Interaction Matrix Element in a Shell Model

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The matrix elements of two-particle interactions between states of many-particle configurations are expressed as products of one-particle reduced matrix elements and of a single recoupling coefficient. Applications are given to the Coulomb interaction of $l^n l'$ configurations and to all three-electron configurations.

1. INTRODUCTION

In a shell-model treatment of a many-particle system one considers initially states of single particles in a central field. In this approximation a many-particle state is constructed by coupling the angular momenta of the various particles according to a definite prescription. In a further approximation one takes into account the interaction between pairs of particles. To this end one has to calculate the two-particle interaction matrix elements between initial many-particle states. Since these initial states are properly symmetrized linear combinations of unsymmetrized states, the matrix elements will be linear combinations of terms constructed from the unsymmetrized states. We shall deal with these unsymmetrized matrix elements in Secs. 2 and 5, and with symmetrized ones in Secs. 3 and 4.

The interaction is conveniently expanded into multipole components. Each of these components is generally the product of a factor depending on radial variables and of another ("angular") factor depending on directional and/or spin variables. We are concerned here only with the angular factor. For example, the electrostatic interaction between two particles, s and t, is expanded into a sum of terms consisting of a radial factor times a spherical function,

$$P_k(\cos\theta_{st}) = \sum_q [4\pi/(2k+1)](-1)^{k-q} \times Y_{k,q}(\theta_s\varphi_s) Y_{k,-q}(\theta_t\varphi_t), \quad (1)$$

of the angle θ_{st} between the directions, $(\theta_s\varphi_s)$ and $(\theta_t\varphi_t)$, of the two particles with respect to the center of the system. In general, the angular factor of each 2^k-pole component of the interaction may be represented as the scalar product

$$\mathfrak{S}^{[k]} \cdot \mathfrak{T}^{[k]} = \sum_q (-1)^{k-q} \mathfrak{S}^{[k]}{}_q \mathfrak{T}^{[k]}{}_{-q}, \quad (2)$$

of two sets of tensorial operators[1] which operate, respectively, on direction (or spin) coordinates s and t.

To calculate the matrix elements of (2) one wants to express them in terms of the matrix elements of the one-particle operators $\mathfrak{S}^{[k]}$ (or $\mathfrak{T}^{[k]}$) between one-particle states with angular momenta j_s', j_s (or j_t', j_t). This requirement led to the development of the Racah algebra. Racah's basic formula,[2] which gives the matrix element of (2) between two-particle states, was interpreted later (FR Chap. 15) in terms of a recoupling of one-particle eigenstates.[3] The matrix element of (2) between states of three or more coupled particles can be reduced to the original Racah formula by a sequence of recouplings. This sequence may be somewhat circuitous, particularly for the exchange portion of an interaction (see, e.g., FR Chap. 16).

In the course of a routine application of this method of multiple recoupling it was noticed that its result could be condensed into a single recoupling coefficient. It was then found that the matrix element of (2) between two many-particle states can be expressed directly as the product of one-particle matrix elements and of a *single* recoupling coefficient. This coefficient arises as the overlap integral—i.e., as the product in Hilbert space—of two wave functions of the same particles with different angular momentum coupling schemes.

The basic new result is given by Eq. (10) in Sec. 2, and applies equally to direct interaction and to exchange matrix elements. This result permits an approach to atomic calculations alternative to that developed by Racah. It is applied in Sec. 3 to obtain the Coulomb interaction energy matrix between symmetrized states of equivalent electrons plus one electron in other subshells. This result relates closely to a formula recently obtained by Judd[4] through the usual approach. Section 4 gives the interaction matrix elements between all possible three-electron states. Section 5 extends Eq. (10) to the matrix elements of nonscalar products of tensorial sets of operators.

2. DERIVATION OF THE MAIN FORMULA

An analytical artifice will be used which replaces each single-particle tensorial operator with a scalar

[1] See, e.g., U. Fano and G. Racah, *Irreducible Tensorial Sets* (Academic Press Inc., New York, 1959), which will be referred to as "FR."

[2] G. Racah, Phys. Rev. **62**, 438 (1942).

[3] Recoupling is an orthogonal transformation between two products of the same angular momentum eigenstates constructed according to alternative coupling schemes. It is a geometric operation which applies not only to angular momentum eigenstates, but also to other irreducible tensorial sets.

[4] B. R. Judd, Phys. Rev. **125**, 613 (1962).

operator. This operator acts on the variables of one particle and simultaneously combines its angular momentum with the angular momentum of an additional mock particle. To this end we introduce a variable κ of a mock particle and wave functions $u(kq)$, or $\mathfrak{u}^{[k]}{}_q$, of this variable pertaining to eigenstates with angular momentum and magnetic quantum numbers k and q. The orthogonality property of these wave functions,

$$\int d\kappa\, u^*(kq')u(kq)=\delta_{q'q}, \tag{3}$$

may be expressed symbolically as

$$\mathfrak{u}^{[k]}{}_{q'}{}^*\mathfrak{u}^{[k]}{}_q=\delta_{q'q}. \tag{3'}$$

This property serves to break up the scalar product of operators in (2) into a product of two separate scalars, each of which involves only $\mathfrak{S}^{[k]}$ or $\mathfrak{T}^{[k]}$:

$$\begin{aligned}\sum_q(-1)^{k-q}\mathfrak{S}^{[k]}{}_q\mathfrak{T}^{[k]}{}_{-q}&=\sum_{qq'}\mathfrak{S}^{[k]}{}_{q'}\delta_{q'q}(-1)^{(k-q)}\mathfrak{T}^{[k]}{}_{-q}\\&=[\sum_{q'}\mathfrak{S}^{[k]}{}_{q'}\mathfrak{u}^{[k]}{}_{q'}{}^*][\sum_q(-1)^{k-q}\mathfrak{u}^{[k]}{}_q\mathfrak{T}^{[k]}{}_{-q}],\end{aligned} \tag{4}$$

that is, in vector notation,

$$\mathfrak{S}^{[k]}\cdot\mathfrak{T}^{[k]}=[\mathfrak{S}^{[k]}\mathbf{u}^{[k]}]^*[\mathbf{u}^{[k]}\cdot\mathfrak{T}^{[k]}]. \tag{5}$$

The notations of FR Chaps. 5 and 6 have been used here. Integration over κ is implied in (4) and (5), in accordance with (3′). The transformation of $\mathfrak{S}^{[k]}\cdot\mathfrak{T}^{[k]}$ in (5) is analogous to the familiar transformation of a product of vectors, $\mathbf{A}\cdot\mathbf{B}$ into a sum of products with unit vectors $\mathbf{u}_i$ directed along the coordinate axes, $\mathbf{A}\cdot\mathbf{B}=\sum_i\mathbf{A}\cdot\mathbf{u}_i\mathbf{u}_i\cdot\mathbf{B}$. (The product $\mathbf{u}^{[k]*}\mathbf{u}^{[k]}$ corresponds to the diadic $\mathbf{u}_i\mathbf{u}_i$ and the integration over κ to the summation over i.)

Call $\psi(\lambda_sj_sm_s)$ the angular momentum eigenfunctions of a particle s on which $\mathfrak{S}^{[k]}{}_q$ operates. (The index λ_s represents all the single-particle quantum numbers other than j_s and m_s.) Application of $\mathfrak{S}^{[k]}{}_q$ from the right on $\psi^*(\lambda_sj_sm_s)$ yields

$$\begin{aligned}\psi^*(\lambda_sj_sm_s)\mathfrak{S}^{[k]}{}_q&=\sum_{\lambda_s''j_s''m_s''}(\lambda_sj_sm_s|\mathfrak{S}^{[k]}{}_q|\lambda_s''j_s''m_s'')\psi^*(\lambda_s''j_s''m_s'')\\&=(2j_s+1)^{-1/2}\sum_{\lambda_s''j_s''m_s''}(\lambda_sj_s\|S^{[k]}\|\lambda_s''j_s'')\\&\quad\times(j_s''kj_sm_s|j_s''m_s''kq)\psi^*(\lambda_s''j_s''m_s''),\end{aligned} \tag{6}$$

where the reduced matrix element $(\lambda_sj_s\|S^{[k]}\|\lambda_s''j_s'')$ has been introduced in accordance with (FR 14.4) and other current references. (The values of the reduced matrix elements of the spherical harmonics and of other usual tensorial operators are given by well-known formulas.) It follows that the application of the whole operator $\mathfrak{S}^{[k]}\mathbf{u}^{[k]*}$ is represented by

$$\begin{aligned}\psi^*(\lambda_sj_sm_s)\mathfrak{S}^{[k]}\mathbf{u}^{[k]*}&=(2j_s+1)^{-1/2}\sum_{\lambda_s''j_s''}(\lambda_sj_s\|S^{[k]}\|\lambda_s''j_s'')\\&\quad\times\bar{\psi}^*((\lambda_s''j_s'',k)j_sm_s),\end{aligned} \tag{7}$$

where the wave function $\bar{\psi}$ pertains to a joint state of the particles s and κ coupled with resultant angular momentum j_s.

Consider now a typical unsymmetrized n-particle wave function with total angular momentum quantum numbers JM. We may represent it in the form

$$\begin{aligned}&\Psi(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots,\lambda_tj_t,\cdots,\lambda_nj_n;\cdots JM)\\&=\sum_{m_1\cdots m_s\cdots m_t\cdots m_n}C^{\cdots j_s\cdots j_t\cdots J}{}_{\cdots m_s\cdots m_t\cdots M}\psi(\lambda_1j_1m_1)\cdots\\&\quad\times\psi(\lambda_sj_sm_s)\cdots\psi(\lambda_tj_tm_t)\cdots\psi(\lambda_nj_nm_n),\end{aligned} \tag{8}$$

where the coefficients C are products of Wigner coefficients which depend on the prescribed coupling of angular momenta. The dots that precede J represent the $n-2$ j numbers required, in addition to J, to specify the coupling of the n one-particle angular momenta (see FR Chap. 8). These j numbers are not listed explicitly here because our treatment does not relate to any specific coupling. Because of Eq. (7), application of the operator $\mathfrak{S}^{[k]}\mathbf{u}^{[k]*}$ to the complex conjugate of Ψ, from the right, is represented by

$$\begin{aligned}&\Psi^*(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots,\lambda_tj_t,\cdots,\lambda_nj_n;\cdots JM)[\mathfrak{S}^{[k]}\mathbf{u}^{[k]*}\\&=(2j_s+1)^{-1/2}\sum_{\lambda_s''j_s''}(\lambda_sj_s\|S^{[k]}\|\lambda_s''j_s'')\Psi^*(\lambda_1j_1,\cdots,(\lambda_s''j_s'',k)j_s,\cdots,\lambda_tj_t,\cdots,\lambda_nj_n;\cdots JM).\end{aligned} \tag{9}$$

The result of the operation is thereby expanded in a series of eigenfunctions of $n+1$ particles—the initial n plus the mock particle—in which the mock particle is coupled to particle s and their resultant is coupled to the other ones exactly as particle s had been before the operation.

Formulas analogous to (6), (7), and (9) are obtained in the process of operating on a wave function (8) with $\mathbf{u}^{[k]}\cdot\mathfrak{T}^{[k]}$ from the left.[5] We have

$$\mathbf{u}^{[k]}\cdot\mathfrak{T}^{[k]}\psi(\lambda_t'j_t'm_t')=\sum_{\lambda_t''j_t''}\Psi((k'',\lambda_t''j_t'')j_t'm_t')(\lambda_t''j_t''\|T^{[k]}\|\lambda_t'j_t')(2j_t'+1)^{-1/2}, \tag{7'}$$

$$\begin{aligned}&\mathbf{u}^{[k]}\cdot\mathfrak{T}^{[k]}\Psi(\lambda_1'j_1',\cdots,\lambda_s'j_s',\cdots,\lambda_t'j_t',\cdots,\lambda_n'j_n';\cdots J'M')\\&=\sum_{\lambda_t''j_t''}\Psi(\lambda_1'j_1',\cdots,\lambda_s'j_s',\cdots,(k,\lambda_t''j_t'')j_t',\cdots,\lambda_n'j_n';\cdots J'M')(\lambda_t''j_t''\|T^{[k]}\|\lambda_t'j_t')(2j_t'+1)^{-1/2}.\end{aligned} \tag{9'}$$

[5] One should, however, conveniently utilize an expression of tensorial operator matrix elements somewhat different from (FR 14.4), namely,

$$(-1)^{k-q}(\lambda_t''j_t''m_t''|\mathfrak{T}^{[k]}{}_{-q}|\lambda_t'j_t'm_t')=(2j_t'+1)^{-1/2}(\lambda_t''j_t''\|T^{[k]}\|\lambda_t'j_t')(j_t''m_t''kq|j_t''kj_t'm_t').$$

Notice that k enters the coupling scheme on the *left* of j_t'' in (7′) and (9′), but on the *right* of j_s'' in (7) and (9).

The desired matrix element is now obtained by multiplying (9) and (9′), with (9) on the left, and integrating over all the $n+1$ variables, $1, \cdots, s, \cdots, \kappa, \cdots, t, \cdots n$. The integral over the product of the left-hand side of (9) and (9′) is the matrix element of $\mathfrak{S}^{[k]}\cdot\mathfrak{T}^{[k]}$, due to (5). On the right-hand side we find, besides numerical coefficients and reduced matrix elements, integrals over products of two wave functions. Each of these integrals vanishes unless it involves a pair of wave functions constructed with products of the same one-particle wave functions. This condition requires that: (a) $(\lambda_s''j_s'')=(\lambda_s'j_s')$ and $(\lambda_t''j_t'')=(\lambda_tj_t)$, so that a single term from each of the summations in (9) and (9′) gives a nonvanishing contribution, and (b) $(\lambda_i'j_i')=(\lambda_ij_i)$ for $i\neq s, t$, so that the whole expression vanishes unless the matrix element on the left-hand side is diagonal in the one-particle quantum numbers other than those of s and t. Moreover, the whole expression also vanishes unless $(JM)=(J'M')$. The residual nonvanishing integral on the right-hand side is the overlap integral mentioned in Sec. 1, which is known as a recoupling coefficient, is independent of the quantum numbers λ and could be expressed as a sum over the products of Wigner coefficients included in the coefficients C of (8). The results of the integration over the product of (9) and (9′) is, therefore,

$$\begin{aligned}(\lambda_1j_1\cdots,\lambda_sj_s,\cdots,\lambda_tj_t,\cdots;JM|\mathfrak{S}^{[k]}\cdot\mathfrak{T}^{[k]}|\lambda_1j_1,\cdots,\lambda_s'j_s',\cdots,\lambda_t'j_t',\cdots;J'M')\\=[(2j_s+1)(2j_t'+1)]^{-1/2}(\lambda_sj_s\|S^{[k]}\|\lambda_s'j_s')(\lambda_tj_t\|T^{[k]}\|\lambda_t'j_t')\\\times(j_1\cdots,(j_s'k)j_s,\cdots,j_t,\cdots|j_1\cdots,j_s',\cdots,(kj_t)j_t',\cdots)^{(J)}\delta_{JJ'}\delta_{MM'}.\end{aligned}\qquad(10)$$

The transformation coefficient on the right-hand side of (10) pertains to the recoupling of $(n+1)$-fold eigenstate products of degree J. The coupling schemes, which are left unspecified on the left and on the right of this coefficient, are understood to be the same as on the corresponding sides of the matrix element on the left-hand side of (10) and to be represented by the same j numbers, with the following *key substitutions*. The quantum number j_t', which represents the angular momentum of the single particle t on the left-hand side of (10), represents, on the right-hand side, the sum of angular momenta k and j_t of the pair of particles κ and t. Similarly, j_s represents the sum of the angular momenta of s and κ on the right-hand side. These substitutions augment the two n-fold products of one-particle states, which identify the matrix elements on the left-hand side of (10), to yield the two $(n+1)$-fold products which identify the recoupling coefficient on the right-hand side. The quantum number k, attributed in our treatment to the mock particle κ, stands, of course, for the degree k of the operators $\mathfrak{S}^{[k]}$ and $\mathfrak{T}^{[k]}$. The factor $[(2j_s+1)(2j_t'+1)]^{-1/2}$ on the right-hand side of (10) contains the quantum numbers that represent the resultant angular momenta of the mock particle and of the particles s and t.

The recoupling coefficient in (10) is, of course, a function only of the j numbers involved in it, namely, (a) the $n+2$ angular momentum quantum numbers $j_1, \cdots, j_{s-1}, j_s, j_s', j_{s+1}, \cdots, j_{t-1}, j_t, j_t', j_{t+1}, \cdots, j_n$, (b) the degree k of the operator sets, (c) the two groups of $n-2$ additional j numbers which specify the (generally different) couplings on the two sides of the recoupling coefficient, (d) the degree J of the products that are being recoupled. The classification and evaluation of recoupling coefficients have not yet received a general treatment. A basic procedure for evaluating any one of them (FR Chap. 9) consists of factorizing it into a sum of products of triple-product recoupling coefficients which are—to within a factor—extensively tabulated under the name of Racah, or 6-j coefficients.[6]

The coupling of many particles is often equal on both sides of the recoupling coefficient in (10), because the interaction operates between two particles only. Thereby the explicit form of the recoupling coefficient may reduce greatly, as will be seen in Sec. 3, since a subgroup of particles with invariant coupling participates in the recoupling as though it consisted of a single particle.

3. EXAMPLE: $l^{n-1}l'$ CONFIGURATIONS

As an example of application of formula (10) we calculate the matrix element

$$(\Psi(\lambda^{\mathrm{I}})|G|\Psi(\lambda^{\mathrm{II}}))\qquad(11)$$

of the interaction

$$G=\sum_{i<j}g_{ij}\quad(i,j=1,2,\cdots,n)$$

between $L-S$ coupling antisymmetric states of n identical particles

$$\begin{aligned}\Psi(\lambda^{\mathrm{I}})&=\Psi(l^{n-1}(\alpha_1S_1L_1)l'SL,JM),\\\Psi(\lambda^{\mathrm{II}})&=\Psi(l^{n-1}(\alpha_1'S_1'L_1')l''S'L',J'M').\end{aligned}\qquad(13)$$

This matrix element is equal to

$$\tfrac{1}{2}n(n-1)(\Psi(\lambda^{\mathrm{I}})|g_{n-1,n}|\Psi(\lambda^{\mathrm{II}})),\qquad(14)$$

where $g_{n-1,n}$ is the interaction between "particle n" and "particle $n-1$." Following Racah[7] we write the

[6] M. Rotenberg, R. Bivins, N. Metropolis, and J. K. Wooten, Jr., *The 3-j and 6-j Symbols* (Technology Press, Cambridge, Massachusetts, 1959).

[7] G. Racah, Phys. Rev. **63**, 367 (1943), Eq. (26).

antisymmetric n-particle states in terms of antisymmetric $n-1$ particle states as

$$\Psi(\lambda^{\mathrm{I}})=(n)^{-1/2}\sum_{i=1}^{n}(-1)^{P_i}\psi(l^{n-1}(\alpha_1S_1L_1)l'_iSL,JM),\quad \Psi(\lambda^{\mathrm{II}})=(n)^{-1/2}\sum_{j=1}^{n}(-1)^{P_j}\psi(l^{n-1}(\alpha_1'S_1'L_1')l''_jS'L',J'M'),\tag{15}$$

where P_i is the parity of the permutation that exchanges i and n, the indexes i, j in l', l'' indicate that the ith and jth particle are in these states and the state $l^{n-1}(\alpha_1S_1L_1)$ is that of particles 1, 2, $\cdots$, $i-1$, $i+1$, $\cdots n$. Substitution of (15) into (14) gives

$$\begin{aligned}(\Psi(\lambda^{\mathrm{I}})|G|\Psi(\lambda^{\mathrm{II}}))&=\tfrac{1}{2}(n-1)\sum_{i,j}(-1)^{P_i+P_j}(l^{n-1}(\alpha_1S_1L_1)l'_iSLJM|g_{n-1,n}|l^{n-1}(\alpha_1'S_1'L_1')l''_jS'L'J'M')\\&=(n-1)\{(l^{n-1}(\alpha_1S_1L_1)l'_nSL,JM|g_{n-1,n}|l^{n-1}(\alpha_1'S_1'L_1')l''_nS'L',J'M')\\&\quad-(l^{n-1}(\alpha_1S_1L_1)l'_{n-1}SL,JM|g_{n-1,n}|l^{n-1}(\alpha_1'S_1'L_1')l''_nS'L',J'M')\}+(\text{core terms if } l'=l''),\end{aligned}\tag{16}$$

after some relabeling which allows one to cancel the $\frac{1}{2}$ factor. [The "core terms" will be ignored in what follows; they are equal to the $n-1$ particles interaction energy $(l^{n-1}(\alpha_1S_1L_1)|G|l^{n-1}(\alpha_1'S_1'L_1'))\times\delta(S_1S_1')\delta(L_1L_1')\delta(l'l'')$.]

Now we separate out the "last" of the l^{n-1} electrons from the other ones utilizing the fractional parentage formula (10) of reference 7,

$$\psi(l^{n-1}\alpha_1S_1L_1)=\sum_{\bar\alpha\bar S\bar L}\psi(l^{n-2}(\bar\alpha\bar S\bar L)lS_1L_1)(l^{n-2}(\bar\alpha\bar S\bar L)lS_1L_1]\!]l^{n-1}\alpha_1S_1L_1).\tag{17}$$

One gets then

$$\begin{aligned}(\Psi(\lambda^{\mathrm{I}})|G|\Psi(\lambda^{\mathrm{II}}))&=(n-1)\sum_{\bar\alpha\bar S\bar L\bar\alpha'\bar S'\bar L'}(l^{n-1}\alpha_1S_1L_1[\![l^{n-2}(\bar\alpha\bar S\bar L)lS_1L_1)\\&\times\{(l^{n-2}(\bar\alpha\bar S\bar L)l_{n-1}S_1L_1l'_nSLJM|g_{n-1,n}|l^{n-2}(\bar\alpha'\bar S'\bar L')l_{n-1}S_1'L_1'l''_nS'L'J'M')\\&-(l^{n-2}(\bar\alpha\bar S\bar L)l_nS_1L_1l'_{n-1}SLJM|g_{n-1,n}|l^{n-2}(\bar\alpha'\bar S'\bar L')l_{n-1}S_1'L_1'l''_nS'L'J'M')\}\\&\times(l^{n-2}(\bar\alpha'\bar S'\bar L')lS_1'L_1']\!]l^{n-1}\alpha_1'S_1'L_1').\end{aligned}\tag{18}$$

The matrix elements of $g_{n-1,n}$ that appear in (18) are now calculated for the case

$$g_{n-1,n}=e^2/r_{n-1,n}.\tag{19}$$

Integration over the space variables yields for the two matrix elements in the right-hand side of (18), respectively, the expressions

$$\begin{aligned}&\sum_k R^k(Nl,N'l';Nl,N''l'')\delta(\bar\alpha\bar\alpha')\delta(\bar S\bar S')\delta(\bar L\bar L')\times\delta(JJ')\delta(MM')\\&\quad\times((\bar S\bar L,l_{n-1})S_1L_1,l'_nSL,JM|\mathfrak{C}^{[k]}(n-1)\cdot\mathfrak{C}^{[k]}(n)|(\bar S\bar L,l_{n-1})S_1'L_1',l''_nS'L',JM),\end{aligned}\tag{20}$$

$$\begin{aligned}&\sum_k R^k(N'l',Nl;Nl,N''l'')\delta(\bar\alpha\bar\alpha')\delta(\bar S\bar S')\delta(\bar L\bar L')\times\delta(JJ')\delta(MM')\\&\quad\times((\bar S\bar L,l_n)S_1L_1,l'_{n-1}SL,JM|\mathfrak{C}^{[k]}(n-1)\cdot\mathfrak{C}^{[k]}(n)|(\bar S\bar L,l_{n-1})S_1'L_1',l''_nS'L',JM),\end{aligned}\tag{21}$$

where the notation of FR for the representation (1) of $P_k(\cos\theta_{n-1,n})$ as a scalar product has been used, the R^k are Slater integrals (N=principal quantum number) and conservation of total angular momentum has been taken into account.

Application of (10) to the matrix elements of the tensorial scalar product in (20) gives

$$\begin{aligned}&((\bar S\bar L,l_{n-1})S_1L_1,l'_nSLJM|\mathfrak{C}^{[k]}(n-1)\cdot\mathfrak{C}^{[k]}(n)|(\bar S\bar L,l_{n-1})S_1'L_1',l''_nS'L'JM)\\&\quad=[(2l+1)(2l''+1)]^{-1/2}(l\|C^{[k]}\|l)(l'\|C^{[k]}\|l'')((\bar S\bar L,(l_{n-1}k)l)S_1L_1,l_n'SL|(\bar S\bar L,l_{n-1})S_1'L_1',(kl_n')l'',S'L')^{(J)}.\end{aligned}\tag{22}$$

Since orbital and spin parts factor out, the recoupling coefficient in (22) is equal to

$$([\bar L,(l_{n-1}k)l]L_1,l_n'|[\bar L,l_{n-1}]L_1',(kl'_n)l'')^{(L)}((\bar S,s_{n-1})S_1,s_n|(\bar S,s_{n-1})S_1',s_n)^{(S)}\delta(LL')\delta(SS').\tag{23}$$

The spin factor is equal to $\delta(S_1,S_1')$ and the orbital part can be expressed as the product of two $\bar W$ functions.

[See FR Eq. (12.4).] With this the right-hand side of Eq. (22) becomes

$$\exp[\pi i(l+l'+\bar{L}+L_1+L_1'+L)][(2L_1+1)(2L_1'+1)]^{1/2}(l\|C^{[k]}\|l)(l'\|C^{[k]}\|l'')$$
$$\times\bar{W}\begin{pmatrix}\bar{L} & l & L_1' \\ k & L_1 & l\end{pmatrix}\bar{W}\begin{pmatrix}L_1' & k & L_1 \\ l' & L & l''\end{pmatrix}\delta(S_1S_1')\delta(LL')\delta(SS'). \quad (24)$$

For the matrix element in (21) (i.e., for the exchange term) application of (10) gives

$$((\bar{S}\bar{L},l_n)S_1L_1,l_{n-1}'SL,JM|\mathfrak{C}^{[k]}(n-1)\cdot\mathfrak{C}^{[k]}(n)|(\bar{S}\bar{L},l_{n-1})S_1'L_1',l_n''S'L',JM)$$
$$=[(2l'+1)(2l''+1)]^{-1/2}(l'\|C^{[k]}\|l)(l\|C^{[k]}\|l'')((\bar{S}\bar{L},l_n)S_1L_1,(l_{n-1}k)l',SL|(\bar{S}\bar{L},l_{n-1})S_1'L_1',(kl_n)l'',S'L')^{(J)}. \quad (25)$$

The recoupling coefficient in (25) is equal to

$$((\bar{L},l_n)L_1,(l_{n-1}k)l'|(\bar{L},l_{n-1})L_1'(kl_n)l'')^{(L)}((\bar{S}s_n)S_1,s_{n-1}|(\bar{S}s_{n-1})S_1',s_n)^{(S)}\delta(LL')\delta(SS'). \quad (26)$$

The spin factor is now a $3-j$ recoupling coefficient that can be written in terms of a $\bar{W}$ function and the orbital part can be expressed in terms of an X function. The right-hand side of Eq. (25) is equal to

$$\exp[\pi i(k+l-l''+2\bar{S}+S_1-S_1')][(2L_1+1)(2L_1'+1)(2S_1+1)(2S_1'+1)]^{1/2}$$
$$\times(l'\|C^{[k]}\|l)(l\|C^{[k]}\|l'')\bar{W}\begin{pmatrix}s & \bar{S} & S_1' \\ s & S & S_1\end{pmatrix}X\begin{Bmatrix}\bar{L} & l & L_1 \\ l & k & l' \\ L_1' & l'' & L\end{Bmatrix}\delta(LL')\delta(SS'). \quad (27)$$

Equations (20) and (21) with (22), (25) and (24), (27) substituted into (18) give, on noticing that

$$\exp[\pi i(k+l-l''+2\bar{S}+S_1-S_1')]=-(-1)^{S_1+S_1'}, \quad (28)$$

$$(\Psi(\lambda^{\mathrm{I}})|G|\Psi(\lambda^{\mathrm{II}}))=(n-1)\sum_{k\bar{\alpha}\bar{S}\bar{L}}(l^{n-1}\alpha_1S_1L_1\{|l^{n-2}(\bar{\alpha}\bar{S}\bar{L})lS_1L_1)$$
$$\times\Bigg\{R^k(Nl,N'l';Nl,N''l'')\exp[\pi i(l+l'+\bar{L}+L_1+L_1'+L)][(2L_1+1)(2L_1'+1)]^{1/2}(l\|C^{[k]}\|l)(l'\|C^{[k]}\|l'')$$
$$\times\bar{W}\begin{pmatrix}\bar{L} & l & L_1' \\ k & L_1 & l\end{pmatrix}\bar{W}\begin{pmatrix}L_1' & k & L_1 \\ l' & L & l''\end{pmatrix}\delta(S_1S_1')+R^k(N'l',Nl;Nl,N''l'')(-1)^{S_1+S_1'}$$
$$\times[(2L_1+1)(2L_1'+1)(2S_1+1)(2S_1'+1)]^{1/2}(l'\|C^{[k]}\|l)(l\|C^{[k]}\|l'')\bar{W}\begin{pmatrix}s & \bar{S} & S_1' \\ s & S & S_1\end{pmatrix}X\begin{Bmatrix}\bar{L} & l & L_1 \\ l & k & l' \\ L_1' & l'' & L\end{Bmatrix}\Bigg\}$$
$$\times(l^{n-2}(\bar{\alpha}\bar{S}\bar{L})lS_1'L_1'|\}l^{n-1}\alpha_1'S_1'L_1')\delta(LL')\delta(SS')\delta(JJ')\delta(MM'). \quad (29)$$

A special case of this formula ($l'=l''$) has been given by Judd[4] and the present one was conjectured by Wybourne.[8]

4. THREE-ELECTRON MATRIX ELEMENTS

In this section Eq. (10) is applied to calculate the Coulomb interaction matrix elements between all possible three electron $L-S$ antisymmetric states. There are three basic types of possible three-electron states, namely, states with three equivalent electrons indicated by $|1)$, states with two equivalent one inequivalent electron, indicated by $|2)$ and states with three inequivalent electrons, indicated by $|3)$.

The matrix elements of an operator,

$$G=\sum_{i<j}g_{ij}=\sum_{i<j}e^2/r_{ij}, \quad (30)$$

are then of the six types

$$\begin{matrix}(1|G|1) & (1|G|2) & (1|G|3) \\ & (2|G|2) & (2|G|3) \\ & & (3|G|3).\end{matrix} \quad (31)$$

Of type $(1|G|1)$ there is only the matrix element

$$(l^3\alpha SL|G|l^3\alpha'SL), \quad (\mathrm{I})$$

[8] B. G. Wybourne (private communication). We thank Dr. Wybourne for communication in advance of publication and for stimulating discussions.

but of type $(1|G|2)$ there are two, according to whether the equivalent electrons in $|2)$ are or are not equivalent to the electrons in $|1)$:

$$(l^3\alpha SL|G|l^2(S'L')l'SL), \qquad \text{(II)}$$

$$(l^3\alpha SL|G|l,l'^2(S'L')SL). \qquad \text{(III)}$$

Matrix elements of the type $(1|G|3)$ vanish unless one of the $l_al_bl_c$ in $|3)$ equals the l of $|1)$. One has then only the two matrix elements

$$(l^3\alpha SL|G|(l_al_b)S_{ab}L_{ab}lSL), \qquad \text{(IV)}$$

$$(l^3\alpha SL|G|(ll_a)S'L'l_bSL). \qquad \text{(V)}$$

Of type $(2|G|2)$ we have

$$(l_a^2(S_aL_a)l_cSL|G|l_a'^2(S_a'L_a')l_c'SL), \qquad \text{(VI)}$$

$$(l_a^2(S_aL_a)l_cSL|G|l_a',l_c'^2(S_cL_c)SL). \qquad \text{(VII)}$$

Of type $(2|G|3)$ there is

$$(l_a^2(S_aL_a)l_cSL|G|(l_a'l_b')S_{ab}L_{ab}l_c'SL), \qquad \text{(VIII)}$$

and of type $(3|G|3)$

$$((l_al_b)S_{ab}L_{ab}l_cSL|G|(l_a'l_b')S_{ab}'L_{ab}'l_c'SL), \qquad \text{(IX)}$$

where l's with the same index letter may be equal but those with different index differ.

The following formulas indicate the main steps and the final explicit form of the matrix elements (I) to (IX) obtained by application of (10). The complete set of formulas is given even though (I), (II), and (III) are special cases (for $n=3$) of (33a, b, and c) of reference 7, and (VI) is a special case of (29). Antisymmetric states of type $|1)$ are represented in terms of fractional parentage, those of types $|2)$ and $|3)$ by formulas of the type (15). Numerical subscripts to quantum numbers l indicate the variable of the one-electron wave function with the given quantum number; thus, e.g., l_{a1}' indicates a wave function of electron 1 with quantum number l_a'.

I.

$$\begin{aligned}(l^3\alpha'SL|G|l^3\alpha SL) &= \sum_{\bar S'\bar L'SL} (l^3\alpha'SL\{\!|l^2(\bar S'\bar L')lSL)(l^2(\bar S'\bar L')lSL|G|l^2(\bar S\bar L)lSL)(l^2(\bar S\bar L)lSL|\!\}l^3\alpha SL)\\ &= 3\sum_{\bar S'\bar L'\bar S\bar L} (l^3\alpha'SL\{\!|l^2(\bar S'\bar L')lSL)(l_1l_2(\bar S'\bar L')l_3SL|g_{12}|l_1l_2(\bar S\bar L)l_3SL)(l^2(\bar S\bar L)lSL|\!\}l^3\alpha SL)\\ &= 3\sum_{k\bar S\bar L} (l^3\alpha'SL\{\!|l^2(\bar S\bar L)lSL)R^k(l^2,l^2)(l\|C^{[k]}\|l)^2 \exp[\pi i(\bar L)]\bar W\begin{pmatrix} l & k & l\\ l & \bar L & l\end{pmatrix}(l^2(\bar S\bar L)lSL|\!\}l^3\alpha SL),\end{aligned}$$

since

$$\begin{aligned}&(l_1l_2(\bar S'\bar L')l_3SL|g_{12}|l_1l_2(\bar S\bar L)l_3SL)\\ &\quad=\sum_k R^k(l^2,l^2)(2l+1)^{-1}(l\|C^{[k]}\|l)^2\big(((l_1k)ll_2)\bar L'l_3|(l_1(kl_2)l)\bar Ll_3\big)^{(L)}((s_1s_2)\bar S's_3|(s_1s_2)\bar Ss_3)^{(S)}\\ &\quad=\sum_k \exp[\pi i(k+\bar L)]R^k(l^2,l^2)(l\|C^{[k]}\|l)^2\bar W\begin{pmatrix} l & k & l\\ l & \bar L & l\end{pmatrix}\delta(\bar L\bar L')\delta(\bar S\bar S'),\end{aligned}$$

and k must be even.

II.

$$\begin{aligned}(l^3\alpha SL|G|l^2(S'L')l'SL) &= 2\sqrt{3}\sum_{\bar S\bar L}(l^3\alpha SL\{\!|l,l^2(\bar S\bar L)SL)(l_1,l_2l_3(\bar S\bar L),SL|g_{23}|l_1l_2(S'L')l'_3SL)\\ &= 2\sqrt{3}\sum_{k\bar S\bar L}(l^3\alpha SL\{\!|l,l^2(\bar S\bar L)SL)R^k(l^2,ll')[(2l+1)(2l'+1)]^{-1/2}(l\|C^{[k]}\|l)(l\|C^{[k]}\|l')\\ &\qquad\times\big(l_1((l_2k)ll_3)\bar L|(l_1l_2)L'(kl_3)l'\big)^{(L)}(s_1(s_2s_3)\bar S|(s_1s_2)S's_3)^{(S)}\\ &= 2\sqrt{3}\sum_{k\bar S\bar L}(l^3\alpha SL\{\!|l,l^2(\bar S\bar L)SL)R^k(l^2,ll')(l\|C^{[k]}\|l)(l\|C^{[k]}\|l')\exp[\pi i(l+\bar L+L+\tfrac{3}{2}+S)]\\ &\qquad\times[(2L'+1)(2\bar L+1)(2S'+1)(2\bar S+1)]^{1/2}\bar W\begin{pmatrix} l & k & l\\ l & \bar L & l'\end{pmatrix}\bar W\begin{pmatrix} l & l & L'\\ l' & L & \bar L\end{pmatrix}\bar W\begin{pmatrix} \frac12 & \frac12 & S'\\ \frac12 & S & \bar S\end{pmatrix}.\end{aligned}$$

III.

$$\begin{aligned}(l^3\alpha SL|G|l,l'^2(S'L')SL) &= \sqrt{3}\sum_{\bar S\bar L}(l^3\alpha SL\{\!|ll^2(\bar S\bar L)SL)(l_3,l_1l_2(\bar S\bar L)SL|g_{12}|l_3,l'_1l'_2(S'L')SL)\\ &= \sqrt{3}(l^3\alpha SL\{\!|ll^2(S'L')SL)(-1)^{L'}\sum_k R^k(l^2,l'^2)(l\|C^{[k]}\|l')^2\bar W\begin{pmatrix} l' & k & l\\ l & L' & l'\end{pmatrix}.\end{aligned}$$

IV.

$$
\begin{aligned}
(l^3\alpha SL|G|l_al_b(S_{ab}L_{ab})lSL) &= (2\times 3)^{1/2}\sum_{\bar S\bar L}(l^3\alpha SL\{|l^2(\bar S\bar L)lSL)\big(l_1l_2(\bar S\bar L)l_3SL|g_{12}|l_{a1}l_{b2}(S_{ab}L_{ab})l_3SL\big)\\
&= 6^{1/2}\sum_{\bar S\bar L}(l^3\alpha SL\{|l^2(\bar S\bar L)lSL)\sum_k R^k(l^2,l_al_b)[(2l+1)(2l_b+1)]^{-1/2}(l\|C^{[k]}\|l_a)(l\|C^{[k]}\|l_b)\\
&\qquad\times\big(((l_{a1}k)ll_2)\bar L l_3|(l_{a1}(kl_2)l_b)L_{ab}l_3\big)^{(L)}\big((s_1s_2)\bar S s_3|(s_1s_2)S_{ab}s_3\big)^{(S)}\\
&= 6^{1/2}(-1)^{L_{ab}}(l^3\alpha SL\{|l^2(S_{ab}L_{ab})lSL)\sum_k R^k(l^2,l_al_b)(l\|C^{[k]}\|l_a)(l\|C^{[k]}\|l_b)\overline{W}\begin{pmatrix}l_a & k & l\\ l & L_{ab} & l_b\end{pmatrix}.
\end{aligned}
$$

V.

$$
\begin{aligned}
(l^3\alpha SL|G|ll_a(S'L')l_bSL) &= 6^{1/2}\sum_{\bar S\bar L}(l^3\alpha SL\{|ll^2(\bar S\bar L)SL)\big(l_1(l_2l_3)\bar S\bar L SL|g_{23}|(l_1l_{a2})S'L'l_{b3}SL\big)\\
&= 6^{1/2}\sum_{k\bar S\bar L}(l^3\alpha SL\{|ll^2(\bar S\bar L)SL)R^k(l^2,l_al_b)[(2l+1)(2l_b+1)]^{-1/2}(l\|C^{[k]}\|l_a)(l\|C^{[k]}\|l_b)\\
&\qquad\times\big(l_1((l_{a2}k)ll_3)\bar L|(l_1l_{a2})L'(kl_3)l_b\big)^{(L)}\big(s_1(s_2s_3)\bar S|(s_1s_2)S's_3\big)^{(S)}\\
&= 6^{1/2}\sum_{k\bar S\bar L}(l^3\alpha SL\{|ll^2(\bar S\bar L)SL)R^k(l^2,l_al_b)(l\|C^{[k]}\|l_a)(l\|C^{[k]}\|l_b)\exp[\pi i(\bar L+l+\tfrac{3}{2}+L+S)]\\
&\qquad\times[(2L'+1)(2S'+1)(2\bar L+1)(2\bar S+1)]^{1/2}\overline{W}\begin{pmatrix}l_a & k & l\\ l & \bar L & l_b\end{pmatrix}\overline{W}\begin{pmatrix}l & l_a & L'\\ l_b & L & \bar L\end{pmatrix}\overline{W}\begin{pmatrix}\frac12 & \frac12 & S'\\ \frac12 & S & \bar S\end{pmatrix}.
\end{aligned}
$$

VI.

$$
\begin{aligned}
&(l_a^2(S_aL_a)l_cSL|G|l_a'^2(S_a'L_a')l_c'SL)\\
&= \sum_k R^k(l_a^2,l_a'^2)\delta(l_cl_c')[(2l_a+1)(2l_a'+1)]^{-1/2}(l_a\|C^{[k]}\|l_a')^2\big(((l_a'{}_1k)l_al_{a2})L_al_{c3}|(l_a'{}_1(kl_{a2})l_a')L_a'l_{c3}\big)^{(L)}\\
&\quad\times((s_1s_2)S_as_3|(s_1s_2)S_a's_3)^{(S)}+2\sum_k R^k(l_al_c,l_a'l_c')\delta(l_al_a')[(2l_a+1)(2l_c'+1)]^{-1/2}(l_a\|C^{[k]}\|l_a')(l_c\|C^{[k]}\|l_c')\\
&\quad\times\big(((l_a'{}_2k)l_al_{a3})L_al_{c1}|(l_a'{}_2l_a'{}_3)L_a'(kl_{c1})l_c'\big)^{(L)}((s_2s_3)S_as_1|(s_2s_3)S_a's_1)^{(S)}+2\sum_k R^k(l_al_c,l_c'l_a')\delta(l_al_a')[(2l_c+1)\\
&\quad\times(2l_c'+1)]^{-1/2}(l_c\|C^{[k]}\|l_a')(l_a\|C^{[k]}\|l_c')((l_{a2}l_{a3})L_a(l_a'{}_1k)l_c|(l_{a3}l_a'{}_1)L_a'(kl_{a2})l_c')^{(L)}((s_2s_3)S_as_1|(s_3s_1)S_a's_2)^{(S)}\\
&= \sum_k R^k(l_a^2,l_a'^2)\delta(l_cl_c')(l_a\|C^{[k]}\|l_a')^2(-1)^{L_a}\overline{W}\begin{pmatrix}l_a' & k & l_a\\ l_a & L_a & l_a'\end{pmatrix}\delta(L_aL_a')\delta(S_aS_a')+2\sum_k R^k(l_al_c,l_al_c')\delta(l_al_a')\\
&\quad\times(l_a\|C^{[k]}\|l_a')(l_c\|C^{[k]}\|l_c')(-1)^{l_c+L}[(2L_a+1)(2L_a'+1)]^{1/2}\overline{W}\begin{pmatrix}l_a & l_a & L_a'\\ k & L_a & l_a\end{pmatrix}\overline{W}\begin{pmatrix}L_a' & k & L_a\\ l_c & L & l_c'\end{pmatrix}\delta(S_aS_a')\\
&\quad+2\sum_k R^k(l_al_c,l_c'l_a')\delta(l_al_a')(l_c\|C^{[k]}\|l_a')(l_a\|C^{[k]}\|l_c')(-1)^{-S_a+S_a'}\\
&\qquad\times[(2S_a+1)(2L_a+1)(2S_a'+1)(2L_a'+1)]^{1/2}X\begin{bmatrix}l_a & l_a & L_a\\ l_a & k & l_c\\ L_a' & l_c' & L\end{bmatrix}\overline{W}\begin{pmatrix}\frac12 & \frac12 & S_a\\ \frac12 & S & S_a'\end{pmatrix}.
\end{aligned}
$$

VII.

$$
\begin{aligned}
&(l_a^2(S_aL_a)l_cSL|G|l_a',l_c'^2(S_cL_c)SL)\\
&= 2\sum_k R^k(l_a^2,l_a'l_c)\delta(l_cl_c')[(2l_a+1)(2l_c+1)]^{-1/2}(l_a\|C^{[k]}\|l_a')(l_a\|C^{[k]}\|l_c)\\
&\qquad\times\big(((l_a'{}_1k)l_al_{a2})L_al_{c3}|l_a'{}_1((kl_{a2})l_cl_{c3})L_c\big)^{(L)}((s_1s_2)S_as_3|s_1(s_2s_3)S_c)^{(S)}\\
&\qquad+2\sum_k R^k(l_al_c,l_c'^2)\delta(l_al_a')[(2l_a+1)(2l_c'+1)]^{-1/2}(l_a\|C^{[k]}\|l_c')(l_c\|C^{[k]}\|l_c')\\
&\qquad\times\big(l_{a3}(l_{c1}'k)l_a)L_al_{c2}|l_{a3}(l_{c1}'(kl_{c2})l_c')L_c\big)^{(L)}((s_3s_1)S_as_2|s_3(s_1s_2)S_c)^{(S)}
\end{aligned}
$$

$$=2\sum_k R^k(l_a{}^2,l_a'l_c)\delta(l_cl_c')(l_a\|C^{[k]}\|l_a')(l_a\|C^{[k]}\|l_c)(-1)^{l_a'+L_a+L+\frac{1}{2}+S}$$

$$\times[(2S_a+1)(2S_c+1)(2L_a+1)(2L_c+1)]^{1/2}\bar{W}\begin{pmatrix}l_a' & l_c & L_a\\ l_c & L & L_c\end{pmatrix}\bar{W}\begin{pmatrix}l_a' & k & l_a\\ l_a & L_a & l_c\end{pmatrix}\bar{W}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & S_a\\ \frac{1}{2} & S & S_c\end{pmatrix}$$

$$+2\sum_k R^k(l_al_c,l_c'^2)\delta(l_al_a')(l_a\|C^{[k]}\|l_c')(l_c\|C^{[k]}\|l_c')(-1)^{l_c+L_c+L+\frac{1}{2}+S}$$

$$\times[(2S_a+1)(2S_c+1)(2L_a+1)(2L_c+1)]^{1/2}\bar{W}\begin{pmatrix}l_a & l_a & L_a\\ l_c & L & L_c\end{pmatrix}\bar{W}\begin{pmatrix}l_c' & k & l_a\\ l_c & L_c & l_c'\end{pmatrix}\bar{W}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & S_a\\ \frac{1}{2} & S & S_c\end{pmatrix}.$$

VIII.

$$(l_a{}^2(S_aL_a)l_cSL|G|l_a'l_b'(S_{ab}'L_{ab}')l_c'SL)$$

$$=\sqrt{2}\sum_k R^k(l_a{}^2,l_a'l_b')\delta(l_cl_c')[(2l_a+1)(2l_b'+1)]^{-1/2}(l_a\|C^{[k]}\|l_a')(l_a\|C^{[k]}\|l_b')$$

$$\times\big(((l_a'{}_1k)l_al_{a2})L_al_{c3}|(l_a'{}_1(kl_{a2})l_b')L_{ab}'l_{c3}\big)^{(L)}((s_1s_2)S_as_3|(s_1s_2)S_{ab}'s_3)^{(S)}$$

$$+\sqrt{2}\sum_k R^k(l_al_c,l_b'l_c')\delta(l_al_a')[(2l_a+1)(2l_c'+1)]^{-1/2}(l_a\|C^{[k]}\|l_b')(l_c\|C^{[k]}\|l_c')$$

$$\times\big((l_{a3}(l_b'{}_2k)l_a)L_al_{c1}|(l_{a3}l_b'{}_2)L_{ab}'(kl_{c1})l_c'\big)^{(L)}((s_3s_2)S_as_1|(s_3s_2)S_{ab}'s_1)^{(S)}$$

$$+\sqrt{2}\sum_k R^k(l_al_c,l_c'l_b')\delta(l_al_a')[(2l_c+1)(2l_c'+1)]^{-1/2}(l_c\|C^{[k]}\|l_b')(l_a\|C^{[k]}\|l_c')$$

$$\times((l_{a2}l_{a3})L_a(l_b'{}_1k)l_c|(l_{a3}l_b'{}_1)L_{ab}'(kl_{a2})l_c')^{(L)}((s_2s_3)S_as_1|(s_3s_1)S_{ab}'s_2)^{(S)}$$

$$=\sqrt{2}\sum_k R^k(l_a{}^2,l_a'l_b')\delta(l_cl_c')(l_a\|C^{[k]}\|l_a')(l_a\|C^{[k]}\|l_b')(-1)^{L_a}\bar{W}\begin{pmatrix}l_a' & k & l_a\\ l_a & L_a & l_b'\end{pmatrix}\delta(L_aL_{ab}')\delta(S_aS_{ab}')$$

$$+\sqrt{2}\sum_k R^k(l_al_c,l_b'l_c')\delta(l_al_a')(l_a\|C^{[k]}\|l_b')(l_c\|C^{[k]}\|l_c')(-1)^{l_c'+L_a+L+L_{ab}'}$$

$$\times[(2L_a+1)(2L_{ab}'+1)]^{1/2}\bar{W}\begin{pmatrix}l_a & l_b' & L_{ab}'\\ k & L_a & l_a\end{pmatrix}\bar{W}\begin{pmatrix}L_{ab}' & k & L_a\\ l_c & L & l_c'\end{pmatrix}\delta(S_aS_{ab}')$$

$$+\sqrt{2}\sum_k R^k(l_al_c,l_c'l_b')\delta(l_al_a')(l_c\|C^{[k]}\|l_b')(l_a\|C^{[k]}\|l_c')(-1)^{S_a+S_{ab}'}$$

$$\times[(2L_a+1)(2L_{ab}'+1)(2S_a+1)(2S_{ab}'+1)]^{1/2}X\begin{Bmatrix}l_a & l_a & L_a\\ l_b' & k & l_c\\ L_{ab}' & l_c' & L\end{Bmatrix}\bar{W}\begin{pmatrix}\frac{1}{2} & \frac{1}{2} & S_a\\ \frac{1}{2} & S & S_{ab}'\end{pmatrix}.$$

IX.

$$(l_al_b(S_{ab}L_{ab})l_cSL|G|l_a'l_b'(S_{ab}'L_{ab}')l_c'SL)$$

$$=(l_{a1}l_{b2}(S_{ab}L_{ab})l_{c3}SL|g_{12}|l_a'{}_1l_b'{}_2(S_{ab}'L_{ab}')l_c'{}_3SL)-(l_{a1}l_{b2}(S_{ab}L_{ab})l_{c3}SL|g_{12}|l_a'{}_2l_b'{}_1(S_{ab}'L_{ab}')l_c'{}_3SL)$$

$$+(l_{a1}l_{b2}(S_{ab}L_{ab})l_{c3}SL|g_{23}|l_a'{}_1l_b'{}_2(S_{ab}'L_{ab}')l_c'{}_3SL)-(l_{a1}l_{b2}(S_{ab}L_{ab})l_{c3}SL|g_{23}|l_a'{}_1l_b'{}_3(S_{ab}'L_{ab}')l_c'{}_2SL)$$

$$+(l_{a1}l_{b2}(S_{ab}L_{ab})l_{c3}SL|g_{31}|l_a'{}_1l_b'{}_2(S_{ab}'L_{ab}')l_c'{}_3SL)-(l_{a1}l_{b2}(S_{ab}L_{ab})l_{c3}SL|g_{31}|l_a'{}_3l_b'{}_2(S_{ab}'L_{ab}')l_c'{}_1SL)$$

$$=\sum_k R^k(l_al_b,l_a'l_b')\delta(l_cl_c')[(2l_a+1)(2l_b'+1)]^{-1/2}(l_a\|C^{[k]}\|l_a')(l_b\|C^{[k]}\|l_b')$$

$$\times\big(((l_a'{}_1k)l_al_{b2})L_{ab}l_{c3}|(l_a'{}_1(kl_{b2})l_b')L_{ab}'l_{c3}\big)^{(L)}((s_1s_2)S_{ab}s_3|(s_1s_2)S_{ab}'s_3)^{(S)}$$

$$-\sum_k R^k(l_al_b,l_b'l_a')\delta(l_cl_c')[(2l_a+1)(2l_a'+1)]^{-1/2}(l_a\|C^{[k]}\|l_b')(l_b\|C^{[k]}\|l_a')$$

$$\times\big(((l_b'{}_1k)l_al_{b2})L_{ab}l_{c3}|((kl_{b2})l_a'l_b'{}_1)L_{ab}'l_c'{}_3\big)^{(L)}((s_1s_2)S_{ab}s_3|(s_2s_1)S_{ab}'s_3)^{(S)}$$

$$+\sum_k R^k(l_bl_c,l_b'l_c')\delta(l_al_a')[(2l_b+1)(2l_c'+1)]^{-1/2}(l_b\|C^{[k]}\|l_b')(l_c\|C^{[k]}\|l_c')$$

$$\times\big((l_{a1}(l_b'{}_2k)l_b)L_{ab}l_{c3}|(l_{a1}l_b'{}_2)L_{ab}'(kl_{c3})l_c'\big)^{(L)}((s_1s_2)S_{ab}s_3|(s_1s_2)S_{ab}'s_3)^{(S)}$$

$$-\sum_k R^k(l_cl_b,l_b'l_c')\delta(l_al_a')[(2l_c+1)(2l_c'+1)]^{-1/2}(l_c\|C^{[k]}\|l_b')(l_b\|C^{[k]}\|l_c')$$

$$\times((l_{a1}l_{b2})L_{ab}(l_b{}'_3k)l_c|(l_{a1}l_b{}'_3)L_{ab}{}'(kl_{b2})l_c{}')^{(L)}((s_1s_2)S_{ab}s_3|(s_1s_3)S_{ab}{}'s_2)^{(S)}$$

$$+\sum_k R^k(l_cl_a,l_c{}'l_a{}')\delta(l_bl_b{}')[(2l_c+1)(2l_a{}'+1)]^{-1/2}(l_c\|C^{[k]}\|l_c{}')(l_a\|C^{[k]}\|l_a{}')$$

$$((l_{a1}l_{b2})L_{ab}(l_c{}'_3k)l_c|((kl_{a1})l_a{}'l_{b2})L_{ab}{}'l_c{}'_3)^{(L)}((s_1s_2)S_{ab}s_3|(s_1s_2)S_{ab}{}'s_3)^{(S)}$$

$$-\sum_k R^k(l_cl_a,l_a{}'l_c{}')\delta(l_bl_b{}')[(2l_c+1)(2l_c{}'+1)]^{-1/2}(l_c\|C^{[k]}\|l_a{}')(l_a\|C^{[k]}\|l_c{}')$$

$$\times((l_{a1}l_{b2})L_{ab}(l_a{}'_3k)l_c|(l_a{}'_3l_b{}'_2)L_{ab}{}'(kl_{a1})l_c{}')^{(L)}((s_1s_2)S_{ab}s_3|(s_3s_2)S_{ab}{}'s_1)^{(S)}$$

$$=\sum_k R^k(l_al_b,l_a{}'l_b{}')\delta(l_cl_c{}')(l_a\|C^{[k]}\|l_a{}')(l_b\|C^{[k]}\|l_b{}')(-1)^{l_a+l_b+L_{ab}}\overline{W}\begin{pmatrix} l_a & l_a{}' & k \\ l_b{}' & l_b & L_{ab}\end{pmatrix}\delta(L_{ab}L_{ab}{}')\delta(S_{ab}S_{ab}{}')$$

$$+\sum_k R^k(l_al_b,l_b{}'l_a{}')\delta(l_cl_c{}')(l_a\|C^{[k]}\|l_b{}')(l_b\|C^{[k]}\|l_a{}')(-1)^{S_{ab}}\overline{W}\begin{pmatrix} l_a & l_b{}' & k \\ l_a{}' & l_b & L_{ab}\end{pmatrix}\delta(L_{ab}L_{ab}{}')\delta(S_{ab}S_{ab}{}')$$

$$+\sum_k R^k(l_bl_c,l_b{}'l_c{}')\delta(l_al_a{}')(l_b\|C^{[k]}\|l_b{}')(l_c\|C^{[k]}\|l_c{}')(-1)^{l_a+l_b+l_c{}'+L_{ab}+L_{ab}{}'+L}$$

$$\times[(2L_{ab}+1)(2L_{ab}{}'+1)]^{1/2}\overline{W}\begin{pmatrix} k & L_{ab} & L_{ab}{}' \\ L & l_c{}' & l_c\end{pmatrix}\overline{W}\begin{pmatrix} k & L_{ab} & L_{ab}{}' \\ l_a & l_b{}' & l_b\end{pmatrix}\delta(S_{ab}S_{ab}{}')$$

$$+\sum_k R^k(l_bl_c,l_c{}'l_b{}')\delta(l_al_a{}')(l_c\|C^{[k]}\|l_b{}')(l_b\|C^{[k]}\|l_c{}')(-1)^{S_{ab}+S_{ab}{}'}$$

$$\times[(2L_{ab}+1)(2L_{ab}{}'+1)(2S_{ab}+1)(2S_{ab}{}'+1)]^{1/2}\overline{W}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & S_{ab} \\ \frac{1}{2} & S & S_{ab}{}'\end{pmatrix}X\begin{bmatrix} l_a & l_b & L_{ab} \\ l_b{}' & k & l_c \\ L_{ab}{}' & l_c{}' & L\end{bmatrix}$$

$$+\sum_k R^k(l_cl_a,l_c{}'l_a{}')\delta(l_bl_b{}')(l_c\|C^{[k]}\|l_c{}')(l_a\|C^{[k]}\|l_a{}')(-1)^{l_a+l_b-l_c+L}$$

$$\times[(2L_{ab}+1)(2L_{ab}{}'+1)]^{1/2}\overline{W}\begin{pmatrix} k & L_{ab} & L_{ab}{}' \\ L & l_c{}' & l_c\end{pmatrix}\overline{W}\begin{pmatrix} k & L_{ab} & L_{ab}{}' \\ l_b & l_a{}' & l_a\end{pmatrix}\delta(S_{ab}S_{ab}{}')$$

$$+\sum_k R^k(l_cl_a,l_a{}'l_c{}')\delta(l_bl_b{}')(l_c\|C^{[k]}\|l_a{}')(l_a\|C^{[k]}\|l_c{}')(-1)^{l_c+l_c{}'+L_{ab}+L_{ab}{}'}$$

$$\times[(2L_{ab}+1)(2L_{ab}{}'+1)(2S_{ab}+1)(2S_{ab}{}'+1)]^{1/2}X\begin{bmatrix} l_b & l_a & L_{ab} \\ l_a{}' & k & l_c \\ L_{ab}{}' & l_c{}' & L\end{bmatrix}\overline{W}\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & S_{ab} \\ \frac{1}{2} & S & S_{ab}{}'\end{pmatrix}.$$

5. EXTENSION OF EQUATION (10)

The matrix elements of nonscalar products of tensorial sets of operators, such as the product $[\mathfrak{S}^{[k_1]}\times\mathfrak{T}^{[k_2]}]^{[k]}$ considered in FR Chap. 15, are given by a formula analogous to (10). An operator of this product set is

$$[\mathfrak{S}^{[k_1]}\times\mathfrak{T}^{[k_2]}]^{[k]}{}_q=\sum_{q_1q_2}\mathfrak{S}^{[k_1]}{}_{q_1}\mathfrak{T}^{[k_2]}{}_{q_2}(k_1q_1k_2q_2|k_1k_2kq). \tag{32}$$

We may factor out this operator by introducing wave functions of two mock particles, $\mathfrak{u}^{[k_1]}{}_{q_1}(\kappa_1)$ and $\mathfrak{u}^{[k_2]}{}_{q_2}(\kappa_2)$, with angular momenta k_1 and k_2, as well as wave functions $\mathfrak{u}^{[k_1k_2,k]}{}_q(\kappa_1,\kappa_2)$ of the same particles coupled in a state with angular momentum k. The Wigner coefficient in (32) can now be represented, in the notation of (4), by $\mathfrak{u}^{[k_1]*}{}_{q_1}\mathfrak{u}^{[k_2]*}{}_{q_2}\mathfrak{u}^{[k_1k_2,k]}{}_q$, from which follows

$$[\mathfrak{S}^{[k_1]}\times\mathfrak{T}^{[k_2]}]^{[k]}{}_q=[\mathfrak{S}^{[k]}\mathfrak{u}^{[k_1]*}(\kappa_1)][\mathfrak{T}^{[k_2]}\mathfrak{u}^{[k_2]*}(\kappa_2)]\mathfrak{u}^{[k_1k_2,k]}{}_q(\kappa_1,\kappa_2), \tag{33}$$

where integration over κ_1 and κ_2 is implied as in (3′) and (5). Both operators $\mathfrak{S}^{[k_1]}\mathfrak{u}^{[k_1]*}$ and $\mathfrak{T}^{[k_2]}\mathfrak{u}^{[k_2]*}$ may be applied to the complex conjugate of (8), using (9) twice to yield the analog of (9)

$$\Psi^*(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots,\lambda_tj_t,\cdots;JM)\mathfrak{S}^{[k_1]}\mathfrak{u}^{[k_1]*}\mathfrak{T}^{[k_2]}\mathfrak{u}^{[k_2]*}$$
$$=(2j_s+1)^{-1/2}(2j_t+1)^{-1/2}\sum_{\lambda_s{}''j_s{}''\lambda_t{}''j_t{}''}(\lambda_sj_s\|S^{[k_1]}\|\lambda_s{}''j_s{}'')(\lambda_tj_t\|T^{[k_2]}\|\lambda_t{}''j_t{}'')$$
$$\times\Psi^*(\lambda_1j_1,\cdots,(\lambda_s{}''j_s{}'',k_1)j_s,\cdots,(\lambda_t{}''j_t{}'',k_2)j_t,\cdots;JM). \tag{34}$$

The wave function $\mathfrak{u}^{[k_1k_2,k]}{}_q$ from (33) may be multiplied with a wave function (8) and expanded into coupled wave functions

$$\mathfrak{u}^{[k_1k_2,k]}{}_q\Psi(\lambda_1'j_1',\cdots,\lambda_s'j_s',\cdots,\lambda_t'j_t',\cdots;J'M')$$
$$=\sum_{J''M''}\Psi((\lambda_1'j_1',\cdots,\lambda_s'j_s',\cdots,\lambda_t'j_t',\cdots)J',(k_1k_2)k;J''M'')(J'kJ''M''|J'M'kq). \quad (35)$$

Multiplication of (34) and (35) in analogy with the multiplication of (9) and (9′), with integration over the variables and consideration of the orthonormality condition, yields the matrix element

$$(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots,\lambda_tj_t,\cdots;JM|[\mathfrak{S}^{[k_1]}\times\mathfrak{T}^{[k_2]}]^{[k]}{}_q|\lambda_1j_1,\cdots,\lambda_s'j_s',\cdots,\lambda_t'j_t',\cdots;J'M')$$
$$=[(2j_s+1)(2j_t+1)]^{-1/2}(\lambda_sj_s\|S^{[k_1]}\|\lambda_s'j_s')(\lambda_tj_t\|T^{[k_1]}\|\lambda_t'j_t')$$
$$\times(j_1,\cdots,(j_s'k_1)j_s,\cdots,(j_t'k_2)j_t,\cdots|(j_1,\cdots,j_s',\cdots j_t',\cdots)J'(k_1k_2)k)^{(J)}(J'kJM|J'M'kq). \quad (36)$$

The reduced matrix element of the operator product is then, according to the definition (FR 14.4),

$$(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots,\lambda_tj_t,\cdots;J\|[\mathfrak{S}^{[k_1]}\times\mathfrak{T}^{[k_2]}]^{[k]}\|\lambda_1j_1,\cdots,\lambda_s'j_s',\cdots,\lambda_t'j_t',\cdots;J')$$
$$=[(2J+1)/(2j_s+1)(2j_t+1)]^{1/2}(\lambda_sj_s\|S^{[k_1]}\|\lambda_s'j_s')(\lambda_tj_t\|T^{[k_2]}\|\lambda_t'j_t')$$
$$\times(j_1,\cdots,(j_s'k_1)j_s,\cdots,(j_t'k_2)j_t,\cdots|(j_1,\cdots j_s',\cdots,j_t',\cdots)J'(k_1k_2)k)^{(J)}. \quad (37)$$

Problems also occur where $\mathfrak{S}^{[k_1]}$ and $\mathfrak{T}^{[k_2]}$ operate on the same variable s rather than on two different variables s and t. Results analogous to (10) and (37) are then obtained, the main difference being than an intermediate state of the particle s occurs, whose quantum numbers λ_s'', j_s'' do not coincide with either λ_s, j_s or λ_s', j_s'. Therefore, a summation over λ_s'', j_s'' appears in the following formulas:

$$(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots;JM|\mathfrak{S}^{[k]}\cdot\mathfrak{T}^{[k]}|\lambda_1j_1,\cdots,\lambda_s'j_s',\cdots;J'M')$$
$$=[(2j_s+1)(2j_s'+1)]^{-1/2}\sum_{\lambda_s''j_s''}(\lambda_sj_s\|S^{[k]}\|\lambda_s''j_s'')(\lambda_s''j_s''\|T^{[k]}\|\lambda_s'j_s')$$
$$\times(j_1,\cdots,(j_s''k)j_s,\cdots|j_1,\cdots,(kj_s'')j_s',\cdots)^{(J)}\delta_{JJ'}\delta_{MM'}, \quad (38)$$

$$(\lambda_1j_1,\cdots,\lambda_sj_s,\cdots;J\|[\mathfrak{S}^{[k_1]}\times\mathfrak{T}^{[k_2]}]^{[k]}\|\lambda_1j_1,\cdots,\lambda_s'j_s',\cdots;J')$$
$$=[(2J+1)/(2j_s+1)(2j_s''+1)]^{1/2}\sum_{\lambda_s''j_s''}(\lambda_sj_s\|S^{[k_1]}\|\lambda_s''j_s'')(\lambda_s''j_s''\|T^{[k_2]}\|\lambda_s'j_s')$$
$$\times(j_1,\cdots,[(j_s'k_2)j_s''k_1]j_s,\cdots|(j_1,\cdots,j_s',\cdots)J'(k_1k_2)k)^{(J)}. \quad (39)$$

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