New identities for matrix elements of spin-dependent interactions in $l^N l'$ configurations

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Formulas for the matrix elements of the spin-dependent interactions, such as spin-spin, spin-other-orbit, and effective electrostatic spin-orbit, were constructed for $l^N l'$ configurations, including the two special cases $N=1$ and $4l+1$. Since these interactions are described by two-electron operators, they comprise, in analogy with the electrostatic interaction, both direct and exchange parts. For each of these interactions, 12 angular momenta participate in the orbital part, as well as in the spin part, of the corresponding matrix element. In the formula representing the direct part, both orbital and spin angular momenta are connected according to the identity of Arima, Horie, and Tanabe; in this identity, a double sum of three $6j$ symbols and one $9j$ symbol is expressed as a simple product of one $6j$ symbol and one $9j$ symbol. In the exchange part, all orbital (spin) angular momenta are grouped in one $12j$ symbol of the first kind, according to a newly discovered identity; in this identity, the $12j$ symbol is expressed as a double sum of three $6j$ symbols and one $9j$ symbol. All the above-mentioned results were also reproduced by using graphical methods. It can thus be concluded that the identity of Arima, Horie, and Tanabe and the new identity, respectively, represent the symmetry properties of the direct and exchange parts of the two-electron spin-dependent interactions. For the purpose of obtaining simple and closed formulas in the special case $N=4l+1$, namely, for configurations comprising a hole and an electron, additional new identities were constructed.

I. INTRODUCTION

It has recently been shown that the introduction of the "additional spin-dependent interactions (additional SDI)" in the energy-level calculations of nl^N (Refs. 1–6) and $nln'l'$ (Refs. 4, 5, 7 and 8) configurations greatly improves the fit between observed and calculated multiplet splittings. The interactions considered were the spin-spin (SS), the spin-other-orbit (SOO), and the effective electrostatic spin-orbit (effective EL-SO) interactions. The first two interactions belong to the category of the mutual magnetic interactions and, respectively, represent the mutual interaction between the magnetic dipole moments of the electrons and between the dipole moment of one electron and the orbital motion of another. The effective EL-SO interaction represents, to second order of perturbation theory, the mixed electrostatic spin-orbit interaction with distant configurations.

In order to include these interactions in more complex configurations, such as $nl^N n'l'$, one must first express them in tensor-operator form and then calculate the angular parts of their matrix elements between states belonging to the desired configuration. Only after the completion of these two steps can one proceed by evaluating the radial integrals (parameters) describing these interactions, and comparing the theory with experiment.

The tensor-operator form of all the additional SDI, for $nl^N n'l'$ configurations, is by now well known, and given by the following formulas:[9,10,5]

$$H_{\rm SS}=-\frac{\beta^2}{\sqrt{5}}\sum_k(-1)^k\left[\frac{(2k+5)!}{(2k)!}\right]^{1/2}\times\sum_{\substack{i,j\\(i\neq j)}}\left[\frac{r_j^k}{r_i^{k+3}}([\underline{C}_i^{(k+2)}\times\underline{C}_j^{(k)}]^{(2)}\cdot[\underline{s}_i\times\underline{s}_j]^{(2)})+\frac{r_i^k}{r_j^{k+3}}([\underline{C}_i^{(k)}\times\underline{C}_j^{(k+2)}]^{(2)}\cdot[\underline{s}_i\times\underline{s}_j]^{(2)})\right] \tag{1}$$

with $\beta=e\hbar/2mc$, and[5]

$$H_{\rm SOO}=\frac{2\beta^2}{\sqrt{3}}\sum_k(-1)^k\sum_{\substack{i,j\\(i\neq j)}}\left[\frac{r_i^{k-2}}{r_j^{k+1}}(2k+1)(2k-1)^{1/2}[\underline{C}_j^{(k)}\times[\underline{C}^{(k)}\times\underline{l}]_i^{(k-1)}]^{(1)}-\frac{r_j^k}{r_i^{k+3}}(2k+1)(2k+3)^{1/2}[\underline{C}_j^{(k)}\times[\underline{C}^{(k)}\times\underline{l}]_i^{(k+1)}]^{(1)}\right.$$

$$-\frac{r_i^{k-2}}{r_j^{k+1}}(k+1)(2k+1)^{1/2}[\underline{C}_j^{(k)}\times[\underline{C}^{(k)}\times\underline{l}]_i^{(k)}]^{(1)}$$

$$+\frac{r_j^{k}}{r_i^{k+3}}k(2k+1)^{1/2}[\underline{C}_j^{(k)}\times[\underline{C}^{(k)}\times\underline{l}]_i^{(k)}]^{(1)}$$

$$+\frac{r_i^{k-1}}{r_j^{k+1}}\frac{\partial}{\partial r_i}[k(k+1)(2k+1)]^{1/2}[\underline{C}_j^{(k)}\times\underline{C}_i^{(k)}]^{(1)}$$

$$+\frac{r_j^{k}}{r_i^{k+2}}\frac{\partial}{\partial r_i}[k(k+1)(2k+1)]^{1/2}[\underline{C}_j^{(k)}\times\underline{C}_i^{(k)}]^{(1)}\Bigg]\cdot(\underline{s}_i+2\underline{s}_j)\ , \tag{2}$$

and also[5,11]

$$H_{\text{EL-SO}}=\sum_{\substack{k\ \text{even}\\ t\ \text{odd}}}\sum_{\substack{i,j\\(i\neq j)}}\frac{2}{\sqrt{3}}(2t+1)\Bigg[S^k(nln'l',nln''l')[l'(l'+1)(2l'+1)]^{1/2}\begin{Bmatrix}1&k&t\\ l'&l'&l'\end{Bmatrix}([\underline{u}_i^{(k)}\times\underline{v}_j^{(t)}]^{(1)}\cdot\underline{s}_j)$$

$$+S^k(nln'l',n'''ln'l')[l(l+1)(2l+1)]^{1/2}\begin{Bmatrix}1&k&t\\ l&l&l\end{Bmatrix}(\underline{s}_i\cdot[\underline{u}_i^{(t)}\times\underline{v}_j^{(k)}]^{(1)})\Bigg]$$

$$+\sum_{\substack{k(P_k=P_{l+l'})\\ t}}\sum_{\substack{i,j\\(i\neq j)}}\frac{1}{\sqrt{3}}(2t+1)\Bigg[T^k(nln'l',n''l'nl)[l'(l'+1)(2l'+1)]^{1/2}(-1)^{1+t}\begin{Bmatrix}1&k&t\\ l&l'&l'\end{Bmatrix}$$

$$+T^k(nln'l',n'l'n'''l)[l(l+1)(2l+1)]^{1/2}(-1)^{k}\begin{Bmatrix}1&k&t\\ l'&l&l\end{Bmatrix}\Bigg]$$

$$\times\{(\underline{s}_i\cdot[\underline{z}_i^{(t)}\times\underline{\tilde{z}}_j^{(k)}]^{(1)})+([\underline{z}_i^{(k)}\times\underline{\tilde{z}}_j^{(t)}]^{(1)}\cdot\underline{s}_j)\}\ , \tag{3}$$

where $\underline{u}^{(k)}$, $\underline{v}^{(k)}$, $\underline{z}^{(k)}$, and $\underline{\tilde{z}}^{(k)}$ are unit tensor operators defined as follows:[11,12]

$$(l||\underline{u}^{(k)}||l)=1,\quad (l'||\underline{v}^{(k)}||l')=1\ ,$$
$$(l||\underline{z}^{(k)}||l')=1,\quad (l'||\underline{\tilde{z}}^{(k)}||l)=1\ ; \tag{4}$$

and $k(P_k=P_{l+l'})$ in the last summation means that k may only take values having the same parity as $l+l'$.

By inspecting formulas (1)—(3), the following conclusions are drawn.

(i) All the additional SDI are described by two-electron operators, that is, by operators of the type

$$G=\sum_{\substack{i,j\\(i\neq j)}}g_{ij}\ .$$

Consequently, for nl^Nnl' configurations, these interactions comprise both *direct* and *exchange* parts, in analogy with the electrostatic interaction. For the SS interaction these parts are, respectively, expressed in terms of the radial integrals $M^k(nl,n'l')$, $M^k(n'l',nl)$, and $N^k(nl,n'l')$ defined by Marvin.[13] The exchange part of the SOO interaction includes, in addition, the radial integrals $K^{k\pm}$, in which derivatives of the radial functions appear under the integral sign [see the last two terms in formula (2)]. These integrals were defined by Jucys *et al.*[14] The direct and exchange parts of the effective EL-SO interactions are, respectively, represented by $S^k(nln'l',nln''l')$, $S^k(nln'l',n'''ln'l')$ and $T^k(nln'l',n''l'nl)$, $T^k(nln'l',n'l'n'''l)$, defined by Goldschmidt and Mallow.[5,11] The definitions of all these parameters as well as the relations holding between them are included in Ref. 5.

(ii) For all these interactions the angular part of each of the terms included in g_{ij} is given as a scalar product of two irreducible tensor operators, which operate, respectively, on the orbital and spin spaces.

$$G=\sum_{\substack{i,j\\(i\neq j)}}g_{ij}$$

can thus be written (up to constant factors which include

TABLE I. Ranks of the various operators describing the additional SDI as compared to the electrostatic interaction.

Interaction \ Rank	K	κ_1		κ_2
SS	2	1		1
SOO	1	0	and/or	1
EL-SO	1	1	and/or	0
electrostatic	0	0		0

also the corresponding reduced matrix elements) in the following form.

The direct part can be written as

$$D=\sum_{\substack{i,j\\(i\neq j)}} D_{ij}=\sum_{\substack{i,j\\(i\neq j)}} ([\underline{u}_i^{(k_1)}\times\underline{v}_j^{(k_2)}]^{(K)}\cdot[\underline{s}_i^{(\kappa_1)}\times\underline{s}_j^{(\kappa_2)}]^{(K)})\ , \tag{5}$$

while the exchange part can be written as

$$E=\sum_{\substack{i,j\\(i\neq j)}} E_{ij}=\sum_{\substack{i,j\\(i\neq j)}} ([\underline{z}_i^{(k_1)}\times\underline{\widetilde{z}}_j^{(k_2)}]^{(K)}\cdot[\underline{s}_i^{(\kappa_1)}\times\underline{s}_j^{(\kappa_2)}]^{(K)})\ . \tag{6}$$

In the last two expressions k_i, κ_i, and K constitute a representative set of the ranks of the various tensor operators describing the additional SDI. For simplicity, the summations over k_i of κ_i which appear in the original formulas (1)—(3) are omitted. The values taken by K, κ_1, and κ_2 in the various additional SDI, and, for comparison, in the electrostatic interaction as well, are gathered in Table I.

In the present work explicit formulas were derived for the matrix elements of D and E, for $nl^Nn'l'$ configurations (including the two special cases $N=1$ and $4l+1$). These formulas were obtained by using two different algebraic methods. At the outset, the calculations by two different methods were devised for checking the final results. It turned out that the results obtained by the two methods, while leading indeed to identical numerical values, differ in form, in the following ways.

(a) For the direct part of each of the additional SDI, these results constitute the two sides of the identity of Arima, Horie, and Tanabe (AHT);[15] in this identity, a double sum of three $6j$ symbols and one $9j$ symbol is expressed as a simple product of one $6j$ symbol and one $9j$ symbol.

(b) For the exchange part, these results constitute the two sides of a newly discovered identity, in which a double sum of three $6j$ symbols and one $9j$ symbol equals one $12j$ symbol of the first kind.[16–19]

Conclusions (a) and (b) hold for both the spin and orbital parts of D and E.

All the above-mentioned results were then reproduced by using graphical methods. These were first introduced by Jucys *et al.*[18] and further developed by a number of authors.[19–22] In the present work the phase conventions of Lindgren and Morrison[22] are used.

It can thus be concluded that the AHT and the new identity, respectively, represent the symmetry properties of the direct and exchange parts of the additional SDI. Each of these identities reduces to a simpler identity whenever one, or more, of the κ_i and/or K vanish; this occurs for the spin part of the SOO and the effective EL-SO interactions, and, of course, for the electrostatic interaction. The various simpler identities will be discussed in a separate paper.

For the purpose of obtaining simple and closed formulas for the matrix elements of the additional SDI, for configurations $nl^{4l+1}n'l'$ comprising a hole and an electron, additional new identities were constructed; these identities enable the performance of summations over the quantum numbers S_2 and L_2, which represent, respectively, the total spin and orbital angular momentum of the grandparent configurations nl^{4l}. These summations cannot be carried out independently, since S_2 and L_2 are connected through the requirement that S_2+L_2 be even, in accordance with the Pauli principle.

II. MATRIX ELEMENTS

A. General expressions

The matrix elements to be calculated are $(l^N(\alpha_1S_1L_1)l'SLJM\{\,|D+E|\,\}l^N(\alpha_1'S_1'L_1')l'S'L'JM)$. The $\{|\ |\}$ sign on both sides of the operator indicates a matrix element between antisymmetric eigenfunctions, whereas a sign $|\ |$ will indicate a matrix element between nonantisymmetrized eigenfunctions. An antisymmetric function for $nl^Nn'l'$ can be written in the form[23]

$$(1,2,\ldots,N+1\,|\,\}l^N(\alpha_1S_1L_1)l'SLJM)$$
$$=(N+1)^{-1/2}\sum_{i=1}^{N+1}(-1)^{P_i}(1,2,\ldots,i-1,N+1,i+1,\ldots,N,i\,|\,l^N(\alpha_1S_1L_1)l'SLJM)\ , \tag{7}$$

where P_i is the parity of the permutation which exchanges i with $N+1$. Utilization of the fact that D and E are symmetric operators whereas the eigenfunctions are antisymmetric leads to the following expressions for the matrix elements of the direct and exchange parts:

$$\{\,|D|\,\}=N(l_{(N)}^N(\alpha_1S_1L_1)l'_{N+1}SLJM\,|\,[\underline{u}_N^{(k_1)}\times\underline{v}_{N+1}^{(k_2)}]^{(K)}\cdot[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}\,|\,l_{(N)}^N(\alpha_1'S_1'L_1')l'_{N+1}S'L'JM)\ , \tag{8}$$

$$\{\,|E|\,\}=-N(l_{(N)}^N(\alpha_1S_1L_1)l'_{N+1}SLJM\,|\,[\underline{z}_N^{(k_1)}\times\underline{\widetilde{z}}_{N+1}^{(k_2)}]^{(K)}\cdot[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}\,|\,l_{(N+1)}^N(\alpha_1'S_1'L_1')l'_NS'L'JM)\ . \tag{9}$$

The factor N on the right-hand side of these equations is a product of the three numbers $N(N+1)$, $(N+1)^{-1/2}$, $(N+1)^{-1/2}$; $N(N+1)$ is the number of pairs of electrons included in each of the summations

$$\sum_{\substack{i,j\\(i\neq j)}} D_{ij},\quad \sum_{\substack{i,j\\(i\neq j)}} E_{ij}\ ,$$

whereas $(N+1)^{-1/2}$ are the normalization factors of the eigenfunctions on each side of the matrix elements. The subscript (N) $[(N+1)]$ in $l^N_{(N)}$ $(l^N_{(N+1)})$ is written to indicate that the Nth $[(N+1)$th$]$ electron is included in the group l^N. Factoring out their J dependence, both $\{\,|D|\,\}$ and $\{\,|E|\,\}$ can be written in the following forms:

$$\{\,|D|\,\}=(-1)^{L+S'+J}\begin{Bmatrix} S & S' & K\\ L' & L & J\end{Bmatrix}||D||\ , \tag{10}$$

$$\{\,|E|\,\}=(-1)^{L+S'+J}\begin{Bmatrix} S & S' & K\\ L' & L & J\end{Bmatrix}||E||\ , \tag{11}$$

where the reduced matrix elements $||D||$ and $||E||$ are given by

$$||D||=N(l^N_{(N)}(\alpha_1S_1L_1)l'_{N+1}SL\,||[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}[\underline{u}_N^{(k_1)}\times\underline{v}_{N+1}^{(k_2)}]^{(K)}||\,l^N_{(N)}(\alpha'_1S'_1L'_1)l'_{N+1}S'L') \tag{12}$$

and

$$||E||=-N(l^N_{(N)}(\alpha_1S_1L_1)l'_{N+1}SL\,||[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}[\underline{z}_N^{(k_1)}\times\underline{\tilde{z}}_{N+1}^{(k_2)}]^{(K)}||\,l^N_{(N+1)}(\alpha'_1S'_1L'_1)l'_NS'L')\ . \tag{13}$$

$[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}[\underline{u}_N^{(\kappa_1)}\times\underline{v}_{N+1}^{(\kappa_2)}]^{(K)}$ and $[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}[\underline{z}_N^{(\kappa_1)}\times\underline{\tilde{z}}_{N+1}^{(\kappa_2)}]^{(K)}$ are both double-tensor operators, acting on the Nth and $(N+1)$th electrons. The problem, therefore, remains to calculate $||D||$ and $||E||$.

B. The configuration $nln'l'$ $(N=1)$

For the two-electron configuration $nln'l'$, formula (12) takes the form

$$\begin{aligned}||D_{ij}||&=(ll'\bar{S}\bar{L}\,||[\underline{s}_i^{(\kappa_1)}\times\underline{s}_j^{(\kappa_2)}]^{(K)}[\underline{u}_i^{(k_1)}\times\underline{v}_j^{(k_2)}]^{(K)}||\,ll'\bar{S}'\bar{L}')\\ &=(\tfrac{1}{2}\tfrac{1}{2}\bar{S}\,||[\underline{s}_i^{(\kappa_1)}\times\underline{s}_j^{(\kappa_2)}]^{(K)}||\,\tfrac{1}{2}\tfrac{1}{2}\bar{S}')(ll'\bar{L}\,||[\underline{u}_i^{(k_1)}\times\underline{v}_j^{(k_2)}]^{(K)}||\,ll'\bar{L}')\ ,\end{aligned}$$

where $\bar{S}\bar{L}$ $(\bar{S}'\bar{L}')$ have been chosen to stand for the total spin and orbital angular momenta of ll', instead of SL $(S'L')$, for later use. By using formula (15.4) of Ref. 24 for both the spin and orbital reduced matrix elements, and also taking into account the definitions (4) above, one obtains

$$||D_{ij}||=[K]([\bar{S},\bar{S}',\bar{L},\bar{L}'])^{1/2}(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & \kappa_2\\ \bar{S} & \bar{S}' & K\end{Bmatrix}\begin{Bmatrix} l & l & k_1\\ l' & l' & k_2\\ \bar{L} & \bar{L}' & K\end{Bmatrix}, \tag{14}$$

where $[K]$ stands for $2k+1$, etc., $[\bar{S},\bar{S}',\bar{L},\bar{L}']$ stands for $[\bar{S}][\bar{S}'][\bar{L}][\bar{L}']$ and

$$(\tfrac{1}{2}||\underline{s}^{(\kappa)}||\tfrac{1}{2})=\begin{cases}\sqrt{3/2} & \text{for } \kappa=1\ ,\\ \sqrt{2} & \text{for } \kappa=0\ .\end{cases} \tag{15}$$

In a similar manner, the expression for $||E_{ij}||$ is found to be

$$\begin{aligned}||E_{ij}||&=-(l_il'_j\bar{S}\bar{L}\,||[\underline{s}_i^{(\kappa_1)}\times\underline{s}_j^{(\kappa_2)}]^{(K)}[\underline{z}_i^{(k_1)}\times\underline{\tilde{z}}_j^{(k_2)}]^{(K)}||\,l_jl'_i\bar{S}'\bar{L}')\\ &=(l_il'_j\bar{S}\bar{L}\,||[\underline{s}_i^{(\kappa_1)}\times\underline{s}_j^{(\kappa_2)}]^{(K)}[z_i^{(k_1)}\times\underline{\tilde{z}}_j^{(k_2)}]^{(K)}||\,l'_il_j\bar{S}'\bar{L}')(-1)^{\bar{S}'+l+l'+\bar{L}'}\end{aligned}$$

according to formula (13.19) of Ref. 24. By using again formula (15.4) of Ref. 24, one obtains

$$||E_{ij}||=(-1)^{\bar{S}'+l+l'+\bar{L}'}[K]([\bar{S},\bar{S}',\bar{L},\bar{L}'])^{1/2}(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & \kappa_2\\ \bar{S} & \bar{S}' & K\end{Bmatrix}\begin{Bmatrix} l & l' & k_1\\ l' & l & k_2\\ \bar{L} & \bar{L}' & K\end{Bmatrix}. \tag{16}$$

C. The configuration $nl^N n'l'$

As mentioned in the introduction, the formulas for the matrix elements of the additional SDI, for $nl^N n'l'$ configurations, were obtained by using two different algebraic methods. The first method utilizes the expressions obtained above for $||D_{ij}||$ and $||E_{ij}||$ in the two-electron case [see formulas (14) and (16)]; it can thus be referred to as the two-electron method. The second method uses, successively, formulas which transform $||D||$ and $||E||$ from the scheme of the combined eigenfunctions of the $nl^N n'l'$ configuration to the one-electron schemes of the Nth and $(N+1)$th electrons. It can thus be referred to as the one-electron method.

1. Method 1

In this method, the derivation of explicit formulas for $||D||$ and $||E||$ is carried out by taking the following steps.

(i) Expansion of the nl^N part of the eigenfunctions appearing on both sides of the reduced matrix elements in terms of fractional parentage coefficients

$$(l^N(\alpha_1 S_1 L_1)| = \sum_{\alpha_2,S_2,L_2} (l^N \alpha_1 S_1 L_1\{|l^{N-1}(\alpha_2 S_2 L_2) l S_1 L_1) \times (l^{N-1}(\alpha_2 S_2 L_2) l (S_1 L_1)| \;.$$

By using the abbreviated notations

$$(l^N(\alpha_1 S_1 L_1)| \equiv (\psi_1| \;,$$

$$(l^{N-1}(\alpha_2 S_2 L_2)| \equiv (\psi_2| \;,$$

etc., and

$$(l^N \alpha_1 S_1 L_1\{|l^{N-1}(\alpha_2 S_2 L_2) l S_1 L_1) \equiv (\psi_1\{|\psi_2) \;,$$

this formula can be written as

$$(\psi_1| = \sum_{\psi_2} (\psi_1\{|\psi_2)(\psi_2, l(S_1 L_1)| \;.$$

(ii) Recoupling of each of these functions between the two schemes of angular momenta

$$l^{N-1}(\alpha_2 S_2 L_2), l(S_1 L_1), l'SL \quad \text{and} \quad l^{N-1}(\alpha_2 S_2 L_2), ll'(\bar{S}\bar{L}), SL \;,$$

which gives

$$(\psi_1 l', SL| = \sum_{\psi_2,\bar{S},\bar{L}} (\psi_1\{|\psi_2)(\psi_2, ll'(\bar{S}\bar{L}), SL|(S_2 L_2, ll'(\bar{S}\bar{L}), SL|S_2 L_2, l(S_1 L_1), l', SL)$$

$$= \sum_{\psi_2,\bar{S},\bar{L}} (\psi_1\{|\psi_2)(\psi_2, ll'(\bar{S}\bar{L}), SL|([S_1,\bar{S},L_1,\bar{L}])^{1/2}(-1)^{S_2+1/2+1/2+S+L_2+l+l'+L} \begin{Bmatrix} S_2 & \frac{1}{2} & S_1 \\ \frac{1}{2} & S & \bar{S} \end{Bmatrix} \begin{Bmatrix} L_2 & l & L_1 \\ l' & L & \bar{L} \end{Bmatrix} .$$

(iii) Transformation of the reduced matrix elements $||D||$ and $||E||$ from the scheme $l^{N-1}(\alpha_2 S_2 L_2), ll'(\bar{S}\bar{L}), SL$ to the scheme $ll'(\bar{S}\bar{L})$, through the use of formula (15.7′) of Ref. 24 for both spin and orbital parts.

(iv) Substitution for $||D_{N,N+1}||$ and $||E_{N,N+1}||$ of the corresponding expressions obtained in formulas (14) and (16) above.

By performing these steps, the following expressions are obtained for $||D||$ and $||E||$:

$$||D|| = N \sum_{\psi_2} (\psi_1\{|\psi_2)(\psi_2|\}\psi_1')(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S_1,S_1',S,S',L_1,L_1',L,L'])^{1/2}$$

$$\times \sum_{\bar{S},\bar{S}'} (-1)^{\bar{S}'+2S+S'-S_2}[\bar{S},\bar{S}'] \begin{Bmatrix} S_2 & \frac{1}{2} & S_1 \\ \frac{1}{2} & S & \bar{S} \end{Bmatrix} \begin{Bmatrix} S_2 & \frac{1}{2} & S_1' \\ \frac{1}{2} & S' & \bar{S}' \end{Bmatrix} \begin{Bmatrix} K & S' & S \\ S_2 & \bar{S} & \bar{S}' \end{Bmatrix} \begin{Bmatrix} \kappa_1 & \frac{1}{2} & \frac{1}{2} \\ \kappa_2 & \frac{1}{2} & \frac{1}{2} \\ K & \bar{S} & \bar{S}' \end{Bmatrix}$$

$$\times \sum_{\bar{L},\bar{L}'} (-1)^{\bar{L}'+L'-L_2}[\bar{L},\bar{L}'] \begin{Bmatrix} L_2 & l & L_1 \\ l & L & \bar{L} \end{Bmatrix} \begin{Bmatrix} L_2 & l & L_1' \\ l' & L' & \bar{L}' \end{Bmatrix} \begin{Bmatrix} K & L' & L \\ L_2 & \bar{L} & \bar{L}' \end{Bmatrix} \begin{Bmatrix} k_1 & l & l \\ k_2 & l' & l' \\ K & \bar{L} & \bar{L}' \end{Bmatrix}, \tag{17}$$

$$||E|| = N \sum_{\psi_2} (\psi_1\{|\psi_2)(\psi_2|\}\psi_1')(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S_1,S_1',S,S',L_1,L_1',L,L'])^{1/2}$$

$$\times \sum_{\bar{S},\bar{S}'} (-1)^{2\bar{S}'+2S+S'-S_2}[\bar{S},\bar{S}'] \begin{Bmatrix} S_2 & \frac{1}{2} & S_1 \\ \frac{1}{2} & S & \bar{S} \end{Bmatrix} \begin{Bmatrix} S_2 & \frac{1}{2} & S_1' \\ \frac{1}{2} & S' & \bar{S}' \end{Bmatrix} \begin{Bmatrix} K & S' & S \\ S_2 & \bar{S} & \bar{S}' \end{Bmatrix} \begin{Bmatrix} \kappa_1 & \frac{1}{2} & \frac{1}{2} \\ \kappa_2 & \frac{1}{2} & \frac{1}{2} \\ K & \bar{S} & \bar{S}' \end{Bmatrix}$$

$$\times \sum_{\bar{L},\bar{L}'} (-1)^{2\bar{L}'+L'-L_2+l+l'} [\bar{L},\bar{L}'] \begin{Bmatrix} L_2 & l & L_1 \\ l' & L & \bar{L} \end{Bmatrix} \begin{Bmatrix} L_2 & l & L_1' \\ l' & L' & \bar{L}' \end{Bmatrix} \begin{Bmatrix} K & L' & L \\ L_2 & \bar{L} & \bar{L}' \end{Bmatrix} \begin{Bmatrix} k_1 & l & l' \\ k_2 & l' & l \\ K & \bar{L} & \bar{L}' \end{Bmatrix} . \tag{18}$$

2. *Method 2*

The direct part $||D||$. For calculating $||D||$ in method 2 the following steps are taken.

(i) Use of formula (15.4) of Ref. 24 and of the definitions (4) above, which results in

$$||D|| = N(l^N\alpha_1 S_1 L_1 || \underline{s}_N^{(\kappa_1)} \underline{u}_N^{(k_1)} || l^N \alpha_1' S_1' L_1') \times (\tfrac{1}{2} || \underline{s}^{(\kappa_2)} || \tfrac{1}{2})[K]([S,S',L,L'])^{1/2} \begin{Bmatrix} S_1 & S_1' & \kappa_1 \\ \frac{1}{2} & \frac{1}{2} & \kappa_2 \\ S & S' & K \end{Bmatrix} \begin{Bmatrix} L_1 & L_1' & k_1 \\ l' & l' & k_2 \\ L & L' & K \end{Bmatrix} ,$$

where $\underline{s}^{(\kappa_1)}u^{(k_1)}$ is the double-tensor operator $\underline{v}^{(\kappa_1 k_1)}$ defined by Racah.[12]

(ii) Use of formula (8.23) of Ref. 22 for the reduced matrix element of $\underline{v}^{(\kappa_1 k_1)}$ leads to the following formula for $||D||$:

$$||D|| = N(\tfrac{1}{2} || \underline{s}^{(\kappa_1)} || \tfrac{1}{2})(\tfrac{1}{2} || \underline{s}^{(\kappa_2)} || \tfrac{1}{2})[K]([S_1,S_1',S,S',L_1,L_1',L,L'])^{1/2}$$
$$\times \sum_{\psi_2} (-1)^{S_1+S_2+1/2+\kappa_1+L_1+L_2+l+k_1} (\psi_1\{|\psi_2)(\psi_2|\}\psi_1')$$
$$\times \begin{Bmatrix} S_1 & \kappa_1 & S_1' \\ \frac{1}{2} & S_2 & \frac{1}{2} \end{Bmatrix} \begin{Bmatrix} S_1 & S_1' & \kappa_1 \\ \frac{1}{2} & \frac{1}{2} & \kappa_2 \\ S & S' & K \end{Bmatrix} \begin{Bmatrix} L_1 & k_1 & L_1' \\ l & L_2 & l \end{Bmatrix} \begin{Bmatrix} L_1 & L_1' & k_1 \\ l' & l' & k_2 \\ L & L' & K \end{Bmatrix} . \tag{19}$$

The exchange part $||E||$. The calculation of $||E||$ through the use of method 2 is accomplished by carrying out the following steps.

(i) Expansion of the eigenfunctions of l^N, on both sides of $||E||$, in terms of fractional parentage coefficients.

(ii) Transformation of the eigenfunction on the right-hand side of $||E||$ from the scheme

$$l^{N-1}(\alpha_2 S_2 L_2) l_{N+1}(S_1' L_1') l_N'(S'L')$$

to the scheme

$$l^{N-1}(\alpha_2 S_2 L_2) l_N'(S_3 L_3) l_{N+1}(S'L') .$$

The recoupling coefficient representing this transformation is given by

$$(j_1 j_2(j_{12}) j_3 J \,|\, j_1 j_3(j_{13}) j_2 J) = (-1)^{j_2+j_3+j_{12}+j_{13}} ([j_{12}][j_{13}])^{1/2} \begin{Bmatrix} j_3 & j_1 & j_{13} \\ j_2 & J & j_{12} \end{Bmatrix} , \tag{20}$$

with

$$S_2,L_2 \leftrightarrow j_1, \quad \tfrac{1}{2},l \leftrightarrow j_2, \quad \tfrac{1}{2},l' \leftrightarrow j_3 ,$$

$$S',L' \leftrightarrow J, \quad S_1',L_1' \leftrightarrow j_{12}, \quad S_3,L_3 \leftrightarrow j_{13} .$$

One obtains

$$||E|| = N \sum_{\psi_2,S_3,L_3} (l^{N-1}(\alpha_2 S_2 L_2) l_N(S_1 L_1) l_{N+1}' SL || [\underline{s}_N^{(\kappa_1)} \times \underline{s}_{N+1}^{(\kappa_2)}]^{(K)} [\underline{z}_N^{(k_1)} \times \tilde{\underline{z}}_{N+1}^{(k_2)}]^{(K)} || l^{N-1}(\alpha_2 S_2 L_2) l_N'(S_3 L_3) l_{N+1} S'L')$$
$$\times (\psi_1\{|\psi_2)(\psi_2|\}\psi_1')(-1)^{l+l'+S_1'+L_1'+S_3+L_3} ([S_1',L_1',S_3,L_3])^{1/2} \begin{Bmatrix} \frac{1}{2} & S_2 & S_3 \\ \frac{1}{2} & S' & S_1' \end{Bmatrix} \begin{Bmatrix} l' & L_2 & L_3 \\ l & L' & L_1' \end{Bmatrix} .$$

(iii) Use of formula (15.4) of Ref. 24 and formulas (4) above results in

$$||E||=N\sum_{\psi_2,S_3,L_3}(l^{N-1}(\alpha_2S_2L_2)lS_1L_1||\underline{s}_N^{(\kappa_1)}\underline{z}_N^{(k_1)}||l^{N-1}(\alpha_2S_2L_2)l'S_3L_3)$$
$$\times(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S,S',L,L',S_1',L_1',S_3,L_3])^{1/2}(\psi_1\{|\psi_2)(\psi_2|\}\psi_1')(-1)^{l+l'+S_1'+L_1'+S_3+L_3}$$
$$\times\begin{Bmatrix}\frac{1}{2} & S_2 & S_3\\ \frac{1}{2} & S' & S_1'\end{Bmatrix}\begin{Bmatrix}S_1 & S_3 & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & \kappa_2\\ S & S' & K\end{Bmatrix}\begin{Bmatrix}l' & L_2 & L_3\\ l & L' & L_1'\end{Bmatrix}\begin{Bmatrix}L_1 & L_3 & k_1\\ l' & l & k_2\\ L & L' & K\end{Bmatrix}.$$

(iv) Use of formula (15.7′) of Ref. 24 and performance of odd permutations of the columns of both $9j$-symbols result in

$$||E||=N\sum_{\psi_2,S_3,L_3}(\psi_1\{|\psi_2)(\psi_2|\}\psi_1')(-1)^{3/2+2S_3+2S_1+S_1'+S_2+S+S'+\kappa_2+l'+2L_3+2L_1+L_1'+L_2+L+L'+k_2}$$
$$\times[S_3,L_3,K]([S,S',L,L',S_1,S_1',L_1L_1'])^{1/2}(\tfrac{1}{2}||\underline{s}^{(K_1)}||\tfrac{1}{2})(\tfrac{1}{2}||s^{(K_2)}||\tfrac{1}{2})$$
$$\times\begin{Bmatrix}\frac{1}{2} & S' & S_1'\\ \frac{1}{2} & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}\frac{1}{2} & \kappa_1 & \frac{1}{2}\\ S_1 & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}K & S & S'\\ \kappa_2 & \frac{1}{2} & \frac{1}{2}\\ \kappa_1 & S_1 & S_3\end{Bmatrix}\begin{Bmatrix}l' & L' & L_1'\\ l & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}l' & k_1 & l\\ L_1 & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}K & L & L'\\ k_2 & l' & l\\ k_1 & L_1 & L_3\end{Bmatrix}.$$

(v) By using now the definition of the $12j$ symbol of the first kind, given by Jahn and Hope,[16] as well as its symmetry relations found by Ord-Smith,[17] the summations over S_3 and L_3 can be carried out as follows:

$$\sum_{S_3}(-1)^{2S_3}[S_3]\begin{Bmatrix}\frac{1}{2} & S' & S_1'\\ \frac{1}{2} & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}\frac{1}{2} & \kappa_1 & \frac{1}{2}\\ S_1 & S_2 & S_3\end{Bmatrix}\begin{Bmatrix}K & S & S'\\ \kappa_2 & \frac{1}{2} & \frac{1}{2}\\ \kappa_1 & S_1 & S_3\end{Bmatrix}=(-1)^{1/2+S'+S_1+\kappa_1}\left\{\begin{array}{cccccccc}\frac{1}{2} & & \kappa_2 & & \kappa_1 & & \frac{1}{2} & \\ & \frac{1}{2} & & K & & \frac{1}{2} & & S_2\\ S_1 & & S & & S' & & S_1' & \end{array}\right\},\tag{21a}$$

$$\sum_{L_3}(-1)^{2L_3}[L_3]\begin{Bmatrix}l' & L' & L_1'\\ l & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}l' & k_1 & l\\ L_1 & L_2 & L_3\end{Bmatrix}\begin{Bmatrix}K & L & L'\\ k_2 & l' & l\\ k_1 & L_1 & L_3\end{Bmatrix}=(-1)^{l+L'+L_1+k_1}\left\{\begin{array}{cccccccc}l & & k_2 & & k_1 & & l & \\ & l' & & K & & l' & & L_2\\ L_1 & & L & & L' & & L_1' & \end{array}\right\}.\tag{21b}$$

The expression for $||E||$ then takes the following form:

$$||E||=N\sum_{\psi_2}(\psi_1\{|\psi_2)(\psi_2|\}\psi_1')(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S_1,S_1',S,S',L_1,L_1',L,L'])^{1/2}$$
$$\times(-1)^{l+l'+L_1+L_1'+k_1+k_2+L_2+L+1+S_1+S_1'+\kappa_1+\kappa_2+S_2+S}$$
$$\times\left\{\begin{array}{cccccccc}\frac{1}{2} & & \kappa_2 & & \kappa_1 & & \frac{1}{2} & \\ & \frac{1}{2} & & K & & \frac{1}{2} & & S_2\\ S_1 & & S & & S' & & S_1' & \end{array}\right\}\left\{\begin{array}{cccccccc}l & & k_2 & & k_1 & & l & \\ & l' & & K & & l' & & L_2\\ L_1 & & L & & L' & & L_1' & \end{array}\right\}.\tag{22}$$

III. IDENTITIES

A. The identity of Arima, Horie, and Tanabe: a representative of the symmetry properties of the direct part of the additional SDI in l^Nl' configurations

The two expressions obtained for $||D||$ through the use of methods 1 and 2 [see formulas (17) and (19), respectively] should be equal to each other. Indeed, each of the double summations, over $\bar{S},\bar{S}'$ and $\bar{L},\bar{L}'$, appearing in formula (17) can be carried out through the use of the identity of AHT (Refs. 15, 18, and 10) given in formula (23) below, this resulting in a simple product of one $6j$ symbol and one $9j$ symbol, as given in formula (19). Since both the spin and orbital parts of $||D||$ can be expressed by either the left-hand side or the right-hand side of the identity of Arima, Horie, and Tanabe, it is hereby concluded that this identity represents the symmetry properties of the direct part of the additional SDI, in $l^N l'$ configurations.

The AHT identity[15] is given by the following formula:

$$\sum_{x,y}[x][y](-1)^{y-j_2+j_1'+j_2'-j-k-k_1+l_2}\begin{Bmatrix}k' & j_2 & l_2\\ j_2' & k_2 & x\end{Bmatrix}\begin{Bmatrix}k' & j_1 & l_1\\ j_1' & k_1 & y\end{Bmatrix}\begin{Bmatrix}k & k_1 & k_2\\ k' & x & y\end{Bmatrix}\begin{Bmatrix}j & j_2 & j_1\\ j' & j_2' & j_1'\\ k & x & y\end{Bmatrix}$$
$$=\begin{Bmatrix}l_2 & l_1 & j\\ j_1 & j_2 & k'\end{Bmatrix}\begin{Bmatrix}l_2 & l_1 & j\\ j_2' & j_1' & j'\\ k_2 & k_1 & k\end{Bmatrix}. \qquad (23)$$

Twelve angular momenta participate in this identity. These are arranged in the following ten triads, four in the $6j$ symbol and six in the $9j$ symbol appearing on the right-hand side of (23); however, since two of these ten triads are identical, only nine different triads are involved: (l_2l_1j), (l_2j_2k'), (j_1l_1k'), (j_1j_2j), $(j_1'j_2'j')$, (k_1k_2k), $(k_2l_2j_2')$, $(k_1l_1j_1')$, $(jj'k)$. An algebraic proof of this identity was, of course, given by its first discovers; a different algebraic proof was given by Judd;[10] a graphical proof of this identity was given by Jucys *et al.*[18]

B. The new identity: represents the symmetry properties of the exchange part of the additional SDI, in $l^N l'$ configurations

The two expressions obtained for $||E||$ through the use of methods 1 and 2 are given in formulas (18) and (22). The requirement that these two expressions be equal leads to the following new identity:

$$\sum_{x,y}[x][y](-1)^{2y+j_1-j_2+l_1-l_2+j-j'+k_1+k_2}\begin{Bmatrix}k' & j_2 & l_2\\ j_2' & k_2 & x\end{Bmatrix}\begin{Bmatrix}k' & j_1 & l_1\\ j_1' & k_1 & y\end{Bmatrix}\begin{Bmatrix}k & k_1 & k_2\\ k' & x & y\end{Bmatrix}\begin{Bmatrix}j & j_2 & j_1'\\ j' & j_2' & j_1\\ k & x & y\end{Bmatrix}$$
$$=\begin{Bmatrix}j_1 & & j' & & j & & j_2 & \\ & j_2' & & k & & j_1' & & k'\\ l_2 & & k_2 & & k_1 & & l_1 & \end{Bmatrix}. \qquad (24)$$

In this identity, one $12j$ symbol of the first kind[19–22] is expressed as a double sum of a product of three $6j$ symbols and one $9j$ symbol. All $3nj$ symbols written on the left-hand side of this identity coincide with those appearing in the identity of AHT, except for the exchange of j_1 and j_1' in the last column of the $9j$ symbol. The twelve angular momenta participating in the $12j$ symbol are arranged in the following eight triads: $(j_1j_2'j')$, $(j'kj)$, $(jj_1'j_2)$, (l_2j_2k'), $(l_2j_2'k_2)$, (k_1k_2k), $(k_1l_1j_1')$, (j_1l_1k').

This eight-triad structure leads to sixteen symmetry relations of the $12j$ symbol of the first kind, first given by Ord-Smith.[17]

Since both the spin and the orbital parts of $||E||$ can be expressed by either the left-hand side or the right-hand side of the new identity it is thus concluded that this identity represents the symmetry properties of the exchange part of the additional SDI, in $l^N l'$ configurations.

C. Algebraic proof of the new identity

The left-hand side of (24) can be written in the following form [transforming all phase factors except $(-1)^{2y}$ to its right-hand side]:

$$\sum_x[x]\begin{Bmatrix}k' & j_2 & l_2\\ j_2' & k_2 & x\end{Bmatrix}\sum_y[y](-1)^{2y}\begin{Bmatrix}k' & j_1 & l_1\\ j_1' & k_1 & y\end{Bmatrix}\begin{Bmatrix}k & k_1 & k_2\\ k' & x & y\end{Bmatrix}\begin{Bmatrix}j & j_2 & j_1'\\ j' & j_2' & j_1\\ k & x & y\end{Bmatrix}. \qquad (25)$$

In the last expression, the summation over y is carried out first, through the use of formula (21), written below in the following form:[16]

$$\sum_y [y](-1)^{2y} \begin{Bmatrix} k_1 & j_1' & l_1 \\ j_1 & k' & y \end{Bmatrix} \begin{Bmatrix} k_1 & k & k_2 \\ x & k' & y \end{Bmatrix} \begin{Bmatrix} j & j_2 & j_1' \\ j' & j_2' & j_1 \\ k & x & y \end{Bmatrix} = (-1)^{x+k+j_1+j_1'} \begin{Bmatrix} l_1 & & j_1' & & j_2 & & x & \\ & k_1 & & j & & j_2' & & k' \\ k_2 & & k & & j' & & j_1 & \end{Bmatrix}. \tag{21c}$$

Substitution of the right-hand side of (21c) in (25) results in the following expression:

$$\sum_x [x](-1)^{x+k+j_1+j_1'} \begin{Bmatrix} j_1 & & l_1 & & j_1' & & j_2 & \\ & k' & & k_1 & & j & & j_2' \\ x & & k_2 & & k & & j & \end{Bmatrix} \begin{Bmatrix} k' & k_2 & x \\ j_2' & j_2 & l_2 \end{Bmatrix}. \tag{25a}$$

Using formula (A.6.40) of Ref. 18, (25a) can be transformed into the following expression:

$$\begin{Bmatrix} j_1 & & l_1 & & k_1 & & k_2 & \\ & k' & & j_1' & & k & & j_2' \\ l_2 & & j_2 & & j & & j' & \end{Bmatrix} (-1)^{2k+2j_1'+j_1+j_2+l_1-l_2+k_1+k_2+j+j'}. \tag{25b}$$

By using the symmetry relations of the $12j$ symbol,[17] and the fact that $(-1)^{2k+2j_1'} = (-1)^{2k+2j+2j_2} = (-1)^{2j'+2j_2}$, (25b) can be written

$$\begin{Bmatrix} j_1 & & j' & & j & & j_2 & \\ & j_2' & & k & & j_1' & & k' \\ l_2 & & k_2 & & k_1 & & l_1 & \end{Bmatrix} (-1)^{j_1-j_2+l_1-l_2+j-j'+k_1+k_2}, \tag{25c}$$

which proves the new identity (24).

IV. GRAPHICAL METHODS

The present section comprises A, derivation of a graphical representation of the $12j$ symbol of the first kind, in accord with the phase conventions of Lindgren and Morrison[22] used herein; B, graphical proof of the new identity; and C, graphical derivation of the formulas for the reduced matrix elements $||D||$ and $||E||$, for $nl^N n'l'$ configurations.

A. Graphical representation of the 12j symbol of the first kind

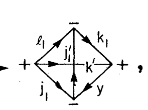
The graphical representation of the $12j$ symbol of the first kind is obtained by starting out from formula (21c), which constitutes its first definition,[16]

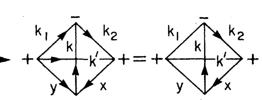
$$\sum_y [y](-1)^{2y} \begin{Bmatrix} l_1 & j_1 & k' \\ y & k_1 & j_1' \end{Bmatrix} \begin{Bmatrix} k_1 & y & k' \\ x & k_2 & k \end{Bmatrix} \begin{Bmatrix} j & j_2 & j_1' \\ j' & j_2' & j_1 \\ k & x & y \end{Bmatrix} = \begin{Bmatrix} l_1 & & j_1' & & j_2 & & x & \\ & k_1 & & j & & j_2' & & k' \\ k_2 & & k & & j' & & j_1 & \end{Bmatrix} (-1)^{x+k+j_1+j_1'} \tag{21d}$$

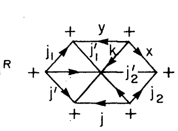
and then taking the following steps.

(i) Describing the $6j$ and $9j$ symbols appearing on the left-hand side of (21d) in graphical form (chapter 3 of Ref. 22); (ii) multiplying them according to the rules of Jucys *et al.*,[18] listed also in chapter 4 of Ref. 22; (iii) performing the summation over y (see again Ref. 18 and chapter 4 of Ref. 22). In these steps and also in further graphical derivations, useful graphical rules are used, which enable (1) the addition (or removal) of arrows to all three lines of a vertex, (2) the reversal of the direction of an arrow, and (3) a change of sign of a vertex (chapter 3 of Ref. 22). These rules will be referred to as "fundamental graphical rules."

(i) The graphical representations of the $6j$ and the $9j$ symbols are

$\begin{Bmatrix} l_1 & j_1 & k' \\ y & k_1 & j_1' \end{Bmatrix} \longleftrightarrow$  , (26a)

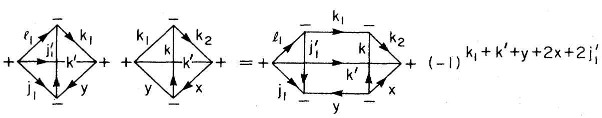
$\begin{Bmatrix} k_1 & y & k' \\ x & k_2 & k \end{Bmatrix} \longleftrightarrow$  , (26b)

$\begin{Bmatrix} j & j_2 & j_1' \\ j' & j_2' & j_1 \\ k & x & y \end{Bmatrix} \longleftrightarrow (-1)^R$  , (27) where $R = j + j_2 + j_1' + j' + j_2' + j_1 + k + x + y$.

(ii) The product

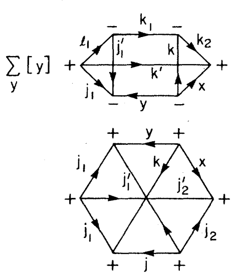
$$\begin{Bmatrix} l_1 & j_1 & k' \\ y & k_1 & j_1' \end{Bmatrix} \begin{Bmatrix} k_1 & y & k' \\ x & k_2 & k \end{Bmatrix}$$

is graphically represented by



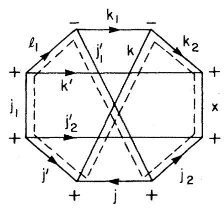
$$(-1)^{k_1+k'+y+2x+2j_1'} . \qquad (28)$$

The last diagram was obtained through the use of formula (4.7) of Ref. 22, which is referred to as the Jucys, Levinson, and Vanagas third theorem (JLV3), in addition to the use of the fundamental graphical rules. The graphical representation of the left-hand side of (21d) thus takes the following form:



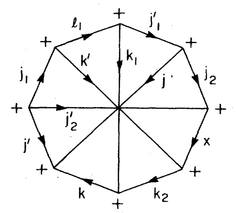
$$\times (-1)^{k_1+k'+k+j+j'+j_1+j_2-j_1'+j_2'-x} . \qquad (29)$$

This graphical expression can now be transformed according to formula (4.9) of Ref. 22 (which is referred to as JLV4) to give (solid line)



$$(-1)^{k_1+k'+k+j+j'+j_1+j_2-j_1'+j_2'-x} . \qquad (30)$$

By drawing the Hamilton line [dotted line in diagram (30)], pulling the graph apart so that this Hamilton line lies along the edges of the octagon, and using the fundamental graphical rules, one obtains



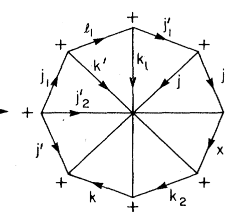
$$(-1)^{x+k+j_1+j_1'} . \qquad (31)$$

Since (31) equals the right-hand side of (21d), which can be written as

$$\begin{Bmatrix} j_1 & & l_1 & & j_1' & & j_2 & \\ & k' & & k_1 & & j & & j_2' \\ x & & k_2 & & k & & j' & \end{Bmatrix} (-1)^{x+k+j_1+j_1'} ,$$

it is hereby concluded that the graphical representation of the 12j symbol of the first kind is given by the following diagram:

$$\begin{Bmatrix} j_1 & l_1 & j_1' & j_2 \\ k' & k_1 & j & j_2' \\ x & k_2 & k & j' \end{Bmatrix} \longleftrightarrow$$



$$. \qquad (32)$$

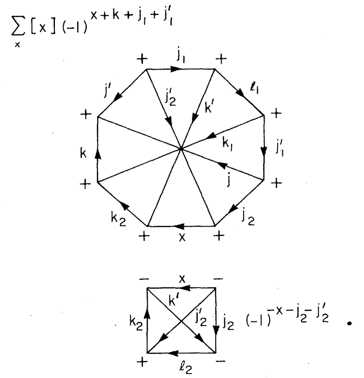
B. Graphical proof of the new identity

The new identity is given by formula (24),

$$\sum_x [x] \begin{Bmatrix} k' & j_2 & l_2 \\ j_2' & k_2 & x \end{Bmatrix} \sum_y [y](-1)^{2y} \begin{Bmatrix} k' & j_1 & l_1 \\ j_1' & k_1 & y \end{Bmatrix} \begin{Bmatrix} k & k_1 & k_2 \\ k' & x & y \end{Bmatrix} \begin{Bmatrix} j & j_2 & j_1' \\ j' & j_2' & j_1 \\ k & x & y \end{Bmatrix}$$

$$= \begin{Bmatrix} j_1 & & j' & & j & & j_2 & \\ & j_2' & & k & & j_1' & & k' \\ l_2 & & k_2 & & k_1 & & l_1 & \end{Bmatrix} (-1)^{j_1-j_2+l_1-l_2+j-j'+k_1+k_2} . \qquad (24')$$

The graphical proof of this identity could be carried out in a straightforward manner, similar to the one taken in Sec. IV A above; that is, by "calculating" graphically the product of the four $3nj$ symbols written in the left-hand side of (24′), and then performing the double sum over x,y—according to the rules of JLV.[18,22] Instead, a short-cut in the proof is made, by exploiting the results already obtained in Sec. IV A. According to these results, all the y-dependent factors on the left-hand side of formula (24′) can be substituted by one 12j symbol of the first kind and a phase factor [see formula (31)]. The left-hand side of (24′) is thus written graphically in the following form:

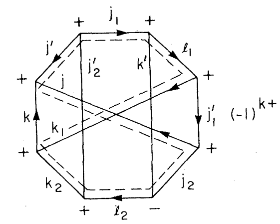


(33)

The last row of (33) constitutes a graphical representation of

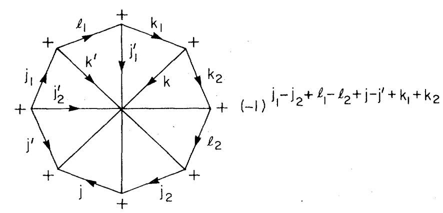
$$\begin{Bmatrix} k' & j_2 & l_2 \\ j_2' & k_2 & x \end{Bmatrix} .$$

The summation over x in (33) can be carried out according to formula (4.9) of Ref. 22 (JLV4). The following result is obtained (solid line):



(34)

By drawing the Hamilton (dotted) line, pulling the diagram apart so that this line lies along the edges of the polygon, and making use of the fundamental graphical rules, one obtains



(35)

which completes the graphical proof of the new identity.

C. Graphical derivation of the direct and exchange matrix element

1. Direct matrix element

The direct matrix element to be graphically calculated is given by formula (8),

$$\{\,|D\,|\,\}=N(l_{(N)}^N(\alpha_1S_1L_1)l'_{N+1}SLJM\,|\,[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}\cdot[\underline{u}_N^{(k_1)}\times\underline{v}_{N+1}^{(k_2)}]^{(K)}\,|\,l_{(N)}^N(\alpha_1'S_1'L_1')l'_{N+1}S'L'JM) . \quad (8')$$

The antisymmetric wave function on each side of (8′) is expressed in terms of vector-coupling and fractional-parentage coefficients. For instance, for the left-hand-side wave function one can write

$$(nl^N(\alpha_1S_1L_1)n'l'SLJM\,|$$

$$=\sum_{M_S,M_L}(JM\,|\,SM_S,LM_L)(nl^N(\alpha_1S_1L_1)n'l'SM_SLM_L\,|$$

$$=\sum_{\substack{M_S,M_L,\\ M_{S_1},m_{s'},\\ M_{L_1},m_{l'}}}(JM\,|\,SM_S,LM_L)(SM_S\,|\,S_1M_{S_1},\tfrac{1}{2}m_{s'})(LM_L\,|\,L_1M_{L_1},l'm_{l'})(nl^N\alpha_1S_1M_{S_1}L_1M_{L_1}\,|\,(n'l'm_{s'}m_{l'}\,|$$

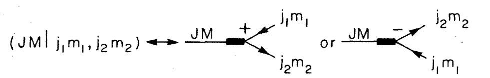
$$=\sum_{\substack{\alpha_2,S_2L_2,\\ M_S,M_L,\\ M_{S_1},m_{s'},\\ M_{L_1},m_{l'}}}(JM\,|\,SM_S,LM_L)(SM_S\,|\,S_1M_{S_1},\tfrac{1}{2}m_{s'})(LM_L\,|\,L_1M_{L_1},l'm_{l'})$$

$$\times(l^N(\alpha_1S_1L_1)\{\,|\,l^{N-1}(\alpha_2S_2L_2)l,S_1L_1)(nl^{N-1}(\alpha_2S_2L_2)nl,S_1M_{S_1}L_1M_{L_1}\,|\,(n'l'm_{s'}m_{l'}\,|$$

$$=\sum_{\substack{\alpha_2,S_2,L_2,\\ M_S,M_L,\\ M_{S_1},m_{s'},\\ M_{L_1},m_{l'},\\ M_{S_2},m_s,\\ M_{L_2},m_l,}}(JM\,|\,SM_S,LM_L)(SM_S\,|\,S_1M_{S_1},\tfrac{1}{2}m_s)(LM_L\,|\,L_1M_{L_1},l'm_{l'})(S_1M_{S_1}\,|\,S_2M_{S_2},\tfrac{1}{2}m_s)(L_1M_{L_1}\,|\,L_2M_{L_2},lm_l)$$

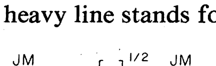
$$\times(l^N(\alpha_1S_1L_1)\{\,|\,l^{N-1}(\alpha_2S_2L_2)l,S_1L_1)(nl^{N-1}\alpha_2S_2M_{S_2}L_2M_{L_2}\,|\,(nlm_sm_l\,|\,(n'l'm_{s'}m_{l'}\,|\ . \tag{36}$$

A vector-coupling coefficient is graphically represented by



(37)

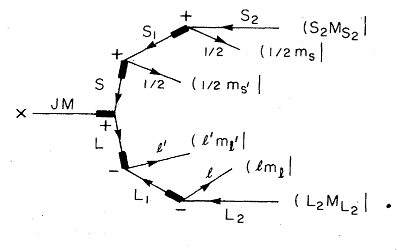
(in each of these diagrams the direction of the arrows are determined so that the "initial" state j_1m_1 scatters off the heavy line into the "final" state j_2m_2. The sign at the vertex of the vector-coupling coefficient is chosen so that the angular momenta are always read in the order Jj_2j_1; the heavy line stands for



(38)

[see formulas (3.11)—(3.16) of Ref. 22]). Now, if one substitutes for each of the five vector-coupling coefficients in (36) its corresponding graphical diagram (37) and then joins the free lines having the same quantum numbers (which means performing summations over the corresponding m's), the left-hand-side wave function takes the following form:

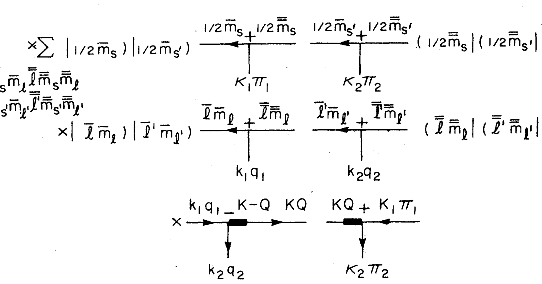
$$(nl^N(\alpha_1S_1L_1)n'l'SLJM\,| = \sum_{\substack{\alpha_2,S_2,L_2,\\ m_{s'},m_s,M_{S_2},\\ m_{l'},m_l,M_{L_2}}} (l^N(\alpha_1S_1L_1)\{\,|\,l^{N-1}(\alpha_2S_2L_2)l,S_1L_1)$$



(39)

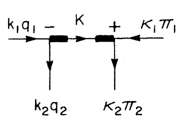
The wave function on the right-hand side of (8′) can be drawn in a similar manner. By expressing the scalar product of two operators in terms of their components, the operator appearing in (8′) is written in the form

$$[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}\cdot[\underline{u}_N^{(k_1)}\times\underline{v}_{N+1}^{(k_2)}]^{(K)}$$
$$=(-1)^K\sum_Q(-1)^{K-Q}[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]_Q^{(K)}[\underline{u}_N^{(k_1)}\times\underline{v}_{N+1}^{(k_2)}]_{-Q}^{(K)}$$
$$=(-1)^K\sum_{\substack{Q,\\ \pi_1,\pi_2,q_1,q_2,}}(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})$$



(40)

by using formulas (4.12) and (4.16)—(4.18) of Ref. 22, for both the spin and orbital operators; it should be noted that the diagram before last in (40) includes the phase factor $(-1)^{K-Q}$ [formula (3.3a) of Ref. 22]. The sum over Q can now be performed, by joining the corresponding free lines, in the last two vector-coupling coefficients; one obtains

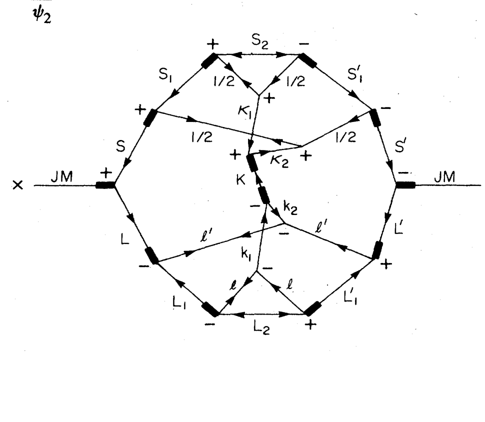


(41)

[formula (3.21b) of Ref. 22].

The matrix element (8′) can now be formed by joining the corresponding lines of the left- and right-hand wave functions and of the operator standing between them (using the orthogonality properties of the wave functions); the following graphical expression is obtained:

$$N(-1)^K\sum_{\psi_2}(\psi_1\{\,|\,\psi_2)(\psi_2\,|\,\}\psi_1')(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})$$

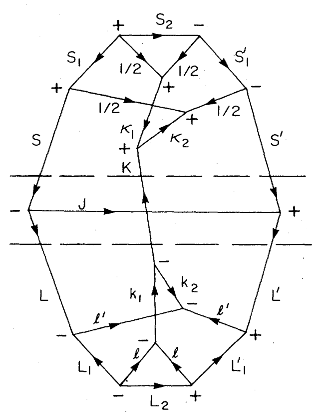


(42)

Since this matrix element is independent of M, the two free lines may be joined together—meaning summation over M, that is, multiplication by $(2J+1)$. This action can be compensated for by removing the two factors $(2J+1)^{1/2}$ (heavy parts of these lines). By substituting also for the remaining heavy lines with the corresponding factors, and using the fundamental graphical rules, the following expression is obtained:

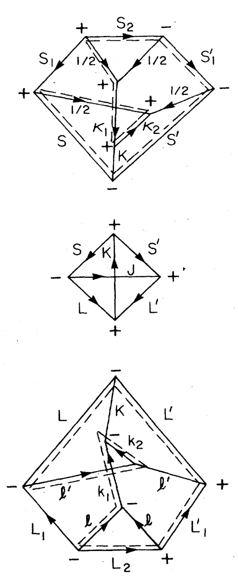
$$N(-1)^K \sum_{\psi_2} (\psi_1\{\,|\,\psi_2)(\psi_2\,|\,\}\psi_1')(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})$$

$$\times[K]([S,S',S_1,S_1',L,L',L_1,L_1'])^{1/2}$$



(43)

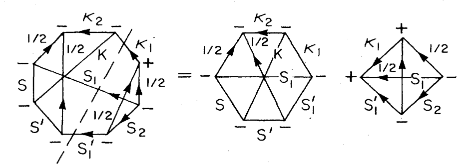
The last diagram may be cut twice on three lines, as shown by the dotted lines, to give the following three diagrams:



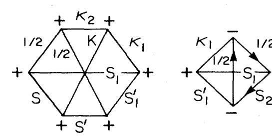
(44)

The second of these diagrams includes all the J dependence of the matrix elements, whereas the first and the third ones depend only on the spin and orbital quantum numbers, respectively. By drawing Hamilton (dotted) lines in the first and third diagrams, pulling them apart so that these lines lie along the edges of the corresponding polygons, and subsequently cutting each of these diagrams in three lines, the following result is obtained.

The spin part is



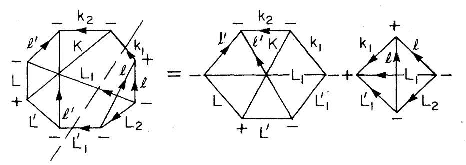
and on changing both $3nj$ symbols to their standard forms we have



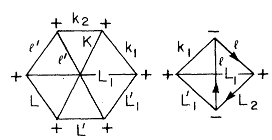
$(-1)^{\kappa_1+1/2+1/2+1/2+S_1+S_2+1}$ (45a)

$$=\begin{Bmatrix} S_1 & S_1' & \kappa_1 \\ \frac{1}{2} & \frac{1}{2} & \kappa_2 \\ S & S' & K \end{Bmatrix}\begin{Bmatrix} S_1 & \kappa_1 & S_1' \\ \frac{1}{2} & S_2 & \frac{1}{2} \end{Bmatrix}(-1)^{S_1+S_2+1/2+\kappa_1}\,. \tag{45b}$$

The orbital part is



and on transforming both $3nj$ symbols to their standard forms we have

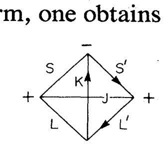


$(-1)^{L_1+L_2+l+k_1+L+L'+K}$ (46a)

$$=\begin{Bmatrix} L_1 & L_1' & k_1 \\ l' & l' & k_2 \\ L & L' & K \end{Bmatrix}\begin{Bmatrix} L_1 & k_1 & L_1' \\ l & L_2 & l \end{Bmatrix}$$

$$\times(-1)^{L_1+L_2+l+k_1+L+L'+K}\,. \tag{46b}$$

On transforming the J-dependent diagram to its standard form, one obtains



$$(-1)^{S'+L'+J} = \begin{Bmatrix} S & L & J \\ L' & S' & K \end{Bmatrix}(-1)^{S'+L'+J}\,. \tag{47}$$

By collecting the contribution of all diagrams the following result is obtained for $\{\,|\,D\,|\,\}$:

$$\{\,|\,D\,|\,\}=(-1)^{L+S'+J}\begin{Bmatrix} S & S' & K \\ L' & L & J \end{Bmatrix}||D||\;,$$

where $||D||$ is identical to the expression given in formula (19).

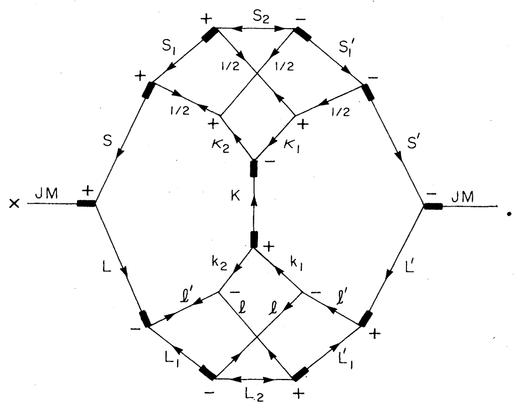
2. *Exchange matrix element*

The exchange matrix element to be graphically calculated is given by formula (9),

$$E=-N(l_{(N)}^N(\alpha_1S_1L_1)l'_{N+1}SLJM\,|\,[\underline{s}_N^{(\kappa_1)}\times\underline{s}_{N+1}^{(\kappa_2)}]^{(K)}\cdot[\underline{z}_N^{(k_1)}\times\tilde{\underline{z}}_{N+1}^{(k_2)}]^{(K)}\,|\,l_{(N+1)}^N(\alpha'_1S'_1L'_1)l'_NS'L'JM)\,. \tag{9'}$$

By proceeding in the same manner as for $\{\,|D|\,\}$, but taking into account that, on the right-hand side of the matrix element, the Nth and $(N+1)$th electrons are characterized by l' and l, respectively, one obtains for $\{\,|E|\,\}$ the following graphical expression:

$$\{\,|E|\,\}=N(-1)^{K+1}\sum_{\psi_2}(\psi_1\{\,|\psi_2)(\psi_2|\,\}\psi'_1)(\tfrac12||\underline{s}^{(\kappa_1)}||\tfrac12)(\tfrac12||\underline{s}^{(\kappa_2)}||\tfrac12)$$



(48)

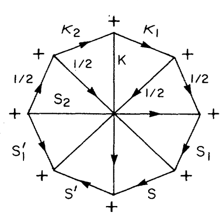
By joining together the two free lines, substituting the heavy lines by the corresponding factors and cutting the resulting diagram into three separate diagrams, the following result is obtained:

$$\{\,|E|\,\}=N(-1)^{K+1}\sum_{\psi_2}(\psi_1\{\,|\psi_2)(\psi_2|\psi'_1)(\tfrac12||\underline{s}^{(\kappa_1)}||\tfrac12)(\tfrac12||\underline{s}^{(\kappa_2)}||\tfrac12)$$

$$\times[K]([S,S',S_1,S'_1,L,L',L_1,L'_1])^{1/2}\times(\text{spin part})\times(\text{orbital part})\times(J\text{-dependent part})\,. \tag{49}$$

The last three factors are given by the following graphical expressions.

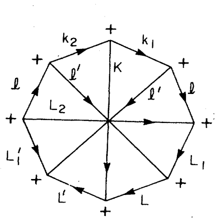
The spin part is equal to



$$(-1)^{K+1+1+S_1+S'_1+\kappa_1+\kappa_2+S_2+S} \tag{50a}$$

$$=\begin{Bmatrix} 1/2 & \kappa_2 & \kappa_1 & 1/2 & \\ & 1/2 & K & 1/2 & S_2 \\ S_1 & S & S' & S'_1 & \end{Bmatrix}(-1)^{K+1+1+S_1+S'_1+\kappa_1+\kappa_2+S_2+S}\,. \tag{50b}$$

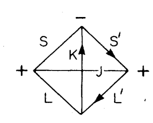
The orbital part is



$$(-1)^{\ell+\ell'+L_1+L'_1+k_1+k_2+L_2+L'+2L} \tag{51a}$$

$$=\begin{Bmatrix} \ell & k_2 & k_1 & \ell & \\ & \ell' & K & \ell' & L_2 \\ L_1 & L & L' & L'_1 & \end{Bmatrix}(-1)^{\ell+\ell'+L_1+L'_1+k_1+k_2+L_2+L'+2L}\,. \tag{51b}$$

The J-dependent part is



$$(-1)^{S'+L'+J}=\begin{Bmatrix} S & L & J \\ L' & S' & K \end{Bmatrix}(-1)^{S'+L'+J}\,. \tag{52}$$

On collecting all terms of $\{\,|E|\,\}$ included in (49), one obtains

$$\{\,|E|\,\}=(-1)^{L+S'+J}\begin{Bmatrix} S & S' & K \\ L' & L & J \end{Bmatrix}||E||\,,$$

where $||E||$ is identical to the expression given in formula (22).

V. THE CONFIGURATION $nl^{4l+1}n'l'$ $(N=4l+1)$

In order to obtain the formulas for $||D||$ and $||E||$ for configurations $nl^{4l+1}n'l'$, comprising a hole (h) and an electron (e), one should start from formulas (19) and (22), respectively, and therein make the following substitutions:

$$N=4l+1, S_1=S'_1=\tfrac12, L_1=L'_1=l$$

$$(l^{4l+1}{}^2l\{\,|\,l^{4l}(S_2L_2)l\,{}^2l)(l^{4l}(S_2L_2)l\,{}^2l\,|\,\}l^{4l+1}{}^2l)=\frac{[S_2][L_2]}{(4l+1)(2l+1)} \qquad (53)$$

[the explicit expression for the coefficients of fractional parentage was obtained through the use of formula (19) of Ref. 23].

The following results are obtained:

$$||D_{he}||=(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S,S',L,L'])^{1/2}\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & \kappa_2\\ S & S' & K\end{Bmatrix}\begin{Bmatrix}l & l & k_1\\ l' & l' & k_2\\ L & L' & K\end{Bmatrix}(-1)^{1+\kappa_1+k_1}$$

$$\times 2\sum_{S_2,L_2}[S_2][L_2](-1)^{S_2+L_2}\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & S_2\end{Bmatrix}\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}, \qquad (54)$$

$$||E_{he}||=(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S,S',L,L'])^{1/2}(-1)^{l+l'+\kappa_1+\kappa_2+k_1+k_2+S+L}$$

$$\times 2\sum_{S_2,L_2}[S_2][L_2](-1)^{S_2+L_2}\begin{Bmatrix}\frac{1}{2} & & \kappa_2 & & \kappa_1 & & \frac{1}{2} & \\ & \frac{1}{2} & & K & & \frac{1}{2} & & S_2\\ \frac{1}{2} & & S & & S' & & \frac{1}{2} & \end{Bmatrix}\begin{Bmatrix}l & & k_2 & & k_1 & & l & \\ & l' & & K & & l' & & L_2\\ l & & L & & L' & & l & \end{Bmatrix}. \qquad (55)$$

In the last three formulas S_2 and L_2 stand, respectively, for the total spin and orbital angular momenta of the l^{4l} configuration; they are thus connected through the requirement that their sum, S_2+L_2, be even, in accordance with the Pauli Principle. Consequently, the summations over S_2,L_2 cannot be carried out independently. In order to perform these summations, the following identities are used [Eqs. (A.6.17), (A.6.18), (A.6.23), and (A.6.24) of Ref. 18]:

(i) $\displaystyle\sum_{L_2}[L_2]\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}=1$,

(ii) $\displaystyle\sum_{L_2}(-1)^{L_2}[L_2]\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}=\delta(k_1,0)[l]=0$

(the last equality on the right is valid for $k_1\neq 0$),

(iii) $$\sum_{L_2}[L_2]\begin{Bmatrix}l & & k_2 & & k_1 & & l & \\ & l' & & K & & l' & & L_2\\ l & & L & & L' & & l & \end{Bmatrix}=\frac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]},$$

(iv) $$\sum_{L_2}(-1)^{L_2}[L_2]\begin{Bmatrix}l & & k_2 & & k_1 & & l & \\ & l & & K & & l & & L_2\\ l & & L & & L' & & l & \end{Bmatrix}=\begin{Bmatrix}l' & K & l'\\ k_1 & l & k_2\end{Bmatrix}\begin{Bmatrix}l' & K & l'\\ L' & l & L\end{Bmatrix}.$$

A. Direct part

Use of the first two identities results in the following equalities, already obtained in a previous paper:[25]

$$\sum_{L_2\text{ even}}[L_2]\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}=\sum_{L_2\text{ odd}}[L_2]\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}=\frac{1}{2}\quad(k_1\neq 0)\,. \qquad (56)$$

Consequently,

$$2\sum_{S_2,L_2}[S_2][L_2]\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & S_2\end{Bmatrix}\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}$$

$$=2\sum_{\substack{L_2\text{ even}\\(S_2=0)}}[L_2]\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & 0\end{Bmatrix}\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}$$

$$+2\sum_{\substack{L_2\text{ odd}\\(S_2=1)}}3[L_2]\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & 1\end{Bmatrix}\begin{Bmatrix}l & l & k_1\\ l & l & L_2\end{Bmatrix}$$

$$=\frac{(-1)^{1+\kappa_1}}{2}+3\begin{Bmatrix}\frac{1}{2} & \frac{1}{2} & \kappa_1\\ \frac{1}{2} & \frac{1}{2} & 1\end{Bmatrix}=1\quad(k_1\neq 0) \qquad (57)$$

for both cases $\kappa_1=0,1$.

Substituting this last result in formula (54), one obtains the following final, explicit, form of $||D_{he}||$:

$$||D_{he}||=(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S,S',L,L'])^{1/2} \times \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \kappa_1 \\ \frac{1}{2} & \frac{1}{2} & \kappa_2 \\ S & S' & K \end{Bmatrix} \begin{Bmatrix} l & l & k_1 \\ l' & l' & k_2 \\ L & L' & K \end{Bmatrix} (-1)^{1+\kappa_1+k_1} . \qquad (58)$$

By comparing formula (58) with formula (14), one obtains the following relation between $||D_{he}||$, for $nl^{4l+1}n'l'$, and $||D_{ee}||$, for $nln'l'$:

$$||D_{he}||=-(-1)^{\kappa_1+k_1}||D_{ee}|| . \qquad (59)$$

Formula (59) is in agreement with Racah's formula (74) of Ref. 12; it leads to the following conclusions concerning the behavior of the direct part of the additional SDI under the conjugation

$$nln'l' \rightarrow nl^{4l+1}n'l' .$$

(i) SS interaction. κ_1+k_1 odd,

$$||D_{he}||=||D_{ee}|| .$$

(ii) Effective EL-SO interaction. κ_1+k_1 even,

$$||D_{he}||=-||D_{ee}|| .$$

(iii) SOO interaction. This interaction splits into two parts. The first, containing the factors $\underline{l}_i,\underline{s}_i$ is characterized by κ_1+k_1 even, in analogy with the spin-orbit interactions, and therefore changes sign under conjugation. The second part, containing $\underline{l}_i$ and $\underline{s}_j$, is represented by κ_1+k_1 odd, and therefore remains invariant under conjugation.

B. Exchange part

Use of identities (iii) and (iv) leads to the following new equalities:

$$2\sum_{L_2 \text{ even}} [L_2] \begin{Bmatrix} l & k_2 & k_1 & l \\ l' & K & l' & L_2 \\ l & L & L' & l \end{Bmatrix} = \frac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]} + \begin{Bmatrix} l' & K & l' \\ k_1 & l & k_2 \end{Bmatrix} \begin{Bmatrix} l' & K & l' \\ L' & l & L \end{Bmatrix} , \qquad (60)$$

$$2\sum_{L_2 \text{ odd}} [L_2] \begin{Bmatrix} l & k_2 & k_1 & l \\ l' & K & l' & L_2 \\ l & L & L' & l \end{Bmatrix} = \frac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]} - \begin{Bmatrix} l' & K & l' \\ k_1 & l & k_2 \end{Bmatrix} \begin{Bmatrix} l' & K & l' \\ L' & l & L \end{Bmatrix} . \qquad (61)$$

These equalities enable the performance of the summation over S_2,L_2 in formula (55) by splitting it into two parts: one over L_2 even ($S_2=0$), and the other over L_2 odd ($S_2=1$). Using also formula (19.8) of Ref. 18 for a $12j$ symbol with one vanishing angular momentum, $||E_{he}||$ is given by the following expression:

$$||E_{he}||=(\tfrac{1}{2}||\underline{s}^{(\kappa_1)}||\tfrac{1}{2})(\tfrac{1}{2}||\underline{s}^{(\kappa_2)}||\tfrac{1}{2})[K]([S,S',L,L'])^{1/2}(-1)^{l+l'+\kappa_1+\kappa_2+k_1+k_2-S+L}$$
$$\times \left[\frac{1}{2} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & \kappa_2 \\ S' & S & K \\ \frac{1}{2} & \frac{1}{2} & \kappa_1 \end{Bmatrix} \left[\frac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]} + \begin{Bmatrix} l' & K & l' \\ k_1 & l & k_2 \end{Bmatrix} \begin{Bmatrix} l' & K & l' \\ L' & l & L \end{Bmatrix} \right] + 3 \begin{Bmatrix} \frac{1}{2} & \kappa_2 & \kappa_1 & \frac{1}{2} \\ \frac{1}{2} & K & \frac{1}{2} & 1 \\ \frac{1}{2} & S & S' & \frac{1}{2} \end{Bmatrix} \left[\frac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]} - \begin{Bmatrix} l' & K & l' \\ k_1 & l & k_2 \end{Bmatrix} \begin{Bmatrix} l' & K & l' \\ L' & l & L \end{Bmatrix} \right] \right] . \qquad (62)$$

The following special cases occur.

(i) SS interaction. In order to calculate the exchange part of the SS interaction in the configuration $nl^{4l+1}n'l'$, one must substitute in (62)

$$\kappa_1=\kappa_2=1, \quad K=2 .$$

The only nonvanishing spin factors are obtained for $S=S'=1$,

$$\frac{1}{2} \begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ 1 & 1 & 2 \\ \frac{1}{2} & \frac{1}{2} & 1 \end{Bmatrix} = 3 \begin{Bmatrix} \frac{1}{2} & 1 & 1 & \frac{1}{2} \\ \frac{1}{2} & 2 & \frac{1}{2} & 1 \\ \frac{1}{2} & 1 & 1 & \frac{1}{2} \end{Bmatrix} = \frac{1}{18} . \qquad (63)$$

Substitution of (63) in the outer square brackets of (62) leads to

$$[\ ]=\frac{1}{9}\frac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]}\delta(S,1)\delta(S',1)\ .$$

Consequently,

$$||E_{he}(\mathrm{SS})||=\frac{5}{2}(-1)^{l+l'+k_1+k_2+1+L}\times\frac{\delta(k_2,L)\delta(k_1,L')}{\sqrt{[k_2][k_1]}}\delta(S,1)\delta(S',1)\ . \quad (64)$$

Now one must take into account the fact that the Hamiltonian representing the SS interaction includes, in addition to (6), also a term with the roles of k_1 and k_2 interchanged. Adding the reduced matrix element of this term to (64), and going over from $||E||$ to $\{\,|\,E\,|\,\}$, according to formula (11) above, the following final, explicit expression for $\{\,|\,E(\mathrm{SS})|\}$ is obtained

$$\{\,|\,E_{he}(\mathrm{SS})\,|\,\}=\tfrac{5}{2}(-1)^{l+l'+k_1+k_2+J}\delta(S,1)\delta(S',1)\times\begin{Bmatrix}1 & 1 & 2\\ k_1 & k_2 & J\end{Bmatrix}\times\frac{\delta(k_2,L)\delta(k_1,L')+\delta(k_1,L)\delta(k_2,L')}{\sqrt{[k_2][k_1]}}\ . \quad (65a)$$

Formula (65a) leads to the following conclusion. In the configuration $nl^{4l+1}n'l'$, for each pair (k_1,k_2), all matrix elements of the SS interaction vanish, except those connecting the levels ${}^3L\,(L=k_2)_J$ and ${}^3L'(L'=k_1)_J$,

$$\begin{aligned}(nl^{4l+1}n'l'{}^3L\,(L=k_2)J\{\,|\,E(\mathrm{SS})\,|\,\}nl^{4l+1}n'l'{}^3L'(L'=k_1)J)\\ =(nl^{4l+1}n'l'{}^3L\,(L=k_1)J\{\,|\,E(\mathrm{SS})\,|\,\}nl^{4l+1}n'l'{}^3L'(L'=k_2)J)\\ =\frac{5}{2}(-1)^{l+l'+k_1+k_2+J}\begin{Bmatrix}1 & 1 & 2\\ k_1 & k_2 & J\end{Bmatrix}\Big/\sqrt{[k_2][k_1]}\ .\end{aligned} \quad (65b)$$

(ii) SOO and effective EL-SO interactions. For these interactions one must substitute

(a) $\kappa_1=0,\ \ \kappa_2=K=1$,

or

(b) $\kappa_2=0,\ \ \kappa_1=K=1$

[in case (b) the roles of k_1 and k_2 are interchanged as compared to case (a), see formulas (2) and (3) above].

(a) The spin factors become

$$\frac{1}{2}\begin{Bmatrix}\frac12 & \frac12 & 1\\ S' & S & 1\\ \frac12 & \frac12 & 0\end{Bmatrix}=\frac{(-1)^{S'}}{2\sqrt6}\begin{Bmatrix}S & S' & 1\\ \frac12 & \frac12 & \frac12\end{Bmatrix}, \quad (66)$$

$$3\begin{Bmatrix}\frac12 & & 1 & & 0 & & \frac12 & \\ & \frac12 & & 1 & & \frac12 & & 1\\ \frac12 & & S & & S' & & \frac12 & \end{Bmatrix}=3\begin{Bmatrix}\frac12 & & \frac12 & & 1 & & 0 & \\ & 1 & & \frac12 & & 1 & & \frac12\\ \frac12 & & \frac12 & & S & & S' & \end{Bmatrix},$$

by using the symmetry relations of the $12j$ symbol,[17]

$$=\frac{3}{\sqrt6}\begin{Bmatrix}\frac12 & \frac12 & 1\\ \frac12 & \frac12 & S'\end{Bmatrix}\begin{Bmatrix}S & S' & 1\\ \frac12 & \frac12 & \frac12\end{Bmatrix}, \quad (67)$$

through the use of formula (19.9) of Ref. 18. Substitution of (66) and (67) in (62) results in

$$\begin{aligned}&||E_{he}(\mathrm{SOO,EL\text{-}SO},\kappa_1=0,\kappa_2=K=1)\\ &=3\sqrt3([S,S',L,L'])^{1/2}(-1)^{l+l'+1+k_1+k_2+S+L}\\ &\times\begin{cases}-\dfrac{1}{6}\begin{Bmatrix}S & S' & 1\\ \frac12 & \frac12 & \frac12\end{Bmatrix}\begin{Bmatrix}L & L' & 1\\ l' & l' & l\end{Bmatrix}\begin{Bmatrix}k_1 & k_2 & 1\\ l' & l' & l\end{Bmatrix} & \text{for } S'=1,\ \ S=0,1\ ,\\[2ex] \left[-\dfrac{1}{6}\begin{Bmatrix}S & S' & 1\\ \frac12 & \frac12 & \frac12\end{Bmatrix}\begin{Bmatrix}L & L' & 1\\ l' & l' & l\end{Bmatrix}\begin{Bmatrix}k_1 & k_2 & 1\\ l' & l' & l\end{Bmatrix}+\dfrac{2}{\sqrt6}\begin{Bmatrix}S & S' & 1\\ \frac12 & \frac12 & \frac12\end{Bmatrix}\dfrac{\delta(k_2,L)\delta(k_1,L')}{[k_2][k_1]}\right] & \text{for } S'=0,\ \ S=1\ .\end{cases}\end{aligned} \quad (68)$$

After subtracting the common term

$$3\sqrt{3}([S,S',L,L'])^{1/2}(-1)^{l+l'+1+k_1+k_2+S+L}$$
$$\times\left[-\frac{1}{6}\begin{Bmatrix} S & S' & 1\\ \frac{1}{2} & \frac{1}{2} & \frac{1}{2}\end{Bmatrix}\begin{Bmatrix} L & L' & 1\\ l' & l' & l\end{Bmatrix}\begin{Bmatrix} k_1 & k_2 & 1\\ l' & l' & l\end{Bmatrix}\right],$$

which is proportional to the reduced matrix element of the spin-orbit interaction of the electron l' in the configuration under discussion, there remains

$$||E_{he}(\text{SOO,EL-SO},\kappa_1=0,\kappa_2=K=1)|| = 3(-1)^{l+l'+k_1+k_2+L}\frac{\delta(k_2,L)\delta(k_1,L')}{\sqrt{[k_2][k_1]}} \times\delta(S,1)\delta(S',0)\ . \quad (69)$$

(b) Following the steps carried out in (a), one obtains for case (b)

$$||E_{he}(\text{SOO,EL-SO},\kappa_2=0,\kappa_1=K=1)|| = 3(-1)^{l+l'+1+k_1+k_2+L}\frac{\delta(k_1,L)\delta(k_2,L')}{\sqrt{[k_2][k_1]}} \times\delta(S,0)\delta(S',1)\ . \quad (70)$$

By multiplying each of these reduced matrix elements by the corresponding factor

$$(-1)^{L+S'+J}\begin{Bmatrix} S & S' & K\\ L' & L & J\end{Bmatrix},$$

the following final expression for $\{\,|\,E(\text{SOO,EL-SO})|\,\}$ is obtained:

$$\{\,|\,E(\text{SOO,EL-SO})\,|\,\} = \sqrt{3}(-1)^{l+l'+k_1+1}\delta(J,k_1) \times[\delta(k_2,L)\delta(k_1,L')\delta(S,1)\delta(S',0) + \delta(k_1,L)\delta(k_2,L')\delta(S,0)\delta(S',1)]/[k_1]\sqrt{[k_2]}\ . \quad (71a)$$

Formula (71a) leads to the following conclusion: In the configuration $nl^{4l+1}n'l'$, for each pair (k_1,k_2), all exchange matrix elements of the SOO and the effective EL-SO interactions vanish, except those connecting the levels $^3L\,(L=k_2)_{J(=k_1)}$ and $^1L'(L'=k_1)_{J(=k_1)}$,

$$(nl^{4l+1}n'l'\,{}^3L\,(L=k_2)J(=k_1)\{\,|\,E\,|\,\}nl^{4l+1}n'l'\,{}^1L'(L'=k_1)J(=k_1)) = (nl^{4l+1}n'l'\,{}^1L(L=k_1)J(=k_1)\{\,|\,E\,|\,\}nl^{4l+1}n'l'\,{}^3L'(L'=k_2)J(=k_1)) = \sqrt{3}(-1)^{l+l'+k_1+1}/[k_1]\sqrt{[k_2]}\ . \quad (71b)$$

It should be emphasized that although exchange matrix elements between two triplet levels are allowed for the SOO and the effective EL-SO interactions, and they indeed occur in the configuration $nln'l'$, this is not the case for $nl^{4l+1}n'l'$; in the latter configuration there are no nonvanishing exchange matrix elements connecting two triplet levels, as in the analogous case of the electrostatic interaction.[12,25] The orbital selection rules, represented by the Kronecker deltas $\delta(k_2,L)\delta(k_1,L')$, etc., are also generalizations of the $\delta(k,L)$ appearing in the electrostatic exchange matrix elements.

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