Microwave Zeeman Effect and Theory of Complex Spectra

F. R. INNES, *Air Force Cambridge Research Center, Bedford, Massachusetts*

AND

C. W. UFFORD, *University of Pennsylvania, Philadelphia, Pennsylvania*

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A treatment in spherical tensors of the microwave Zeeman interaction of Abragam, Kambe, and Van Vleck is given. A calculation of g factors in atomic oxygen is then made and the numerical values compared with those worked out previously. New methods and results are developed for finding matrix elements of one-particle and two-particle operators for wave functions which contain more than one group of equivalent particles. The generality of these results is such that they may be used in the various coupling schemes of atomic and nuclear shell models.

1. INTRODUCTION

THE development of the microwave Zeeman Hamiltonian in spherical tensors, described below in Secs. 2–4, leads to expressions for the pertinent operators which are easy to handle for particular systems and are at the same time free of the quantum numbers of such systems. Procedures are based upon the standard methods of Racah[1] and others.[2] The reader will recall that other interaction operators have been developed along similar lines during recent years,[3] with an expected advantage of ease of computation as compared with the methods to be found, for example, in the text of Condon and Shortley.[4]

In atomic systems, very little attention has been directed to interaction energies involving closed shells except for some Coulomb effects,[5] even though a level-dependent variation is to be found in the angular elements of the spin-other-orbit operator. Also such energies must be included in the two-particle Zeeman effects.[6] Basic approaches in this type of calculation have recently been set down by Elliott, Flowers, and Yanagawa,[7] among others, for the broad problem of elements diagonal in configuration and with wave functions comprising a number of groups of equivalent particles. Further developments are given in the Appendix to this paper. It has been found possible to reduce a number of these expressions to compact forms [see Eqs. (A2), (A6), and (A7)], without specifying a particular coupling scheme.

The application to the Zeeman effect is made in Sec. 5 and to the ground term of oxygen in Sec. 6. Minor corrections to the work of KVV show an improvement in theoretical results over against the available experimental results.[8] It is hoped that the prospect of relatively simple procedures held forth by the formulas derived below will lead to new laboratory determinations of Zeeman splitting. Hartree's atomic units, described in TAS, Appendix,[4] have been used throughout this work.

2. MICROWAVE ZEEMAN HAMILTONIAN

The derivation of the operator is discussed in AVV and KVV.[6] Five parts are distinguished, as follows:

$$\begin{aligned}
\delta Z_{1,2} &= -\tfrac{1}{2}\alpha^3 \textstyle\sum_i \{\mathbf{H}\cdot(\mathbf{l}_i+2\mathbf{s}_i)T_i + Z[\nabla_i(r_i^{-1})\times\mathbf{A}_i]\cdot\mathbf{s}_i\},\\
\delta Z_{3,4} &= +\alpha^3 \textstyle\sum_{i<j}[\nabla_i(r_{ij}^{-1})\times\mathbf{A}_i]\cdot(\mathbf{s}_i+2\mathbf{s}_j), \qquad (1)\\
\delta Z_5 &= -\alpha^3 \textstyle\sum_{i<j}[r_{ij}^{-1}(\mathbf{A}_i\cdot\mathbf{p}_j)+r_{ij}^{-3}(\mathbf{r}_{ij}\cdot\mathbf{A}_i)(\mathbf{r}_{ij}\cdot\mathbf{p}_j)].
\end{aligned}$$

This will now be considered in the form $\delta Z=\mathbf{H}\cdot\delta\mathfrak{y}$. The field, $\mathbf{H}$, is recoupled to the left side of each expression after replacing the potential $\mathbf{A}_i$ by the value $\frac{1}{2}\mathbf{H}\times\mathbf{r}_i$. The moments are

$$\begin{aligned}
\delta\mathfrak{y}_{1,2} &= -\tfrac{1}{2}\alpha^3 \textstyle\sum_i \{(\mathbf{l}_i+2\mathbf{s}_i)T_i - \tfrac{1}{2}Z[\mathbf{s}_i\times\nabla_i(r_i^{-1})]\times\mathbf{r}_i\},\\
\delta\mathfrak{y}_{3,4} &= -\tfrac{1}{2}\alpha^3 \textstyle\sum_{i<j}[(\mathbf{s}_i+2\mathbf{s}_j)\times\nabla_i(r_{ij}^{-1})]\times\mathbf{r}_i, \qquad (2)\\
\delta\mathfrak{y}_5 &= -\tfrac{1}{2}\alpha^3 \textstyle\sum_{i<j}[r_{ij}^{-1}(\mathbf{r}_i\times\mathbf{p}_j)+r_{ij}^{-3}(\mathbf{r}_i\times\mathbf{r}_j)(\mathbf{r}_{ij}\cdot\mathbf{p}_j)].
\end{aligned}$$

The orbital parts of these moments will be expressed in terms of operator forms $\mathbf{C}^{(k)}$, $(\mathbf{C}^{(k)}\mathbf{l})^{(k')}$ and radial operators in r_i and r_j in this and in the following two sections. A standard concise notation for the generalized

[1] G. Racah, Phys. Rev. **62**, 438 (1942); **63**, 367 (1943), denoted RII and RIII, respectively.

[2] Among others, the papers of J. P. Elliott, Proc. Roy. Soc. (London) **A218**, 345 (1953); Biedenharn, Blatt, and Rose, Revs. Modern Phys. **24**, 249 (1952); Arima, Horie, and Tanabe, Progr. Theoret. Phys. Japan **11**, 143 (1954), are useful and give further references.

[3] Five such studies, of spin-dependent interactions, are those of J. Hope and L. W. Longdon, Phys. Rev. **102**, 1124 (1956); H. Horie, Progr. Theoret. Phys. Japan **10**, 296 (1953); I. Talmi, Phys. Rev. **89**, 1065 (1953). F. R. Innes, Phys. Rev. **91**, 31 (1953); R. E. Trees, Phys. Rev. **92**, 308 (1953).

[4] E. U. Condon and G. H. Shortley, *The Theory of Atomic Spectra* (Cambridge University Press, New York, 1951), denoted TAS.

[5] TAS 9[6]. For other effects involving closed shells, see G. Araki, Proc. Phys.-Math. Soc. Japan **19**, 592 (1937), also T. Yamanouchi and H. Horie, J. Phys. Soc. Japan **7**, 52 (1952).

[6] A. Abragam and J. H. Van Vleck, Phys. Rev. **92**, 1448 (1953); K. Kambe and J. H. Van Vleck, Phys. Rev. **96**, 66 (1954), denoted AVV and KVV, respectively. In this work, intergroup effects are of the same order of magnitude as intragroup effects (see Table II of KVV).

[7] Reference 2, above; J. P. Elliott and B. H. Flowers, Proc. Roy. Soc. (London) **A229**, 536 (1955); S. Yanagawa, J. Phys. Soc. Japan **8**, 302 (1953).

[8] E. B. Rawson and R. Beringer, Phys. Rev. **88**, 677 (1952).

product of two or more spherical tensors is used throughout. Composite one-particle and two-particle operators are initially distinguished through the use of parentheses and curly brackets, respectively [see also Innes, reference 3, Eqs. (2) and (11)].

The one-particle interactions require little treatment. The best value of the kinetic energy, T, is found in AVV and KVV. The orbital operator in $\delta\mathfrak{y}_2$ is

$$-r_i^{-1}(\mathbf{s}_i\times\mathbf{C}_i^{(1)})\times\mathbf{C}_i^{(1)}\equiv+2r_i^{-1}((\mathbf{s}\mathbf{C}^{(1)})_i^{(1)}\mathbf{C}_i^{(1)})^{(1)}$$
$$=+\tfrac{1}{3}r_i^{-1}[2\mathbf{s}_i+(\sqrt{2}\times\sqrt{5})(\mathbf{s}\mathbf{C}^{(2)})_i^{(1)}]. \quad (3)$$

Thus the one-particle moment operators are

$$\delta\mathfrak{y}_{1,2}=-\tfrac{1}{2}\alpha^3\sum_i[(\mathbf{l}_i+2\mathbf{s}_i)T_i$$
$$-\tfrac{1}{3}Zr_i^{-1}(\mathbf{s}_i+(\sqrt{\tfrac{5}{2}})(\mathbf{s}\mathbf{C}^{(2)})_i^{(1)})]. \quad (4)$$

3. TWO-PARTICLE SPIN-DEPENDENT INTERACTIONS

After recoupling the expression given in (2), it is found that

$$\delta\mathfrak{y}_{3,4}=+\tfrac{1}{2}\alpha^3\sum_{i<j}\{(\mathbf{s}_i+2\mathbf{s}_j)[-(2/\sqrt{3})\{\mathbf{r}_i\nabla_i(r_{ij}^{-1})\}^{(0)}$$
$$-\{\mathbf{r}_i\nabla_i(r_{ij}^{-1})\}^{(1)}+(5/3)^{\frac{1}{2}}\{\mathbf{r}_i\nabla_i(r_{ij}^{-1})\}^{(2)}]\}^{(1)}. \quad (5)$$

The gradient which occurs here relates to the commutator of the linear momentum [see (9)] and the operand $1/r_{ij}$,

$$\nabla_i\left(\frac{1}{r_{ij}}\right)=+i\left[\mathbf{p}.\frac{1}{r_{ij}}\right]=\frac{\mathbf{r}_{ij}}{r_{ij}^3},$$

$$=-\frac{1}{\sqrt{3}}\sum_k(-)^k\left[\frac{r_i^{k-1}}{r_j^{k+1}}[k(2k-1)(2k+1)]^{\frac{1}{2}}\right.$$
$$\times\{\mathbf{C}_i^{(k-1)}\mathbf{C}_j^{(k)}\}^{(1)}+\frac{r_j^k}{r_i^{k+2}}[(k+1)(2k+1)(2k+3)]^{\frac{1}{2}}$$
$$\left.\times\{\mathbf{C}_i^{(k+1)}\mathbf{C}_j^{(k)}\}^{(1)}\right]. \quad (6)$$

A number of conventions which relate to radial operators have been introduced in this and like expressions to follow. In the expansion of the reciprocal distance in Legendre polynomials, the first (second) mode, $r_j\gtrless r_i(r_i\gtrless r_j)$, leads to the first (second) term of this equation. It is evidently clear, in each equation involving such an expansion [as in (8), (11), and (12) of this paper], which mode is in use. The explicit expression of the pertinent radial integrals proceeds in a standard way.[9] As an example, the radial element of $r_i^k r_j^{-k-1}$ is the integral $(ab|r_i^k r_j^{-k-1}|cd)$, or

$$\int_0^\infty dr_i\,R_{ia}r_i^kR_{ic}\int_{r_i}^\infty dr_j\frac{R_{jb}R_{jd}}{r_j^{k+1}}, \quad (7a)$$

and that of $r_j^k r_i^{-k-1}$ is

$$\int_0^\infty dr_i\frac{R_{ia}R_{ic}}{r_i^{k+1}}\int_0^{r_i}dr_j\,R_{jb}r_j^kR_{jd}. \quad (7b)$$

We have generally avoided the writing of radial operators in terms of $r_<$ and $r_>$ unless real conciseness is obtained by this means (compare KVV, Secs. II and III).

The final result for the two-particle spin-dependent interactions is

$$\delta\mathfrak{y}_{3,4}=+\alpha^3\sum_{i<j}\{(\mathbf{s}_i+2\mathbf{s}_j)\sum_k(-)^k(2k+1)^{\frac{1}{2}}\times\left[\frac{1}{3}\left(k\frac{r_i^k}{r_j^{k+1}}-(k+1)\frac{r_j^k}{r_i^{k+1}}\right)\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(0)}\right.$$
$$+\frac{[k(k+1)]^{\frac{1}{2}}}{2\sqrt{2}\sqrt{3}}\left(\frac{r_i^k}{r_j^{k+1}}+\frac{r_j^k}{r_i^{k+1}}\right)\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(1)}-\frac{[k(k+1)]^{\frac{1}{2}}}{6\sqrt{2}}\left(\left[\frac{2k+3}{2k-1}\right]^{\frac{1}{2}}\frac{r_i^k}{r_j^{k+1}}-\left[\frac{2k-1}{2k+3}\right]^{\frac{1}{2}}\frac{r_j^k}{r_i^{k+1}}\right)\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(2)}$$
$$\left.+\frac{[k(k-1)(2k-3)]^{\frac{1}{2}}}{2\sqrt{3}(2k-1)^{\frac{1}{2}}}\frac{r_i^k}{r_j^{k+1}}\{\mathbf{C}_i^{(k-2)}\mathbf{C}_j^{(k)}\}^{(2)}-\frac{[(k+1)(k+2)(2k+5)]^{\frac{1}{2}}}{2\sqrt{3}(2k+3)^{\frac{1}{2}}}\frac{r_j^k}{r_i^{k+1}}\{\mathbf{C}_i^{(k+2)}\mathbf{C}_j^{(k)}\}^{(2)}\right]\}^{(1)}. \quad (8)$$

4. TWO-PARTICLE SPIN-INDEPENDENT INTERACTION

First the linear momentum, found in (1), (2), and (6), is given the following form:

$$\mathbf{p}=i\sqrt{2}r^{-1}(\mathbf{C}^{(1)}\mathbf{l})^{(1)}-i\partial_r\mathbf{C}^{(1)}. \quad (9)$$

The first part of $\delta\mathfrak{y}_5$ then leads to the first two parts of (10), below. The vector operator in the second part of $\delta\mathfrak{y}_5$ can be altered, by replacing $\mathbf{r}_i\times\mathbf{r}_j$ by $-\mathbf{r}_{ij}\times\mathbf{r}_j$, and recoupled to yield the last four parts. Thus,

$$\frac{2\delta\mathfrak{y}_5}{\alpha^3}=-\frac{2r_i}{r_jr_{ij}}\{\mathbf{C}_i^{(1)}(\mathbf{C}^{(1)}\mathbf{l})_j^{(1)}\}^{(1)}+\sqrt{2}\frac{r_i}{r_{ij}}\partial_{r_j}\{\mathbf{C}_i^{(1)}\mathbf{C}_j^{(1)}\}^{(1)}-\frac{1}{3r_{ij}}\mathbf{l}_j$$
$$-\frac{\sqrt{5}}{2\sqrt{3}}\frac{1}{r_{ij}^3}(\{\mathbf{r}_{ij}\mathbf{r}_{ij}\}^{(2)}\mathbf{l}_j)^{(1)}-\frac{\sqrt{5}}{\sqrt{2}}\frac{1}{r_{ij}^3}(\{\mathbf{r}_{ij}\mathbf{r}_{ij}\}^{(2)}(\mathbf{C}^{(2)}\mathbf{l})_j^{(2)})^{(1)}+\frac{\sqrt{5}}{\sqrt{3}}\frac{r_j}{r_{ij}^3}(\{\mathbf{r}_{ij}\mathbf{r}_{ij}\}^{(2)}\mathbf{C}_j^{(2)})^{(1)}\partial_{r_j}. \quad (10)$$

[9] As in TAS 8[6].

After expansion of r_{ij}^{-3} and recoupling, the useful function of r_{ij} is the (symmetrical) form,

$$\frac{\{\mathbf{r}_{ij}\mathbf{r}_{ij}\}^{(2)}}{r_{ij}^3}=\frac{1}{\sqrt{5}}\sum_k(-)^k\left[\frac{(k+1)(2k+1)}{2k+3}\right]^{\frac{1}{2}}\left\{\frac{2\sqrt{2}}{\sqrt{3}}\left[\frac{k}{2k-1}\right]^{\frac{1}{2}}\left(\frac{r_i^k}{r_j^{k+1}}+\frac{r_j^k}{r_i^{k+1}}\right)\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(2)}\right.$$
$$\left.+[(k+2)(2k+5)]^{\frac{1}{2}}\left[\left(\frac{r_i^k}{r_j^{k+1}}-\frac{r_i^{k+2}}{r_j^{k+3}}\right)\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k+2)}\}^{(2)}+\left(\frac{r_j^k}{r_i^{k+1}}-\frac{r_j^{k+2}}{r_i^{k+3}}\right)\{\mathbf{C}_i^{(k+2)}\mathbf{C}_j^{(k)}\}^{(2)}\right]\right\}. \quad (11)$$

The moment $\delta\mathfrak{y}_5$ expressed in spherical tensors follows after some recouplings:

$$\delta\mathfrak{y}_5=+\frac{\alpha^3}{2\sqrt{3}}\sum_k(-)^k\left[\left(\frac{r_j^k}{r_i^{k+1}}+\frac{r_i^{k+2}}{r_j^{k+3}}\right)\left\{\left[\frac{k(k+3)}{2k+3}\right]^{\frac{1}{2}}[(2k+1)^{\frac{1}{2}}\{\mathbf{C}_i^{(k)}(\mathbf{C}^{(k)}\mathbf{l})_j^{(k)}\}^{(1)}\right.\right.$$
$$-(2k+5)^{\frac{1}{2}}\{\mathbf{C}_i^{(k+2)}(\mathbf{C}^{(k+2)}\mathbf{l})_j^{(k+2)}\}^{(1)}]-2\left[\frac{2k+1}{2k+3}\right]^{\frac{1}{2}}[(2k+1)^{\frac{1}{2}}\{\mathbf{C}_i^{(k)}(\mathbf{C}^{(k)}\mathbf{l})_j^{(k+1)}\}^{(1)}$$
$$\left.+\left[\frac{(k+1)(2k+5)}{k+2}\right]^{\frac{1}{2}}\{\mathbf{C}_i^{(k+2)}(\mathbf{C}^{(k)}\mathbf{l})_j^{(k+1)}\}^{(1)}]\right\}-\left(k\frac{r_j^k}{r_i^{k+1}}-(k+3)\frac{r_i^{k+2}}{r_j^{k+3}}\right)\frac{r_j\partial r_j}{2k+3}$$
$$\left.\times([k(k+1)(2k+1)]^{\frac{1}{2}}\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(1)}-[(k+2)(k+3)(2k+5)]^{\frac{1}{2}}\{\mathbf{C}_i^{(k+2)}\mathbf{C}_j^{(k+2)}\}^{(1)})\right]. \quad (12)$$

The tensor form $(\mathbf{C}^{(t-1)}\mathbf{l})^{(t)}$, which occurs here, is simply related to $(\mathbf{C}^{(t+1)}\mathbf{l})^{(t)}$:

$$(\mathbf{C}^{(t+1)}\mathbf{l})^{(t)}=+[t(2t-1)]^{\frac{1}{2}}[(t+1)(2t+3)]^{-\frac{1}{2}}(\mathbf{C}^{(t-1)}\mathbf{l})^{(t)}. \quad (13)$$

[The form $(\mathbf{C}^{(1)}\mathbf{l})^{(0)}$ must vanish by the parity rule.]

A relation involving quantum numbers which is useful in dealing with some of these expressions is

$$(\mathbf{C}^{(k)}\mathbf{l})^{(k)}=\tfrac{1}{2}[l(l+1)-l'(l'+1)-k(k+1)][k(k+1)]^{-\frac{1}{2}}\mathbf{C}^{(k)}. \quad (14)$$

The general relation is

$$(l\|(\mathbf{T}^{(k_1)}\mathbf{Y}^{(k_2)})^{(k)}\|l')=(-)^{k_1+k_2-k}(2k+1)^{\frac{1}{2}}\sum_{l''}(l\|T^{(k_1)}\|l'')(l''\|Y^{(k_2)}\|l')W(k_1lk_2l';l''k). \quad (15)$$

We append here the two integrals which contain ∂_{rj}, *viz.*,

$$\left(ab\left|\frac{r_j^{k+1}}{r_i^{k+1}}\partial_{rj}\right|cd\right)=\int_0^\infty dr_i\frac{R_{ia}R_{ic}}{r_i^{k+1}}\int_0^{r_i}dr_j\,R_{jb}r_j^{k+2}\partial_{rj}\left(\frac{R_{jd}}{r_j}\right), \quad (16a)$$

$$\left(ab\left|\frac{r_i^{k+2}}{r_j^{k+2}}\partial_{rj}\right|cd\right)=\int_0^\infty dr_i\,R_{ia}r_i^{k+2}R_{ic}\int_{r_i}^\infty dr_j\frac{R_{jb}}{r_j^{k+1}}\partial_{rj}\left(\frac{R_{jd}}{r_j}\right). \quad (16b)$$

Direct elements of this type can be brought to the form of those in (7) by means of an integration by parts.

5. MATRIX ELEMENTS AND THE *g* FACTOR

Submatrix elements in SL coupling which are independent of J, such as those given in the appendix, are related to the entire matrix element as follows[10]:

$$\langle SLJM|T_Q^{(\kappa k\Xi)}|S'L'J'M'\rangle=(-)^{J+M}$$
$$\times V(JJ'\Xi;-MM'Q)$$
$$\times[(2J+1)(2\Xi+1)(2J'+1)]^{\frac{1}{2}}\begin{Bmatrix}S&L&J\\S'&L'&J'\\\kappa&k&\Xi\end{Bmatrix}$$
$$\times\langle SL\|T^{(\kappa k)}\|S'L'\rangle. \quad (17)$$

For elements of the Zeeman interactions, Ξ is equal to unity and Q is zero. After the restriction is made that only diagonal elements are appropriate, one writes

$$\langle SLJM|\mu_0^{(\kappa k1)}|SLJM\rangle=\sqrt{3}M\left[\frac{2J+1}{J(J+1)}\right]^{\frac{1}{2}}\begin{Bmatrix}S&L&J\\S&L&J\\\kappa&k&1\end{Bmatrix}$$
$$\times\langle SL\|\mu^{(\kappa k)}\|SL\rangle=\tfrac{1}{2}\alpha gM, \quad (18)$$

in terms of the Bohr magneton ($\frac{1}{2}\alpha$ in atomic units) and the Landé g factor. It may be noted in passing that this expression vanishes if $\kappa+k$ is an even number. Thus the quantity in (8) which is of rank one in the orbital part makes no contribution.

The general methods for finding matrix elements which are diagonal in configuration are discussed in the Appendix. The two-particle interactions in a configura-

[10] The form given by the Eckart-Wigner theorem is found in RII, Eq. (29).

tion involving more than one group of equivalent particles will involve intergroup and intragroup elements as there described.

In the work to follow, wide use will be made of unit double tensors [see (A1)] which are defined and written in a different way than are those of RII (58), (102), namely, in setting $(sl\|U^{(\kappa k)}\|sl)$ equal to unity. Otherwise stated, this is, for irreducible tensor operators which are properly normalized, the expression

$$\sum_i \mathbf{s}_i^{(\kappa)}\mathbf{T}_i^{(k)}=(s\|s^{(\kappa)}\|s)(l\|T^{(k)}\|l)\mathbf{U}^{(\kappa k)}. \quad (19)$$

A more general type of unit tensor, for elements not diagonal in l, need not be introduced for the present. The fact that we here exclude pairs of wave functions which differ in configuration means that direct elements may be expressed in terms of elements of one-particle operators within a single group, as in (A6b), below. If exchange elements are expanded in direct elements, through the use of (A4), then the unit tensors as given above again suffice for the cases here considered.

6. APPLICATION TO OXYGEN

As a check and an example of calculations, the factors Δg_1 and Δg_2 for normal oxygen (as given in AVV and KVV) have been reworked. If we define $\delta\mathfrak{y}^{(\kappa k)}$ to be one of the operators occurring in (4), (8), or (12) and $\delta g^{(\kappa k)}$ to be the contribution of that operator to the g factor (κ and k are spin and orbital ranks, respectively), then

$$\alpha\delta g_1{}^{(\kappa k)}=3\sqrt{2}\begin{Bmatrix}1&1&1\\1&1&1\\ \kappa&k&1\end{Bmatrix}\times(1s^22s^22p^4\,{}^3P\|\delta\mu^{(\kappa k)}\|1s^22s^22p^4\,{}^3P), \quad (20a)$$

$$\alpha\delta g_2{}^{(\kappa k)}=(\sqrt{10})\begin{Bmatrix}1&1&2\\1&1&2\\ \kappa&k&1\end{Bmatrix}\times(1s^22s^22p^4\,{}^3P\|\delta\mu^{(\kappa k)}\|1s^22s^22p^4\,{}^3P). \quad (20b)$$

In fact, the products of the numerical and the 9-j coefficient take on two values only, for such κ and k as allow a nonzero result. In δg_1 this value is $(3\sqrt{2})^{-1}$ throughout. In δg_2, the same value obtains except for $(\kappa,k)=(1,2)$ in which case it is $-(15\sqrt{2})^{-1}$. Contributions to $\Delta g_2-\Delta g_1$ all originate, then, in the last operator of $\delta\mathfrak{y}_2$, (4), and in the last three operators of $\delta\mathfrak{y}_{3,4}$, (8).

(a) Contribution of $\delta\mathfrak{y}_1$

The submatrix elements of the operator $\delta\mathfrak{y}_1$ of (4) involve only the partially filled shell, $2p^4$. We need the submatrix elements of

$$\sum_i \mathbf{s}_i^{(0)}\mathbf{l}_i^{(1)}=(s\|s^{(0)}\|s)(l\|l^{(1)}\|l)\mathbf{U}^{(01)}. \quad (21a)$$

It is convenient in calculations to relate the unit double tensors $\mathbf{U}^{(\kappa k)}$ to the unit tensors of Racah by

$$\mathbf{V}^{(\kappa k)}=(s\|s^{(\kappa)}\|s)\mathbf{U}^{(\kappa k)}, \quad (22)$$

$$\mathbf{U}^{(k)}=(2s+1)^{\frac{1}{2}}(2S+1)^{-\frac{1}{2}}\mathbf{U}^{(0k)}. \quad (23)$$

Tables of the submatrix elements of these operators are given in RII and RIII or they may be found from RIII (23). Furthermore, the orbital (and spin) angular-momentum vectors are such that $(l\|l\|l)=[l(l+1)\times(2l+1)]^{\frac{1}{2}}$, as may be seen from RIII (24). We also need the submatrix element

$$\sum_i \mathbf{s}_i^{(1)}\mathbf{l}_i^{(0)}=(s\|s^{(1)}\|s)(l\|l^{(0)}\|l)\mathbf{U}^{(10)}. \quad (24a)$$

Putting the values of the submatrix elements in (21a) and (24a) we find

$$(p^4\,{}^3P\|\textstyle\sum_i s_i{}^{(0)}l_i{}^{(1)}\|p^4\,{}^3P)=+3\sqrt{2}, \quad (21b)$$

$$(p^4\,{}^3P\|\textstyle\sum_i s_i{}^{(1)}l_i{}^{(0)}\|p^4\,{}^3P)=+3\sqrt{2}. \quad (24b)$$

With these values in (4) and (20) we obtain for the contribution of $\delta\mathfrak{y}_1$ in atomic units,

$$\delta g_1=-\tfrac{3}{2}\alpha^2\langle T_i\rangle_{\text{Av}}, \quad (25a)$$

$$\delta g_2-\delta g_1=0. \quad (25b)$$

(b) Contribution of $\delta\mathfrak{y}_2$

The operator $\delta\mathfrak{y}_2$ is given in (4). In addition to the submatrix elements of $\sum_i\mathbf{s}_i^{(1)}\mathbf{l}_i^{(0)}$ given for $\delta\mathfrak{y}_1$ by (24b), we need those of $\sum_i(\mathbf{s}^{(1)}\mathbf{C}^{(2)})_i^{(1)}$,

$$\sum_i \mathbf{s}_i^{(1)}\mathbf{C}_i^{(2)}=(s\|s^{(1)}\|s)(l\|C^{(2)}\|l)\mathbf{U}^{(12)}. \quad (26a)$$

If we put the submatrix elements in (26a), we find

$$(p^4\,{}^3P\|\textstyle\sum_i s_i{}^{(1)}C_i{}^{(2)}\|p^4\,{}^3P)=3/\sqrt{5}. \quad (26b)$$

With (24b) and (26b) in (4) and (20), we obtain for the contribution of $\delta\mathfrak{y}_2$, in atomic units,

$$\delta g_1=\tfrac{1}{4}\alpha^2Z\langle 1/r\rangle_{\text{Av}}, \quad (27a)$$

$$\delta g_2=(3/20)\alpha^2Z\langle 1/r\rangle_{\text{Av}}, \quad (27b)$$

$$\delta g_2-\delta g_1=-\tfrac{1}{10}\alpha^2Z\langle 1/r\rangle_{\text{Av}}. \quad (27c)$$

(c) Contributions to $\delta\mathfrak{y}_3$ and $\delta\mathfrak{y}_4$ from the Partially Filled Shell $2p^4$

The operator for $\delta\mathfrak{y}_{3,4}$ is given by (8). As an example we shall calculate the contribution to the first term of $\delta\mathfrak{y}_3$ from the partially filled shell, $2p^4$. We require the submatrix element of $(\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(0)})^{(1)}$. Here k equals 2 only since the factor k in the coefficient eliminates zero, and other values are eliminated by parity and triangle inequality considerations in the submatrix element $(l\|C^{(k)}\|l)$. The intragroup submatrix element is given by (A3), from which we find

$$(p^4\,{}^3P\|\textstyle\sum_{i<j}\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\{\mathbf{C}_i^{(2)}\mathbf{C}_j^{(2)}\}^{(0)}\|p^4\,{}^3P)=(-)^{1+0-1+2+2-0}\,\tfrac{1}{2}\sqrt{3}(s\|s^{(1)}\|s)(s\|s^{(0)}\|s)\times(1\|C^{(2)}\|1)^2[\textstyle\sum_{S''L''}(p^4\,{}^3P\|U^{(12)}\|p^4S''L'')(p^4S''L''\|U^{(02)}\|p^4\,{}^3P)W(1101;S''1)W(2121;L''0)-(p^4\,{}^3P\|U^{(10)}\|p^4\,{}^3P)W(1\tfrac{1}{2}0\tfrac{1}{2};\tfrac{1}{2}1)W(2121;10)]. \quad (28a)$$

The unit-tensor matrix element $(p^4\,{}^3P\|U^{(02)}\|p^4\,{}^3P)$ equals $\sqrt{\frac{3}{2}}$ and is diagonal so that the sum in (28a) reduces to one term. Also

$$(p^4\,{}^3P\|U^{(12)}\|p^4\,{}^3P)=-1, \tag{29a}$$

$$(p^4\,{}^3P\|U^{(10)}\|p^4\,{}^3P)=+2. \tag{29b}$$

With these values in (28a), we obtain

$$(p^4\,{}^3P\|\textstyle\sum_{i<j}\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\{\mathbf{C}_i^{(2)}\mathbf{C}_j^{(2)}\}^{(0)}\|p^4\,{}^3P)=-9/(5\sqrt{10}). \tag{28b}$$

From (8), (20), and the submatrix element from (28b) we obtain the stated contribution of $(\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\times\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(0)})^{(1)}$. In atomic units,

$$\delta g_1=-\tfrac{1}{5}\alpha^2F_<{}^2(2p,2p) \tag{30a}$$

$$=-\tfrac{1}{10}\alpha^2F^2(2p,2p)=\delta g_2, \tag{30b}$$

since $F_<{}^2(2p2p)$ equals $\frac{1}{2}F^2(2p,2p)$.

Similar calculations for the other terms of $\delta\mathfrak{y}_{3,4}$ give for its entire contribution of this kind,

$$\delta g_1=\tfrac{1}{8}\alpha^2[-5F^0(2p,2p)+(11/5)F^2(2p,2p)], \tag{31a}$$

$$\delta g_2=\tfrac{1}{8}\alpha^2[-(31/5)F^0(2p,2p)+F^2(2p,2p)], \tag{31b}$$

$$\delta g_2-\delta g_1=-\tfrac{1}{8}\alpha^2(6/5)[F^0(2p,2p)+F^2(2p,2p)]. \tag{31c}$$

(d) Contribution to $\delta\mathfrak{y}_{3,4}$ from Closed Shells

Since there is one partially filled shell in oxygen, we turn now to the intergroup matrix elements involving a partially filled and a closed shell. We shall take the same term of (8) as in (c), and restrict the treatment to exchange elements. The operator is $(\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(0)})^{(1)}$, and the submatrix element is given by (A7). The configuration consists of three groups and the sum extends over $1s$ and $2s$.

$$\begin{aligned}(1s^22s^22p^4\,{}^3P\|\textstyle\sum_{i<j}\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\{\mathbf{C}_i^{(k)}\mathbf{C}_j^{(k)}\}^{(0)}\|1s^22s^2sp^4\,{}^3P)&=\tfrac{1}{2}(p^4\,{}^3P\|U^{(10)}\|p^4\,{}^3P)\textstyle\sum_n\{-\sqrt{3}W(\frac{1}{2}1\frac{1}{2}0;\frac{1}{2}1)\\ \times W(1k1k;00)[(s\|s^{(1)}\|s)(s\|s^{(0)}\|s)(0\|C^{(k)}\|1)(1\|C^{(k)}\|0)\mathfrak{P}_n(sp,ps)+(-)^{1+0-1+k+k-0}(s\|s^{(1)}\|s)(s\|s^{(0)}\|s)&\\ \times(0\|C^{(k)}\|1)(1\|C^{(k)}\|0)\mathfrak{P}_n(ps,sp)]\}=(1/\sqrt{6})\textstyle\sum_n[\mathfrak{P}_n(sp,ps)+\mathfrak{P}_n(ps,sp)],&\end{aligned} \tag{32}$$

since evidently k equals 1 only. The two energy parameters are the same. From (8), (20), and the submatrix element (32), we obtain the contribution of $(\{\mathbf{s}_i^{(1)}\mathbf{s}_j^{(0)}\}^{(1)}\{\mathbf{C}_i^{(1)}\mathbf{C}_j^{(1)}\}^{(0)})^{(1)}$,

$$\delta g_1=-(1/9)\alpha^2\textstyle\sum_n G_<{}^1(ns,2p)=-(1/18)\alpha^2\sum_n G^1(ns,2p)=\delta g_2 \tag{33}$$

as before, with $G_<{}^1$ equal to $\frac{1}{2}G^1$.

A similar calculation for the other terms of $\delta\mathfrak{y}_3$ and $\delta\mathfrak{y}_4$ in (8) gives as the entire contribution to $\delta\mathfrak{y}_{3,4}$ from intergroup elements, in atomic units,

$$\delta g_1=\alpha^2\textstyle\sum_n[-\frac{1}{2}F_>{}^0(2p,ns)-\frac{2}{3}F_>{}^0(ns,2p)+\frac{1}{3}F_>{}^2(2p,ns)], \tag{34a}$$

$$\delta g_2-\delta g_1=\alpha^2\textstyle\sum_n[\frac{1}{5}F_>{}^0(2p,ns)-\frac{2}{5}F_>{}^2(2p,ns)+\frac{1}{5}G^1(2p,ns)]. \tag{34b}$$

(e) Contributions from $\delta\mathfrak{y}_5$

As an example of the contribution from $\delta\mathfrak{y}_5$, we shall calculate one of the intergroup matrix elements, in particular, the first term given in (12) which contributes only to exchange elements for k equal to 1. One needs submatrix elements of the operator $(\{\mathbf{s}_i^{(0)}\mathbf{s}_j^{(0)}\}^{(0)}\{\mathbf{C}_i^{(1)}(\mathbf{C}^{(1)}\mathbf{l})_j^{(1)}\}^{(1)})^{(1)}$. From (A7), we have

$$\begin{aligned}(1s^22s^22p^4\,{}^3P\|\textstyle\sum_{i<j}\{\mathbf{s}_i^{(0)}\mathbf{s}_j^{(0)}\}^{(0)}\{\mathbf{C}_i^{(1)}(\mathbf{C}^{(1)}\mathbf{l})_j^{(1)}\}^{(1)}\|1s^22s^22p^4\,{}^3P)&\\ =\tfrac{1}{2}(p^4\,{}^3P\|U^{(01)}\|p^4\,{}^3P)\textstyle\sum_n\{-\sqrt{3}W(\frac{1}{2}0\frac{1}{2}0;\frac{1}{2}0)W(1111;01)(-)^{0+0-0+1+1-1}&\\ \times(s\|s^{(0)}\|s)(s\|s^{(0)}\|s)(0\|(\mathbf{C}^{(1)}\mathbf{l})^{(1)}\|1)(1\|C^{(1)}\|0)\mathfrak{P}_n(ps,sp)\}=-(1/\sqrt{2})\textstyle\sum_n\mathfrak{P}_n(ps,sp).&\end{aligned} \tag{35}$$

From (12), (20) and the submatrix element (35), we obtain the contribution of $(\{\mathbf{s}_i^{(0)}\mathbf{s}_j^{(0)}\}^{(0)}\{\mathbf{C}_i^{(1)}(\mathbf{C}^{(1)}\mathbf{l})_j^{(1)}\}^{(1)})^{(1)}$, in atomic units,

$$\delta g_1=(1/30)\alpha^2\textstyle\sum_n[G_1(2p,ns)+G^3(2p,ns)]=\delta g_2. \tag{36}$$

We have seen that $\delta g_1=\delta g_2$ throughout $\delta\mathfrak{y}_5$. In this way we obtain all the terms of this operator.

If one now combines (25), (27), (31), and (34) with the terms of $\delta\mathfrak{y}_5$, one finds

$$\begin{aligned}\Delta g_1=(8mc^2)^{-1}\{&-12\langle T\rangle_{Av}+2Z\langle e^2/r\rangle_{Av}-[5F^0(2p,2p)-(11/5)F^2(2p,2p)\\ &+\textstyle\sum_n(4F_>{}^0(2p,ns)+(16/3)F_>{}^0(ns,2p)-(8/3)F_>{}^2(2p,ns))]\\ &-2[F^0(2p,2p)+F^2(2p,2p)+\textstyle\sum_n\frac{4}{3}(F_>{}^0(ns,2p)+F_>{}^2(2p,ns)-(7/20)G^1(2p,ns)-\frac{1}{4}G^{-1}(2p,ns)\\ &-\tfrac{1}{10}G^3(2p,ns)+\tfrac{3}{4}R(2p,ns))]\},\end{aligned} \tag{37}$$

$$\Delta g_2=\Delta g_1-(5mc^2)^{-1}\{\tfrac{1}{2}Z\langle e^2/r\rangle_{Av}+[\tfrac{3}{4}F^0(2p,2p)+\tfrac{3}{4}F^2(2p,2p)+\textstyle\sum_n(-F_>{}^0(2p,ns)+2F_>{}^2(2p,ns)-G^1(2p,ns))]\}.$$

These equations show the following minor differences with those of KVV. In the first $\sum_n$ of Δg_1, the first term reads $F_>^0(2p,ns)$ instead of $F_>^2(2p,ns)$, and the coefficient of the third term is $-(8/3)$ instead of $-(8/5)$. In the second $\sum_n$ in Δg_1, the second term is $F_>^2(2p,ns)$ instead of $F_>^0(2p,ns)$; and the sign of $\frac{3}{4}R(2p,ns)$ is + rather than −. In Δg_2, the sign before the square bracket is + instead of −; and the coefficient of $F_>^2(2p,ns)$ is 2 instead of $\frac{4}{3}$. The results obtained here may also be obtained from KVV (4), (12), (13), (14), (15), and (16). They have the result, upon insertion of the numerical values for O I ^3P given in KVV, Table I, that

Δg (calc)	Δg (obs)
$\Delta g_1=981\times10^{-6}$	971×10^{-6}
$\Delta g_2=917\times10^{-6}$	905×10^{-6}
$\Delta g_1-\Delta g_2=64\times10^{-6}$	66×10^{-6}.

Thus the difference is given with higher precision than the absolute values themselves, as should indeed be the case (KVV, Sec. IV).

Note added in proof.—The relevant interactions have also been derived by W. Perl [Phys. Rev. **91**, 852 (1953)]. More recent numerical values for normal oxygen have now been published by Radford, Hughes, and Innes [Bull. Am. Phys. Soc. Ser. II, **3**, 8 (1958)]. Apart from the increased precision of observation, they differ from those given in Sec. 6 in that a corrected figure for the electron moment has been adopted [C. M. Sommerfield, Phys. Rev. **107**, 328 (1957); A. Petermann, Helv. Phys. Acta **30**, 407 (1957)]. For reference purposes, the new values are

Δg (calc)	Δg (obs)
$\Delta g_1=996\times10^{-6}$	986×10^{-6}
$\Delta g_2=932\times10^{-6}$	921×10^{-6}
$\Delta g_1-\Delta g_2=64\times10^{-6}$	65×10^{-6}

Finally, the changes in the KVV calculations noted at the end of Sec. 6 have been taken up with the authors. Agreement was also reached on all of these changes in conversations between one of us and K. Kambe. It is now anticipated that new information should be obtained through relaxations of the (restricted) Hartree-Fock method in the determination of the energy parameters [see G. W. Pratt, Phys. Rev. **102**, 1303 (1956)]. We are indebted to the author of the above paper for a number of observations which relate to these techniques.

7. ACKNOWLEDGMENTS

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APPENDIX. SUBMATRIX ELEMENTS INVOLVING A NUMBER OF GROUPS OF EQUIVALENT PARTICLES AND DIAGONAL IN CONFIGURATION

A1. General

The elements of one-particle operators and the intragroup elements of two-particle operators are both derived through the use of one recoupling procedure. The corresponding procedure for intergroup elements (of two-particle operators) is more elaborate. Results for all three sorts of elements are given in Secs. A2 and A3, below, but the mode of derivation is put down only for the intergroup type. From the given description the derivation of the intragroup form may be inferred quite readily. The general approach for all these forms involves (a), the use of RII(44b) after appropriate recoupling in the wave functions, and (b), the expansion of the elements of two-particle operators into weighted sums of products of single-group elements of one-particle operators as given in Eq. (A1). Complete $(T)SL$-coupling matrix elements are found in each case through the use of (17), above, or its jj-coupling equivalent, if that scheme is in use.

Submatrix elements are formulated in a compact way by replacing sets of quantum numbers by a single letter. Thus a group of equivalent particles is written l^nI. In wave functions which appear below, a number of groups are coupled together by adding each succeeding group to the resultant of those preceding, thus $l_1^{n_1}(I_1l_2^{n_2}I_2)(I_{\Sigma 2}\cdots l_t^{n_t}I_t)I_{\Sigma t}$. A null group, $l_0^{n_0}I_0$, may also be inserted for greater clarity in interpreting the results. Omitted particles or groups are indicated by superscripts, e.g., the symbol $I_{\Sigma t}{}^{(p)q}$ is the result of coupling together t groups omitting one particle from group p and the entire group q. The wave function of two particles is written simply $(l_pl_q)I_{(pq)}$. In the SL scheme (used in Secs. 5 and 6, above) the expression $(2S+1)(2L+1)$ corresponds to $(2I+1)$ and $(2s+1)\times(2l+1)$, the number of particles in a closed shell, is written $(2l+1)$ in, e.g., (A7). The abbreviation $[a]\equiv(2a+1)$, now in frequent use, will also be used.

There are also useful conventions for the operators. The general one-particle operator $\mathbf{V}^{(K)}$ is, in the SL scheme, the double tensor, $\sum_i \mathbf{s}_i^{(\kappa)}\mathbf{T}_i^{(k)}$ (see RII, Sec. 5). The two-particle operator $\mathbf{V}^{(K_1K_2K)}$ is the general form $\sum_{i<j}\{\mathbf{s}_i^{(\kappa_1)}\mathbf{s}_j^{(\kappa_2)}\}^{(\kappa)}\{\mathbf{T}_i^{(k_1)}\mathbf{Y}_j^{(k_2)}\}^{(k)}$ instances of which appear frequently in Secs. 3 and 4. Observe that $(s\|s^{(\kappa)}\|s)(l\|T^{(k)}\|l)$ is written $(l\|V^{(K)}\|l)$ and that products of n-j coefficients appear as single coefficients.

The basic submatrix element of the developments to follow is

$$(l^nI\|V^{(K)}\|l^nI')=(l\|V^{(K)}\|l)(l^nI\|U^{(K)}\|l^nI') \quad \text{(A1a)}$$

in terms of a unit double tensor [see (19)], the element of which is [RIII(23)],

$$(l^nI\|U^{(K)}\|l^nI')=n([I][I'])^{\frac{1}{2}}$$
$$\times\sum_{I_1}(l^nI\,[\![l^{n-1}I_1)(l^{n-1}I_1\,]\!]l^nI')W(I_1IlK;\,lI'). \quad \text{(A1b)}$$

Radial terms in both wave functions and operators have frequently been omitted. However, they are contained in the energy parameters of the elements of (A2), (A6), and (A7), below.

A2. Intragroup Elements of One- and Two-Particle Operators

The intragroup elements of two-particle operators correspond to the quantities a and c in the treatment given by Yanagawa,[7] a and d in that given by Elliott.[2] We consider elements in which particles are picked out of one group at a time, either singly or in pairs. The number of groups has been designated t and the number of particles $n=\sum n_p$, $p=0, \cdots, t$. The final form, which can be found through a procedure analogous to that used in the next section, is

$$\begin{aligned}&(I_0 l_1^{n_1} I_1, I_{\Sigma 1} l_2^{n_2} I_2, I_{\Sigma 2} \cdots l_t^{n_t} I_t, I_{\Sigma t} \| V^{(--K)} \| I_0 l_1^{n_1} I_1', I_{\Sigma 1}' l_2^{n_2} I_2', I_{\Sigma 2}' \cdots l_t^{n_t} I_t', I_{\Sigma t}')\\ &\quad = \sum_p ([I_{\Sigma p}][I_{\Sigma p}'] \cdots [I_{\Sigma t}][I_{\Sigma t}'])^{\frac{1}{2}} (l_p^{n_p} I_p \| V^{(--K)} \| l_p^{n_p} I_p')\\ &\quad \times \mathfrak{P}_p W(I_{\Sigma p-1} I_{\Sigma p} I_p' K; I_p I_{\Sigma p}') W(I_{p+1} I_{\Sigma p} I_{\Sigma p+1}' K; I_{\Sigma p+1} I_{\Sigma p}') \cdots W(I_t I_{\Sigma t-1} I_{\Sigma t}' K; I_{\Sigma t} I_{\Sigma t-1}')\\ &\qquad\qquad \times \begin{cases} \delta(I_m, I_m') \text{ for all } m \neq p \\ \delta(I_{\Sigma m'}, I_{\Sigma m'}') \text{ for all } m' < p. \end{cases} \end{aligned} \tag{A2}$$

$\mathfrak{P}$ indicates the pertinent energy parameter (the radial integral and other factors). The resultants $I_{\Sigma 1}$ and $I_{\Sigma 1}'$ appear *pro forma*, merely, since I_0 is the (^1S) term of a null set. If $\mathbf{V}^{(--K)}$ is a one-particle operator, the single-group submatrix elements are given by (A1). If it is a two-particle operator, these elements are

$$\begin{aligned}(l^n I \| V^{(K_1 K_2 K)} \| l^n I') = (-)^{K_1+K_2-K} \tfrac{1}{2}[K]^{\frac{1}{2}} (l \| V_i^{(K_1)} \| l)(l \| V_j^{(K_2)} \| l) [\textstyle\sum_{I''} (l^n I \| U^{(K_1)} \| l^n I'')(l^n I'' \| U^{(K_2)} \| l^n I')\\ \times W(K_1 I K_2 I'; I'' K) - (l^n I \| U^{(K)} \| l^n I') W(K_1 l K_2 l, l K)]. \end{aligned} \tag{A3}$$

The derivation of a slightly less general form of this relation has already been given [Innes, reference 3, Eq. (12), and Horie, reference 3, Eq. (12)].

A3. Intergroup Elements

The intergroup elements correspond to the quantities b and d in the treatment given by Yanagawa[7] and b and c in that by Elliott.[2] There are, in general, two direct and two exchange parts for each pair of groups, and four corresponding energy parameters.

When one of the direct parts of the element has been given, as in (A6b), the corresponding exchange part may be found by expanding the rank-dependent 9-j coefficient[11] and treating each term of the sum separately. Thus, for the first exchange part, as shown in (A6a),

$$(-)^{l_p+l_q-I_{(pq)}'} \begin{Bmatrix} l_p & l_q & I_{(pq)} \\ l_q & l_p & I_{(pq)}' \\ K_1 & K_2 & K \end{Bmatrix} = \sum_{Q_1, Q_2} (-)^{l_p-l_q-K_2+Q_2} [Q_1][Q_2] \begin{Bmatrix} l_p & l_p & Q_1 \\ l_q & l_q & Q_2 \\ K_1 & K_2 & K \end{Bmatrix} \begin{Bmatrix} l_p & l_q & I_{(pq)} \\ l_p & l_q & I_{(pq)}' \\ Q_1 & Q_2 & K \end{Bmatrix}. \tag{A4}$$

Discussion of this method of treating exchange elements will be found in RII, Sec. 5. The two remaining parts involve simply an interchange of K_1 and K_2 with insertion of the factor $(-)^{K_1+K_2-K}$.

When in process of development, the entire intergroup submatrix element is in the form of a combination of two-particle elements. Two one-particle wave functions have been relocated near the right-hand side of each wave function through the use of a double sequence of 6-j coefficients (written below as a single unitary coefficient), and two coefficients of fractional parentage. Another pair of coefficients (a 6-j and a 9-j) has then been employed to recouple the two one-particle wave functions into the form $(l_p l_q) I_{(pq)}$. Step by step displacement of a group within the wave function is accomplished by transformations of the type

$$\langle (ab)e,c,d | (ac)f,b,d \rangle = ([e][f])^{\frac{1}{2}} W(ebcf; ad), \tag{A5}$$

and the unitary coefficient consists of two flights of these, displacing groups q and p, respectively, with sums over intermediate terms. This program leads to the expression

$$\begin{aligned}&(I_0 l_1^{n_1} I_1, I_{\Sigma 1} l_2^{n_2} I_2, I_{\Sigma 2} \cdots l_t^{n_t} I_t, I_{\Sigma t} \| V^{(K_1 K_2 K)} \| I_0 l_1^{n_1} I_1', I_{\Sigma 1}' l_2^{n_2} I_2', I_{\Sigma 2}' \cdots l_t^{n_t} I_t', I_{\Sigma t}')\\ &\quad = \tfrac{1}{2}[K]^{\frac{1}{2}} \textstyle\sum_{p<q} n_p n_q \sum_I ([I_p][I_p'][I_q][I_q'][I_{\Sigma t^q}][I_{\Sigma t^q}'])^{\frac{1}{2}} [I_{(pq)}][I_{(pq)}'][I_{\Sigma t}{}^{(p)q}][I_{\Sigma t}{}^{(pq)}]\\ &\quad \times \langle \cdots I_{\Sigma p-1} I_p, I_{\Sigma p} \cdots I_t, I_{\Sigma t} | \cdots I_{q-1}, I_{\Sigma q-1}{}^p I_{q+1}, I_{\Sigma q+1}{}^{pq} \cdots I_t, I_{\Sigma t}{}^{pq} I_p, I_{\Sigma t}{}^q I_q, I_{\Sigma t} \rangle\\ &\quad \times \text{the primed counterpart of this coefficient}\\ &\quad \times (l_p^{n_p} I_p \{\!| l_p^{n_p-1} I_p{}^{(p)}) (l_p^{n_p} I_p' \{\!| l_p^{n_p-1} I_p{}^{(p)}) (l_q^{n_q} I_q \{\!| l_q^{n_q-1} I_q{}^{(q)}) (l_q^{n_q} I_q' \{\!| l_q^{n_q-1} I_q{}^{(q)}) \end{aligned}$$

[11] See Arima, Horie, and Tanabe, reference 2, Eq. (16).

$$\times W(I_{\Sigma t}{}^{pq}I_p{}^{(p)}I_{\Sigma t}{}^q l_p; I_{\Sigma t}{}^{(p)q}I_p)\begin{Bmatrix} I_{\Sigma t}{}^{(p)q} & l_p & I_{\Sigma t}{}^q \\ I_q{}^{(q)} & l_q & I_q \\ I_{\Sigma t}{}^{(pq)} & I_{(pq)} & I_{\Sigma t}\end{Bmatrix} W(I_{\Sigma t}{}^{pq}I_p{}^{(p)}I_{\Sigma t}{}^{q'}l_p; I_{\Sigma t}{}^{(p)q}I_p{}')\begin{Bmatrix} I_{\Sigma t}{}^{(p)q} & l_p & I_{\Sigma t}{}^{q'} \\ I_q{}^{(q)} & l_q & I_q{}' \\ I_{\Sigma t}{}^{(pq)} & I_{(pq)}{}' & I_{\Sigma t}{}'\end{Bmatrix}$$

$$\times([I_{\Sigma t}][I_{\Sigma t}'])^{\frac{1}{2}}W(I_{\Sigma t}{}^{(pq)}I_{\Sigma t}I_{(pq)}{}'K; I_{(pq)}I_{\Sigma t}')\{+(l_p\|V_i{}^{(K_1)}\|l_p)(l_q\|V_j{}^{(K_2)}\|l_q)\begin{Bmatrix} l_p & l_q & I_{(pq)} \\ l_p & l_q & I_{(pq)}{}' \\ K_1 & K_2 & K\end{Bmatrix}\mathfrak{P}(pqpq)$$

$$+(-)^{2l_p+2l_q-I_{(pq)}-I_{(pq)}{}'}(l_q\|V_i{}^{(K_1)}\|l_q)(l_p\|V_j{}^{(K_2)}\|l_p)\begin{Bmatrix} l_q & l_p & I_{(pq)} \\ l_q & l_p & I_{(pq)}{}' \\ K_1 & K_2 & K\end{Bmatrix}\mathfrak{P}(qpqp)$$

$$-(-)^{l_p+l_q-I_{(pq)}{}'}(l_p\|V_i{}^{(K_1)}\|l_q)(l_q\|V_j{}^{(K_2)}\|l_p)\begin{Bmatrix} l_p & l_q & I_{(pq)} \\ l_q & l_p & I_{(pq)}{}' \\ K_1 & K_2 & K\end{Bmatrix}\mathfrak{P}(pqqp)$$

$$-(-)^{l_p+l_q-I_{(pq)}}(l_q\|V_i{}^{(K_1)}\|l_p)(l_p\|V_j{}^{(K_2)}\|l_q)\begin{Bmatrix} l_q & l_p & I_{(pq)} \\ l_p & l_q & I_{(pq)}{}' \\ K_1 & K_2 & K\end{Bmatrix}\mathfrak{P}(qppq)\}$$

$$\times\begin{cases}\delta(I_m, I_m') \text{ for all } m\neq p, q \\ \delta(I_{\Sigma m'}, I_{\Sigma m'}') \text{ for all } m'<p.\end{cases} \quad \text{(A6a)}$$

The summed parameter sign, I, represents several sets of quantum numbers all of which can, in fact, be removed through the use of identities given in the next section. The sequence of operations for the first direct part is now given in detail. Reference is made to summed parameters and relevant identity for each step of the reduction. It will be noted that the summed parameters $I_{\Sigma t-1}{}^q\cdots I_{\Sigma q+1}{}^q$ and their primed counterparts make no overt appearance in (A6a). They may be found by writing out the unitary coefficients in full, in the manner explained above.

a. Remove $I_{(pq)}$, $I_{(pq)}{}'$ and $I_{\Sigma t}{}^{(pq)}$ with (A9).
b. Insert a submatrix element for group q according to (A1).
c. Remove $I_{\Sigma t}{}^{(p)q}$ with (A11).
d. Insert a submatrix element for group p (see step b).
e. Remove $I_{\Sigma t}{}^{pq}$ with (A11) and $I_{\Sigma t}{}^q$ and $I_{\Sigma t}{}^{q'}$ with (A10). Proceed in this way step by step until $I_{\Sigma q+1}{}^{pq}$, $I_{\Sigma q+1}{}^q$, and $I_{\Sigma q+1}{}^{q'}$ are removed.
f. Remove $I_{\Sigma q-1}{}^p\cdots I_{\Sigma p+1}{}^p$ with successive applications of (A11).

After these steps have been taken, the form given above becomes

$$\tfrac{1}{2}[K]^{\frac{1}{2}}\sum_{p<q}([I_{\Sigma p}][I_{\Sigma p}']\cdots[I_{\Sigma t}][I_{\Sigma t}'])^{\frac{1}{2}}$$
$$\times(l_p{}^{n_p}I_p\|V_i{}^{(K_1)}\|l_p{}^{n_p}I_p')(l_q{}^{n_q}I_q\|V_j{}^{(K_2)}\|l_q{}^{n_q}I_q')W(I_{\Sigma p-1}I_{\Sigma p}I_p'K_1; I_pI_{\Sigma p}')W(I_{p+1}I_{\Sigma p}I_{\Sigma p+1}'K_1; I_{\Sigma p+1}I_{\Sigma p}')$$
$$\times\cdots W(I_{q-1}I_{\Sigma q-2}I_{\Sigma q-1}'K_1; I_{\Sigma q-1}I_{\Sigma q-2}')\begin{Bmatrix} I_{\Sigma q-1} & I_q & I_{\Sigma q} \\ I_{\Sigma q-1}{}' & I_q{}' & I_{\Sigma q}{}' \\ K_1 & K_2 & K\end{Bmatrix}$$
$$\times W(I_{q+1}I_{\Sigma q}I_{\Sigma q+1}'K; I_{\Sigma q+1}I_{\Sigma q}')\cdots W(I_tI_{\Sigma t-1}I_{\Sigma t}'K; I_{\Sigma t}I_{\Sigma t-1}'), \quad \text{(A6b)}$$

also with the same δ functions that appear in (A6a) and the energy parameter, $\mathfrak{P}(pqpq)$, of the first direct part.

One commonly occurring particular instance of this general result is that in which all shells but the last are closed. In fact one may simply write down the entire intergroup element in this case, since the expansion of the exchange parts, by means of (A4), reduces to one term. This element is the useful form, for example, in the application made in Sec. 6.

A portion of the element involving only closed shells may appear if K is zero. It is omitted here since it can be found quite readily as a particular instance of the portion which involves closed shells and an unfilled shell. This portion is

$$\tfrac{1}{2}(l_t{}^{n_t}I_t\|U^{(K)}\|l_t{}^{n_t}I_t')\sum_{p\neq t}\{(2l_p+1)[\delta(K_1,0)(l_t\|V_j{}^{(K)}\|l_t)\mathfrak{P}(ptpt)+\delta(K_2,0)(l_t\|V_i{}^{(K)}\|l_t)\mathfrak{P}(tptp)]$$
$$-(2K+1)^{\frac{1}{2}}W(l_tK_1l_tK_2; l_pK)[(l_p\|V_i{}^{(K_1)}\|l_t)(l_t\|V_j{}^{(K_2)}\|l_p)\mathfrak{P}(pttp)$$
$$+(-)^{K_1+K_2-K}(l_t\|V_i{}^{(K_1)}\|l_p)(l_p\|V_j{}^{(K_2)}\|l_t)\mathfrak{P}(tppt)]\}. \quad \text{(A7)}$$

The known relations TAS 9^612 and 9^613 may be found by using (A3) and (A7), respectively. The spin-other-orbit interaction yields intergroup elements of type (A7),[12] but the spin-spin interaction (tensor force) does not, since the spin rank is too large.

[12] These effects are important in calculations of fine structure (now under study).

A4. Relations in 6-*j* and 9-*j* Coefficients

The process of expanding a given submatrix element into a set of elements in another coupling scheme displays an identity involving *n-j* coefficients. For example, (A4), above, is represented by the submatrix form,

$$\langle (a_2b_1)e \| (\dot{a}_1a_2)\bar{a}(b_1\dot{b}_2)\bar{b},\ \bar{e} \| (\dot{a}_1\dot{b}_2)\dot{e}\rangle = \sum_{\bar{c}_1,\bar{c}_2} \begin{Bmatrix} \dot{a}_1 & a_2 & \bar{a} \\ b_1 & \dot{b}_2 & \bar{b} \\ \bar{c}_1 & \bar{c}_2 & \bar{e} \end{Bmatrix} ([\bar{a}][\bar{b}][\bar{c}_1][\bar{c}_2])^{\frac{1}{2}} \langle (a_2b_1)e \| (\dot{a}_1b_1)\bar{c}_1(a_2\dot{b}_2)\bar{c}_2,\ \bar{e} \| (\dot{a}_1\dot{b}_2)\dot{e}\rangle. \tag{A8}$$

The identities which are needed for removal of sums in (A6a) derive from similar forms, *viz.*, $\langle (a_1a_2)a(b_1b_2)b,\ e \| (\bar{a}_2\bar{b}_2)\bar{e} \| (a_1\dot{a}_2)\dot{a}(b_1\dot{b}_2)\dot{b},\ \dot{e}\rangle$ and the simpler $\langle a_2(b_1b_2)b,\ e \| (\bar{a}_2\bar{b}_2)\bar{e} \| \dot{a}_2(b_1\dot{b}_2)\dot{b},\ \dot{e}\rangle$. These relations are

$$W(a_1a\dot{a}_2\bar{a}_2;\ a_2\dot{a})W(b_1b\dot{b}_2\bar{b}_2;\ b_2\dot{b}) \begin{Bmatrix} a & b & e \\ \dot{a} & \dot{b} & \dot{e} \\ \bar{a}_2 & \bar{b}_2 & \bar{e} \end{Bmatrix}$$

$$= \sum_{c_1,c_2,\dot{c}_2} [c_1][c_2][\dot{c}_2] W(c_1e\dot{c}_2\bar{e};\ c_2\dot{e}) \begin{Bmatrix} a_1 & a_2 & a \\ b_1 & b_2 & b \\ c_1 & c_2 & e \end{Bmatrix} \begin{Bmatrix} a_1 & \dot{a}_2 & \dot{a} \\ b_1 & \dot{b}_2 & \dot{b} \\ c_1 & \dot{c}_2 & \dot{e} \end{Bmatrix} \begin{Bmatrix} a_2 & b_2 & c_2 \\ \dot{a}_2 & \dot{b}_2 & \dot{c}_2 \\ \bar{a}_2 & \bar{b}_2 & \bar{e} \end{Bmatrix}, \tag{A9}$$

and

$$W(b_1b\dot{b}_2\bar{b}_2;\ b_2\dot{b}) \begin{Bmatrix} a_2 & b & e \\ \dot{a}_2 & \dot{b} & \dot{e} \\ \bar{a}_2 & \bar{b}_2 & \bar{e} \end{Bmatrix} = \sum_{c_2,c_2} [c_2][\dot{c}_2] W(b_1e\dot{c}_2\bar{e};\ c_2\dot{e}) W(b_1bc_2a_2;\ b_2e) W(b_1\dot{b}\dot{c}_2\dot{a}_2;\ \dot{b}_2\dot{e}) \begin{Bmatrix} a_2 & b_2 & c_2 \\ \dot{a}_2 & \dot{b}_2 & \dot{c}_2 \\ \bar{a}_2 & \bar{b}_2 & \bar{e} \end{Bmatrix}. \tag{A10}$$

This last is also given by Arima *et al.* [reference 2, Eq. (A3)]. A fundamental (and well-known) relation, which may be deduced from those given above, is

$$W(a_1a\dot{a}_2\bar{a}_2;\ a_2\dot{a})W(b_1a\dot{b}_2\bar{a}_2;\ b_2\dot{a}) = \sum\nolimits_c [c] W(aa_2b_1c;\ a_1b_2) W(\dot{a}\dot{a}_2b_1c;\ a_1\dot{b}_2) W(cb_2\dot{a}_2\bar{a}_2;\ a_2\dot{b}_2). \tag{A11}$$

It is evident that each submatrix form indicates a vector coupling identity in a concise way.