: The summations appearing in the uncontracted formula are treated one by one in reverse order to that of their appearance, i.e., starting with the last and ending with the first. For each summation in its turn, the possibilities of applying the identities are checked one by one in a fixed order. If a certain identity is applicable the corresponding summation is replaced by the right hand side of the identity and the checking process starts from the beginning, i.e., again from the last appearing summation. This procedure is needed since after applying a certain identity it may be possible that another application of an identity which was not possible previously can now be made. The fixed order by which the possibilities of applying the identities are checked enables maximal contraction only when the initial number of summations is not too large. In order to avoid unnecessary summations already in the uncontracted formula we make use of Eq. (10) as was detailed above.

It should be pointed out that the formulas for S^k, which are obtained by inserting the formulas of the appropriate $Z^{(k)}$'s to (4), can in many cases be further contracted removing the summation appearing in (4). However, it was found convenient to calculate the matrices of the Z^k's separately and apply (4) only numerically. This will be further detailed in Section V.

SUMMARY

The method presented above for calculating the algebraic formulas for $(\psi \| Z^{(k)}(l, l') \| \psi')$ is simple to program, being based on just two elementary repeated steps: The removal of a right shell, and the exchange of two neighboring shells. The additional contraction stage also does not introduce any complication in the programming. The computer time in the entire process remains negligible (as will be detailed in Section V).

The procedure of checking the result, which is performed by means of (4), does not require any additional effort in programming since the same routines are used to calculate both (4a) and (4b), owing to their symmetry between the indices a and b.

As was mentioned in the Introduction, magnetic and effective interactions can also be decomposed in terms of one-particle operators. Therefore exactly the same method can be applied for their calculation. Formulas analogous to Eq. (12) for the cases of spin orbit and hyperfine interactions are given in the appendix.

V. THE COMPUTER PROGRAM–GENERAL REVIEW

Input. The input of the program is most simple. It contains only the names of the configurations Γ and Γ' between which the interaction is to be calculated. (It is possible of course that $\Gamma = \Gamma'$).

Main Stages. As a first step the involved parameters (Slater integrals) are determined. The program treats the parameters one at a time performing for every parameter the following steps:

a. The intermediate configurations Γ'' and Γ''' of Eq. (4) are determined. (The order of the shells in the intermediate configurations is determined so that the total number of "exchanges" in the transformation to the recordered scheme is minimal.)

b. The symbols which characterize the quantum numbers appearing in the standard scheme are defined, and the formulas for the involved operators $Z^{(K)}$ are then calculated.

c. The numerical matrices of these formulas are calculated. This part, being independent of the method described in Sections II–IV, will not be detailed in this paper. We only mention here that in this part lists of terms and c.f.p. tables are read from a special file which was prepared for that purpose for the shells s, p, d, f.

d. The matrix elements of (4a) and (4b) are obtained and checked one by one by comparing the results. In fact, in the step c the factors $(-1)^{L-L''-k}[L]$ and $(-1)^{L-L'''-k}[L]$ of (4) are attached to the formulas of the left $Z^{(K)}$ of (4a) and (4b), respectively. Consequently the results of the present step are obtained simply by usual matrix multiplication and addition. Moreover, since the final matrices are diagonal with respect to S and L, these operations are performed for each pair of values of S and L separately, thus saving computer memory.

e. The final step is the construction of the matrices for the different J's appearing in the corresponding problem.

General Characteristics—Possibilities and Limitations

The program is written in Fortran IV for a CDC 6400 computer which has a memory of 64K words.

Memory. For the derivation of the formulas only 20000_8 words are needed and there is no limitation on the configurations involved. For the numerical calculation, the size of the memory needed depends on the length of the lists of terms involved. The program is suitable for configurations containing up to 200 terms where 62000_8 words are sufficient. For bigger configurations the dimension of several vectors in the program should be extended and correspondingly the memory used should be greater.

Computer time. The derivation of the formulas (including the contraction process) takes two seconds at most for each parameter. Therefore there is no need for further improvements of this stage. On the other hand, the process of the numerical calculation is incomparably longer (between a few seconds to 10 min for a parameter, depending on the complexity of the corresponding formula). Here there are many possibilities for improvements, for instance, the calculation of the coefficients of $F^k(l_1, l_1)$ in the configuration $\Gamma = l_1^{N_1} l_2^{N_2} \cdots l_q^{N_q}$ can be performed in a much shorter way with in the configuration $l_1^{N_1}$ and then be extended to Γ. Another possibility of improvement is to do the numerical calculations (in appropriate cases) of the full expressions (4a) and (4b) and not of the involved $Z^{(K)}$'s separately. This shortens the calculation only when a further contraction of the entire formula can be performed, removing the summations of (4). However, as the above described method does not take too much time, it was not found worthwhile complicating the program for such improvements.

We quote characteristic numbers for two cases: The first example is a calculation of d^5p matrices which are of a commonly used size. (Here there are altogether 6 electrostatic and effective two-body parameters. The number of terms is 88 and the number of j's is 9.) The total computer time needed for the calculation is *30 sec.*

The second is the particularly complicated complex:

$$f^2d^2 + f^2ds + f^2s^2 + fd^2p + fdsp + fs^2p + d^4 + d^3s + d^2s^2.$$

The number of electrostatic parameters (including interaction between configurations and two-body effective interactions) in the whole complex is 160. The total number of terms is 603, and the number of j's is 11. The total computer time needed in the construction of the matrices (including checkings) for the whole complex is about 2 hr. Taking into account that a single diagonalization of that complex takes about 90 min, and many dozens of diagonalizations are needed for the interpretation of a single pertinent spectrum, this makes the calculation time very satisfactory.

APPENDIX: FORMULAS FOR ONE-PARTICLE INTERACTION IN THE REORDERED SCHEME

Spin–Orbit Interaction

$$(\bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_r^{N_r}(\alpha_r S_r L_r)\, SLJ \,\|\, \sum_i S_i \cdot l_i \,\|\, \bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_r^{N_r}(\alpha_r{}' S_r{}' L_r{}')\, S'L'J)$$

$$= N_r\{l_r(l_r+1)(2l_r+1)\,3/2\}^{1/2}\,(-1)^{\bar{S}_0+\bar{L}_0+S_r{}'+L_r{}'+S+S'+l_r+J}$$

$$\times\,[S, L, S', L', S_r\,, L_r\,, S_r{}', L_r{}']^{1/2}\begin{Bmatrix} S & S' & 1 \\ L' & L & j \end{Bmatrix}\begin{Bmatrix} S & S' & 1 \\ S_r{}' & S_r & \bar{S}_0 \end{Bmatrix}\begin{Bmatrix} L & L' & 1 \\ L_r{}' & L_r & \bar{L}_0 \end{Bmatrix}$$

$$\times \sum_{l_r^{N_r-1}\alpha'' S'' L''} (-1)^{L_r''+S_r''+S_r+L_r+1/2}\begin{Bmatrix} 1/2 & 1 & 1/2 \\ S_r & S_r'' & S_r{}' \end{Bmatrix}\begin{Bmatrix} l_r & 1 & l_r \\ L_r & L_r'' & L_r{}' \end{Bmatrix}$$

$$\times\,(l_r^{N_r}\alpha_r S_r L_r \,|\}\, l_r^{N_r-1}\alpha_r'' S_r'' L_r'')(l_r^{N_r-1}\alpha_r'' S_r'' L_r'' \,\{|\, l_r^{N_r}\alpha_r{}' S_r{}' L_r{}').$$

Hyperfine Interaction

$$(\bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_r^{N_r}(\alpha_r S_r L_r)\, SLJ \,\|\, \sum_i (SC^{(2)})_i^{(1)} \,\|\, \bar{\alpha}_0\bar{S}_0\bar{L}_0\,,\, l_r^{N_r}(\alpha_r{}' S_r{}' L_r{}')\, S'L'J')$$

$$= 3N_r\{l_r(l_r+1)(2l_r+1)/2(2l_r-1)(2l_r+3)\}^{1/2}$$

$$\times\,(-1)^{\bar{S}_0+\bar{L}_0+S_r{}'+L_r{}'+L_r+S+L+l_r+1}\,[J, J', S, S', L, L', S_r\,, S_r{}', L_r\,, L_r{}']^{1/2}$$

$$\times \begin{Bmatrix} S & S' & 1 \\ S_r{}' & S_r & S_0 \end{Bmatrix}\begin{Bmatrix} L & L' & 2 \\ L_r{}' & L_r & L_0 \end{Bmatrix}\begin{Bmatrix} S & S' & 1 \\ L & L' & 2 \\ J & J' & 1 \end{Bmatrix}$$

$$\times \sum_{l_r^{N_r-1}\alpha_r'' S_r'' L_r''} (l_r^{N_r}\alpha_r S_r L_r \,|\}\, l_r^{N_r-1}\alpha_r'' S_r'' L_r'')(l_r^{N_r-1}\alpha_r'' S_r'' L_r'' \,\{|\, l_r^{N_r}\alpha_r{}' S_r{}' L_r{}')$$

$$\begin{Bmatrix} S_r & S_r{}' & 1 \\ 1/2 & 1/2 & S_r'' \end{Bmatrix}\begin{Bmatrix} L_r & L_r{}' & 2 \\ l_r & l_r & L_r'' \end{Bmatrix}(-)^{S_r''+L_r''+S_r+1/2}$$

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