Extension of the Theory of Complex Spectra

GEORGE H. SHORTLEY AND BERNARD FRIED
Mendenhall Laboratory of Physics, Ohio State University, Columbus, Ohio

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This paper extends the tabular and formular material of the theory of complex spectra to configurations involving f and g electrons. In making these computations it was found that in practically every case significant simplification could be made over the methods previously used. In particular, for the computation of the electrostatic energies for two-electron-like almost-closed-shell configurations a simple closed formula was found which entirely replaces the previous lengthy diagonal-sum calculation. The explicit content of the paper is best exhibited by listing the section headings: I. Extension of Tables of c^k, b^k, and a^k to gp, gd, gf, gg. II. Explanation of the Regularities in the Electrostatic Energies of Two-Electron Configurations and Formulas for gp, gd, gf, gg, g^2. III. Formula Determining the Electrostatic Energies of Two-Electron-Like Configurations with Almost-Closed Shells. Values for p^5g and d^9g. IV. Matrices for Transformation of pf, df, pg, dg from LS to jj Coupling. V. Matrices of Electrostatic Interaction in jj Coupling for p^5f, (d^9p), d^9d, d^9f, d^9g.

SPECTROSCOPIC analysis is beginning more and more to involve configurations with f and g electrons.[1] For this reason we believe it useful to extend the tabular and formular material of the theory of complex spectra to the point where it will handle the simpler of the observed f- and g-electron configurations. This is the purpose of the present paper. The abstract above contains a statement of the contents by sections. In extending this material to the more complicated configurations for which the amount of computational labor is great, it became desirable to re-examine the methods of calculation with a view to simplifying them if possible. It has been found that in practically every case significant simplification could be made over the methods previously used. In one case (the determination of the electrostatic energies for almost-closed-shell configurations) it was possible to find a simple closed formula to replace the previous lengthy diagonal-sum calculation. These simplified methods of computation are discussed at the beginning of each section before the tabular results are given.

I. EXTENSION OF TABLES OF c^k, b^k, AND a^k TO gp, gf, gd, gg (TABLES I AND II)

The a's, b's, and c's are the Slater coefficients needed to compute the matrix of electrostatic interaction.[2] The values of the a's and b's follow at once by 8^614 (TAS) from the values of the c's. The c's represent the following definite integrals:

$$c^k(lm,\, l'm') = \left(\frac{2}{2k+1}\right)^{\frac{1}{2}} \int_0^\pi \Theta(k,\, m-m')\Theta(lm)\Theta(l'm')\sin\theta\, d\theta, \tag{1}$$

$$|l-l'| \leqslant k \leqslant l+l' \qquad k+l+l' = 2g \quad (g \text{ integral}). \tag{2}$$

The direct individual evaluation of these integrals by means of Gaunt's formula 8^611 is very laborious because of the sum occurring in this formula. We find, however, that it is possible to express $c^k(l,\, m;\, l',\, l'-\epsilon)$ as the square root of a polynomial in m and then compute from this polynomial the $2l+1$ entries with $m=l,\, \cdots,\, -l$ with but little more trouble than the direct evaluation of a single entry. We start by noting that an examination of Gaunt's derivation shows that 8^611 is valid for the whole range $-l \leqslant m \leqslant l$; $-l' \leqslant m' \leqslant l'$; $-l'' \leqslant m+m' \leqslant l''$.

[1] Compare, for example, Shenstone's analysis of Cu II, which is discussed theoretically in the paper following this.
[2] See Condon and Shortley, *Theory of Atomic Spectra* [which we shall denote, following Kemble, by TAS], pp. 175–180 for definitions and previous tabulations.

TABLE I. $c^k(lm, l'm')$ and $b^k(lm, l'm')$. We write $c^k = \pm\sqrt{(x/D_k)}$, where D_k depends only on k, l, l'. In the table are listed only the sign preceding the radical and the value of x, D_k being given at the head of each column. Since $b^k = (c^k)^2$, $b^k = +x/D_k$. Note that $c^k(l'm', lm) = (-1)^{m-m'}c^k(lm, l'm')$.

$c^k(lm, l'm')$ FOR $l+l'$ EVEN

ll'	m	m'	$k=$ 0	2	4	6	8
gs	±4	0			$+\sqrt{}$ 1/9		
	±3	0			1		
	±2	0			1		
	±1	0			1		
	0	0			1		
gd	±4	±2		$+\sqrt{}$ 70/245	$-\sqrt{}$168/10672.2	$+\sqrt{}$ 1/4089.8	
	±3	±2		+ 35	− 378	+ 5	
	±2	±2		+ 15	− 540	+ 15	
	±1	±2		+ 5	− 600	+ 35	
	0	±2		+ 1	− 540	+ 70	
	∓1	±2		0	− 378	+ 126	
	∓2	±2		0	− 168	+ 210	
	∓3	±2		0	0	+ 330	
	∓4	±2		0	0	+ 495	
	±4	±1		0	+ 588	− 9	
	±3	±1		+ 35	+ 525	− 32	
	±2	±1		+ 40	+ 243	− 70	
	±1	±1		+ 30	+ 30	− 120	
	0	±1		+ 16	− 30	− 175	
	∓1	±1		+ 5	− 243	− 224	
	∓2	±1		0	− 525	− 252	
	∓3	±1		0	− 588	− 240	
	∓4	±1		0	0	− 165	
	±4	0		0	− 784	+ 45	
	±3	0		0	− 49	+ 108	
	±2	0		+ 15	+ 64	+ 168	
	±1	0		+ 30	+ 289	+ 210	
	0	0		+ 36	+ 400	+ 225	
gg	±4	±4	1	$-\sqrt{}$784/5929	$+\sqrt{}$196/12370$\frac{31}{81}$	$-\sqrt{}$ 16/20449	$+\sqrt{}$ 1/120607$\frac{18}{49}$
	±3	±4	0	− 588	+ 490	− 84	+ 9
	±2	±4	0	− 168	+ 630	− 240	+ 45
	±1	±4	0	0	+ 490	− 480	+ 165
	0	±4	0	0	+ 196	− 720	+ 495
	∓1	±4	0	0	0	− 792	+ 1287
	∓2	±4	0	0	0	− 528	+ 3003
	∓3	±4	0	0	0	0	+ 6435
	∓4	±4	0	0	0	0	+ 12870
	±3	±3	1	− 49	− 441	+ 289	− 64
	±2	±3	0	− 525	− 70	+ 507	− 252
	±1	±3	0	− 378	+ 70	+ 540	− 720
	0	±3	0	0	+ 441	+ 300	− 1650
	∓1	±3	0	0	+ 490	+ 18	− 3168
	∓2	±3	0	0	0	− 198	− 5148
	∓3	±3	0	0	0	− 924	− 6864
	±2	±2	1	+ 64	− 121	− 484	+ 784
	±1	±2	0	− 243	− 360	− 189	+ 1764
	0	±2	0	− 540	− 121	0	+ 3150
	∓1	±2	0	0	+ 70	+ 210	+ 4620
	∓2	±2	0	0	+ 630	+ 504	+ 5544
	±1	±1	1	+ 289	+ 81	− 1	− 3136
	0	±1	0	− 30	− 81	− 210	− 4410
	∓1	±1	0	− 600	− 360	− 420	− 5040
	0	0	1	+ 400	+ 324	+ 400	+ 4900

TABLE I.—*Continued*

$c^k(lm, l'm')$ FOR $l+l'$ ODD

ll'	m	m'	$k=$ 1	3	5	7
gp	±4	±1		$+\sqrt{28/147}$	$-\sqrt{1/363}$	
	±3	±1		+ 21	− 3	
	±2	±1		+ 15	− 6	
	±1	±1		+ 10	− 10	
	0	±1		+ 6	− 15	
	∓1	±1		+ 3	− 21	
	∓2	±1		+ 1	− 28	
	∓3	±1		0	− 36	
	∓4	±1		0	− 45	
	±4	0		0	+ 9	
	±3	0		+ 7	+ 16	
	±2	0		+ 12	+ 21	
	±1	0		+ 15	+ 24	
	0	0		+ 16	+ 25	
gf	±4	±3	$+\sqrt{28/63}$	$-\sqrt{42/847}$	$+\sqrt{420/143143}$	$-\sqrt{1/26291\frac{4}{7}}$
	±3	±3	+ 7	− 63	+ 1575	− 7
	±2	±3	+ 1	− 54	+ 3375	− 28
	±1	±3	0	− 30	+ 5250	− 84
	0	±3	0	− 9	+ 6300	− 210
	∓1	±3	0	0	+ 5670	− 462
	∓2	±3	0	0	+ 3150	− 924
	∓3	±3	0	0	0	− 1716
	∓4	±3	0	0	0	− 3003
	±4	±2	0	+ 70	− 1960	+ 9
	±3	±2	+ 21	+ 14	− 4235	+ 48
	±2	±2	+ 12	− 3	− 4800	+ 147
	±1	±2	+ 3	− 32	− 3125	+ 336
	0	±2	0	− 49	− 700	+ 630
	∓1	±2	0	− 30	+ 210	+ 1008
	∓2	±2	0	0	+ 3360	+ 1386
	∓3	±2	0	0	+ 7350	+ 1584
	∓4	±2	0	0	0	+ 1287
	±4	±1	0	− 42	+ 4704	− 45
	±3	±1	0	+ 14	+ 4802	− 180
	±2	±1	+ 15	+ 40	+ 1849	− 420
	±1	±1	+ 15	+ 15	+ 15	− 735
	0	±1	+ 6	− 1	− 1210	− 1050
	∓1	±1	0	− 32	− 3584	− 1260
	∓2	±1	0	− 54	− 3402	− 1260
	∓3	±1	0	0	− 294	− 990
	∓4	±1	0	0	+ 5880	− 495
	±4	0	0	0	− 7056	+ 165
	±3	0	0	− 63	− 1764	+ 480
	±2	0	0	− 3	+ 84	+ 840
	±1	0	+ 10	+ 15	+ 2166	+ 1120
	0	0	+ 16	+ 36	+ 3600	+ 1225

If in $8^6 11$ we substitute l', $l'-\epsilon$ for lm; k, $m-l'+\epsilon$ for $l'm'$; lm for l'', $m+m'$; we can obtain the formula

$$c^k(l, m; l', l'-\epsilon) = \frac{(-1)^{g+l+\epsilon} g!}{(g-l)!(g-l')!(g-k)!(2g+1)!} \left[\frac{(2l+1)(2l'+1)}{\epsilon!(2l'-\epsilon)!} \frac{(k+l'-\epsilon-m)!}{(l-m)!} \frac{(l+m)!}{(k-l'+\epsilon+m)!} \right]^{\frac{1}{2}}$$

$$\times \sum_s (-1)^s \binom{\epsilon}{s} (2l'-s)!(2g-2l'+s)! \frac{(2g-2k)!}{(2g-2k-s)!} \frac{(k-l'+m+\epsilon)!}{(k-l'+m+s)!}. \quad (3A)$$

In the sum, $\binom{\epsilon}{s}$ is the binomial coefficient, and s runs from 0 to the lesser of ϵ and $2g-2k$.

TABLE II. $a^k(lm, l'm')$. *The value of this coefficient is independent of the signs of m and m'. As in the preceding table, we print the common denominator of several related values but once at the beginning of each group. For* $l=0$, $a^k(00, l'm')=\delta(k, 0)$ *for all* l', m'; *for* $k=0$, $a^0(lm, l'm')=1$ *for all values of the arguments; in the table we give values only for* l, l', $k>0$. *Note that* $a^k(l'm', lm)=a^k(lm, l'm')$.

ll'	$\vert m\vert$	$\vert m'\vert$	$k=$ 2	4	6	8
gp	4	1	+28/385			
	3	1	+7			
	2	1	−8			
	1	1	−17			
	0	1	−20			
	4	0	−56			
	3	0	−14			
	2	0	+16			
	1	0	+34			
	0	0	+40			
gd	4	2	+56/539	+14/2335$\frac{2}{3}$		
	3	2	+14	−21		
	2	2	−16	−11		
	1	2	−34	+9		
	0	2	−40	+18		
	4	1	−28	−56		
	3	1	−7	+84		
	2	1	+8	+44		
	1	1	+17	−36		
	0	1	+20	−72		
	4	0	−56	+84		
	3	0	−14	−126		
	2	0	+16	−66		
	1	0	+34	+54		
	0	0	+40	+108		
gf	4	3	+140/1155	+42/3670$\frac{1}{3}$	+4/12269.4	
	3	3	+35	−63	−17	
	2	3	−40	−33	+22	
	1	3	−85	+27	+1	
	0	3	−100	+54	−20	
	4	2	0	−98	−24	
	3	2	0	+147	+102	
	2	2	0	+77	−132	
	1	2	0	−63	−6	
	0	2	0	−126	+120	
	4	1	−84	+14	+60	
	3	1	−21	−21	−255	
	2	1	+24	−11	+330	
	1	1	+51	+9	+15	
	0	1	+60	+18	−300	
	4	0	−112	+84	−80	
	3	0	−28	−126	+340	
	2	0	+32	−66	−440	
	1	0	+68	+54	−20	
	0	0	+80	+108	+400	
gg	4	4	+784/5929	+196/12370$\frac{31}{81}$	+16/20449	+1/1206071$\frac{8}{49}$
	3	4	+196	−294	−68	−8
	2	4	−224	−154	+88	+28
	1	4	−476	+126	+4	−56
	0	4	−560	+252	−80	+70
	3	3	+49	+441	+289	+64
	2	3	−56	+231	−374	−224
	1	3	−119	−189	−17	+448
	0	3	−140	−378	+340	−560
	2	2	+64	+121	+484	+784
	1	2	+136	−99	+22	−1568
	0	2	+160	−198	−440	+1960
	1	1	+289	+81	+1	+3136
	0	1	+340	+162	−20	−3920
	0	0	+400	+324	+400	+4900

Alternatively if in $8^6 11$ we substitute k, $m-l'+\epsilon$ for lm; l', $l'-\epsilon$ for $l'm'$; lm for l'', $m+m'$, we can obtain

$$c^k(l,m;l',l'-\epsilon)=\frac{(-1)^{g+l}g!}{(g-l)!(g-l')!(g-k)!(2g+1)!}\left[\frac{(2l+1)(2l'+1)}{\epsilon!(2l'-\epsilon)!}\frac{(k+l'-\epsilon-m)!}{(l-m)!}\frac{(l+m)!}{(k-l'+\epsilon+m)!}\right]^{\frac{1}{2}}$$

$$\times\sum_s(-1)^s\binom{\epsilon}{s}(2l'-s)!(2g-2l'+s)!\frac{(2g-2l)!}{(2g-2l-s)!}\frac{(l-m)!}{(l-m-\epsilon+s)!},\quad (3B)$$

where s runs from 0 to the lesser of ϵ and $2g-2l$.

These formulas are good for the full range $-l\leqslant m\leqslant l$; hence we need consider only $\epsilon\leqslant l$ since the negative values of $l'-\epsilon$ may be covered by the formula $c^k(l,m;l',m')=c^k(l,-m;l',-m')$. For $\epsilon\leqslant l$, it may be seen that formula (3A) gives *directly* for $(c^k)^2$ a polynomial of order $2l'$ in m if $\epsilon>2g-2k$; formula (3B) gives *directly* a polynomial of order $2l'$ in m if $\epsilon>2g-2l$; while if $\epsilon<2g-2k$ and $\epsilon<2g-2l$ both formulas give polynomials of order $2l'$ *directly*. By *directly* we mean that the numerator and denominator of the rational function which these formulas give for $(c^k)^2$ come ready factorized so that the denominator may be canceled at once.[3]

The procedure for calculating the entries of Table I is then the following. In (3A) or (3B) take $l\geqslant l'$ to minimize the number of polynomials required. Then for each value of k occurring in (2), and for $\epsilon=0,1,\cdots,l'$, compute the c's as functions of m, using, in order to simplify the computation and make the sums as short as possible, (3A) if $\epsilon>2g-2k$, (3B) if $\epsilon>2g-2l$ (these inequalities are mutually exclusive), and either formula if $\epsilon<2g-2l$ and $\epsilon<2g-2k$. For example, one gets all the entries for gd from nine formulas, of which the following three are typical:

$$c^2(gm;d2)=+[(4+m)(3+m)(2+m)(1+m)/24\cdot 49\cdot 5]^{\frac{1}{2}}=c^2(g,-m;d,-2),$$
$$c^4(gm;d1)=+(2m-1)[5(5-m)(4+m)/6\cdot 121\cdot 49]^{\frac{1}{2}}=c^4(g,-m;d,-1),$$
$$c^6(gm;d0)=+[5(36-m^2)(25-m^2)/4\cdot 169\cdot 121]^{\frac{1}{2}}=c^6(g,-m;d,0).$$

These are valid for $-4\leqslant m\leqslant 4$.

II. Explanation of the Regularities in the Electrostatic Energies of Two-Electron Configurations amd Formulas for gp, gd, gf, gg, g^2

Inspection of the formulas for the electrostatic energies of two-electron configurations (TAS §5[7]) reveals a number of striking regularities to which attention has been called but for which, so far as we know, no proofs have been given. In order that we may justifiably take advantage of these regularities in our computations, we first indicate their general proofs.

(*a*) *In the case of* ll' (two nonequivalent electrons, cf. gp, gd, gf, gg below), ${}^1L$ *and* ${}^3L$ *have equal coefficients of the F's and equal but opposite coefficients of the G's.*

Consider a table, such as $1^7 2$ of TAS, in which the orbital functions are classified according to M_S and M_L. The sum of the diagonal elements of electrostatic energy for the states in the box $(1,M_L)$, with $M_S=1$, $M_L=M_L$, gives the sum of the energies of the N triplets of largest L value, if there are N states in this box. This sum is a certain linear combination of F's and G's. Consider now the diagonal sum for the corresponding box $(0,M_L)$ with $M_S=0$. This box contains $2N$ states and the diagonal sum gives the total energy of the N triplets and N singlets of highest L value. We see from the arrangement of the spins that the coefficients of the F's for this box are just twice those for $(1,M_L)$, while the coefficients of the G's vanish. The difference between the diagonal sum for $(0,M_L)$ and $(1,M_L)$ is the energy sum for the N singlets, and this sum therefore has the same F coefficients but the negative of the G coefficients of the triplet sum. By starting now with

[3] The ratio of two factorials involving m should here be treated like the ratio of two Γ functions, ignoring the fact that the factorials may be meaningless for certain values of m, for the resulting polynomials will always vanish properly for such m.

the highest M_L value, which involves only one singlet and one triplet, and working down, we prove the statement (*a*) by induction.

(*b*) *In the case of nln′l* (nonequivalent electrons of the same l value, cf. *gg* below) *in addition to* (*a*) *one finds that for those terms which are permitted in* nl^2 *by the exclusion principle the coefficients of the F's equal those of the corresponding G's, while for the terms excluded in* nl^2, *corresponding coefficients of F's and G's are equal and opposite.*

(*c*) *One can obtain the electrostatic energies for* nl^2 *from those for nln′l by setting* $F^k=G^k$ *and dividing by 2.*

The proof of (*c*) follows at once from the fact (TAS p. 232) that the Russell-Saunders eigenfunctions of nl^2, both the vanishing and the nonvanishing ones, may be obtained from the corresponding eigenfunctions of $nln'l$ by setting $n=n'$ and dividing by $\sqrt{2}$. Then, since $G^k(nl^2)\equiv F^k(nl^2)$, a diagonal electrostatic matrix element of nl^2 in LS coupling is obtained from that of $nln'l$ by setting $G^k=F^k$ and dividing by 2; as stated in (*c*). If this is done for one of the terms of ll which is excluded from l^2, the resulting energy must vanish; this requires that for such terms of ll the coefficients of F^k and G^k be equal and opposite. This proves one of the statements of (*b*), the other statement now follows at once from (*a*), which says that the unexcluded member of the pair of terms, ${}^1L$, ${}^3L$, has opposite G coefficients from the excluded member, and hence will have G coefficients equal to its F coefficients.

We give now the electrostatic energies of two-electron configurations involving g electrons. We also give the $\zeta(SL)$ which determine the absolute first-order Landé splitting (cf. TAS §4[7]). [We do not go on and calculate the complete matrices of spin-orbit interaction in LS coupling for these configurations because so far no one has wanted to use these matrices—even the known ones (TAS, pp. 268–269) for pd, d^2, dd—for intermediate-coupling computations because of the extreme complexity of the equations involved. Most of the complex configurations for which intermediate-coupling computations have been made involve almost-closed shells, and for these the jj-coupling matrices, which we do obtain, are of most interest.]

gp:

$$
\begin{aligned}
{}^1F,\ {}^3F &= F_0+55\,F_2\pm(G_3+55\,G_5) & \zeta({}^3F) &= \tfrac{5}{8}\,\zeta_g-\tfrac{1}{8}\,\zeta_p\\
{}^1G,\ {}^3G &= F_0-77\,F_2\mp(7\,G_3-11\,G_5) & \zeta({}^3G) &= \tfrac{19}{40}\,\zeta_g+\tfrac{1}{40}\,\zeta_p\\
{}^1H,\ {}^3H &= F_0+28\,F_2\pm(28\,G_3+G_5) & \zeta({}^3H) &= \tfrac{2}{5}\,\zeta_g+\tfrac{1}{10}\,\zeta_p
\end{aligned}
$$

gd:

$$
\begin{aligned}
{}^1D,\ {}^3D &= F_0+110\,F_2+143\,F_4\pm(G_2+330\,G_4+715\,G_6) & \zeta({}^3D) &= \tfrac{5}{6}\,\zeta_g-\tfrac{1}{3}\,\zeta_d\\
{}^1F,\ {}^3F &= F_0+11\,F_2-286\,F_4\mp(5\,G_2+957\,G_4-286\,G_6) & \zeta({}^3F) &= \tfrac{13}{24}\,\zeta_g-\tfrac{1}{24}\,\zeta_d\\
{}^1G,\ {}^3G &= F_0-65\,F_2+234\,F_4\pm(15\,G_2+883\,G_4+78\,G_6) & \zeta({}^3G) &= \tfrac{17}{40}\,\zeta_g+\tfrac{3}{40}\,\zeta_d\\
{}^1H,\ {}^3H &= F_0-70\,F_2-91\,F_4\mp(35\,G_2-798\,G_4-13\,G_6) & \zeta({}^3H) &= \tfrac{11}{30}\,\zeta_g+\tfrac{2}{15}\,\zeta_d\\
{}^1I,\ {}^3I &= F_0+56\,F_2+14\,F_4\pm(70\,G_2+168\,G_4+G_6) & \zeta({}^3I) &= \tfrac{1}{3}\,\zeta_g+\tfrac{1}{6}\,\zeta_d
\end{aligned}
$$

gf:

$$
\begin{aligned}
{}^1P,\ {}^3P &= F_0+275\,F_2+429\,F_4+715\,F_6\pm(G_1+33\,G_3+10725\,G_5+5005\,G_7) & \zeta({}^3P) &= \tfrac{5}{4}\,\zeta_g-\tfrac{3}{4}\,\zeta_f\\
{}^1D,\ {}^3D &= F_0+165\,F_2-143\,F_4-1287\,F_6\mp(3\,G_1+77\,G_3+12155\,G_5-3003\,G_7) & \zeta({}^3D) &= \tfrac{7}{12}\,\zeta_g-\tfrac{1}{12}\,\zeta_f\\
{}^1F,\ {}^3F &= F_0+30\,F_2-299\,F_4+1170\,F_6\pm(6\,G_1+97\,G_3-2990\,G_5+1365\,G_7) & \zeta({}^3F) &= \tfrac{5}{12}\,\zeta_g+\tfrac{1}{12}\,\zeta_f\\
{}^1G,\ {}^3G &= F_0-94\,F_2+39\,F_4-650\,F_6\mp(10\,G_1+63\,G_3-9594\,G_5-455\,G_7) & \zeta({}^3G) &= \tfrac{7}{20}\,\zeta_g+\tfrac{3}{20}\,\zeta_f\\
{}^1H,\ {}^3H &= F_0-159\,F_2+289\,F_4+225\,F_6\pm(15\,G_1-23\,G_3+8779\,G_5+105\,G_7) & \zeta({}^3H) &= \tfrac{19}{60}\,\zeta_g+\tfrac{11}{60}\,\zeta_f\\
{}^1I,\ {}^3I &= F_0-105\,F_2-203\,F_4-45\,F_6\mp(21\,G_1-91\,G_3-3115\,G_5-15\,G_7) & \zeta({}^3I) &= \tfrac{25}{84}\,\zeta_g+\tfrac{17}{84}\,\zeta_f\\
{}^1K,\ {}^3K &= F_0+140\,F_2+42\,F_4+4\,F_6\pm(28\,G_1+42\,G_3+420\,G_5+G_7) & \zeta({}^3K) &= \tfrac{2}{7}\,\zeta_g+\tfrac{3}{14}\,\zeta_f
\end{aligned}
$$

gg:

$$
\begin{aligned}
{}^1S,\ {}^3S &= F_0+1540\,F_2+2002\,F_4+2860\,F_6+24310\,F_8\pm(G_0+1540\,G_2+2002\,G_4+2860\,G_6+24310\,G_8)\\
{}^1P,\ {}^3P &= F_0+1309\,F_2+1001\,F_4-143\,F_6-19448\,F_8\mp(G_0+1309\,G_2+1001\,G_4-143\,G_6-19448\,G_8)\\
{}^1D,\ {}^3D &= F_0+883\,F_2-299\,F_4-1469\,F_6+12376\,F_8\pm(G_0+883\,G_2-299\,G_4-1469\,G_6+12376\,G_8)\\
{}^1F,\ {}^3F &= F_0+334\,F_2-949\,F_4+442\,F_6-6188\,F_8\mp(G_0+334\,G_2-949\,G_4+442\,G_6-6188\,G_8)\\
{}^1G,\ {}^3G &= F_0-230\,F_2-467\,F_4+1030\,F_6+2380\,F_8\pm(G_0-230\,G_2-467\,G_4+1030\,G_6+2380\,G_8)\\
{}^1H,\ {}^3H &= F_0-665\,F_2+581\,F_4-1205\,F_6-680\,F_8\mp(G_0-665\,G_2+581\,G_4-1205\,G_6-680\,G_8)\\
{}^1I,\ {}^3I &= F_0-791\,F_2+721\,F_4+601\,F_6+136\,F_8\pm(G_0-791\,G_2+721\,G_4+601\,G_6+136\,G_8)\\
{}^1K,\ {}^3K &= F_0-392\,F_2-784\,F_4-152\,F_6-17\,F_8\mp(G_0-392\,G_2-784\,G_4-152\,G_6-17\,G_8)\\
{}^1L,\ {}^3L &= F_0+784\,F_2+196\,F_4+16\,F_6+F_8\pm(G_0+784\,G_2+196\,G_4+16\,G_6+G_8)
\end{aligned}
$$

$$\zeta({}^3P)=\zeta({}^3D)=\zeta({}^3F)=\zeta({}^3G)=\zeta({}^3H)=\zeta({}^3I)=\zeta({}^3K)=\zeta({}^3L)=\tfrac{1}{4}\,\zeta_{ng}+\tfrac{1}{4}\,\zeta_{n'g}.$$

***g*²:** The formulas for the allowed terms, ${}^1S$, ${}^3P$, ${}^1D$, ${}^3F$, ${}^1G$, ${}^3H$, ${}^1I$, ${}^3K$, ${}^1L$, are obtained from *gg* by omitting the expressions in the G's. The intervals are given by $\zeta({}^3P)=\zeta({}^3F)=\zeta({}^3H)=\zeta({}^3K)=\tfrac{1}{2}\zeta_{ng}$.

TABLE III. *The integral* C_{uvw} [cf. (6)].*

$C_{000}=2$	$C_{112}=4/15$	$C_{222}=4/35$	$C_{334}=4/77$
$C_{011}=2/3$	$C_{123}=6/35$	$C_{224}=4/35$	$C_{336}=200/3003$
$C_{022}=2/5$	$C_{134}=8/63$	$C_{233}=8/105$	$C_{345}=40/1001$
$C_{033}=2/7$	$C_{145}=10/99$	$C_{235}=20/231$	$C_{347}=70/1287$
$C_{044}=2/9$		$C_{244}=40/693$	$C_{444}=36/1001$
		$C_{246}=10/143$	$C_{446}=40/1287$
			$C_{448}=980/21879$

* The table gives all nonvanishing integrals for u and $v\leq 4$. The values are independent of the order of the three subscripts.

III. FORMULA DETERMINING THE ELECTROSTATIC ENERGIES OF TWO-ELECTRON-LIKE CONFIGURATIONS WITH ALMOST-CLOSED SHELLS. VALUES FOR p^5g AND d^9g

In §1[13] (TAS) it is shown that *the coefficients of the F's in the electrostatic energies for the configuration* $l^{m-1}l'$, which has one electron missing from the l shell, *are the negatives of those for the related two-electron configuration* ll'. It is also shown that *the coefficients of the G's vanish for the triplets*, so that if the formulas for ll' are known the computation is reduced to a determination of the coefficients of the G's for the singlets. These G singlet coefficients, in the cases where they have been previously obtained, by the lengthy diagonal-sum calculation, turn out to have the strikingly simple form shown by the formulas of p. 299, TAS. We show below the reason for this form and give for the nonvanishing G coefficients an explicit formula whose use eliminates completely the necessity for a diagonal-sum calculation for configurations of this type.

The start of the table (similar to 1[13]5, TAS) which classifies the orbital functions for $l^{m-1}l'$ according to the values of M_S and M_L is, for $M_S=0$:

$$
\begin{array}{ll}
M_L=l+l' & (-l^+, l'^+)(-l^-, l'^-),\\
M_L=l+l'-1 & (-l+1^+, l'^+)(-l+1^-, l'^-)\\
 & (-l^+, l'-1^+)(-l^-, l'-1^-),\\
M\ =l+l'-2 & (-l+2^+, l'^+)(-l+2^-, l'^-)\\
 & (-l+1^+, l'-1^+)(-l+1^-, l'-1^-)\\
 & (-l^+, l'-2^+)(-l^-, l'-2^-).
\end{array}
$$

(The first entry in each parenthesis gives the quantum number m_l, m_s of the electron *missing* from the l shell, the second entry the quantum numbers of the l' electron.) The table continues in this fashion down to $M_L=|l-l'|$, and the G terms in the energies of all the singlets may be obtained by using just this part of the table.

In the diagonal sum for the box characterized by $M_S=0$, $M_L=M_L$, the coefficient of $G^k(ll')$, according to 1[13]4 (TAS), is seen to be

$$+\sum_m 2b^k(l, m; l', M_L+m). \qquad (4)$$

Now we shall presently prove that

$$
\begin{aligned}
\sum_m b^k(l, m; l', M+m)
&=\frac{(2l+1)(2l'+1)}{2(2k+1)}C_{ll'k} \quad \text{if } k\geq |M|\\
&=0 \quad \text{if } k<|M|,
\end{aligned}
\qquad (5)
$$

so that the sum (4), when it is nonvanishing, is independent of M_L. The factor $C_{ll'k}$ is the integral of the product of three Legendre polynomials:

$$C_{ll'k}=\int_0^\pi P_l(\cos\theta)P_{l'}(\cos\theta)P_k(\cos\theta)\sin\theta\, d\theta. \qquad (6)$$

Its values, which may be readily obtained from 9[6]9 (TAS) are given in Table III. From (4) and (5), and the usual diagonal-sum procedure which starts with the box with $M_S=0$, $M_L=l+l'$ and works down the table we see at once that

In the electrostatic energy for ^1L *the coefficients of all* G^k*'s vanish except that for* $k=L$, *which has the value*

$$\frac{(2l+1)(2l'+1)}{2L+1}C_{ll'L}.$$

Since $C_{ll'k}$ *vanishes unless the triangular conditions (2) are satisfied, only alternate singlets, those with* $L=l+l'$, $l+l'-2$, $l+l'-4$, $\cdots$, $|l-l'|$ *have any nonvanishing G coefficients. The intermediate singlets, with* $L=l+l'-1$, $l+l'-3$, $\cdots$ *have the same electrostatic energies as the triplets of the same L value.*

From this rule and those enunciated at the beginning of this section we may at once write down the electrostatic energy formulas, in particular the formulas for d^9g which we shall need in our applications to Cu II in the succeeding paper. In p^5g and d^9g the only nonvanishing terms in the G's are given by

$$
\begin{array}{ll}
p^5g \ \text{ or } \ g^{17}p & \begin{cases} {}^1H: & 90G_5\\ {}^1F: & 72G_3 \end{cases}\\
d^9g \ \text{ or } \ g^{17}d & \begin{cases} {}^1I: & 990G_6\\ {}^1G: & 3080G_4\\ {}^1D: & 252G_2. \end{cases}
\end{array}
\qquad (7)
$$

Note that these are written in terms of G_k rather than G^k ($G_k=G^k/D_k$, cf. Table I).

Proof of (5).—By the definition of $b^k=(c^k)^2$,

$$\sum_m b^k(l,\ m;\ l',\ M+m)=\sum_m b^k(l',\ M+m;\ l,\ m)$$

$$=\sum_m \frac{2}{2k+1}\int\int[\Theta_1(k,\ M)\Theta_1(l',\ M+m)\Theta_1(l,\ m)][\Theta_2(k,\ M)\Theta_2(l',\ M+m)\Theta_2(l,\ m)]\sin\theta_1\sin\theta_2\,d\theta_1\,d\theta_2,$$

if $k\geqslant|M|$. *b^k and hence the sum vanish by definition for $k<|M|$.* We now introduce integrals over φ_1 and φ_2, involving a quantum number m', which vanish unless $m'=M+m$, in which case they equal $(2\pi)^{-\frac{1}{2}}$. We may then write m' for $M+m$ in the Θ factors if we introduce a sum over m'. In this way the above expression becomes

$$=\sum_m\sum_{m'}\frac{4\pi}{2k+1}\int\int\int\int[\Theta_1(kM)\Theta_2(kM)\Phi_1(M)\bar{\Phi}_2(M)][\Theta_1(l'm')\Theta_2(l'm')\bar{\Phi}_1(m')\Phi_2(m')]$$
$$\times[\Theta_1(lm)\Theta_2(lm)\Phi_1(m)\bar{\Phi}_2(m)]\sin\theta_1\sin\theta_2\,d\theta_1\,d\theta_2\,d\varphi_1\,d\varphi_2.$$

The sums over m and m' may now be evaluated by means of the spherical-harmonic addition theorem to give

$$=\frac{(2l'+1)(2l+1)}{4\pi(2k+1)}\int\int\int\int\Theta_1(kM)\Theta_2(kM)\Phi_1(M)\bar{\Phi}_2(M)P_{l'}(\cos\omega)P_l(\cos\omega)\sin\theta_1\sin\theta_2\,d\theta_1\,d\theta_2\,d\varphi_1\,d\varphi_2,$$

where ω is the angle between the directions θ_1, φ_1 and θ_2, φ_2. Now express the product $P_{l'}(\cos\omega)P_l(\cos\omega)$ as a series in

TABLE IV. Matrices for transformation from LS to jj coupling.

df

	$^3H_6$
$\frac{5}{2}\ \frac{7}{2}$	1

	$^3H_5$	$^3G_5$	$^1H_5$	
$\frac{5}{2}\ \frac{7}{2}$	1	12	$\sqrt{30}$	
$\frac{5}{2}\ \frac{5}{2}$	$3\sqrt{10}$	$\sqrt{10}$	$-5\sqrt{3}$	$\frac{1}{5\sqrt{7}}$
$\frac{3}{2}\ \frac{7}{2}$	$2\sqrt{21}$	$-\sqrt{21}$	$\sqrt{70}$	

	$^3H_4$	$^3G_4$	$^3F_4$	$^1G_4$	
$\frac{5}{2}\ \frac{7}{2}$	$-4\sqrt{2}$	$\sqrt{33}$	$-5\sqrt{55}$	$2\sqrt{165}$	
$\frac{5}{2}\ \frac{5}{2}$	$2\sqrt{55}$	$6\sqrt{30}$	$-10\sqrt{2}$	$-10\sqrt{6}$	$\frac{1}{10\sqrt{21}}$
$\frac{3}{2}\ \frac{7}{2}$	$-2\sqrt{22}$	$18\sqrt{3}$	$10\sqrt{5}$	$6\sqrt{15}$	
$\frac{3}{2}\ \frac{5}{2}$	$4\sqrt{110}$	$-\sqrt{15}$	5	$10\sqrt{3}$	

	$^3G_3$	$^3F_3$	$^3D_3$	$^1F_3$	
$\frac{5}{2}\ \frac{7}{2}$	$-3\sqrt{5}$	$\sqrt{35}$	$-4\sqrt{30}$	$2\sqrt{105}$	
$\frac{5}{2}\ \frac{5}{2}$	$10\sqrt{2}$	$6\sqrt{14}$	$-6\sqrt{3}$	$-2\sqrt{42}$	$\frac{1}{14\sqrt{5}}$
$\frac{3}{2}\ \frac{7}{2}$	$-2\sqrt{15}$	$2\sqrt{105}$	$6\sqrt{10}$	$2\sqrt{35}$	
$\frac{3}{2}\ \frac{5}{2}$	$15\sqrt{3}$	$-\sqrt{21}$	$4\sqrt{2}$	$6\sqrt{7}$	

	$^3F_2$	$^3D_2$	$^3P_2$	$^1D_2$	
$\frac{5}{2}\ \frac{7}{2}$	-4	$\sqrt{15}$	$-3\sqrt{6}$	$3\sqrt{10}$	
$\frac{5}{2}\ \frac{5}{2}$	$3\sqrt{6}$	$3\sqrt{10}$	-4	$-\sqrt{15}$	$\frac{1}{5\sqrt{7}}$
$\frac{3}{2}\ \frac{7}{2}$	-3	$2\sqrt{15}$	$4\sqrt{6}$	$\sqrt{10}$	
$\frac{3}{2}\ \frac{5}{2}$	$4\sqrt{6}$	$-\sqrt{10}$	3	$2\sqrt{15}$	

	$^3P_0$
$\frac{5}{2}\ \frac{5}{2}$	1

pf

	$^3G_5$
$\frac{3}{2}\ \frac{7}{2}$	1

	$^3G_4$	$^3F_4$	$^1G_4$	
$\frac{3}{2}\ \frac{7}{2}$	2	$2\sqrt{15}$	$2\sqrt{5}$	
$\frac{3}{2}\ \frac{5}{2}$	$3\sqrt{5}$	$\sqrt{3}$	-6	$\frac{1}{2\sqrt{21}}$
$\frac{1}{2}\ \frac{7}{2}$	$\sqrt{35}$	$-\sqrt{21}$	$2\sqrt{7}$	

	$^3G_3$	$^3F_3$	$^3D_3$	$^1F_3$	
$\frac{3}{2}\ \frac{7}{2}$	-6	$6\sqrt{7}$	$-12\sqrt{5}$	$6\sqrt{21}$	
$\frac{3}{2}\ \frac{5}{2}$	$9\sqrt{5}$	$5\sqrt{35}$	-8	$-2\sqrt{105}$	$\frac{1}{42}$
$\frac{1}{2}\ \frac{7}{2}$	$-3\sqrt{3}$	$5\sqrt{21}$	$8\sqrt{15}$	$6\sqrt{7}$	
$\frac{1}{2}\ \frac{5}{2}$	36	$-4\sqrt{7}$	$2\sqrt{5}$	$4\sqrt{21}$	

	$^3F_2$	$^3D_2$	$^1D_2$	
$\frac{3}{2}\ \frac{7}{2}$	$-\sqrt{3}$	$2\sqrt{6}$	6	
$\frac{3}{2}\ \frac{5}{2}$	$4\sqrt{2}$	5	$-\sqrt{6}$	$\frac{1}{3\sqrt{7}}$
$\frac{1}{2}\ \frac{5}{2}$	$2\sqrt{7}$	$-\sqrt{14}$	$\sqrt{21}$	

	$^3D_1$
$\frac{3}{2}\ \frac{5}{2}$	1

	$^3D_1$	$^3P_1$	$^1P_1$	
$\frac{5}{2}\ \frac{7}{2}$	$-\sqrt{5}$	$\sqrt{10}$	$2\sqrt{5}$	
$\frac{5}{2}\ \frac{5}{2}$	4	$3\sqrt{2}$	-1	$\frac{1}{\sqrt{35}}$
$\frac{3}{2}\ \frac{5}{2}$	$\sqrt{14}$	$-\sqrt{7}$	$\sqrt{14}$	

pg

	$^3H_6$
$\frac{3}{2}\ \frac{9}{2}$	1

	$^3H_5$	$^3G_5$	$^1H_5$	
$\frac{3}{2}\ \frac{9}{2}$	$\sqrt{3}$	$4\sqrt{2}$	$\sqrt{10}$	
$\frac{3}{2}\ \frac{7}{2}$	$2\sqrt{6}$	1	$-2\sqrt{5}$	$\frac{1}{3\sqrt{5}}$
$\frac{1}{2}\ \frac{9}{2}$	$3\sqrt{2}$	$-2\sqrt{3}$	$\sqrt{15}$	

	$^3H_4$	$^3G_4$	$^3F_4$	$^1G_4$	
$\frac{3}{2}\ \frac{9}{2}$	-8	$9\sqrt{11}$	$-5\sqrt{77}$	$6\sqrt{55}$	
$\frac{3}{2}\ \frac{7}{2}$	$4\sqrt{77}$	$18\sqrt{7}$	-10	$-6\sqrt{35}$	$\frac{1}{18\sqrt{15}}$
$\frac{1}{2}\ \frac{9}{2}$	$-2\sqrt{11}$	36	$20\sqrt{7}$	$12\sqrt{5}$	
$\frac{1}{2}\ \frac{7}{2}$	$8\sqrt{55}$	$-9\sqrt{5}$	$\sqrt{35}$	30	

	$^3G_3$	$^3F_3$	$^1F_3$	
$\frac{3}{2}\ \frac{9}{2}$	-1	$\sqrt{15}$	$2\sqrt{5}$	
$\frac{3}{2}\ \frac{7}{2}$	$2\sqrt{5}$	$2\sqrt{3}$	-2	$\frac{1}{6}$
$\frac{1}{2}\ \frac{7}{2}$	$\sqrt{15}$	-3	$2\sqrt{3}$	

	$^3F_2$
$\frac{3}{2}\ \frac{7}{2}$	1

dg

	$^3I_7$
$\frac{5}{2}\ \frac{9}{2}$	1

	$^3H_6$	$^3I_6$	$^1I_6$	
$\frac{5}{2}\ \frac{9}{2}$	$4\sqrt{7}$	$\sqrt{2}$	$\sqrt{21}$	
$\frac{5}{2}\ \frac{7}{2}$	$\sqrt{5}$	$\sqrt{70}$	$-2\sqrt{15}$	$\frac{1}{3\sqrt{15}}$
$\frac{3}{2}\ \frac{9}{2}$	$-3\sqrt{2}$	$3\sqrt{7}$	$3\sqrt{6}$	

	$^3I_5$	$^3H_5$	$^3G_5$	$^1H_5$	
$\frac{5}{2}\ \frac{9}{2}$	$-4\sqrt{5}$	$\sqrt{286}$	$-3\sqrt{546}$	$\sqrt{2145}$	
$\frac{5}{2}\ \frac{7}{2}$	$\sqrt{910}$	$7\sqrt{77}$	$-12\sqrt{3}$	$-\sqrt{2310}$	$\frac{1}{15\sqrt{33}}$
$\frac{3}{2}\ \frac{9}{2}$	$-\sqrt{195}$	$7\sqrt{66}$	$12\sqrt{14}$	$6\sqrt{55}$	
$\frac{3}{2}\ \frac{7}{2}$	$4\sqrt{390}$	$-2\sqrt{33}$	$3\sqrt{7}$	$3\sqrt{110}$	

	$^3H_4$	$^3G_4$	$^3F_4$	$^1G_4$	
$\frac{5}{2}\ \frac{9}{2}$	$-2\sqrt{7}$	$6\sqrt{2}$	$-2\sqrt{110}$	$6\sqrt{10}$	
$\frac{5}{2}\ \frac{7}{2}$	$4\sqrt{14}$	21	$-\sqrt{55}$	$-6\sqrt{5}$	$\frac{1}{30}$
$\frac{3}{2}\ \frac{9}{2}$	$-4\sqrt{2}$	$7\sqrt{7}$	$\sqrt{385}$	$2\sqrt{35}$	
$\frac{3}{2}\ \frac{7}{2}$	$2\sqrt{154}$	$-2\sqrt{11}$	$2\sqrt{5}$	$2\sqrt{55}$	

	$^3G_3$	$^3F_3$	$^3D_3$	$^1F_0$	
$\frac{5}{2}\ \frac{9}{2}$	$-6\sqrt{6}$	$2\sqrt{154}$	$-10\sqrt{11}$	$2\sqrt{462}$	
$\frac{5}{2}\ \frac{7}{2}$	$3\sqrt{165}$	$7\sqrt{35}$	$-4\sqrt{10}$	$-2\sqrt{105}$	$\frac{1}{6\sqrt{105}}$
$\frac{3}{2}\ \frac{9}{2}$	$-3\sqrt{11}$	$7\sqrt{21}$	$20\sqrt{6}$	$6\sqrt{7}$	
$\frac{3}{2}\ \frac{7}{2}$	$6\sqrt{55}$	$-2\sqrt{105}$	$2\sqrt{30}$	$6\sqrt{35}$	

	$^3D_1$
$\frac{5}{2}\ \frac{7}{2}$	1

	$^3F_2$	$^3D_2$	$^1D_2$	
$\frac{5}{2}\ \frac{9}{2}$	$-\sqrt{10}$	$5\sqrt{2}$	$5\sqrt{3}$	
$\frac{5}{2}\ \frac{7}{2}$	$4\sqrt{5}$	7	$-\sqrt{6}$	$\frac{1}{3\sqrt{15}}$
$\frac{3}{2}\ \frac{7}{2}$	$3\sqrt{5}$	-6	$3\sqrt{6}$	

TABLE V. Matrices of electrostatic energy in jj coupling.

d^9f

a: $\frac{5}{2}, \frac{7}{2}$ c: $\frac{3}{2}, \frac{7}{2}$
b: $\frac{5}{2}, \frac{5}{2}$ d: $\frac{3}{2}, \frac{5}{2}$

	0b
0b	$-24F_2-66F_4$

	6a
6a	$-10F_2-3F_4$

	3a	3b	3c	3d
3a	$\frac{1}{7}(20F_2+132F_4+360G_3)$	$\frac{\sqrt{10}}{7}(-\frac{48}{5}F_2+66F_4-72G_3)$	$\frac{\sqrt{3}}{7}(30F_2-264F_4+120G_3)$	$\frac{\sqrt{15}}{7}(\frac{13}{5}F_2-66F_4+72G_3)$
3b		$\frac{1}{7}(\frac{348}{5}F_2-209F_4+144G_3)$	$\frac{\sqrt{30}}{7}(\frac{19}{5}F_2-55F_4-24G_3)$	$\frac{\sqrt{6}}{7}(\frac{36}{5}F_2+66F_4-72G_3)$
3c			$5F_2+\frac{120}{7}G_3$	$\sqrt{5}(-\frac{6}{5}F_2+\frac{72}{7}G_3)$
3d				$\frac{66}{5}F_2+\frac{216}{7}G_3$

	5a	5b	5c
5a	$\frac{74}{7}F_2+\frac{123}{7}F_4+72G_5$	$\sqrt{10}(\frac{12}{7}F_2+\frac{12}{7}F_4-36G_5)$	$\sqrt{21}(-\frac{12}{7}F_2-\frac{12}{7}F_4+24G_5)$
5b		$-\frac{60}{7}F_2-\frac{11}{7}F_4+180G_5$	$\sqrt{210}(-\frac{1}{7}F_2-\frac{1}{7}F_4-12G_5)$
5c			$-7F_2+168G_5$

	2a	2b	2c	2d
2a	$-10F_2+33F_4$	$-\frac{12}{5}\sqrt{6}F_2$	$\frac{60}{7}F_2+\frac{396}{7}F_4$	$\frac{\sqrt{6}}{7}(-\frac{22}{5}F_2+165F_4)$
2b		$-\frac{12}{5}F_2+33F_4$	$\frac{\sqrt{6}}{7}(\frac{27}{5}F_2+165F_4)$	$\frac{288}{35}F_2-\frac{396}{7}F_4$
2c			$-15F_2$	$-\frac{12}{5}\sqrt{6}F_2$
2d				$\frac{12}{5}F_2$

	4a	4b	4c	4d
4a	$12F_2-36F_4$	$-2\sqrt{110}F_4$	$\frac{\sqrt{11}}{7}(2F_2+72F_4)$	$\frac{\sqrt{55}}{7}(3F_2+10F_4)$
4b		$12F_2+11F_4$	$\frac{\sqrt{10}}{7}(5F_2+33F_4)$	$\frac{\sqrt{2}}{7}(-36F_2-22F_4)$
4c			$13F_2$	$2\sqrt{5}F_2$
4d				$-6F_2$

	1a	1b	1d
1a	$-\frac{150}{7}F_2-\frac{297}{7}F_4+40G_1$	$\sqrt{5}(-\frac{72}{35}F_2-\frac{132}{7}F_4-4G_1)$	$\sqrt{70}(-\frac{18}{35}F_2-\frac{33}{7}F_4+4G_1)$
1b		$-\frac{552}{35}F_2+\frac{66}{7}F_4+2G_1$	$\sqrt{14}(\frac{72}{35}F_2+\frac{132}{7}F_4-2G_1)$
1d			$-\frac{84}{5}F_2+28G_1$

d^9g

a: $\frac{5}{2}, \frac{9}{2}$ c: $\frac{3}{2}, \frac{9}{2}$
b: $\frac{5}{2}, \frac{7}{2}$ d: $\frac{3}{2}, \frac{7}{2}$

	1b
1b	$-110F_2-143F_4$

	7a
7a	$-56F_2-14F_4$

	4a	4b	4c	4d
4a	$28F_2+\frac{91}{3}F_4+1232G_4$	$\sqrt{2}(-\frac{48}{5}F_2+\frac{130}{3}F_4-616G_4)$	$\frac{\sqrt{14}}{3}(28F_2-182F_4+616G_4)$	$\frac{\sqrt{22}}{3}(\frac{23}{5}F_2-65F_4+616G_4)$
4b		$\frac{308}{5}F_2-\frac{364}{3}F_4+616G_4$	$\frac{\sqrt{7}}{3}(\frac{67}{5}F_2-130F_4-616G_4)$	$\frac{\sqrt{11}}{3}(\frac{22}{5}F_2+104F_4-616G_4)$
4c			$\frac{98}{3}F_2+\frac{4312}{9}G_4$	$\sqrt{77}(-\frac{14}{15}F_2+\frac{616}{9}G_4)$
4d				$\frac{1001}{15}F_2+\frac{6776}{9}G_4$

	6a	6b	6c
6a	$\frac{728}{15}F_2+\frac{658}{9}F_4+154G_6$	$\sqrt{35}(\frac{56}{15}F_2+\frac{28}{9}F_4-44G_6)$	$\sqrt{14}(-\frac{56}{5}F_2-\frac{28}{3}F_4+66G_6)$
6b		$-\frac{154}{3}F_2-\frac{91}{9}F_4+440G_6$	$\sqrt{10}(-\frac{14}{5}F_2-\frac{7}{3}F_4-132G_6)$
6c			$-\frac{196}{5}F_2+396G_6$

	3a	3b	3c	3d
3a	$-\frac{532}{15}F_2+\frac{1183}{9}F_4$	$\sqrt{110}(-\frac{32}{15}F_2+\frac{26}{9}F_4)$	$\sqrt{66}(\frac{28}{5}F_2+\frac{182}{9}F_4)$	$\sqrt{330}(-\frac{1}{5}F_2+\frac{65}{9}F_4)$
3b		$\frac{44}{3}F_2+\frac{572}{9}F_4$	$\sqrt{15}(\frac{11}{5}F_2+\frac{286}{9}F_4)$	$\sqrt{3}(22F_2-\frac{1144}{9}F_4)$
3c			$-\frac{1078}{15}F_2$	$-\frac{1078}{105}\sqrt{5}F_2$
3d				$\frac{77}{3}F_2$

	5a	5b	5c	5d
5a	$\frac{196}{3}F_2-\frac{1127}{9}F_4$	$\sqrt{182}(\frac{4}{15}F_2-\frac{40}{9}F_4)$	$\frac{196}{9}\sqrt{39}F_4$	$\sqrt{78}(\frac{7}{5}F_2+\frac{35}{9}F_4)$
5b		$\frac{814}{15}F_2+\frac{533}{9}F_4$	$\sqrt{42}(\frac{6}{5}F_2+\frac{65}{9}F_4)$	$\sqrt{21}(-\frac{44}{5}F_2-\frac{52}{9}F_4)$
5c			$\frac{196}{3}F_2$	$\frac{196}{15}\sqrt{2}F_2$
5d				$-\frac{539}{15}F_2$

	2a	2b	2d
2a	$-\frac{308}{3}F_2-\frac{1001}{9}F_4+140G_2$	$\sqrt{2}(-\frac{44}{3}F_2-\frac{572}{9}F_4-28G_2)$	$\sqrt{2}(-11F_2-\frac{143}{3}F_4+84G_2)$
2b		$-\frac{154}{3}F_2+\frac{1001}{9}F_4+\frac{56}{5}G_2$	$44F_2+\frac{572}{3}F_4-\frac{168}{5}G_2$
2d			$-77F_2+\frac{504}{5}G_2$

d^9d

a: $\frac{5}{2}, \frac{5}{2}$ c: $\frac{3}{2}, \frac{5}{2}$
b: $\frac{5}{2}, \frac{3}{2}$ d: $\frac{3}{2}, \frac{3}{2}$

	0a	0d
0a	$-\frac{56}{5}F_2-42F_4+6G_0$	$\sqrt{6}(-\frac{7}{5}F_2-42F_4+2G_0)$
0d		$-\frac{49}{5}F_2+4G_0$

	2a	2b	2c	2d
2a	$\frac{7}{25}(-4F_2+75F_4+48G_2)$	$\frac{12}{25}(-8F_2+75F_4-14G_2)$	$\frac{12}{25}(8F_2-75F_4+14G_2)$	$\frac{2\sqrt{21}}{25}(F_2-75F_4+28G_2)$
2b		$\frac{28}{25}(F_2+3G_2)$	$\frac{1}{25}(47F_2-900F_4-84G_2)$	$\frac{14\sqrt{21}}{25}(F_2-2G_2)$
2c			$\frac{28}{25}(F_2+3G_2)$	$\frac{14\sqrt{21}}{25}(-F_2+2G_2)$
2d				$\frac{49}{25}(3F_2+4G_2)$

	1a	1b	1c	1d
1a	$-\frac{184}{25}F_2+6F_4$	$\sqrt{14}(-\frac{24}{25}F_2-12F_4)$	$\sqrt{14}(\frac{24}{25}F_2+12F_4)$	$\sqrt{14}(-\frac{13}{25}F_2+18F_4)$
1b		$-\frac{196}{25}F_2$	$\frac{21}{25}F_2+84F_4$	$\frac{98}{25}F_2$
1c			$-\frac{196}{25}F_2$	$-\frac{98}{25}F_2$
1d				$-\frac{49}{25}F_2$

	3a	3b	3c	3d
3a	$\frac{116}{25}F_2-19F_4$	$\sqrt{6}(-\frac{12}{25}F_2-6F_4)$	$\sqrt{6}(\frac{12}{25}F_2+6F_4)$	$\frac{54}{25}F_2+6F_4$
3b		$\frac{154}{25}F_2$	$\frac{46}{25}F_2+9F_4$	$-\frac{28}{25}\sqrt{6}F_2$
3c			$\frac{154}{25}F_2$	$\frac{28}{25}\sqrt{6}F_2$
3d				$-\frac{49}{25}F_2$

	5a
5a	$-4F_2-F_4$

	4a	4b	4c
4a	$\frac{28}{5}F_2+7F_4+28G_4$	$\sqrt{2}(\frac{12}{5}F_2+2F_4-28G_4)$	$\sqrt{2}(-\frac{12}{5}F_2-2F_4+28G_4)$
4b		$-\frac{14}{5}F_2+56G_4$	$-\frac{6}{5}F_2-F_4-56G_4$
4c			$-\frac{14}{5}F_2+56G_4$

p^5f

a: $\frac{3}{2}, \frac{7}{2}$
b: $\frac{3}{2}, \frac{5}{2}$
c: $\frac{1}{2}, \frac{7}{2}$
d: $\frac{1}{2}, \frac{5}{2}$

	5a
5a	$-5F_2$

	1b
1b	$-12F_2$

	3a	3b	3c	3d
3a	$\frac{25}{7}F_2$	$-\frac{6}{7}\sqrt{5}F_2$	$\frac{50}{7}\sqrt{3}F_2$	$\frac{30}{7}F_2$
3b		$\frac{66}{7}F_2$	$\frac{9}{7}\sqrt{15}F_2$	$-\frac{24}{7}\sqrt{5}F_2$
3c			0	0
3d				0

	2a	2b	2d
2a	$-\frac{75}{7}F_2+72G_2$	$\sqrt{6}(-\frac{12}{7}F_2-12G_2)$	$\sqrt{21}(-\frac{6}{7}F_2+12G_2)$
2b		$\frac{12}{7}F_2+12G_2$	$\sqrt{14}(\frac{24}{7}F_2-6G_2)$
2d			$42G_2$

	4a	4b	4c
4a	$\frac{65}{7}F_2+\frac{40}{3}G_4$	$\sqrt{5}(\frac{10}{7}F_2-8G_4)$	$\sqrt{35}(-\frac{10}{7}F_2+\frac{8}{3}G_4)$
4b		$-\frac{30}{7}F_2+24G_4$	$\sqrt{7}(-\frac{5}{7}F_2-8G_4)$
4c			$\frac{56}{3}G_4$

$P_\lambda(\cos\omega)$, and then expand $P_\lambda(\cos\omega)$ by the addition theorem:

$$P_{l'}(\cos\omega)P_l(\cos\omega)=\sum_\lambda\frac{2\lambda+1}{2}C_{ll'\lambda}P_\lambda(\cos\omega)=\sum_\lambda 2\pi C_{ll'\lambda}\sum_\mu\Theta_1(\lambda\mu)\Theta_2(\lambda\mu)\bar{\Phi}_1(\mu)\Phi_2(\mu)$$

to give

$$\sum_m b^k(l,m;l',M+m)=\frac{(2l'+1)(2l+1)}{2(2k+1)}\sum_{\lambda,\mu}C_{ll'\lambda}\int\int\Theta_1(kM)\Phi_1(M)\Theta_1(\lambda\mu)\bar{\Phi}_1(\mu)\sin\theta_1\,d\theta_1\,d\varphi_1$$
$$\cdot\int\int\Theta_2(kM)\bar{\Phi}_2(M)\Theta_2(\lambda\mu)\Phi_2(\mu)\sin\theta_2\,d\theta_2\,d\varphi_2.$$

These integrals vanish unless $\lambda\mu\equiv kM$, in which case they give the value 1, so the sum over λ, μ gives finally the result (5).

IV. Matrices for Transformation of pf, df, pg, dg from LS to jj Coupling (Table IV)

In order to find the electrostatic energy matrices needed to handle configurations like p^5f of the rare gases, d^9f and d^9g of spectra like Cu II, in jj coupling, we need the transformations from LS to jj coupling. The transformation matrix for the almost-closed-shell configuration $l^{m-1}l'$ is the same as that for the two-electron configuration ll' when the states are correlated as in Chapter XII, TAS. We obtain these matrices by simultaneous diagonalization of the jj-coupling matrices of $\boldsymbol{L}_1\cdot\boldsymbol{L}_2$ (or $\boldsymbol{L}^2$) and $\boldsymbol{S}_1\cdot\boldsymbol{S}_2$ (or $\boldsymbol{S}^2$) as sketched in §6[12], TAS. We may note one simplification in connection with this diagonalization which was not noticed when previous computations were made. In no two-electron configuration will more than four levels of the same J value occur, so the transformation factorizes into matrices of at most fourth order. For a typical J value, the four Russell-Saunders levels are ${}^1J_J$, ${}^3J+1_J$, ${}^3J_J$, ${}^3J-1_J$. The state ${}^1J_J$ may be obtained directly from the matrix $\boldsymbol{S}_1\cdot\boldsymbol{S}_2$ since it has a value of $\boldsymbol{S}_1\cdot\boldsymbol{S}_2$ different from the other three. The states ${}^3J+1_J$ and ${}^3J-1_J$ may be obtained directly from the matrix of $\boldsymbol{L}_1\cdot\boldsymbol{L}_2$ since they possess unique values of this quantity. The state ${}^3J_J$ however has the same value of $\boldsymbol{S}_1\cdot\boldsymbol{S}_2$ as the other triplets and the same $\boldsymbol{L}_1\cdot\boldsymbol{L}_2$ as the singlet. To obtain it directly involves the *simultaneous* diagonalization of the two matrices with its attendant inconvenient intermediate matrix multiplications. But this may be avoided by noting that after ${}^1J_J$, ${}^3J+1_J$, ${}^3J-1_J$ have been found, the eigenfunction for ${}^3J_J$ is the unique function orthogonal to the other three.

The phases of the LS-coupling states in the transformation matrices of Table IV are arbitrary but the jj-coupling phases are chosen in accordance with the conventions of §6[12], TAS.

V. Matrices of Electrostatic Interaction in jj Coupling for p^5f, (d^9p), d^9d, d^9f, d^9g (Table V)

We finally give the results of transforming the electrostatic energies of section III to jj coupling by means of the matrices of section IV for cases of interest in the paper following this. The electrostatic matrices for p^5p and p^5d are given on pp. 307, 313 of TAS. We note that since the electrostatic energies and the LS-jj transformations are the same, the jj electrostatic-energy matrix for d^9p is the same as that for p^5d, when the d^9 and the p j values are correlated with the d and the p^5 j values respectively. Hence we do not need to give the d^9p matrix. Note however, that to conform to the jj-coupling phase conventions of TAS, a phase factor $(-1)^{j_1+j_2-J}$ must be applied in switching from pd to dp or from p^5d to d^9p.