1985

Group theoretical analysis of in-shell interaction in atoms

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GROUP THEORETICAL ANALYSIS
OF IN-SHELL INTERACTION IN ATOMS

A Thesis
Presented to
the Faculty of the Department of Physics
College of the Pacific
University of the Pacific

In Partial Fulfillment of
the Requirements for the Degree of Master
of Science in Physics

by
Yanfang Ho
April, 1985
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Dated April 9, 1985
ACKNOWLEDGMENTS

I am grateful to many individuals who have given me much help during the course of my research.

To Dr. Reuben Smith, Dean of the Graduate School at University of the Pacific, my thanks for his sponsorship of my study program.

To Professor Carl Wulfman, I owe more than words can describe for his thoughtful advice, guidance and zealous encouragement in the process of my research, my sincere appreciation for giving me a chance to study at the University of the Pacific and to join him at Princeton University as well as at the University of Canterbury in New Zealand.

To Professor Brian Wybourne, my sincere appreciation for giving me a chance to visit the University of Canterbury and his advice and guidance in the preparation of this thesis, and especially for help with recoupling techniques.

To Professor Herschel Rabitz, my thanks for giving me an opportunity to visit Princeton University, and to use the powerful computer and fine library of Princeton University.

To the Professors in the Physics Department, I am grateful for the considerable help they gave to me during my stay at the University of the Pacific.

I wish to express my extreme gratitude to Mrs. Carl Wulfman and Mrs. Catherine Bruner, my English teachers and motherly
friends, for their generous hospitality during my stay with them.

I am deeply indebted to Mrs. Celia Nathe for her assistance in typing this thesis.
Group theoretical analysis
of in-shell interaction in atoms

Abstract

A group theoretic approach to Layzer's 1/Z expansion method is explored. In part this builds on earlier work of Wulfman(2), of Moshinsky et al(14), and of Sinanoglu, Herrick(15), and Kellman (16) on second row atoms.

I investigate atoms with electrons in the 3s-3p-3d shell and find:

1. Wulfman's constant of motion accurately predicts configuration mixing for systems with two to eight electrons in the 3s-3p subshell.

2. The same constant of motion accurately predicts configuration mixing for systems with two electrons in the 3s-3p-3d shell.

3. It accurately predicts configuration mixing in systems of high angular momentum L and of high spin angular momentum S containing three electrons in the 3s-3p-3d shell, but gives less accurate results when L and S are both small.

I also show how effective nuclear charges may be calculated by a group theoretical approach. In addition I explore several new methods for expressing electron repulsion operators in terms of operators of the S0(4,2) dynamical group of one - electron atoms.
GROUP THEORETICAL ANALYSIS
OF IN-SHELL INTERACTION IN ATOMS

TABLE OF CONTENTS

ABSTRACT

I. INTRODUCTION PART 1: 1/Z EXPANSION METHOD...............(1)

II. INTRODUCTION PART 2: GROUP THEORETICAL ANALYSIS OF
THE 1/Z METHOD FOR THE HELIUM SERIES......................(3)

1. USING GROUP THEORY TO DETERMINE COEFFICIENTS OF
CONFIGURATION MIXING...........................................(3)

2. USING GROUP THEORY TO DETERMINE EFFECTIVE NUCLEAR
CHARGES..............................................................(4)

III. TWO AND THREE ELECTRON CONFIGURATION MIXING WITHIN
THE 3s-3p-3d SHELL............................................(13)

1. INTRODUCTION..................................................(13)

(1) IRREDUCIBLE TENSOR OPERATORS AND THEIR MATRIX
ELEMENTS; WIGNER-ECKART THEOREM...............................(13)

(2) SCALAR PRODUCT OF TENSORS, COULOMB INTERACTION
IN RUSSELL SAUNDERS TERMS (SL SCHEME) FOR TWO
ELECTRONS..........................................................(17)

(3) COUPLING OF THREE ANGULAR MOMENTA......................(24)
(4) COULOMB INTERACTION IN RUSSELL SAUNDERS TERMS
FOR THREE ELECTRONS........................................(29)

2. CALCULATION OF CONFIGURATION MIXING WITHIN THE
3s-3p-3d SHELL...................................................(35)

(1) TWO ELECTRON MATRIX ELEMENTS OF COULOMB
INTERACTION AND OF A₁, A₂ WITHIN THE 3s-3p-3d
SHELL.................................................................(35)

(2) RECOUPLING COEFFICIENTS WITHIN THE 3s-3p-3d
SHELL FOR THREE ELECTRONS..............................(39)

(3) MATRIX ELEMENTS OF COULOMB INTERACTION AND OF
Σ_{i<j} (L_i L_j - A_i A_j) WITHIN IN THE 3s-3p-3d SHELL
FOR THREE ELECTRON SYSTEMS.........................(39)

(4) RESULTS..............................................................(47)

TABLE 1. MATRIX ELEMENTS FOR A₁, A₂ IN THE
3s-3p-3d SHELL...................................................(47)

TABLE 2. MATRIX ELEMENTS FOR THE COULOMB
INTERACTION IN THE 3s-3p-3d SHELL...........(48)

TABLE 3. RECOUPLING COEFFICIENTS WITHIN THE
3s-3p-3d SHELL FOR THREE ELECTRONS.....(53)

TABLE 4. COEFFICIENTS OF FRACTIONAL PARENTAGE
FOR p.................................................................(63)

TABLE 5. COEFFICIENTS OF FRACTIONAL PARENTAGE
FOR d.................................................................(63)
TABLE 6. COMPARISON OF EXACT AND APPROXIMATE
CONFIGURATION MIXING......................(64)

3. EXPLORATIONS.................................................(86)

IV. THE EXPRESSION FOR THE INTERACTION BETWEEN TWO
ELECTRONS IN THE n = 2 SHELL IN TERMS OF GENERATORS
OF SO(4).........................................................(86)

1. AN EXPRESSION FOR COULOMB INTERACTIONS IN TERMS OF
A AND L...........................................................(87)

(1) EVALUATION OF RATIOS OF REDUCED MATRIX ELEMENTS
FOR THE n = 2 AND FOR THE n = 3 SHELL..............(88)

(2) THE SYMMETRIZED FORM FOR y (A) THAT SATISFIES

\[ (Y_{\ell m}(A))^+ = (-1)^m Y_{\ell -m}(A) \] ..................(91)

(3) DISCUSSION....................................................(93)

2. AN EXPRESSION FOR COULOMB INTERACTIONS IN TERMS OF
A AND B...........................................................(94)

(1) FINDING \[ \sum_m (-1)^m Y_{\ell m}(\xi_1) Y_{\ell -m}(\xi_2) \] IN TERMS OF
PRODUCT OF \(\xi_1\) AND \(\xi_2\).........................(96)

(2) A METHOD FOR EVALUATING THE MATRIX ELEMENTS......(98)

V. APPENDICES......................................................(100)

APPENDIX 1. SOME EXAMPLES OF CALCULATIONS OF THE
MATRIX ELEMENTS OF \[ \sum_{\xi_1, \xi_2} (L_1 \cdot L_2 - A_1 \cdot A_2) \].....(100)
APPENDIX 2. SOME EXAMPLES OF CALCULATIONS OF
THE RATIO OF REDUCED MATRIX ELEMENTS....(101)

APPENDIX 3. SOME EXAMPLES OF CALCULATIONS OF THE
MATRIX ELEMENTS OF V.................(104)

APPENDIX 4. THE SLATER INTEGRALS WITH EFFECTIVE
NUCLEAR CHARGES IN (II-2-7)..........(106)

VI. REFERENCES.................................(110)
I. Introduction part 1; $1/Z$ expansion method

A promising theoretical scheme for describing atomic spectra was developed by David Layzer some time ago (1). This scheme emphasizes the importance of the interaction between configurations that are degenerate in hydrogenic approximation, and the importance of changes in the wave functions that can be expressed as changes in effective nuclear charges. The theory is in some respects simpler than the one based on the central-field approximation and Hartree-Fock wave functions. It also gives more direct explanations of the systematics of atomic spectra.

In a nonrelativistic approximation the Hamiltonian for an $N$-electron atom of nuclear charge $Z$ is given (in atomic units) by:

$$H(N,Z) = \sum \frac{1}{2} p_i^2 - \frac{Z}{r_i} + \sum \frac{1}{r_{ij}}, \quad (I-0-1)$$

If we adopt a new unit of length equal to the old one divided by $Z$, so $r_i = \overline{r}_i/Z$, $p = Z \overline{p}_i$, then:

$$H(N,Z) = \sum \frac{1}{2} Z^2 \overline{p}_i^2 - \overline{Z}^2 / \overline{r}_i + \sum Z / \overline{r}_{ij},$$

$$= Z^2 \left[ (\overline{p}_i^2/2 - 1/\overline{r}_i + \sum Z^{-2} / \overline{r}_{ij} ) = Z^2 \overline{H} \right], \quad (I-0-2)$$

where

$$H(N,Z) = \sum \frac{1}{2} (\overline{p}_i^2/2 - 1/\overline{r}_i) + \sum Z^{-2} / \overline{r}_{ij} = \overline{H}^o + \lambda \overline{V},$$

and

$$\overline{H}^o = \sum \frac{1}{2} (\overline{p}_i^2/2 - 1/\overline{r}_i) = \sum \overline{H}_i^o \quad \overline{H}_i^o = \frac{\overline{p}_i^2}{2} - 1/\overline{r}_i.$$
\[ \lambda = \frac{1}{Z}, \quad \vec{V} = \sum_{i<j} \frac{1}{r_{ij}}. \]

Layzer uses perturbation theory with \( \lambda = \frac{1}{Z} \) as the perturbation parameter. Because of the degeneracy of levels of different \( \ell \) but the same principal quantum number \( n \) he must use degenerate perturbation theory to determine the approximate eigenvectors and eigenvalues from which the effective nuclear charge is determined. This gives a term in the wave function of zero order in \( \frac{1}{Z} \). He then uses effective nuclear charges to deal with changes in wave functions of first order in \( \frac{1}{Z} \). For the treatment of terms of higher order in \( \frac{1}{Z} \) we refer the reader to Layzer's papers (1).
II. Introduction part 2; group theoretical analysis of the 1/Z method for the helium series

1. Using group theory to determine the coefficient of configuration mixing

According to Wulfman's work (2) for two electron atoms we have:

\[(A_{ij} + \mu_{ij}) \Psi_{PQLM} = \left[ P(P + 2) + Q \right] \Psi_{PQLM}, \]

\[(L_{ij} \cdot A_{ij}) \Psi_{PQLM} = \left[ Q(P + 1) \right] \Psi_{PQLM}, \]

\[L_{ij} \Psi_{PQLM} = L(L + 1) \Psi_{PQLM}, \quad \text{(II-1-1)} \]

\[(L_{ij})_{\mu} \Psi_{PQLM} = M \Psi_{PQLM}. \]

where \( A_{ij} = A_x - A_y, \quad L_{ij} = L_x + L_y, \quad A_j \) being the Runge Lenz vector of particle \( j \), and \( L_j \) being the angular momentum of particle \( j \).

The functions satisfying (II-1-1) are:

\[
\Psi_{PQLM} = \left| PQLM(n, n_j) \right> = \sum_{L_x, L_y} (-1)^{L_x - n_x} \left[ (2L_x + 1)(2L_y + 1)(P + Q + 1) \right]^{1/2} 
\]

\[
\left\{ \frac{(n_x - 1)/2, (n_x - 1)/2, \ell_x}{\left( \frac{P + Q}{2}, \frac{P - Q}{2}, L \right)} x \left\{ \frac{(n_j - 1)/2, (n_j - 1)/2, \ell_j}{\left( \frac{P + Q}{2}, \frac{P - Q}{2}, L \right)} \right\} \right. \]

\[
\left. L_{ij}^{+} L_{ij} L_{ij}^{-} L_{ij} \right\}^{25}(n_x, \ell_x, n_j, \ell_j) \quad \text{(II-1-2)}
\]
where \( j_\alpha = (n_i - 1)/2 \), \( j_\beta = (n_j - 1)/2 \),

\[ J_\alpha = j_i + j_z, \ldots j_z - j_i, \]

\[ J = j_i + j_z, \ldots j_z - j_i, \]

\[ P = J_\alpha + J_\beta, \]

\[ Q = J_\alpha - J_\beta. \]

\( ^{2S+1}L(n_i, l_i; n_j l_j) \) is a two electron configuration with definite S, L, n and l quantum numbers.

When \( n_i = 2, n_j = 2, L = 0, \eta = +, \) from (II-1-2) the states are:

\[ 000(22) = -0.500 S(s) + 0.866 S(p^2); \]

\[ 200(22) = -0.866 S(s) - 0.500 S(p^2). \]

The states obtained by the degenerate perturbation method i.e. by diagonalization are:

\[ -0.476 S(s^2) + 0.880 S(p^2), \]

\[ -0.880 S(s^2) - 0.476 S(p^2). \]

One can see the first set is very close to the second set and Wulfman's method is simpler than the 1/Z method for finding the coefficients of configuration mixing. It is found to accurately predict most in-shell configuration mixing in doubly excited states of two electron atoms (2).

2. Using group theory to determine the effective nuclear charge
We have used a new way of looking at effective nuclear charges that utilizes their group theoretic interpretation as scale factors. We find the effective nuclear charges in doubly excited states of helium by using group operators of SO(4,2). In this we make use of a representation of SO(4,2), derived by Bednar (13), which has considerable advantages in atomic and molecular studies. The generators in this realization are defined as follows:

\[ J_k = (-i/2) \epsilon_{ijk} \left( x_i \frac{\partial}{\partial x_j} - x_j \frac{\partial}{\partial x_i} \right), \]

\[ A_k = -1/2 (x_k \Delta - 2 \frac{\partial}{\partial x_k} - 2x_j \frac{\partial^2}{\partial x_j \partial x_k} + x_k), \]

\[ B_k = -1/2 (x_k \Delta - 2 \frac{\partial}{\partial x_k} - 2x_j \frac{\partial^2}{\partial x_j \partial x_k} - x_k), \]

\[ T_1 = -1/2 (r \Delta + r), \]

\[ T_2 = -i (1 + x_j \frac{\partial}{\partial x_j}) = -i (1 + r \frac{\partial}{\partial r}), \]

\[ T_3 = 1/2 (r \Delta - r), \]

\[ \Gamma_k = i r \frac{\partial}{\partial x_k}. \]

where:

\[ \Delta = \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_j}, \quad r = (x_j x_j)^{1/2}. \]

These generators are self-adjoint with the scalar product:

\[ \int X^{*}_{n'k'm'}(x) \frac{1}{r} X_{nkm}(x) r^2 \sin \theta \, dO = \delta_{n'n'} \delta_{k'k} \delta_{m'm}. \]
The wave functions \( \chi_{n\ell m}(\mathbf{x}) \) can be expressed in spherical coordinates as:

\[
\chi_{n\ell m}(r, \theta, \varphi) = \frac{2}{\sqrt{(n-\ell-l)! (n+l)!}} (2r)^{\ell} L_{n-\ell-1 \ell}^{2\ell}(2r) \psi_{\ell m}(\theta, \varphi)
\]

where the \( L_{n-\ell-1 \ell}^{2\ell}(2r) \) are Laguerre polynomials. In this realization, the operators \( J, A, B, T \) form the Lie algebra of the subgroup \( SO(4,1) \) with the following commutation relations:

\[
\begin{align*}
[ J_+, J_- ] &= i \epsilon_{+k} J_k, \\
[ A_+, A_- ] &= i \epsilon_{+k} J_k, \\
[ J_+, A_- ] &= i \epsilon_{+k} A_k, \\
[ B_+, B_- ] &= -i \epsilon_{+k} J_k, \\
[ J_+, B_- ] &= i \delta_{j} B_k, \\
[ A_+, B_- ] &= i \delta_{j} T_2, \\
[ A_+, T_- ] &= -i B_2, \\
[ B_+, T_- ] &= -i A_2, \\
[ J_+, T_- ] &= 0.
\end{align*}
\]

The operators \( T, T_1, T_2, T_3 \) obey the following commutation relations:

\[
\begin{align*}
[ T_1, T_2 ] &= -i T_3, \\
[ T_2, T_3 ] &= i T_1.
\end{align*}
\]
\[ [T_3, T_1] = i T_2 \]

They therefore form the Lie algebra of an SO(2,1) subgroup. This realization is particularly convenient because the position operators in it have the following simple form:

\[ x_i = B_i - A_i , \]

\[ r = T_3 - T_1 . \quad (II-2-4) \]

Also the matrix representation of the generators \( J, A, B, T \) is quite simple. We emphasize that the scalar product in Bednar representation is different from the usual one in Schrödinger's representation. For example we can show that the generator:

\[ T_2 = -i(r \frac{\partial}{\partial r} + 1) , \]

is self-adjoint with the scalar product:

\[ \int X_{n'l'm'}^* (x) \frac{1}{r} X_{n'lm} (x) r^2 \, dr \, d\Omega . \]

By using integration by parts, we have:

\[ \int X_{n'l'm'}^* T_2 X_{n'lm} \, r \, dr \, d\Omega = \int X_{n'l'm'}^* [-i (r \frac{\partial}{\partial r} + 1)] X_{n'lm} \, r \, dr \, d\Omega \]

\[ = -i X_{n'l'm'}^* r^2 X_{n'lm} \bigg|_0^\infty + i \int X_{n'l'm'} \frac{1}{r} \left( \frac{\partial X_{n'lm}^*}{\partial r} \right) \, dr \, d\Omega \]

\[ + 2i \int r X_{n'l'm'} \frac{\partial X_{n'lm}^*}{\partial r} \, dr \, d\Omega - i \int X_{n'l'm'}^* X_{n'lm} \, r \, dr \, d\Omega , \]
We have:

\[
\int \chi^*_{n'k'm'} T_2 \chi_{nkm} r \, dr \, d\Omega = \int (T_2 \chi^*_{n'k'm'}) \chi_{nkm} r \, dr \, d\Omega.
\]

So, \( T_2 = -i (r \frac{\partial}{\partial r} + 1) \) is self-adjoint with the scalar product:

\[
\int \chi^*_{n'k'm'} \chi_{nkm} r \, dr \, d\Omega.
\]

Also we can show that the generator

\[
T_2 = -i (r \frac{\partial}{\partial r} + 3/2).
\]

is self-adjoint with the scalar product:

\[
\int \psi^*_{n'k'm'} \psi_{nkm} r^2 \, dr \, d\Omega.
\]

Using integration by parts, we have:

\[
\int \psi^*_{n'k'm'} \psi_{nkm} r^2 \, dr \, d\Omega = \int \psi^*_{n'k'm'} i \left[ r \frac{\partial}{\partial r} + \frac{3}{2} \right] \psi_{nkm} r \, dr \, d\Omega,
\]

\[
= -i \psi^*_{n'k'm'} \psi_{nkm} \bigg|_0^\infty + 3i \int \psi^*_{n'k'm'} r^2 \psi_{nkm} r \, dr \, d\Omega.
\]
Therefore we have:

\[ \int \Psi_{n \ell m}^* \nabla^2 \Psi_{n \ell m} \, r \, d \mathbf{r} \, d \Omega = \int (T_a \Psi_{n \ell m})^* \Psi_{n \ell m} \, r \, d \mathbf{r} \, d \Omega, \]

so, \( T_a = -i(r \frac{\partial}{\partial r} + 3/2) \) is self-adjoint when the scalar product is:

\[ \int \Psi_{n \ell m}^* \Psi_{n \ell m} \, r \, d \mathbf{r} \, d \Omega. \]

We make use of the operators \( \exp(i \alpha T_a) \). We have:

\[ \exp(i \alpha T_a) f(r) = \exp(3\alpha/2) f(e^{3/2}r) \]

If \( \int \Psi(r) \Psi(r) dv = 1 \), and then:

\[ \int e^{3\alpha/2} \Psi^* (e^{3/2}r) e^{3\alpha/2} \Psi (e^{3/2}r) dv = \int \Psi^* (e^{3/2}r) \Psi (e^{3/2}r) d(e^{3/2}r) = 1 \]

Thus we may interpret \( e^{3/2} \) as \( z \), \( \ln z = \alpha \), where \( z \) is the effective nuclear charge.

We see one can use the operator \( \exp(i \alpha T_a) \) to set the effective nuclear charge in the eigenvector 

\[ |PQLM;Z_a Z_b> = |2000>. \]
\[ |PQLM; Z_a Z_b > = 10000 > \]. We have:

\[
2000Z_a Z_b > = \frac{1}{\sqrt{15}} \left[-(3/2) \right] S(2s, Z_a, 2s Z_b) \\
- (1/2) \left[ S(2p, Z_a, 2p Z_b) \right] \\
+ 1/\sqrt{15} \left[-(5/2) \right] S(2s, Z_b, 2s Z_a) \\
- (1/2) \left[ S(2p, Z_b, 2p Z_a) \right].
\]

Where D is a normalization constant.

We find the effective nuclear charge by varying the \( Z_a, Z_b \) to minimize the energy of the system:

\[
<2000Z_a Z_b | H | 2000Z_a Z_b > \text{ where } H = H^0 + H_z^0 + 1/r_{12}
\]

\[
<2000Z_a Z_b | H | 2000Z_a Z_b > = <2000Z_a Z_b | H^0 | 2000Z_a Z_b > \\
+ <2000Z_a Z_b | H_z^0 | 2000Z_a Z_b > + <2000Z_a Z_b | 1/r_{12} | 2000Z_a Z_b >.
\]

By using the formula \( 1/r_{12} = \sum_{k=0}^{\infty} \frac{r_{12}^k}{r_{12}^{k+1}} P_k(\cos \theta_{12}) \).

When \( r_1 > r_2 \),

\[
1/r_{12} = \sum_{k=0}^{\infty} \frac{r_2^k}{r_1^{k+1}} P_k(\cos \theta_{12})
\]

When \( r_1 < r_2 \),

\[
1/r_{12} = \sum_{k=0}^{\infty} \frac{r_1^k}{r_2^{k+1}} P_k(\cos \theta_{12}) \quad (II-2-5)
\]

and the relation

\[
< l, l' | m | P_k(\cos \theta_{12}) | l, l, m > = (-1)^l l' l + l
\]

\[
x \left( \frac{2 \ell_+ 1}{2 \ell_+ 1} \right) \left( \frac{2 \ell_+ 1}{2 \ell_+ 1} \right)
\]

\[
x \left( \frac{2 \ell_+ 1}{2 \ell_+ 1} \right) \left( \frac{2 \ell_+ 1}{2 \ell_+ 1} \right)
\]

We obtain:
$$W(Z_a, Z_b) = \langle 2000Z_a, Z_b | 1/r_{ij} | 2000Z_a, Z_b \rangle$$

$$= \left\{ 1 \frac{F_{ss} (Z_a, Z_b Z) + F_{sSsE} (Z_a, Z_b Z)}{8 + 6D_{sSsE} (Z_a, Z_b) + 2D_{pP} (Z_a, Z_b)} \right\}$$

Here:

$$F_{i j m} (Z_a, Z_b k) = \int_0^\infty R_{i k} (Z_a, Z_b x) x^{1-k} \int_0^\infty R_{j m} (Z_b, Z_b y) y^{2+k} \mathrm{d}x \mathrm{d}y$$

$$F_{i j m} (Z_a, Z_b k) = \int_0^\infty R_{i k} (Z_a, Z_b x) x^{1-k} \int_0^\infty R_{j m} (Z_b, Z_b y) y^{2+k} \mathrm{d}x \mathrm{d}y$$

By using a Macsyma computer we calculated all these integrals (which are given in appendix 4) and substituted them into (II-2-7). We found the minimum of $E(Z_a, Z_b)$ by a numerical method. The minimum occurs for $E(Z_a = 1.8, Z_b = 1.8)$ and $D(Z_a = 1.8, Z_b = 1.8) = 4$.

The eigenvector and eigenvalue with effective nuclear charge $Z_a = 1.8, Z_b = 1.8$ are:
\[ |PQLM_{z_a z_b} > = -(3/2)^{1/2} S(2s 1\&, 2s 1\&) - (1/2)^{1/2} S(2p 1\& , 2p 1\&) \]

here, \( P = 2 , \ Q = 0 , \ L = 0 , \ M = 0 \),

\[ E(Z_a = 1.8, Z_b = 1.8) = -0.76851562 \text{ (A. U.).} \]

Here, where we only consider configuration mixing within a shell, the effective nuclear charge is independent of the angular momentum quantum number. For the same doubly-excited state \( 2'S(2s^2, 2p^2) \) the energy calculated from D. R. Herrick's formula (20)(21) is -0.7575757(A.U.) and the energy calculated by J. R. Jasperse and M. H. Friedman (22) is -0.758100(A.U.). Our result is lower because we have used better configuration mixing and have found the effective nuclear charge that gives the lowest extremum in \( E(Z_a, Z_b) \).

So far we have not found a general formula that gives the effective nuclear charge directly for \( n > 2 \) and \( N > 2 \). Also there exists no general relation analogous to (II-1-2) which predicts configuration mixing when \( N > 2 \). To prepare the way for the development of such a formula we will, in this thesis, concern ourselves with the configuration mixing problem for three electrons in the 3s-3p-3d shell. We will in this work test the validity of using a known approximate constant of motion for 2s-2p and 3s-3p as an approximate constant of motion for 3s-3p-3d systems.
It was recently found by Wulfman (3), that the operator $C^* = \sum (A_i - A_j)^2 + (L_i + L_j)^2$, a sum of particle-pair $O(4)$ Casimir operators, is a surprisingly good approximate constant of motion for $N$-electrons in the 2s-2p shell (16). Ho and Wulfman established that this constant also accurately fixes configuration mixing within the entire 3s-3p subshell (4). We here investigate the use of $C^*$ in approximating configuration mixing within the 3s-3p-3d shell. We calculate both approximate and exact in-shell configuration mixing for two and three electron systems.

There are many methods for dealing with configuration mixing for many electrons. We here use the group theoretic methods developed by Racah (5) for dealing with complicated configurations in Russell Saunders approximation. We first introduce some important concepts and the mathematical formalism presented by Racah in his series of papers (5).
The concept of irreducible tensor operator occupies a central position in the modern theory of angular momentum. Its importance was first emphasized by Racah (5) who derived the algebra of these operators and applied them to the study of atomic spectroscopy. Pioneering work had also been done by Wigner.

The matrix components of electrostatic interaction between electrons depend on the matrix elements of the spherical harmonics. The spherical harmonics play the role of operators and not of eigenfunctions, and it is convenient to consider in a general way the algebra of such operators. Suppose \( J_x, J_y, J_z \) are the components of angular-momentum which satisfy the commutation relations.

\[
\begin{align*}
[J_x, J_y] &= iJ_z, \\
[J_y, J_z] &= iJ_x, \\
[J_z, J_x] &= iJ_y
\end{align*}
\]

and satisfy \( J^+ = J \). It is easy to show (6) that the nonvanishing matrix elements of the operators \( J_x = J_x + iJ_y \) and \( J_z \) are given by the equations

\[
\begin{align*}
\langle j \, m + 1 | J_x^+ | j \, m \rangle &= \sqrt{j(j + 1) - m(m + 1)}, \\
\langle j \, m | J_z | j \, m \rangle &= m.
\end{align*}
\] (III-1-1)

Racah considered a set of operators \( t^q_0(q = k, k - 1, k - 2, \ldots, -k) \) which satisfy analogous relations when acted on by the angular momentum operators. Such operators are called spherical tensor
operators of rank $k$. They are defined by means of the commutation relations

\[
\left[ J^z, t^K_\theta \right] = q \cdot t^K_\phi
\]

\[
\left[ J^z, t^K_\phi \right] = \left[ k(k + 1) - q(q + 1) \right] t^K_\phi. \quad (III-1-2)
\]

In order to compare (III-1-1) and (III-1-2) we first recall an elementary result from quantum mechanics. The $z$ component of the orbital angular momentum operator in spherical polar coordinates is:

\[
J^z = J^z_0 = -i \frac{\partial}{\partial \phi}. \quad (III-1-3)
\]

Assuming $f$ and $\Psi$ to be ordinary functions, we have:

\[
J^z_2(f\Psi) = -i(\frac{\partial}{\partial \phi} f) - i f(\frac{\partial}{\partial \phi} \Psi) = (J^z_2 f)\Psi + f(J^z_2 \Psi), \quad (III-1-4)
\]

and solving for $(J^z_2 f)\Psi$ we obtain:

\[
(J^z_2 f)\Psi = (J^z_2 f - f J^z_2)\Psi.
\]

Since the function is arbitrary, this leads to the identity:

\[
J^z_2 f = [J^z_2, f] \quad (III-1-5)
\]

It is seen that equations (III-1-1) are the analogs of the corresponding relations (III-1-2) for the angular momentum operators. This implies that the components of a spherical tensor operator transform among themselves as do the corresponding angular momentum states when operated upon by the rotation operator $e^{i \theta \cdot \hat{J}}$. It was for
this reason that Racah gave the general definition for irreducible tensors as follows: The set $T_{J\ell M}$ constitutes a spherical irreducible tensor if the commutation relationships:

$$[J_x \pm iJ_y, T_{J\ell M}] = (J \mp M)(J \pm M + 1) T_{J\ell M}$$

$$[J_x, T_{J\ell M}] = M T_{J\ell M}$$

(III-1-6)

are fulfilled.

One can also directly define irreducible tensor operators by their transformation properties under rotation:

$$R T_{J\ell M} R^{-1} = \sum_{\ell'} \sum_{m'} D_{\ell m'}^{\ell'}(\alpha \beta \gamma) T_{J\ell M}$$

(III-1-7)

where $R = e^{i\alpha J_x} e^{i\beta J_y} e^{i\gamma J_z}$ is the rotation operator and $\alpha, \beta, \gamma$ are the Euler angles defining the rotation. $D_{\ell m'}^{\ell'}(\alpha \beta \gamma)$ are the matrix elements of $R$ in the $J M$ representation. The definition (III-1-7) is equivalent to (III-1-6)(6). Using group theoretical language (III-1-7) implies that both the angular momentum eigenfunctions $Y_{\ell \ell'}$ and the tensor operators $T_{J\ell M}$ form a basis for a representation of the rotation group. The representation is said to be "irreducible", because it is not possible to form any linear combination of the basis functions which gives a representation of lower dimensionality.

Having defined the components $T_{J\ell M}$ of an irreducible tensor in (III-1-6) and (III-1-7), we now will discuss the matrix elements of such tensor components between
states of sharp angular momentum. The general result was discovered independently by Eckart and by Wigner. The Wigner-Eckart theorem states that the dependence of the matrix element $<j' m' | T_{jm} | j m>$ on the projection quantum numbers is entirely contained in the Clebsch Gordan coefficient $C(j' L j; m' M m)$, i.e. that:

$$<j' m' | T_{jm} | j m> = C(j' J j; m' M m) <j' || T_{j} || j> . \quad (I I I - 1 - 8)$$

The quantity $<j' || T_{j} || j>$ is called the reduced matrix element of the set of tensor operators $T_{jm}$. It is independent of $M, m, m$. Therefore the W-E theorem permits a separation of those features of a physical process depending on the geometry of the system from those depending on the detailed physical dynamics. One can find the proof of this theorem in general books about angular momentum (7).

(2) Scalar product of tensors; Coulomb interaction for two electrons in Russell-Saunders terms ($S L$ scheme)

The Coulomb interaction energy between two electrons at $r_1$ and $r_2$ may be expanded in terms of scalar products of spherical harmonics. In order to calculate the matrix elements of $1/r_{12}$, we therefore consider the coupling of tensor operators.

A. Tensor product of irreducible tensors (12)

A product of two tensors $A^{(k)}$ and $B^{(l)}$ is a quantity built out of an ensemble of $(2k + 1)(2l + 1)$ bilinear
products $A^{(k)}_k B^{(\ell)}_\ell$ for the full range of values of $k$ and $\lambda$.

The tensor built out of all these components is reducible. This is an extension of the result about the product of two vectors $A^{(n)}_n B^{(n)}_n$, which has nine components. These nine components can be regarded as three distinct irreducible tensor products: One component belongs to the usual scalar product $A \cdot B$; three more belong to the usual vector product $A \times B$; and the other five belong to the symmetrical tensor product $1/2(A \otimes B + B \otimes A) - A \cdot B \mathbb{I}/3$ in which $\mathbb{I}$ is the unit second order tensor whose Cartesian expression is $(\hat{i} \cdot \hat{i} + \hat{j} \cdot \hat{j} + \hat{k} \cdot \hat{k})$.

The product elements $A^{(k)}_k B^{(\ell)}_\ell$ may be transformed to a set of irreducible tensor products of order $n$, given by the usual vector coupling values:

$$n = k + l', k + l - 1, \ldots |k - l| \quad \text{(III-1-9)}$$

We adopt the notation $[A \times B]^{(n)}$ for the irreducible tensor of order $n$, which is one of the products of $A^{(n)}_n$ and $B^{(n)}_n$. The rule of transformation of the basic components on making a rotation $R$ of the coordinate frame is:

$$A^{(k)}_k B^{(\ell)}_\ell = \sum_{k' \lambda'} A^{(k)}_{k'} B^{(\ell)}_{\lambda'} D^{(k')}_{k \lambda'}(R) D^{(\ell)}_{\lambda' \lambda}(R) \quad \text{.}$$

By using $D^{(j)}_{m', m} D^{(j')}_{m'', m''} = \sum_{j, m} <m, m'| j, m> D^{(j)}_{m, m'} <j, m' | \mu, \mu'>$ the products of the $D$'s can be replaced by a series of single $D$'s giving:

$$A^{(k)}_k B^{(\ell)}_\ell = \sum_{k' + \lambda = \mu} A^{(k)}_{k'} B^{(\ell)}_{\lambda'} <k, \lambda'| (k, l) j \gamma > \sum_{m = k + \lambda} D^{(j)}_{m, \mu} (j, \mu(k, l) | K, \lambda) \quad \text{.}$$
Multiplying by \( \langle K, \lambda | (k, l) n, \mu \rangle \), summing over \((k, \lambda)\) and using the orthogonality property of the coupling coefficients

\[
\sum_{j m} \langle m'_i, m'_j | j m \rangle < j m | m, m'_i > = \delta(m_i', m_i) \delta(m'_j, m_j),
\]

we find:

\[
\sum_{K + \lambda = \mu} A_K B_\lambda \langle K, \lambda | (k, l) n, \mu \rangle = \sum_{K' + \lambda' = \mu} A_{K'} B_{\lambda'} \langle K', \lambda' | (k, l) n, \mu \rangle D_{\mu}^{(n)}
\]

This shows that the quantities on the left transform as the components of an irreducible tensor of order \( n \).

Therefore the \( n \)th-order irreducible tensor product has components:

\[
\left[ A \times B \right]^{(n)} \mu = \sum_{K + \lambda = \mu} A_K B_\lambda < K, \lambda | (k, l) n, \mu >
\]

in which \( \mu = n, n-1, \ldots, -n \). This general result shows that a scalar product \((n = 0)\) exists only for two tensors of equal order \( k = 1 \). In this case, we have:

\[
<j, m, j, m_1 | j_1, j_2, j - m_1 > = (-1)^j (2j + 1)^{1/2} \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & m_3 \end{pmatrix}
\]

let \( j_3 = 0, m_3 = 0, j_1 = j_2 = k, m_1 = K, m_2 = \lambda \)

\[
< K, \lambda | (k, k) | 0, 0 > = \begin{pmatrix} k & k & 0 \\ K & \lambda & 0 \end{pmatrix} = \left[ (-1)^{K-K} / (2k + 1)^{1/2} \right] \delta(\lambda, -\lambda)
\]

and therefore the scalar product is:

\[
\left[ A \times B \right]_0 = \left[ (-1)^{k} / (2k + 1)^{1/2} \right] \sum_{K} A_K (-1)^k B_K
\]

B. Matrix elements of the tensor product of two tensor operators (12).
To calculate the matrix elements of the mixed tensor operator \( X^\kappa_{\mathcal{A}} = \{ T^{(k)} x U^{(k\mathcal{A})}\} \) in the L S M scheme it is convenient to suppose that the system can be separated into two independent parts: part 1 and part 2 if it is a two particle system. \( T \) could be a function of position and spin coordinates of the first particle and \( U \) a similar function for the second particle. By using the Wigner-Eckart theorem (III-1-8) we have:

\[
\langle \alpha j, j_z; J M | X^\kappa_{\mathcal{A}} | j'; j'_z; J' M' \rangle = (-1)^{J-Z-M} \begin{pmatrix} J & K & J' \\ -M & -M \end{pmatrix} (\mathcal{A}) \]

\[
x < \kappa j, j_z; J | X^\kappa_{\mathcal{A}} | \alpha j', j'_z; J > . \tag{III-1-12}
\]

This follows from (III-1-10) because \( X^\kappa_{\mathcal{A}} \) is defined as a tensor product of two irreducible tensor operators, each acting on the separate parts of the system. We may write:

\[
X^\kappa_{\mathcal{A}} = \sum_{\mathcal{B}^{\mathcal{A}}} (-) ^{\kappa_1 - \kappa_2 + \mathcal{A}} (2K+1)^{1/2} \begin{pmatrix} \kappa_1, \kappa_2, K \\ \mathcal{B}, \mathcal{B}^{\mathcal{A}} \end{pmatrix} \begin{pmatrix} \kappa_1 \kappa_2, \kappa_1 \kappa_2 \\ \mathcal{B}, \mathcal{B}^{\mathcal{A}} \end{pmatrix} T^{(k\mathcal{B})} U^{(k\mathcal{B}^{\mathcal{A}})} . \tag{III-1-13}
\]

Equation (III-1-12) then becomes:

\[
\langle \alpha j, j_z; J M | X^\kappa_{\mathcal{A}} | j', j'_z; J' M' \rangle = \langle \omega j, j_z; J M | \sum_{\mathcal{B}, \mathcal{B}^{\mathcal{A}}} (-)^{\kappa_1 - \kappa_2 + \mathcal{A}} (2K+1)^{1/2} \begin{pmatrix} \kappa_1, \kappa_2, K \\ \mathcal{B}, \mathcal{B}^{\mathcal{A}} \end{pmatrix} T^{(k\mathcal{B})} U^{(k\mathcal{B}^{\mathcal{A}})} \alpha j', j'_z; J' M > .
\]

If we use
\[ \alpha j, j_2; J M = \sum_{m, m_1} (-)^{j, j_2 + m} (2J + 1)^{1/2} \left( \begin{array}{ccc} j & j_2 & J \\ m & m_1 & m \end{array} \right) j, m_1; j_2 m_2 \]

and use the Wigner-Eckart theorem individually for \( T_{\tilde{j}}^{(k)} \) and \( U_{\tilde{g}_2}^{(k_2)} \) we have:

\[ (-)^{J - M} \left( \begin{array}{ccc} J & K & J' \\ -M & Q & M' \end{array} \right) <\alpha j, j_2; J || X^{(k)} || \tilde{\alpha} j', j_2'; J' > = \sum_{m, m_2} \sum_{m_2, m_2'} (-)^{j, j_2 - M}
\]

\[ \times (-)^{j', j_2 + m' + k_2, k_2 + Q + j, j_2 - m_2} \left( \begin{array}{ccc} (2K + 1)(2J + 1)(2J' + 1) \end{array} \right)^{1/2} \left( \begin{array}{ccc} j & k & j_2 \\ -m_2 & \tilde{g}_2 & m_2 \end{array} \right)
\]

\[ \left( \begin{array}{ccc} j & j_2 & J \\ m & m_2 & -M \end{array} \right) \left( \begin{array}{ccc} j' & j_2' & J' \\ m' & m_2' & -M' \end{array} \right) \left( \begin{array}{ccc} k & k & k \\ \tilde{g}_2 & \tilde{g}_2 & -Q \end{array} \right) \left( \begin{array}{ccc} j & k & j_2 \\ -m_2 & \tilde{g}_2 & m_2 \end{array} \right)
\]

\[ x <\alpha j || T_{(k)} || j_2, \alpha' > <\alpha' j_2 || U_{(k_2)} || j > = (III-1-14)
\]

When both sides are multiplied by \( (-)^{J - M} \left( \begin{array}{ccc} J & K & J' \\ -M & Q & M' \end{array} \right) \)

and summed over \( M, M, Q, \) the left side, by the orthogonality property of \( 3j \) symbols (8), gives:

\[ <\alpha j, j_2; J || X^{(k)} || \tilde{\alpha} j', j_2'; J' > = \left( (2J' + 1)(2J + 1)(2K + 1) \right)^{1/2}
\]

\[ \left( \begin{array}{ccc} j & j_2 & J \\ j' & j_2' & J' \\ k_1 & k_2 & K \end{array} \right) \sum_{\alpha''} <\alpha j || T_{(k)} || j_2 > <\tilde{\alpha} j_2 || U_{(k_2)} || j > (III-1-15)
\]

The scalar product of two irreducible vector operators \( T^{(k)} \) and \( U^{(k)} \) is defined as:
Expressed in terms of the tensor operator product this is:

\[(T^{(k)} \cdot U^{(k)}) = (-)^{k} (2k + 1)^{1/2} [T^{(k)} \times U^{(k)}]^{0}.\]

Its matrix elements are obtained by using (III-1-12) and (III-1-15):

\[<\alpha j, j' j'; J \ M | T^{(k)} U^{(k)} | \alpha' j', j' j'; J' \ M'> = (-)^{J-M+k} \]

\[\times [(2k + 1)(2k + 1)(2J + 1)(2J' + 1)]^{1/2} \left( \begin{array}{ccc} J & 0 & J' \\ M & 0 & M' \end{array} \right)\]

\[\times \sum_{\alpha''} \langle \alpha'' j' \parallel T^{(k)} \parallel \alpha'' j' \rangle \langle \alpha'' j' \parallel U^{(k)} \parallel \alpha'' j' \rangle \left( \begin{array}{ccc} j_j & j_j & J \\ j_j & j_j & J' \\ K & K & 0 \end{array} \right).\]

Because \((J, 0, J') = \delta(J, J') \delta(M, M') (-1)^{J-M} (2J + 1)^{1/2}\) and

\[\left( \begin{array}{ccc} j_j & j_j & J \\ j_j & j_j & J' \\ K & K & 0 \end{array} \right) = (-)^{J+J'+K} \left( \begin{array}{ccc} J \parallel (2J + 1)(2k + 1) \right)^{1/2} \left( \begin{array}{ccc} j_j & j_j & J \\ j_j & j_j & J' \\ K & K & 0 \end{array} \right)\]

(III-1-16) reduces to:

\[<\alpha j, j' j'; J \ M | T^{(k)} U^{(k)} | \alpha' j', j' j'; J' \ M'> = (-)^{j_j + j_j + J} \delta(J, J') \delta(M, M')\]

\[\times \left\{ \begin{array}{ccc} j_j & j_j & J \\ j_j & j_j & J' \\ K & K & 0 \end{array} \right\} \langle \alpha'' j' \parallel T^{(k)} \parallel \alpha'' j' \rangle \langle \alpha'' j' \parallel U^{(k)} \parallel \alpha'' j' \rangle .\]

From classical physics we know the Coulomb interaction
between two electrons can be expressed as:

\[
\frac{1}{r_{12}} = \sum_{k=0}^{\infty} \frac{Y_{l}^{l} \frac{4\pi}{l+1}}{r^{l+1}} \sum_{\ell} \frac{Y_{\ell}^{k}(\hat{n}_{1}, \hat{n}_{2}) Y_{\ell}^{k}(\hat{n}_{1}, \hat{n}_{2})}{r^{\ell}}.
\]

If we define a "C tensor" having components

\[
C_{\ell}^{k} = (4\pi/2k + 1)^{\frac{1}{2}} Y_{\ell}^{k}(\psi)
\]

then:

\[
\frac{1}{r_{12}} = \sum_{k} C_{\ell}^{k} / r_{\ell}^{k+1} C(1) \cdot C(2) . 
\] (III-1-17')

In order to calculate the matrix elements of \(1/r_{12}\), we can use (III-1-17) to easily calculate the matrix elements of \(C(1) \cdot C(2)\):

\[
<\alpha j_1 j_2 ; J M | C_{\ell}^{k} (1) C_{\ell}^{k} (2) | \alpha' j_1' j_2' J' M' > = (-)^{j_1' + j_2' + J} \delta_{(J, J') \delta (M, M')}
\]

\[
X \left\{ j, j_1, J \right\} \sum_{\alpha''} <\alpha' j_1 j_2 | C_{\ell}^{k} (1) | \alpha'' j_1' > <\alpha'' j_2 | C_{\ell}^{k} (2) | \alpha' > . 
\] (III-1-18)

Here the reduced matrix elements of \(C_{\ell}^{k}\) can be shown to be:

\[
< j | C_{\ell}^{k} | j' > = (-)^{j} \left( \frac{2j + 1}{2} \right)^{\frac{1}{2}} \left\{ \begin{array}{ccc} j & k & j' \\ 0 & 0 & 0 \end{array} \right\} \) (III-1-19)
\]

The 3-j symbol here is zero unless \(\ell + k + \ell'\) is even.

The calculation of matrix elements of \(A(1) \cdot A(2)\) is similar to that of \(C_{\ell}^{k}(1) \cdot C_{\ell}^{k}(2)\) because the Runge-Lenz vector is a tensor of rank \(k = 1\), hence:

\[
<\alpha j_1 j_2 ; J M | A_{\ell}^{(1)} A_{\ell}^{(2)} | \alpha' j_1' j_2' J' M' > = (-)^{j_1' + j_2' + J} \left\{ \begin{array}{ccc} j_1 & j_2 & J \\ j_1' & j_2' & J' \end{array} \right\} \left\{ \begin{array}{ccc} j & k & j' \\ 0 & 0 & 0 \end{array} \right\} \) (III-1-19)
It is known that (9):

\[ <n, j|A''|n, j + 1> = -\left[ (n - j - 1)(n + j + 1)(j + 1) \right]^{\frac{1}{2}}, \]  

(III-1-21a)

\[ <n, j|A^o|n, j> = 0, \]  

(III-1-21b)

\[ <n, j + 1|A''|n, j> = \left[ (n - j)(n + j + 1) \right]^{\frac{1}{2}}. \]  

(III-1-21c)

These results differ from the results of Biedenharn by a factor \(-(2j + 3)^{-\frac{1}{2}}\) in (III-1-21c) and a factor \(-(2j - 1)^{-\frac{1}{2}}\) in (III-1-21a) because the m-dependent part is expressed as a W-E coefficient by Biedenharn and it is expressed as a 3-j symbol here.

(3) Coupling of three angular momenta

We have set forth the coupling of two angular momenta \(j_1\) and \(j_2\) to give a resultant \(j = j_1 + j_2\). There is a unitary transformation from the representation in which \(j_1^i, j_1^j\) and \(j_2^i, j_2^j\) are diagonal to the representation in which \(j_2^2, j_2^j\) and \(j_1^2, j_1^j\) are diagonal.

The elements of this unitary transformation are Clebsch Gordan coefficients \(<j, m, j_1, m_1|j, j_2, j m>:\n
\[ |\gamma j, j_1, j_2, j m> = \sum_{m, m_2} |\gamma j, m, j_2, m_2><j, m, j_2, m_2| j, j_2, j m>, \]  

(III-1-22)
C-G coefficients are closely related to the 3-\(j\) symbol of Wigner which is defined by:

\[
\begin{align*}
(j, j_2, j_3) &= (-1)^{j_2-j_2-m_3} (2j_2 + 1)^{1/2} <j, m, j_2 | j, j_2, j_3 - m_3> \\
&\quad \text{(III-1-23)}
\end{align*}
\]

We now consider the addition of three angular momenta \(j, j_2, j_3\) to form the total angular momentum \(j = j + j_2 + j_3\) and we shall study the coefficients of the unitary transformations connecting different coupling schemes for three angular momenta. The necessity for this generalization arises from the fact that this simple type of coupling occurs in almost every problem of interest to us here. The unitary transformations referred to represent a recoupling since they connect different ways of forming the resultant from the three angular momenta.

For three angular momenta there are several sets of commuting operators which may be diagonalized simultaneously. Each set contains six operators, as may be seen from the uncoupled representation, in which \(j, j_2, j_3\) are diagonal. If a representation is desired in which the square and z-component of the total angular momentum are diagonal, this can be obtained by compounding any two of the angular momenta into an intermediate angular momentum, and then compounding this intermediate angular momentum with the third member of the original set. Thus the six operators which may be diagonalized are \(j^{\pm}, j_2^{\pm}, j_3^{\pm}, j^{\pm}, j_2^{\pm}, j_3^{\pm}\). There are three such representations, since \(j\) can be either \(j + j_2\),
Let us consider the connection between the first two representations characterized by the intermediate angular momenta. These two representations are related by a unitary transformation, the elements of which we write as:

\[ \langle (j_1, j_2, j_3) ; j_{12}, j_2, j_3 ; JM \rangle = \sum_{j_{12}} \langle j_{12} (j_1, j_2) ; j_{12}, j_3 ; JM \rangle \langle j_{12} (j_2, j_3) ; j_{12}, j_3 ; JM \rangle \]

Then

\[ \sum_{j_{12}} \langle j_{12} (j_1, j_2) ; j_{12}, j_3 ; JM \rangle = \sum_{j_{12}} \langle j_{12} (j_2, j_3) ; j_{12}, j_3 ; JM \rangle \]

By using the rules for coupling two angular momenta (III-1-4), the two types of eigenfunction in (III-1-24) can easily be written as:

\[ \langle j_{12} (j_1, j_2, j_3) ; JM \rangle = \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]

Substitution of (III-1-25) and (III-1-26) into (III-1-24) gives:

\[ \sum_{m_1, m_2, m_3} \langle j_1, m_1 ; j_2, m_2, m_3 ; j_3, j_4 m_4 \rangle \langle j_1, j_2, m_4 ; j_3, j_4, j_5 m_5 \rangle \]
We take the scalar product of both sides of (III-1-27) with \( |j, \mu_1, \mu_2, \mu_3 \rangle \) and obtain:

\[
\sum_{m_2 m_3} \langle j, m_2 j_3 \rangle M M |j_1, m_1 j_2 j_3 j M > |j, m_2 j_3 j M > \delta_{M-m_2, \mu_1} \delta_{M-m_3, \mu_2} \delta_{M-m_3, \mu_3} \]

or

\[
\sum_{m_1 m_2} \langle j_1, j_2 j_3 j M |j_1, j_2 j_3 j M > |j_1, j_2 j_3 j M > \delta_{M-m_1, \mu_1} \delta_{M-m_2, \mu_2} \delta_{M-m_3, \mu_3} \]

The symbols \( \delta \) can be eliminated by replacing \( \mu_1 + \mu_2 + \mu_3 \) by \( M \). We can, from Edmonds' book, equation (5.3.2), show that the transformation coefficients are independent of \( M \), so we can drop the argument \( M \) in the transformation coefficient. This gives:

\[
\langle j_3, \mu_3 j_3 \rangle M |j_2 j_3 j M > |j_1, j_2 j_3 j M > = 
\sum_{j_1 j_2} \langle j_1, j_2 j_3 j M |j_1, j_2 j_3 j M > |j_1, j_2 j_3 j M > \delta_{j_1 + j_2 + j_3, M} \]

Multiplication (III-1-30) by \( |j_1, j_2 j_3 j M > \) and summation over \( j_3 \) keeping \( j_2 + j_3 \) fixed, and use of the
orthogonality of the C-G coefficients gives:

$$\sum_{M_2} \langle j_1 j_2 j_3 j_4 M_2 | j_2 j_3 j_4 M_2 \rangle \langle j_1 j_2 j_3 j_4 M_2 | j_1 j_2 j_3 j_4 M_2 \rangle = \langle (j_1, j_2) j_3 j_4 M | j_1, (j_2, j_3) j_4 M \rangle \langle j_1 j_2 j_3 M | j_1 j_2 j_3 M \rangle.$$

(III-1-31)

Similarly multiplication by $$\langle j_1 j_2 j_3 j_4 M | j_1 j_2 j_3 M \rangle$$, summation over $$M_3$$ keeping $$M_1, M_2, M_3$$ fixed and replacing $$j_4$$ by $$j$$ gives:

$$\langle (j_1, j_2) j_3 j_4 M | j_1, (j_2, j_3) j_4 M \rangle = \sum_{M_3} \langle j_1 j_2 j_3 j_4 M_3 | j_1 j_2 j_3 j_4 M_3 \rangle \times \langle j_1 j_2 j_3 j_4 M_3 | j_1 j_2 j_3 j_4 M_3 \rangle$$

$$\langle j_1 j_2 j_3 j_4 M | j_1 j_2 j_3 M \rangle \times \langle j_1 j_2 j_3 j_4 M | j_1 j_2 j_3 M \rangle.$$

(III-1-31')

The elements of the unitary matrix are, within a multiplicative factor, the Racah coefficients $$W$$ which are defined by the following relation:

$$\langle (j_1, j_2) j_3 j_4 M | j_1 j_2 j_3 j_4 M \rangle = \left[ (2j_1 + 1)(2j_2 + 1) \right]^{1/2} W(j_1, j_2; j_3, j_4).$$

(III-1-32)

Racah coefficients are closely related to the 6-j symbol of Wigner. The relation is given by:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{pmatrix} = (-)^{j_1 + j_2 + j_3 + J} W(j_1, j_2; j_3, j_4).$$

(III-1-33)

Thus we get the useful result:
$$\langle j_1 j_2 j_3 ; J \mid j_1 (j_2 j_3) j_{123} ; J \rangle = (-) \frac{j_1 + j_2 + j_3 + J}{2} \left[ (2j_{12} + 1)(2j_{23} + 1) \right] \frac{1}{2} \left\{ j_1 \quad j_2 \quad j_3 \right\} \left\{ j_{12} \quad j_{23} \right\} \ .$$

It is sometimes useful to consider the changing of the coupling together with a change in the order of the vectors. Proceeding as before yields:

$$\langle j_1 j_2 j_3 ; J \mid j_1 (j_2 j_3) j_{123} ; J \rangle = (-) \frac{j_1 + j_2 + j_3 + j_4}{2} \left[ (2j_{12} + 1)(2j_{13} + 1) \right] \frac{1}{2} \left\{ j_{12} \quad j_{13} \quad J \right\} \left\{ j_{12} \quad j_{13} \quad j_4 \right\} \ .$$

(4) Coulomb interaction in Russell Saunders terms for three electrons

(a) Recoupling coefficients where the electrons are not equivalent

The case in which all three electrons are not equivalent is considered here. By repeated application of the coupling procedure (see (III-1-22) and (III-1-23)), the L S M wave function for three electron systems with a specified coupling order is found to be

$$\langle ab \mid L_{ab} S_{ab} c ; SM_{ab} ; LM \rangle = (-) \frac{1}{2} + \frac{\epsilon}{2} + \frac{\epsilon}{2} + L_{ab} - L_{ab} - S_{ab} - M_{ab} - M_{ab}$$

$$\left[ (2S + 1)(2L + 1)(2S_{ab} + 1)(2L_{ab} + 1) / N_{ab} \right] ^{1/2}$$
Here \( N = 1 \) if \( a = b \), and \( N = 2 \) if \( a = b \) and \( \phi(a,b,c,l,2,3) \) is a Slater determinant. The matrix elements for Coulomb interaction in the general case |(ab)c will now be found as:

\[
\langle (ab)L_{ab}S_{ab},c;S L \mid \sum_{ij} \frac{e^2}{r_{ij}} \mid (ab)L_{ab}S_{ab},c;S L \rangle =
\]

\[
= \langle S M_5 L M \mid \frac{e^2}{r_{1a}} \mid S'M'L'M \rangle + \langle S M_5 L M \mid \frac{e^2}{r_{1b}} \mid S'M'L'M \rangle
\]

+ \langle S M_5 L M \mid \frac{e^2}{r_{1\alpha}} \mid S'M'L'M \rangle

Letting \( \langle S M_5 L M \rangle \) stand for \( \langle (ab)L_{ab}S_{ab},c;S L \rangle \) for pithiness, then by (III-1-17')

\[
\langle (ab)L_{ab}S_{ab},c;S L \mid \sum_{ij} \frac{e^2}{r_{ij}} \rangle =
\]

\[
e^2 \langle S M_5 L M \mid \sum_{k} \frac{C(1)\cdot C(2)}{r_{i}^{k+1}} \mid S'M'L'M \rangle
\]

\[
e^2 \langle S M_5 L M \mid \sum_{k} \frac{C(1)\cdot C(3)}{r_{i}^{k+1}} \mid S'M'L'M \rangle
\]

\[
e^2 \langle S M_5 L M \mid \sum_{k} \frac{C(2)\cdot C(3)}{r_{i}^{k+1}} \mid S'M'L'M \rangle \quad (III-1-37)
\]

By using the orthogonality relation of the C-G coefficients and the orthogonality of the
wavefunction \( | \ell_c m_c 1/2 m_{sc} > \), the first term on (III-1-37)’s right side gives:

\[
\begin{align*}
& \langle S_{M_s} L M | \sum_{\kappa} r_{\kappa} \langle \kappa | C (1) \cdot C (2) | S_{M_s} L M > = \\
& \quad x \delta (L, L') \delta (M_s, M_s') \delta (M_s, M_s') \delta (S, S') e^2 \\
& \quad x \langle S_{ab} M_{ab} L_{ab} M_{ab} | \sum_{\kappa} r_{\kappa} \langle \kappa | C (1) \cdot C (2) | S_{ab} M_{ab} L_{ab} M_{ab} > .
\end{align*}
\]

In order to evaluate the second and third terms of (III-1-37), it is necessary to recouple the state \( | (ab) c > \) in such a way that the quantum labels \( a, b, c \) are associated with coordinate labels 1, 2, 3 respectively. The two electrons that are coupled first are indicated by the arguments of the spherical tensor operators forming the scalar products. Taking the second term in (III-1-37) and recoupling the state \( | (ab) c > \) by (III-1-35) to give \( | (ac) b > \) and using the orthogonality relation one has:

\[
\begin{align*}
& \langle S_{M_s} L M | \sum_{\kappa} r_{\kappa} \langle \kappa | C (1) \cdot C (2) | S_{M_s} L M > = \delta (LL') \delta (SS') \delta (MM') \delta (M_s, M_s') \\
& \quad x e^2 \left[ (2L_{ab} + 1)(2L_{ab} + 1)(2S_{ab} + 1)(2S_{ab} + 1) \right] \frac{1}{2} (-1)^{L_{ab} + L_{ab} + 2S + 1} \\
& \quad x \left[ (2L_{ac} + 1)(2S_{ac} + 1)(2L_{ac} + 1)(2S_{ac} + 1) \right] \frac{1}{2} (-1)^{L_{ac} + L_{ac} + 2S - 1} \\
& \quad \left\{ \begin{array}{c}
L_{ab} L_c L \\
L_{ac} L_b L_a
\end{array} \right\} \left\{ \begin{array}{c}
S_{ab} \frac{1}{2} S \\
S_{ac} \frac{1}{2} \frac{1}{2}
\end{array} \right\} \\
& \quad \left\{ \begin{array}{c}
L_{ab} L_c L \\
L_{ac} L_b L_a
\end{array} \right\} \left\{ \begin{array}{c}
S_{ab} \frac{1}{2} S \\
S_{ac} \frac{1}{2} \frac{1}{2}
\end{array} \right\} \\
& \quad x < S_{ac} M_{sac} L_{ac} M_{ac} | \sum_{\kappa} r_{\kappa} \langle \kappa | C (1) \cdot C (3) | S_{ac} M_{sac} L_{ac} M_{ac} > .
\end{align*}
\]
We can also see that \((2S + 1)(2S - 1)\) is even for a three electron system. The third term on the right side of (III-1-37) is evaluated in the same way by using (III-1-34) to recouple the state \(|(ab)c>\) to yield
\[|(a(bc)>:\]
\[
e^<(SM_{\alpha},L_M)(x^k)C(2)C(3)|SM_{\alpha}',L_M'> = S(L_{\alpha})S(S_{\alpha})δ(m_km')δ(m_km')
\]
\[\times\sum_{L_{bc},S_{bc}}((2L_{bc} + 1)(2S_{bc} + 1)(2S_{bc} + 1))\frac{1}{2}((-1)^{L_{bc} + S_{bc} + 2S_1-1})\times (((2L_{ab} + 1)(2L_{ab} + 1)(2S_{ab} + 1)(2S_{ab} + 1))\frac{1}{2}((-1)^{L_{ab} + L_{ab}})
\]
\[x<\left\{\begin{array}{ccc} l_a & l_b & l_{ab} \\ l_c & l_{bc} & l_{bc} \end{array}\right\}\times \left\{\begin{array}{ccc} l_a & l_b & l_{ab} \\ l_c & l_{bc} & l_{bc} \end{array}\right\}\times \left\{\begin{array}{ccc} \frac{1}{2} \frac{1}{2} S_{ab} \\ \frac{1}{2} S_{bc} \end{array}\right\}\times \left\{\begin{array}{ccc} \frac{1}{2} \frac{1}{2} S_{ab}' \\ \frac{1}{2} S_{bc}' \end{array}\right\}\times S_{bc} M_{bc} L_{bc} M_{bc} > .
\]

The elements of the energy matrix for other configurations, for example \(|a^2c>\), can be deduced from the previous results for the general three electron configuration \(|(ab)c>\), which can be verified by changing all \(b\)'s to \(a\)'s. Then by using the recoupling procedure, we can reduce the calculations for three electrons to those for two electrons.

(b) Equivalent electron orbitals; Coefficients of fractional parentage

If we couple two equivalent electrons with the usual
vector coupling formulas we obtain anti-symmetric or symmetric eigenfunctions according to whether $S + L$ is even or odd (10). The eigenfunctions of states with $S + L$ even are therefore the normalized eigenfunctions of allowed states of $\ell^i$. If we add, in the same way, to the allowed states of $\ell^i$ a third $\ell$ electron, the eigenfunctions obtained are in general anti-symmetric only with respect to the first two electrons, but not with respect to the third. Therefore, $|\ell'(S' L') SL>\) is not an exchange anti-symmetric eigenfunction of $\ell'$. We can see this from the transformation:

$$|\ell'(S' L) lSL> = \sum_{S'' L''} \ell L(S'' L''), SL<\ell , \ell (S'' L''), SL |\ell^2(S'L') \ell , SL>,$$

(III-1-40)

where the transformation coefficients are given by (III-1-34). In (III-1-34), $S + L$ can be even and odd. Therefore we obtain in general, in the sum (III-1-34), allowed and forbidden values of $S L$ and therefore $|\ell'(S' L') l, SL>\) is not antisymmetric with respect to the second and third electrons.

The wave function for three equivalent orbitals can be written as a linear combination of the states $|\ell'(S' L) l, SL>,\) i.e. as:

$$|\ell'; SL> = \sum_{S'L'} \ell'(S' L') l; SL<\ell^i (S' L') ; SL |\ell^3, SL>. \) (III-1-41)

Application of (III-1-34) gives:
\[
\left| \ell^3; S \ L > = \sum_{S'' L''} \ell, \ell (S'' L''); S \ L >
\]
\[
x \ < \ell, \ell (S'' L'') S \ L > \mid \ell^2 (S' L'), \ell; S \ L > < \ell^2 (S' L'') S \ L > \ell, \ell (S' L') S \ L > \ell^3; S \ L > ,
\]
\[
(III-1-42)
\]

where \(< \ell^2 (S' L') S L > \ell^3; S L >\), called the coefficients of fractional parentage satisfy the equation system (5):
\[
\sum_{S'' L''} < \ell, \ell (S'' L'') S L > \mid \ell^2 (S' L'), \ell; S \ L > < \ell^2 (S' L'') S \ L > \ell, \ell (S' L') S \ L > \ell^3; S \ L > = 0 .
\]
\[
(III-1-43)
\]

when \(S + L\) is odd. Then, the coefficients of \(\left| \ell, \ell (S'' L'') S L >\) vanish for every forbidden value of \(S'' L'\) \((S'' + L'\) is odd). Since \(Q^3; S L >\), in (III-1-41), satisfies the condition (III-1-43), it is a function anti-symmetric with respect to the electrons 1 and 2 and also with respect to the electrons 2 and 3; hence it is anti-symmetric with respect to all three electrons. The condition (III-1-43) is necessary and sufficient for the determination of the coefficients of fractional parentage of the terms of \(l^3\). The fractional parentage of the terms of \(p^3\) and \(d^3\) calculated with this method are given in (5c) and table 3. Some useful properties of the coefficients of fractional parentage are:
\[
< \ell^3; S L > \mid \ell, \ell; S L > = 1/2 \left[ 1 + (-)^{L+S} \right] .
\]
\[
(III-1-44)
\]
\[
< \ell^n; S L > \mid \ell^{-1}, \ell'; S L > = \ell (\alpha' S' L'), \ell; S L > \ell^n \alpha S L > .
\]
\[
(III-1-44')
\]
\[
\sum_{\alpha' L' S'} < \ell^n; S L > \mid \ell^{-1} (\alpha' S' L'), \ell; S L > < \ell^n (\alpha' S' L'), \ell; S L > \ell^n \alpha'' S L > = \delta (\alpha \alpha'') .
\]
\[
(III-1-45)
\]
By using the coefficients of fractional parentage we can calculate the matrix element of the scalar operator $G = \sum g_{ij}$ for $l^3$ configurations. The following results were derived by Racah (5c):

$$< l^3; SL \mid G \mid l^3; SL > = 3 \sum_{S_1 L_1} < l^3; SL \mid l (\alpha, S_1 L_1), l^3 (S_2 L_2) \mid SL >$$

$$x < l^3; S_2 L_2 \mid g_{ij} \mid l^3 S_1 L_1 > < l (\alpha, S_1 L_1), l^3 (S_2 L_2), S_2 L_2 \mid l^3 \alpha' S L > .$$

(III-1-47)

$$< l^3; SL \mid G \mid l' (\alpha' S' L' ) \mid l'; SL > = 2 \sqrt{3} \sum_{S_1' L_1'} < l^3; SL \mid l (\alpha, S_1 L_1), l' (S_2 L_2) \mid SL >$$

$$x < l' (\alpha' S' L' ) \mid l' SL > l, l' (S_1' L_2') < l; g_{ij} \mid l' i \Delta j \mid S_2' L_2 > .$$

(III-1-48)

$$< l^3; SL \mid G \mid l (\alpha, S_1 L_1), l' (S_2 L_2) \mid SL > = \sqrt{3} x$$

$$\sum_{S_1' L_2'} < l^3; SL \mid l (\alpha, S_1 L_1), l' (S_2 L_2) \mid SL > < l' S_2 L_2 \mid l' S_1' L_1 > .$$

(III-1-49)

2. Calculation of configuration mixing within the 3s-3p-3d shell

(1) Matrix elements of Coulomb interaction and $A_1, A_2$ within the 3s-3p-3d shell for two electrons

We know from section 1(4) that we can reduce the
calculations for three electrons to those for two electrons. It is necessary to consider the matrix elements for two electrons in detail. We consider first a system of two electrons in \( S \) \( L \) coupling. The antisymmetric wave function of two electrons with quantum numbers \( l_a \) and \( l_b \) is:

\[
\begin{align*}
\{ l_{a b} \} S M_5 L M &= (\frac{1}{\sqrt{2}})[ l_{a(1)} l_{b(2)} SM_5 LM > \pm l_{a(2)} l_{b(1)} SM_5 LM_5 > ] \\
&= \text{(III-2-1)}
\end{align*}
\]

The subscripts 1 and 2 refer to the individual electrons (the curly brackets are used to denote an antisymmetric combination.) In the second term, the coordinates are mixed. To align the coordinates properly we should exchange the quantum labels \( a \) and \( b \) because the wave function in \( S \) \( L \) coupling is obtained by coupling the angular and spin parts of the one electron spin orbitals independently. To exchange the quantum labels \( a \) and \( b \) corresponds to interchanging two columns of two \( 3j \)-symbols and introduces a phase factor \((-)^{l_a + l_b - L}
\)

\((-)^{\frac{1}{2} + \frac{1}{2} - S}(8)\). Thus equation (III-2-1) can be written as:

\[
\begin{align*}
\{ l_{a b} \} & SM_5 LM > = \frac{1}{\sqrt{2}}[ l_{a(1)} l_{b(2)} SM_5 LM > + (-)^{l_a + l_b + L + S} \\
& \times l_{a(2)} l_{b(1)} SM_5 LM > ] \\
&= \text{(III-2-2)}
\end{align*}
\]

If \( l_a = l_b \) the electrons are equivalent. Equation (III-2-2) reduces to:

\[
\begin{align*}
\{ l_{a a} \} & SM_5 LM > = N[1 + (-)^{L+S}] l_{a(1)} l_{a(2)} SM_5 LM > \\
&= \text{(III-2-3)}
\end{align*}
\]

This will vanish if \( S + L \) is odd, and hence only
functions where $S + L$ is even correspond to physical states. The normalization factor $N$ is then equal to 1/2 and the antisymmetric function becomes:

$$\left| \{ l_{a}^{2}\} S_{a}L_{a} \right> = \left| \lambda_{a}(1) \lambda_{b}(2), S_{a}L_{a} \right>, \quad S + L \text{ even} .$$

(III-2-3)

We can now use the wave function (III-2-3) to obtain the Coulomb interaction for a state of two equivalent electrons in LS-coupling. Using the formula (III-1-18) gives:

$$\langle \{ l' \} S L | 1/R_{a} | \{ l'' \} S'L' \rangle = \sum_{k} F^{k}(\ell \ell) (-)^{k} \left\{ \begin{array}{ccc} \ell & \ell & L \\ \ell & \ell & k \end{array} \right\}$$

$$\times \langle \ell || C^{k} | l' \rangle \langle \ell || C^{k} | l \rangle > \delta(\ell \ell') \delta(SS').$$

(III-2-4)

Because $C^{(1)}$ and $C^{(2)}$ act only on the space coordinates, the spin part can be separated to give:

$$\langle SM_{s} | 1 | SM'_{s} \rangle = (-)^{S-M_{s}} \left( S', S, 0 \right)_{(M'_{s}, -M_{s}, 0)} < S || 1 || S > = \delta(SS') \delta(M_{s}, M'_{s}).$$

(III-2-5)

For the general case the Coulomb interaction for a state of two nonequivalent electrons becomes:

$$\langle \{ l_{a} \lambda_{b} \} S_{a}L_{a} | r_{a}^{-1} || \ell_{c} \lambda_{d} \} S_{a}L_{a} \rangle = 1/2 \left\{ \langle \lambda_{a}(1) \lambda_{b}(2) S_{a}L_{a} | c_{a}^{-1} | \lambda_{c}(1) \lambda_{d}(2) S_{a}L_{a} \rangle \\ - \langle l_{a}(1) \lambda_{b}(2) S_{a}L_{a} | r_{a}^{-1} | \lambda_{c}(2) \lambda_{d}(1) S_{a}L_{a} \rangle - \langle \lambda_{a}(2) \lambda_{b}(1) S_{a}L_{a} | r_{a}^{-1} | \lambda_{c}(1) \lambda_{d}(2) S_{a}L_{a} \rangle \\ + \langle \lambda_{a}(2) \lambda_{b}(1) S_{a}L_{a} | r_{a}^{-1} | \lambda_{c}(2) \lambda_{d}(1) S_{a}L_{a} \rangle \right\} .$$

There are two direct terms and two exchange terms. Since the two-electron interaction is symmetric with
respect to an interchange of the coordinates of two electrons we have:

\[
\langle \{ \ell_a, \ell_b \} SL | \tilde{r}_{\ell}^{-1} | \{ \ell_c, \ell_d \} S'L \rangle = \langle \ell_a(1) \ell_b(2) SL | \tilde{r}_{\ell}^{-1} | \ell_c(1) \ell_d(2) S'L \rangle
\]

- \[\langle \ell_d(1) \ell_b(2) S L | \tilde{r}_{\ell}^{-1} | \ell_c(2) \ell_d(1) S'L \rangle\]

= \[\langle \ell_a(1) \ell_b(2) S L | \tilde{r}_{\ell}^{-1} | \ell_c(1) \ell_d(2) S'L \rangle + (-) \ell_c + \ell_d + L' + S'\]

\[\times \langle \ell_a(1) \ell_b(2) S L | \tilde{r}_{\ell}^{-1} | \ell_d(1) \ell_c(2) S L \rangle.\]  \hspace{1cm} (III-2-6)

Using (III-1-18), (III-2-6) becomes:

\[
\langle \{ \ell_a, \ell_b \} SL | \tilde{r}_{\ell}^{-1} | \{ \ell_c, \ell_d \} S'L \rangle = \sum_{\ell} (-) \ell_b + \ell_c + L \delta_{L, L'} \delta_{S, S'} \left\{ \ell_a \ell_b \ell_c \ell_d \right\}
\]

\[\times \langle \ell_a \| \mathbf{C}^k(1) \| \ell_c \rangle < \ell_b \| \mathbf{C}^k(2) \| \ell_d \rangle \mathbf{F}^k + (-) \ell_c + \ell_d + S \sum_{\ell} \delta_{L, L'} \delta_{S, S'} \left\{ \ell_a \ell_b \ell_c \ell_d \right\}
\]

\[\times \langle \ell_a \| \mathbf{C}^k(1) \| \ell_d \rangle < \ell_b \| \mathbf{C}^k(2) \| \ell_c \rangle \mathbf{F}^k.\]  \hspace{1cm} (III-2-7)

If \( \ell_a = \ell_b = \ell \) then \( L + S \) is even and:

\[
\langle \{ \ell \ell \} SL | \tilde{r}_{\ell}^{-1} | \{ \ell_c, \ell_d \} SL \rangle = \left(1/\sqrt{2}\right) <\ell(1) \ell(2) SL | \tilde{r}_{\ell}^{-1} | \ell_c(1) \ell_d(2) S'L \rangle
\]

+ (-) \\[\ell_c + \ell_d + L + S \] \langle \ell(1) \ell(2) SL | \tilde{r}_{\ell}^{-1} | \ell_d(1) \ell_c(2) S'L \rangle

\[= \sum_{\ell} \left(1/\sqrt{2}\right) (-) \ell + \ell_c + L \left\{ \ell_a \ell_c \ell \right\} <\ell \| \mathbf{C}^k(1) \| \ell_d \rangle < \ell \| \mathbf{C}^k(2) \| \ell_c \rangle \mathbf{F}^k + (-) \ell_c + \ell_d + L
\]

\[- (-) \ell_c + \ell_d + L + S \left\{ \ell_a \ell_c \ell \right\} <\ell \| \mathbf{C}^k(1) \| \ell_d \rangle < \ell \| \mathbf{C}^k(2) \| \ell_c \rangle \mathbf{F}^k
\]

\[= \sum_{\ell} \left(2/\sqrt{2}\right) (-) \ell + \ell_c \left\{ \ell_a \ell_c \ell \right\} <\ell \| \mathbf{C}^k(1) \| \ell_d \rangle < \ell \| \mathbf{C}^k(2) \| \ell_c \rangle \mathbf{F}^k.\]

If \( L + S \) is even then:
Similarly, we have:

\[
\langle \{l\ell\} SL | r_{z2}^l | \{l\ell'\} SL \rangle = \sum_k (\frac{2}{\sqrt{2}})^l \frac{\ell + \ell' + \ell + \ell'}{\ell_d \ell_e \ell_e \ell_k} \left\{ \frac{\ell \ell \ell \ell}{\ell \ell \ell \ell} \right\} \times \langle \ell \ell'|c^k(1)|\ell \ell' \rangle R \langle \ell \ell'|c^k(2)|\ell \ell' \rangle R^k .
\]

(III-2-8)

Similarly, we have:

\[
\langle \{l\ell\} SL | r_{z2}^l | \{l\ell'\} SL \rangle = \langle (1) (2) SL | r_{z2}^l | (1) (2) SL \rangle \]

\[
= \sum_k (-)^{\ell + \ell' + \ell} \left\{ \frac{\ell \ell \ell \ell}{\ell \ell \ell \ell} \right\} \langle \ell \ell'|c^k(1)|\ell \ell' \rangle R \langle \ell \ell'|c^k(2)|\ell \ell' \rangle R^k .
\]

(III-2-9)

We can use (III-2-4), (III-2-7), (III-2-8) and (III-2-9) to calculate the matrix elements for two electrons. We have worked out all the matrix elements for the Coulomb interaction and for \(A \cdot A\). (\(A\) is the Runge-Lenz vector.) These are given in table 1 and table 2.

(2) Recoupling coefficients within 3s-3p-3d shell for three electrons.

By using the recoupling procedure, we can reduce the calculations for three electrons to two electron calculations. It is necessary to work out all the recoupling coefficients within the 3s-3p-3d shell for three electrons. These are given in table 3. We also give the coefficients of fractional parentage for \(p^3\) and \(d^3\) in table 4 and 5.

(3) Matrix elements of Coulomb interaction and

\[
\sum_{\ell j} (L_j L_j - A_j A_j) \text{ within the 3s-3p-3d shell for three}
\]
electrons.

In order to compare approximate and exact configuration mixing we have to calculate the matrix elements of both \( \sum_{i<j} (L_i \cdot L_j - A_i \cdot A_j) \) and \( 1/r_{ij} \). We can rewrite the approximate constant of the motion for \( N \)-electrons \( C_2^- = \sum (A_i - A_j)^2 + (L_i - L_j)^2 \) as follows:

\[
C_{2}^{ij} = (A_i - A_j)^2 + (L_i + L_j)^2 = (A_i)^2 + (A_j)^2 + (L_i)^2 + (L_j)^2 + 2(L_i \cdot L_j - A_i \cdot A_j)
\]

By using the identity

\[
\left[(A_i)^2 + (L_j)^2\right]|n \ell m(j)\rangle = (n^2 - 1)|n \ell m(j)\rangle,
\]

we have:

\[
C_{2}^{ij} = 2(n^2 - 1) + 2(L_i \cdot L_j - A_i \cdot A_j).
\]

Thus

\[
C_2^- = \sum_{i<j} C_{2}^{ij} = 2(n^2 - 1)N(N - 1)/2 + 2 \sum_{i<j} (L_i \cdot L_j - A_i \cdot A_j).
\]

As \( n \) and \( N \) are fixed, if \( C_2^- \) is a approximate constant of motion then it follows that \( \Omega = \sum_{i<j} (L_i \cdot L_j - A_i \cdot A_j) \) is an approximate constant of motion. Then \( C_2^- \) can be replaced by \( \Omega \) for convenience.

(a) Matrix elements of

\[
\mathcal{L} = \sum_{i<j} L_i \cdot L_j = 1/2 \sum_{i<j} L_i \cdot L_j = 1/2 \left[ \sum_{i<j} L_i \cdot L_j - \sum_{i<j} L_i \cdot L_j \right].
\]
Using $L^2 = \sum_j (\ell_j)^2 + \sum_{\lambda} \ell_\lambda \cdot \ell_\lambda$ gives
\[
< \ell'_{\lambda_1 s_1 \lambda}, \ell'_{\lambda_2 s_2 \lambda} \mid L \mid \ell'_{\lambda_1' s_1' \lambda'}, \ell'_{\lambda_2' s_2' \lambda'} > S' L = [L_1(L_1 + 1) - \ell \ell (\ell + 1)]/2
- \left[ L_2(L_2 + 1) - \ell' \ell' (\ell' + 1) \right]/2 \delta_{S_1 S_1'} \delta_{L_1 L_1'} \delta_{S_2 S_2'} \delta_{L_2 L_2'}
+ < \ell'_{\lambda_1 s_1 \lambda}, \ell'_{\lambda_2 s_2 \lambda} \mid S L \mid \sum_{\lambda_1} \sum_{j=N+1}^K \ell_j \cdot \ell_j' \mid \ell'_{\lambda_1' s_1' \lambda'}, \ell'_{\lambda_2' s_2' \lambda'} \mid S L > . \tag{III-2-13}
\]

By using (III-1-17) the last matrix element equates to:
\[
(-1)^{L_1'+L_1+1} \left[ \begin{array}{ccc} L_1 & L_2 & L \\ L_1' & L_2' & 1 \end{array} \right] < \ell'_{\lambda_1 s_1 \lambda}, \ell'_{\lambda_2 s_2 \lambda} \mid \sum_{\lambda_1} \sum_{j=N+1}^K \ell_j \cdot \ell_j' \mid \ell'_{\lambda_1' s_1' \lambda'}, \ell'_{\lambda_2' s_2' \lambda'} > \delta_{\lambda_1 \lambda_1'} \delta_{\lambda_2 \lambda_2'} .
\]

By using the formula (8),
\[
< \ell' \mid L \mid \ell > = \frac{1}{\ell} \delta_{\ell \ell'} (2\ell + 1) (\ell + 1) \ell \]^{1/2}
\]
the last matrix element of (III-2-13) equates to:
\[
(-1)^{L_1'+L_1+1} \left[ \begin{array}{ccc} L_1 & L_2 & L \\ L_1' & L_2' & 1 \end{array} \right] \left[ L_1(L_1 + 1)(2L_1 + 1) \right]^{1/2} \left[ L_2(L_2 + 1)(2L_2 + 1) \right]^{1/2} \delta_{\lambda_1 \lambda_1'} \delta_{\lambda_2 \lambda_2'} .
\]

By using the formula for the 6-j symbol (8) we find this becomes:
\[
\frac{(-1)^{L_1+L_2+L+L_1+L_2+L_1+1} 2 \left[ L_2 (L_2 + 1) + L_1 (L_1 + 1) - L (L + 1) \right]}{\left[ 2 L_1 (2L_1 + 1) (2L_1 + 2) 2 L_2 (2L_2 + 1) (2L_2 + 2) \right]^{1/2}}
\]
\[
\times \left[ L_1 (L_1 + 1) (2L_1 + 1) L_2 (L_2 + 1) (2L_2 + 1) \right]^{1/2}
\]
Finally we have:

\[
\langle l_{ij}^\nu , l_{kl}^\kappa \mid L \mid l_{ij}^\nu , l_{kl}^\kappa \mid S L \rangle = \delta_{\nu \mu} \delta_{\kappa \kappa} \delta_{l_j l_k} \delta_{l_i l_k} \delta_{l_i l_k} \delta_{l_i l_k} \\
\times [L(L+1) - N\ell(\ell + 1) - K \ell(\ell + 1)]/2.
\]

(III-2-14)

Since \( \langle l \| l \| L \rangle = \delta_{\ell \ell}[(\ell + 1)(2\ell + 1)]^{1/2} \)

there can be no off-diagonal matrix elements of \( L \). In general the matrix elements of \( \sum_{i<j} l_{ij} \) in any configuration of \( N_e \) electrons are:

\[
1/2 \left[ L(L+1) - \sum_{\ell} N_e \ell(\ell + 1) \right]
\]

(b) Matrix elements of \( \sum_{i<j} A_i A_j \) and Coulomb interaction

The calculation of \( \sum_{i<j} A_i A_j \) and \( \sum_{i<j} e^2/\mathbf{r}_{ij} \) are similar. There are 299 matrix elements in each case within the 3s-3p-3d shell for three electrons, but only twelve different types. We will give an example for each type. Making use of the recoupling technique and the results in table 1, 2, 3, 4, 5 we obtain:

1. \[ \langle l^3; S L \mid \sum_{i<j} g_{ij}^\kappa \mid l^3; S L \rangle \]

\[
\langle \rho^3; S L \mid \sum_{i<j} g_{ij}^\kappa \mid \rho^3; S L \rangle = 3 \sum_{\kappa} \langle \rho^3; S_L \| \rho(S_\ell L_\ell) \rho^3 \| \rho(S_L) \rangle \]

\[
\times \langle \rho^3; S_L \| g_{ij}^\kappa \| \rho^3; S_L \rangle.
\]

2. \[ \langle l^3; S L \mid \sum_{i<j} g_{ij}^\kappa \mid l' l^2 S L \rangle \]
\[
\begin{align*}
&\langle p^3; SL \sum_{k} g_k^k \mid d^2 (SL) p; SL \rangle = \langle p^3; SL \sum_{k} g_k^k \mid p d^2 (SL) ; SL \rangle (-^{S+L+\rho+\frac{\lambda}{2} - s_l - L}) \\
&= \sqrt{3} \sum_{L} p^3; SL \{p^3 (SL) ; SL \langle p^3 (SL) \mid g^k \mid d^2 (SL) \rangle (-^{S+L+\rho+\frac{\lambda}{2} - s_l - L}) \}
\end{align*}
\]

\[
S, L, L, L
\]

\[
\begin{align*}
&= \sqrt{3} \sum_{L} p^3; SL \{p^3 (SL) ; SL \langle p^3 (SL) \mid g^k \mid d^2 (SL) \rangle (-^{S+L+\rho+\frac{\lambda}{2} - s_l - L}) \}
\end{align*}
\]

\[
S, L, L
\]

\[
\begin{align*}
&= \sum_{S} \langle p^3; SL \mid p^3 (S, L) , p; SL \rangle \langle p^3; SL \mid g^k \mid d^2 (S, L) \rangle (-^{S+L+\rho+\frac{\lambda}{2} - s_l - L}) \}
\end{align*}
\]

\[
S, L, L
\]

\[
\begin{align*}
&= \sqrt{3} \langle p^3; SL \mid p^3 (S, L) , p; SL \rangle \langle p^3; SL \mid g^k \mid d^2 (S, L) \rangle (-^{S+L+\rho+\frac{\lambda}{2} - s_l - L}) \}
\end{align*}
\]

\[
S, L, L
\]

\[
\begin{align*}
&= \sqrt{3} \langle p^3; SL \mid p^3 (S, L) , p; SL \rangle \langle p^3; SL \mid g^k \mid d^2 (S, L) \rangle (-^{S+L+\rho+\frac{\lambda}{2} - s_l - L}) \}
\end{align*}
\]

\[
S, L, L
\]
\[ x \langle p^2 S_x L_x \mid g_{i_4} \mid s d \sigma_\lambda \rangle (-\frac{1}{2}) - s - L + 2 + L_k + s + L - \frac{1}{2} - p \]

\[ = -\sqrt{3} \sum_{k} \langle p^2 \mid p S_x L_x, p \mid s d \sigma_\lambda \rangle \langle (p s) \mid S, L, d, s L \rangle \langle p (s d) \sigma_\lambda \mid s L \rangle \]

\[ x \langle p^2 S L \mid g_{i_4} \mid s d \sigma_\lambda \rangle . \]

5. \[ \langle \ell' (L, S) l' ; S L \mid \sum_{k} g_{i_4}^k \mid \ell^2 (S_x L_x), l' ; S L \rangle \]

\[ \langle d^2 (S L), p ; S L \mid \sum_{k} g_{i_4}^k \mid d^2 (S_x L_x) \mid p ; S L \rangle = \sum_{k} \langle d^2 (S, L) \mid g_{i_4}^k \mid d^2 S_x L_x \rangle \]

\[ + 2 \sum_{k} \langle (dd) S L, p ; S L \mid g_{i_4}^k \mid (dd) S_x L_x, p ; S L \rangle \]

\[ = 2 \sum_{k} \langle (dd) S L, p ; S L \mid d (dp) \sigma_\lambda \mid S L \rangle \langle d (dp) \sigma_\lambda \mid (dd) S_x L_x, p ; S L \rangle \]

\[ x \langle dp \sigma_\lambda \mid g_{i_4}^k \mid dp \sigma_\lambda \rangle + \sum_{k} \langle d^2 S L, L \mid g_{i_4}^k \mid d^2 S_x L_x \rangle . \]

6. \[ \langle \ell'' \ell', L S L \mid \sum_{k} g_{i_4}^k \mid \ell'' \ell', L S L \rangle \]

\[ \langle d^2 (S L), L s ; S L \mid \sum_{k} g_{i_4}^k \mid p^2 (S_x L_x), s ; S L \rangle \]

\[ = \sum_{k} \langle d^2 , S L \mid g_{i_4}^k \mid p^2 S_x L_x \rangle . \]

7. \[ \langle \ell' \ell', S L \mid \sum_{k} g_{i_4}^k \mid \ell' \ell', S L \rangle \]

\[ \langle d^2 (S L), S L \mid \sum_{k} g_{i_4}^k \mid d, p^2 (S_x L_x) ; S L \rangle \]

\[ = \sqrt{2} \langle (dd) S L, L s ; S L \mid \sum_{k} g_{i_4}^k \mid dp^2 (S_x L_x) ; S L \rangle . \]
\[
= 2 \sum_{\lambda} \langle(dd)S, L, s; SL|d, (ds)_{\sigma\lambda}; SL\rangle \langle p^2 S, L_2| g_{ik}^l| ds_{\sigma\lambda} \rangle
\]

8. \( \langle l^2, l'; SL| \sum_{i,j} g_{ij}^k| l^2, l''; SL \rangle \)

\[
\langle p^2 (S, L_1), d; SL| \sum_{i,j} g_{ij}^k| p^2 S, L_2, s; SL \rangle =
\]

\[
= 2 \langle (pp)S, L_1, d; SL| \sum_{i,j} g_{ij}^k| (pp)S, L_2, s; SL \rangle
\]

\[
= 2 \sum_{\lambda} \langle (pp)S, L_1, d; SL| p, (pd)_{\sigma\lambda}; SL\rangle \langle pd_{\sigma\lambda}| g_{ik}^l| ps_{\sigma\lambda} \rangle
\]

\[
x \langle p, (ps)_{\sigma\lambda}; S, L| (pp)S, L_2, s; SL \rangle.
\]

9. \( \langle l^2, l'; SL| \sum_{i,j} g_{ij}^k| l, l''; SL \rangle \)

\[
\langle d^2 (S, L_1), s; SL| \sum_{i,j} g_{ij}^k| d, s^2 S, L_2; SL \rangle =
\]

\[
\sqrt{2} \langle(dd)S, L_1, s; SL| \sum_{i,j} g_{ij}^k| d, s^2 S, L_2; SL \rangle
\]

\[
= \sqrt{2} \sum_{\lambda} \langle(dd)S, L_1, s; SL| d, (ds)_{\sigma\lambda}; SL\rangle \langle ds_{\sigma\lambda}| g_{ik}^l| s^2 S_2 L_2 \rangle
\]

\[
+ \sqrt{2} \sum_{\lambda'} \langle(ds)_{\sigma\lambda'}, s; SL| d, s^2 S_2 L_2; SL\rangle \langle d^2 S, L_1| g_{ik}^l| ds_{\sigma\lambda'} \rangle
\]

10. \( \langle l(l', l''); S, L| \sum_{i,j} g_{ij}^k| l'', l''; S, L \rangle \)

\[
\langle d(sp)S, L_1, s; SL| \sum_{i,j} g_{ij}^k| p, d^2 (S, L_2); SL \rangle
\]

\[
= \langle d(sp)S, L_1, s; SL| \sum_{i,j} g_{ij}^k| d^2 (S_2 L_2), p; SL \rangle \langle -) S_2 + L_2 + p + \lambda' - s - \lambda
\]
\[
= \sqrt{2} \sum_{\kappa} \langle (d \sigma \lambda) S_1 L_1, p; SL | d(p \sigma \lambda) g_\kappa \rangle | sp S_1 L_1 \rangle (-)^{p + \frac{1}{2} - s - L} \\
+ \sum_{\kappa} \langle d(s \sigma \lambda) S_2 L_2, SL | (d s \sigma \lambda) p; SL \rangle < d \sigma \lambda g_\kappa \rangle | d^2 S_2 L_2 \rangle (-)^{p + \frac{1}{2} - s - L} \\
\]
(4) Results

Table 1: Matrix elements for $A_1 \cdot A_2$ in the 3s-3p-3d shell

(A) $< l' S L | A_1 \cdot A_2 | l'' S L >$

1. $< d^1 S | A_1 \cdot A_2 | p^1 S > = 2\sqrt{15}/3$

2. $< d^1 P | A_1 \cdot A_2 | p^2 P > = -\sqrt{5}$

3. $< d^1 D | A_1 \cdot A_2 | p^2 D > = -\sqrt{21}/3$

4. $< p^2 S | A_1 \cdot A_2 | s^2 S > = -8\sqrt{3}/3$

(B) $< l' S L | A_1 \cdot A_2 | l'' S L >$

1. $< p^2 D | A_1 \cdot A_2 | s d D > = 4\sqrt{6}/3$

(C) $< l' l'' S L | A_1 \cdot A_2 | l'''' S L >$

1. $< p d' P | A_1 \cdot A_2 | s p' P > = -4\sqrt{5}/3$

2. $< p d^3 P | A_1 \cdot A_2 | s p^3 P > = -4\sqrt{5}/3$

3. $< s p' P | A_1 \cdot A_2 | d p' P > = -4\sqrt{5}/3$

4. $< s p^3 P | A_1 \cdot A_2 | d p^3 P > = 4\sqrt{5}/3$

5. $< p d' P | A_1 \cdot A_2 | p s' P > = -4\sqrt{5}/3$

6. $< p d^3 P | A_1 \cdot A_2 | p s^3 P > = 4\sqrt{5}/3$

7. $< p s' P | A_1 \cdot A_2 | p s' P > = 8/3$

8. $< p s^3 P | A_1 \cdot A_2 | p s^3 P > = -8/3$
(9) \[ <dp^3P|A_1 \cdot A_2|dp^3P> = \frac{1}{3} \]

(10) \[ <dp^3P|A_3 \cdot A_4|dp^3P> = -\frac{1}{3} \]

(11) \[ <dp^3D|A_3 \cdot A_4|dp^3D> = -1 \]

(12) \[ <dp^3D|A_1 \cdot A_2|dp^3D> = 1 \]

(13) \[ <dp^3F|A_1 \cdot A_2|dp^3F> = 2 \]

(14) \[ <dp^3F|A_3 \cdot A_4|dp^3F> = -2 \]

(15) \[ <dp^3F|A_3 \cdot A_4|dp^3F> = <dp^3F|A_1 \cdot A_2|dp^3F> \]

(16) \[ <dp^3F|A_1 \cdot A_2|dp^3F> = <dp^3F|A_3 \cdot A_4|dp^3F> \]

(17) \[ <dp^3F|A_3 \cdot A_4|dp^3F> = -<dp^3F|A_1 \cdot A_2|dp^3F> \]

Table 2: Matrix elements for Coulomb interaction in the 3s-3p-3d shell (18)

\[
(A) \quad <l' S, L, \ell | C^k, C^{\ell'} | l' S, L, >
\]

(1) \[ <s^2'S | l/r_{12} | s^2'S> = R^2(3s3s;3s3s) = .066406 \]

(2) \[ <p^2 'S | l/r_{12} | p^2 'S> = R^2(3p3p;3p3p) \]

\[
+ 2R^2(3p3p;3p3p)/5 = .086263
\]

(3) \[ <p^2 ^3P | l/r_{12} | p^2 ^3P> = R^0(3p3p;3p3p) \]

\[
- R^2(3p3p;3p3p)/5 = .064670
\]

(4) \[ <p^2 'D | l/r_{12} | p^2 'D> = R^0(3p3p;3p3p) \]

\[
+ R^2(3p3p;3p3p)/25 = .073307
\]
(5) \[
\langle d^2 'S \mid 1/r_{12} \mid d^2 'S \rangle = R^0 (3d3d;3d3d) \\
+ 14 R^2 (3d3d;3d3d)/49 \\
+ 126 R^4 (3d3d;3d3d)/441 = 0.107486
\]

(6) \[
\langle d^2 'D \mid 1/r_{12} \mid d^2 'D \rangle = R^0 (3d3d;3d3d) \\
- 3 R^2 (3d3d;3d3d)/49 \\
+ 36 R^4 (3d3d;3d3d)/441 = 0.085683
\]

(7) \[
\langle d^2 'P \mid 1/r_{12} \mid d^2 'P \rangle = R^0 (3d3d;3d3d) \\
+ 7 R^2 (3d3d;3d3d)/49 \\
- 84 R^4 (3d3d;3d3d)/441 = 0.086892
\]

(8) \[
\langle d^2 'F \mid 1/r_{12} \mid d^2 'F \rangle = R^0 (3d3d;3d3d) \\
- 8 R^2 (3d3d;3d3d)/49 \\
- 9 R^4 (3d3d;3d3d)/441 = 0.078025
\]

(9) \[
\langle d^1 'G \mid 1/r_{12} \mid d^1 'G \rangle = R^0 (3d3d;3d3d) \\
+ 4 R^2 (3d3d;3d3d)/49 \\
+ R^4 (3d3d;3d3d)/441 = 0.089821
\]

(B) \[
\langle L^2 S L \mid C^\dagger C \mid L^2 S L \rangle
\]

(1) \[
\langle p^2 'S \mid 1/r_{12} \mid s^2 'S \rangle = -\sqrt{3} R' (3p3p;3s3s)/3 = -0.024432
\]

(2) \[
\langle d^2 'S \mid 1/r_{12} \mid s^2 'S \rangle = R^2 (3d3d;3s3s)/\sqrt{5} = 0.010190
\]

(3) \[
\langle p^2 'S \mid 1/r_{12} \mid d^2 'S \rangle = -2\sqrt{15} R' (3p3p;3d3d)/15 \\
- 3\sqrt{15} R^2 (3p3p;3d3d)/35 = -0.025634
\]

(4) \[
\langle p^2 'P \mid 1/r_{12} \mid d^2 'P \rangle = -5 R' (3p3p;3d3d)/5 \\
+ 3\sqrt{5} R (3p3p;3d3d)/35 = -0.010675
\]
(5) $\langle p^2 'D | l/r_d | d^4 'D \rangle = -\sqrt{21} R(3p3p;3d3d)/15$
$- 3\sqrt{21} R(3p3p;3d3d)/245 = -0.01179$

C. $\langle l^2 S L | C_k \cdot C_k' | l'' l'' S L \rangle$

(1) $\langle d^2 'D | 1/r_{1a} | d's 'D \rangle = -2\sqrt{35} R(3d3d;3d3s)/35 = 0.008235$
(2) $\langle p^2 'D | 1/r_{1a} | sd 'D \rangle = 2\sqrt{15} R(3p3p;3s3p)/15 = 0.0186235$
(3) $\langle s^2 'S | 1/r_n | ds 'D \rangle = 0$
(4) $\langle p^2 'D | 1/r_{1a} | d's 'D \rangle = 0.018605$

D. $\langle l' l'S L | C_k \cdot C_k' | l'' l'' S L \rangle$

(1) $\langle pd 'P | 1/r_{1a} | ps 'P \rangle = -\sqrt{2} R(3p3d;3p3s)/5$
$- \sqrt{2} R(3p3d;3s3p)/3 = -0.024262$

(2) $\langle pd 'P | 1/r_{1a} | ps 'P \rangle = -\sqrt{2} R(3p3d;3p3s)/5$
$+\sqrt{2} R(3p3d;3s3p)/3 = 0.009705$

(3) $\langle dp 'P | 1/r_{1a} | sp 'P \rangle = \langle pd 'P | 1/r_{1a} | ps 'P \rangle$
$= -0.024262$

(4) $\langle dp 'P | 1/r_{1a} | sp 'P \rangle = \langle pd 'P | 1/r_{1a} | ps 'P \rangle$
$= 0.009705$

(5) $\langle pd 'P | 1/r_{1a} | sp 'P \rangle = \langle pd 'P | 1/r_{1a} | ps 'P \rangle$
$= -0.024262$

(6) $\langle pd 'P | 1/r_{1a} | sp 'P \rangle = -\langle pd 'P | 1/r_{1a} | ps 'P \rangle$
$= -0.009705$

(7) $\langle sp 'P | 1/r_{1a} | sp 'P \rangle = R(3s3p;3s3p)$
\[
+ R^I (3s3p;3p3s)/3 = 0.082899
\]

(8) \[
<\text{sp}^3P \left| 1/r_{1z} \right| \text{sp} \ P> = R^o (3s3p;3s3p) - R^I (3s3p;3s3p)/3 = 0.054687
\]

(9) \[
<\text{ds}^1D \left| 1/r_{1z} \right| \text{ds}^1D> = R^o (3d3s;3d3s) + R^d (3d3s;3s3d)/5 = 0.077691
\]

(10) \[
<\text{ds}^3D \left| 1/r_{1z} \right| \text{ds}^3D> = R^o (3d3s;3d3s) - R^d (3d3s;3s3d)/5 = 0.068576
\]

(11) \[
<\text{pd}^1P \left| 1/r_{1z} \right| \text{pd}^1P> = R^o (3p3d;3p3d) + R^d (3p3d;3p3d)/5 + R^I (3p3d;3d3p)/15 + 9R^3 (3p3d;3d3p)/35 = 0.092621
\]

(12) \[
<\text{pd}^3P \left| 1/r_{1z} \right| \text{pd}^3P> = R^o (3p3d;3p3d) + R^d (3p3d;3p3d)/5 - R^I (3p3d;3d3p)/15 - 9R^3 (3p3d;3d3p)/35 = 0.075694
\]

(13) \[
<\text{pd}^1D \left| 1/r_{1z} \right| \text{pd}^1D> = R^o (3p3d;3p3d) - R^d (3p3d;3p3d)/5 - R^I (3p3d;3d3p)/5 + 3R^3 (3p3d;3d3p)/35 = 0.064930
\]

(14) \[
<\text{pd}^3D \left| 1/r_{1z} \right| \text{pd}^3D> = R^o (3p3d;3p3d) - R^d (3p3d;3p3d)/5 + R^I (3p3d;3d3p)/5 - 3R^3 (3p3d;3d3p)/35 = 0.074479
\]

(15) \[
<\text{pd}^1F \left| 1/r_{1z} \right| \text{pd}^1F> = R^o (3p3d;3p3d) + 2R^d (3p3d;3p3d)/35 + 2R^I (3p3d;3d3p)/5 + 3R^3 (3p3d;3d3p)/245 = 0.092962
\]
\begin{align*}
(16) \langle \text{pd}^3 F \mid \frac{1}{r_{ik}} \mid \text{pd}^4 F \rangle &= R^2 (3p3d; 3p3d) + \frac{2R^2 (3p3d; 3p3d)}{35} \\
&- \frac{2R (3p3d; 3d3p)}{5} \\
&- \frac{3R^3 (3p3d; 3d3p)}{245} \\
&= 0.065029
\end{align*}
Table 3: Recoupling coefficients within the 3s-3p-3d shell for three electrons

\[ \langle (dd)S, L, p ; SL | d(dp)_{\sigma \lambda} ; SL \rangle \]

(1) \[ \langle (dd)S, L, p ; ^2S | d(dp)_{\sigma \lambda} ; ^2S \rangle \]

<table>
<thead>
<tr>
<th>( s, l )</th>
<th>( ^1D )</th>
<th>( ^3D )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ^3P )</td>
<td>( \sqrt{3}/2 )</td>
<td>1/2</td>
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</tbody>
</table>

(2) \[ \langle (dd)S, L, p ; ^2P | d(dp)_{\sigma \lambda} ; ^2P \rangle \]

<table>
<thead>
<tr>
<th>( s, l )</th>
<th>( ^1P )</th>
<th>( ^3P )</th>
<th>( ^1D )</th>
<th>( ^3D )</th>
<th>( ^1F )</th>
<th>( ^3F )</th>
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<tbody>
<tr>
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<td>( -\sqrt{105} )</td>
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<td>( \sqrt{105} )</td>
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</table>

(3) \[ \langle (dd)S, L, p ; ^4D | d(dp)_{\sigma \lambda} ; ^2D \rangle \]

<table>
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<th>( ^1D )</th>
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<th>( ^1F )</th>
<th>( ^3F )</th>
</tr>
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<td>20</td>
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<td>10</td>
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<td>( ^3F )</td>
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</table>
(4) $\langle (dd)S, L, \epsilon, p; ^3F | d(dp)_{\sigma \lambda}; ^3F \rangle$

<table>
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<tr>
<th>$^3\epsilon \lambda$</th>
<th>$^1p$</th>
<th>$^3p$</th>
<th>$^1d$</th>
<th>$^3d$</th>
<th>$^1f$</th>
<th>$^3f$</th>
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<td>$\sqrt{14}$</td>
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<td>$-\sqrt{210}$</td>
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</table>

(5) $\langle (dd)S, L, \epsilon, p; ^2G | d(dp)_{\sigma \lambda}; ^2G \rangle$

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</table>

(6) $\langle (dd)S, L, \epsilon, p; ^2H | d(dp)_{\sigma \lambda}; ^2H \rangle$

<table>
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</table>
(7) \[ \langle (dd)S, L, p; ^4S | d(dp)\sigma; ^4S \rangle \]

\[
\begin{array}{ccc}
\sigma & ^3D \\
S, L & ^3P \\
\end{array}
\]

\[
\begin{array}{ccc}
& ^3D \\
^3P & 1 \\
\end{array}
\]

(8) \[ \langle (dd)S, L, p; ^4P | d(dp)\sigma; ^4P \rangle \]

\[
\begin{array}{ccc}
\sigma & ^3P & ^3D & ^3F \\
S, L & ^3P & -\sqrt{35} & \sqrt{3} & \sqrt{105} \\
& & 10 & 6 & 15 \\
\end{array}
\]

(9) \[ \langle (dd)S, L, p; ^4D | d(dp)\sigma; ^4D \rangle \]

\[
\begin{array}{ccc}
\sigma & ^3P & ^3D & ^3F \\
S, L & ^3P & 3 & -\sqrt{35} & \sqrt{14} \\
& & 10 & 10 & 5 \\
& \sqrt{14} & \sqrt{10} & 1 \\
\end{array}
\]

(10) \[ \langle (dd)S, L, p; ^4F | d(dp)\sigma; ^4F \rangle \]

\[
\begin{array}{ccc}
\sigma & ^3P & ^3D & ^3F \\
S, L & ^3F & -\sqrt{5} & \sqrt{2} & \sqrt{30} \\
& & 5 & 2 & 10 \\
\end{array}
\]

(11) \[ \langle (dd)S, L, p; ^4G | d(dp)\sigma; ^4G \rangle \]

\[
\begin{array}{ccc}
\sigma & ^3D & ^3F \\
S, L & ^3F & -\sqrt{6} & \sqrt{30} \\
& & 6 & 6 \\
\end{array}
\]
\[
\langle dp^2 (S, L,) ; SL \mid (dp)_{\sigma \lambda} p; SL \rangle
\]

(1) \quad \langle dp^2 (S, L,) ; s \mid (dp)_{\sigma \lambda} p; s \rangle

<table>
<thead>
<tr>
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<th>( ^3 P )</th>
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</table>

(2) \quad \langle dp^2 (S, L,) ; \( ^3 P \mid (dp)_{\sigma \lambda} p; \( ^3 P \rangle

<table>
<thead>
<tr>
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<th>( ^3 P )</th>
<th>( ^1 D )</th>
<th>( ^3 D )</th>
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<tr>
<td>( ^1 D )</td>
<td>-( \sqrt{3} )</td>
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<td>-1</td>
<td>( \sqrt{3} )</td>
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(3) \quad \langle dp^2 (S, L,) ; \( ^1 D \mid (dp)_{\sigma \lambda} p; \( ^2 D \rangle

<table>
<thead>
<tr>
<th>S, L,</th>
<th>( ^1 P )</th>
<th>( ^3 P )</th>
<th>( ^1 D )</th>
<th>( ^3 D )</th>
<th>( ^1 F )</th>
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<td>4</td>
<td>12</td>
<td>10</td>
<td>30</td>
</tr>
<tr>
<td>( ^1 S )</td>
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<td>( \sqrt{15} )</td>
<td>( \sqrt{3} )</td>
<td>-1</td>
<td>-( \sqrt{105} )</td>
<td>( \sqrt{35} )</td>
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<td>( ^1 D )</td>
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<td>( \sqrt{7} )</td>
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</table>
(4) \[ \langle \sigma \lambda (S, L_1) ; ^2F | (dp) \sigma \lambda p ; ^2F \rangle \]

<table>
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<th>( \sigma \lambda )</th>
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<th>('F'</th>
<th>('3D'</th>
<th>('3F'</th>
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(5) \[ \langle \sigma \lambda (S, L_1) ; ^2G | (dp) \sigma \lambda p ; ^2G \rangle \]

<table>
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(6) \[ \langle \sigma \lambda (S, L_1) ; ^4P | (dp) \sigma \lambda p ; P \rangle \]

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(7) \[ \langle \sigma \lambda (S, L_1) ; ^4D | (dp) \sigma \lambda p ; ^4D \rangle \]

<table>
<thead>
<tr>
<th>( \sigma \lambda )</th>
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<th>( ^3D )</th>
<th>( ^3F )</th>
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<td>( \sqrt{105} )</td>
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<tr>
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<td>15</td>
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</tbody>
</table>
\[
\begin{align*}
(8) \quad & \langle \text{dp}^2(S, L_1); \text{F} | (\text{dp}) \sigma \lambda; \text{p} \rangle \text{F} > \\
& \begin{array}{c|cc}
\sigma \lambda & 3\text{D} & 3\text{F} \\
\hline
3\text{p} & \sqrt{3} & \sqrt{6} \\
& 3 & 3 \\
\end{array} \\
& \langle \text{d}^2(S, L_1); \text{SL} | \text{d}(\text{ds}) \sigma \lambda; \text{SL} > \\
(1) \quad & \langle \text{d}^4(S, L_1); \text{S} | \text{d}(\text{ds}) \sigma \lambda; \text{S} > \\
& \begin{array}{c|cc}
\sigma \lambda & 1\text{D} & 3\text{D} \\
\hline
1\text{S} & -1 & \sqrt{3} \\
& 2 & 2 \\
\end{array} \\
(2) \quad & \langle \text{d}^4(S, L_1); \text{P} | \text{d}(\text{ds}) \sigma \lambda; \text{P} > \\
& \begin{array}{c|cc}
\sigma \lambda & 1\text{D} & 3\text{D} \\
\hline
3\text{p} & \sqrt{3} & 1 \\
& 2 & 2 \\
\end{array} \\
(3) \quad & \langle \text{d}^4(S, L_1); \text{D} | \text{d}(\text{ds}) \sigma \lambda; \text{D} > \\
& \begin{array}{c|cc}
\sigma \lambda & 1\text{D} & 3\text{D} \\
\hline
1\text{D} & -1 & \sqrt{3} \\
& 2 & 2 \\
\end{array} \\
(4) \quad & \langle \text{d}^3(S, L_1); \text{F} | \text{d}(\text{ds}) \sigma \lambda; \text{F} > \\
& \begin{array}{c|cc}
\sigma \lambda & 1\text{D} & 3\text{D} \\
\hline
3\text{F} & \sqrt{3} & 1 \\
& 2 & 2 \\
\end{array}
\end{align*}
\]
\[
\begin{array}{c|cc}
\sigma & {^1D} & {^3D} \\
\hline
{^1G} & -1 & \sqrt{3} \\
& 2 & \frac{1}{2} \\
\hline
\end{array}
\]

\[
\begin{array}{c|c}
\sigma & {^3D} \\
\hline
{^3P} & 1 \\
\hline
\end{array}
\]

\[
\begin{array}{c|c}
\sigma & {^3D} \\
\hline
{^3F} & 1 \\
\hline
\end{array}
\]

\[
\langle p^2(S, L_s) s; S| p(ps) \sigma; S \rangle
\]

\[
\begin{array}{c|cc}
\sigma & {^1P} & {^3P} \\
\hline
{^1S} & -1 & \sqrt{3} \\
& 2 & \frac{1}{2} \\
\hline
\end{array}
\]

\[
\begin{array}{c|cc}
\sigma & {^1P} & {^3P} \\
\hline
{^3P} & \sqrt{3} & 1 \\
& 2 & \frac{1}{2} \\
\hline
\end{array}
\]
\[ <p^2(S, L, \sigma) s; ^2D | p(ps) \sigma \chi; ^2D > \]

\[
\begin{array}{c|cc}
\sigma \chi & 1^P & 3^P \\
S, L & \hline
1^D & -1 & \sqrt{3} \\
2 & 2 & 2 \\
\end{array}
\]

\[ <p^2(SL_1) s; ^4P | p(ps) \sigma \chi; ^4P > \]

\[
\begin{array}{c|c}
\sigma \chi & 3^P \\
S, L_1 & \hline
3^P & 1 \\
\end{array}
\]

\[ <ds^2(S, L_1); SL | (ds) \sigma \chi s; SL > \]

\[ <ds^2(S, L_1); ^2D | (ds) \sigma \chi s; ^2D > \]

\[
\begin{array}{c|cc}
\sigma \chi & 1^D & 3^D \\
S, L & \hline
1^S & -1 & \sqrt{3} \\
2 & 2 & 2 \\
\end{array}
\]

\[ <ps^2(S, L_1); ^2P | (ps) \sigma \chi s; ^2P > \]

\[
\begin{array}{c|cc}
\sigma \chi & 1^P & 3^P \\
S, L_1 & \hline
1^P & -1 & \sqrt{3} \\
2 & 2 & 2 \\
\end{array}
\]

\[ <d(sp)S, L_1; SL | (ds) \sigma \chi p; SL > \]
(1) \[ \langle d(sp)S, L; \ ^2P \mid (ds)_{\sigma_x} P; \ ^2P \rangle \]

<table>
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<td>(-)</td>
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<td>( \sqrt{3} )</td>
<td>( \sqrt{3} )</td>
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<td>( \quad )</td>
<td>( \sqrt{3} )</td>
<td>( \sqrt{3} )</td>
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<tr>
<td>( \quad )</td>
<td>( -)</td>
<td>(-)</td>
</tr>
<tr>
<td>( \quad )</td>
<td>( -)</td>
<td>(-)</td>
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<tr>
<td>( ^3P )</td>
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<td>(-)</td>
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<tr>
<td>( \quad )</td>
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</table>

(2) \[ \langle d(sp) S, L; \ ^4D \mid (ds)_{\sigma_x} P; \ ^2D \rangle \]

<table>
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<td>( ^3P )</td>
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</tbody>
</table>

(3) \[ \langle d(sp) S, L; \ ^2F \mid (ds)_{\sigma_x} P; \ ^2F \rangle \]

<table>
<thead>
<tr>
<th>( S, L )</th>
<th>( ^1D )</th>
<th>( ^3D )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( ^1P )</td>
<td>(-1)</td>
<td>( \sqrt{3} )</td>
</tr>
<tr>
<td>( \quad )</td>
<td>(-)</td>
<td>(-)</td>
</tr>
<tr>
<td>( \quad )</td>
<td>( \sqrt{3} )</td>
<td>( \sqrt{3} )</td>
</tr>
<tr>
<td>( \quad )</td>
<td>( \sqrt{3} )</td>
<td>( \sqrt{3} )</td>
</tr>
<tr>
<td>( \quad )</td>
<td>(-)</td>
<td>(-)</td>
</tr>
<tr>
<td>( \quad )</td>
<td>(-)</td>
<td>(-)</td>
</tr>
<tr>
<td>( ^3P )</td>
<td>( -)</td>
<td>(-)</td>
</tr>
<tr>
<td>( \quad )</td>
<td>( -)</td>
<td>(-)</td>
</tr>
</tbody>
</table>

(4) \[ \langle d(sp)^3P; \ ^4P \mid (ds)^3D P; \ ^4P \rangle = 1 \]

(5) \[ \langle d(sp)^3P; \ ^4F \mid (ds)^3D P; \ ^4F \rangle = 1 \]
\[ \langle d(sp)^3 P; ^4 D | (ds)^3 Dp; ^4 D \rangle = -1 \]

\[ \langle (sp)S, L, d; sL | s(pd) \sigma_x; sL \rangle \]

\[ \begin{array}{c|cc}
\sigma_x & \bar{1}P & \bar{3}P \\
\hline
\bar{1}P & -1 & \sqrt{3} \\
& 2 & 2 \\
\bar{3}P & \sqrt{3} & 1 \\
& 2 & 2 \\
\end{array} \]

\[ \langle (sp)S, L, d; ^2 D | s(pd) \sigma_x; ^2 D \rangle \]

\[ \begin{array}{c|cc}
\sigma_x & \bar{1}D & \bar{3}D \\
\hline
\bar{1}P & -1 & \sqrt{3} \\
& 2 & 2 \\
\bar{3}P & \sqrt{3} & 1 \\
& 2 & 2 \\
\end{array} \]

\[ \langle (sp)S, L, d; ^2 F | s(pd) \sigma_x; ^2 F \rangle \]

\[ \begin{array}{c|cc}
\sigma_x & \bar{1}F & \bar{3}F \\
\hline
\bar{1}P & -1 & \sqrt{3} \\
& 2 & 2 \\
\bar{3}P & \sqrt{3} & 1 \\
& 2 & 2 \\
\end{array} \]

\[ \langle (sp)^3 Pd; ^4 P | s(pd)^3 P; ^4 P \rangle = 1 \]
\[(5) \quad <(sp)^3Pd; ^4D \mid s(pd)^3D; ^4D> = 1\]

\[(6) \quad <(sp)^3Pd; ^4F \mid s(pd)^3F; ^4F> = 1\]

Table 4: Coefficients of fractional parentage for \(p^3(5C)\)

<table>
<thead>
<tr>
<th>(p^3)</th>
<th>(N)</th>
<th>'S'</th>
<th>'P'</th>
<th>'D'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^4S)</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>(^2P)</td>
<td>18(^{-\frac{1}{2}})</td>
<td>2</td>
<td>-3</td>
<td>-(5)(^\frac{1}{2})</td>
</tr>
<tr>
<td>(^2D)</td>
<td>2(^{-\frac{1}{2}})</td>
<td>0</td>
<td>1</td>
<td>-1</td>
</tr>
</tbody>
</table>

Table 5: Coefficients of fractional parentage for \(d^3(5C)\)

<table>
<thead>
<tr>
<th>(d^3)</th>
<th>(N)</th>
<th>'S'</th>
<th>'P'</th>
<th>'D'</th>
<th>'F'</th>
<th>'G'</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^3P)</td>
<td>30(^{-\frac{1}{2}})</td>
<td>0</td>
<td>7(^{\frac{1}{2}})</td>
<td>15</td>
<td>-8(^{\frac{1}{2}})</td>
<td>0</td>
</tr>
<tr>
<td>(^3P)</td>
<td>15(^{-\frac{1}{2}})</td>
<td>0</td>
<td>-(8)(^{\frac{1}{2}})</td>
<td>0</td>
<td>-7(^{\frac{1}{2}})</td>
<td>0</td>
</tr>
<tr>
<td>(^3D)</td>
<td>60(^{-\frac{1}{2}})</td>
<td>4</td>
<td>-(3)</td>
<td>-(5)(^{\frac{1}{2}})</td>
<td>-21(^{\frac{1}{2}})</td>
<td>-(3)</td>
</tr>
<tr>
<td>(^3D)</td>
<td>140(^{-\frac{1}{2}})</td>
<td>0</td>
<td>-(7)</td>
<td>45(^{\frac{1}{2}})</td>
<td>21(^{\frac{1}{2}})</td>
<td>-(5)</td>
</tr>
<tr>
<td>(^3F)</td>
<td>70(^{-\frac{1}{2}})</td>
<td>0</td>
<td>28(^{\frac{1}{2}})</td>
<td>-(10)(^{\frac{1}{2}})</td>
<td>7(^{\frac{1}{2}})</td>
<td>-(5)</td>
</tr>
<tr>
<td>(^3F)</td>
<td>5(^{\frac{1}{2}})</td>
<td>0</td>
<td>-1</td>
<td>0</td>
<td>2</td>
<td>0</td>
</tr>
<tr>
<td>(^3G)</td>
<td>42(^{-\frac{1}{2}})</td>
<td>0</td>
<td>0</td>
<td>-(10)(^{\frac{1}{2}})</td>
<td>21(^{\frac{1}{2}})</td>
<td>11(^{\frac{1}{2}})</td>
</tr>
<tr>
<td>(^3H)</td>
<td>2(^{-\frac{1}{2}})</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>1</td>
</tr>
</tbody>
</table>
Table 6: Comparison of exact and approximate configuration mixing (19)

I. Matrix elements of $\sum_{i<j} 1/r_{ij}$ (indicated in the first line of each box) and matrix elements of $\sum_{i<j}(L_i \cdot L_j - A_i \cdot A_j)$ (indicated in the second line of each box). The overlap between the eigenstates of these two operators is lined below each matrix.

(1) Matrix elements for $n = 3$ $N = 2$:

<table>
<thead>
<tr>
<th>$d^2 \frac{3}{2} \frac{1}{2}$</th>
<th>$p^2 \frac{3}{2} \frac{1}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.086892</td>
<td>-0.010675</td>
</tr>
<tr>
<td>$-5$</td>
<td>$\sqrt{5}$</td>
</tr>
<tr>
<td>-0.010675</td>
<td>0.064670</td>
</tr>
<tr>
<td>$\sqrt{5}$</td>
<td>-1</td>
</tr>
</tbody>
</table>

overlap: 0.999

<table>
<thead>
<tr>
<th>$d \frac{1}{2} \frac{3}{2} \frac{1}{2}$</th>
<th>$p \frac{1}{2} \frac{3}{2} \frac{1}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.092621</td>
<td>-0.024262</td>
</tr>
<tr>
<td>$-10/3$</td>
<td>$4\sqrt{5}/3$</td>
</tr>
<tr>
<td>-0.024262</td>
<td>0.082899</td>
</tr>
<tr>
<td>$4\sqrt{5}/3$</td>
<td>$-8/3$</td>
</tr>
</tbody>
</table>

overlap: 0.999

<table>
<thead>
<tr>
<th>$d \frac{3}{2} \frac{1}{2}$</th>
<th>$p \frac{3}{2} \frac{1}{2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.075694</td>
<td>-0.009705</td>
</tr>
<tr>
<td>$-8/3$</td>
<td>$4\sqrt{5}/3$</td>
</tr>
<tr>
<td>-0.009705</td>
<td>0.054687</td>
</tr>
<tr>
<td>$4\sqrt{5}/3$</td>
<td>$8/3$</td>
</tr>
</tbody>
</table>

overlap: 0.996
(2) Matrix elements for $n = 3 \ N = 3$:

\[
\begin{array}{c|c|c}
\langle d^2 3p, ^4S \rangle & \langle p^3, ^4S \rangle \\
\hline
\langle d^2 3p \rangle & .235850 & -.018971 \\
\langle d^2 3p \rangle & -9 & \sqrt{15} \\
\langle p^3 3s \rangle & .194010 & -3 \\
\end{array}
\]

overlaps: .996
<table>
<thead>
<tr>
<th>\langle d^3 \bar{P} p; ^4 P \rangle</th>
<th>\langle d^{sp} \bar{P} p; ^4 P \rangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.228120</td>
<td>-0.009210</td>
</tr>
<tr>
<td>-4</td>
<td>\sqrt{2}</td>
</tr>
<tr>
<td>-0.009210</td>
<td>0.198960</td>
</tr>
<tr>
<td>2\sqrt{2}</td>
<td>0</td>
</tr>
</tbody>
</table>

Overlap: 0.983

<table>
<thead>
<tr>
<th>\langle d^3 \bar{F} p; ^4 F \rangle</th>
<th>\langle d^{sp} \bar{P} p; ^4 F \rangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.221790</td>
<td>-0.006140</td>
</tr>
<tr>
<td>-2/3</td>
<td>4\sqrt{2}/3</td>
</tr>
<tr>
<td>-0.006140</td>
<td>0.188290</td>
</tr>
<tr>
<td>4\sqrt{2}/3</td>
<td>20/3</td>
</tr>
</tbody>
</table>

Overlap: 0.998

<table>
<thead>
<tr>
<th>\langle pd^2 \bar{F}; ^2 G \rangle</th>
<th>\langle pd^{2s} \bar{F}; ^2 G \rangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.243760</td>
<td>-0.012090</td>
</tr>
<tr>
<td>3/2</td>
<td>\sqrt{15}/2</td>
</tr>
<tr>
<td>-0.012090</td>
<td>0.233970</td>
</tr>
<tr>
<td>\sqrt{15}/2</td>
<td>5/2</td>
</tr>
</tbody>
</table>

Overlap: 0.998

<table>
<thead>
<tr>
<th>\langle d^4 \bar{F} \rangle</th>
<th>\langle d^4 \bar{s} F \rangle</th>
<th>\langle dp^4 \bar{F} \rangle</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.239390</td>
<td>0</td>
<td>0.008000</td>
</tr>
<tr>
<td>-3</td>
<td>0</td>
<td>-\sqrt{3}</td>
</tr>
<tr>
<td>0</td>
<td>0.214000</td>
<td>0</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.008000</td>
<td>0</td>
<td>0.201000</td>
</tr>
<tr>
<td>-\sqrt{3}</td>
<td>0</td>
<td>3</td>
</tr>
</tbody>
</table>

Overlap: 0.998 0.998 1
\[
\begin{array}{c|c|c}
| d^2 'S \rangle & dp^2 'D \rangle & p^2 'S \rangle \\
\hline
\langle d^2 'S \rangle & 0.24910 & -0.01315 & -0.02563 \\
\hline
& 6 & 4/3 & 2/15/3 \\
\langle dp^2 'D \rangle & -0.01315 & 0.23316 & 0.002420 \\
\hline
& 4/3 & -14/3 & -4/15/3 \\
\langle p^2 'S \rangle & -0.02563 & 0.002420 & 0.20774 \\
\hline
& 2/15/3 & -4/5/3 & 2/3 \\
\end{array}
\]
overlap: 0.963 0.832 0.869

\[
\begin{array}{c|c|c}
| pd^2 'P^4D \rangle & pd^2 'P^4D \rangle & d(sp)^3 'P^4D \rangle \\
\hline
\langle pd^2 'P^4D \rangle & 0.225480 & -0.002280 & 0.004111 \\
\hline
& -12/5 & 2/14/5 & -2/10/5 \\
\langle pd^2 'P^4D \rangle & -0.002280 & 0.227580 & 0.01027 \\
\hline
& 2/14/5 & 64/15 & -8/35/15 \\
\langle d(sp)^3 'P^4D \rangle & 0.004110 & 0.010270 & 0.197740 \\
\hline
& -2/10/5 & -8/35/15 & 2/3 \\
\end{array}
\]
overlap: 0.975 0.967 0.992

\[
\begin{array}{c|c|c|c}
| d^3 'G \rangle & d^2 'Gs^2 G \rangle & dp^2 'D^1 G \rangle \\
\hline
\langle d^3 'G \rangle & 0.248810 & -0.004920 & 0.009960 \\
\hline
& 1 & 0 & -15/3 \\
\langle d^2 'Gs^2 G \rangle & -0.004920 & 0.231530 & -0.01315 \\
\hline
& 0 & 4 & 4\sqrt{3}/3 \\
\langle dp^2 'D^1 G \rangle & 0.009960 & -0.013150 & 0.217330 \\
\hline
& -15/3 & 4\sqrt{3}/3 & 7 \\
\end{array}
\]
overlap: 0.971 0.999 0.971
### Table 1

| $| d^3 F \rangle$ | $| d^{3/2} F \rangle$ | $| d^3 P^2 F \rangle$ | $| d^2 P^3 D F \rangle$ |
|-----------------|-----------------|-----------------|-----------------|
| $\langle d^2 F |$ | $-0.00660$ | $0.01169$ | $-0.00772$ |
| $-3$ | $0$ | $\sqrt{6}$ | $1$ |
| $\langle d^{3/2} F |$ | $0.22885$ | $0.00000$ | $0.02278$ |
| $0$ | $0$ | $0$ | $-4$ |
| $\langle d^3 P^2 F |$ | $0.01169$ | $0.22418$ | $-0.01530$ |
| $-\sqrt{6}$ | $0$ | $0$ | $\sqrt{6}$ |
| $\langle d^3 D^2 F |$ | $0.007720$ | $0.02278$ | $-0.01530$ |
| $1$ | $-4$ | $\sqrt{6}$ | $1$ |

Overlap: $0.958$ $0.965$ $0.959$ $0.977$

### Table 2

| $| d^3 P \rangle$ | $| d^{3/2} P^4 \rangle$ | $| d^3 P^4 P \rangle$ | $| p^3 P^4 P \rangle$ |
|-----------------|-----------------|-----------------|-----------------|
| $\langle d^4 P |$ | $0$ | $0.013500$ | $0$ |
| $-8$ | $0$ | $-\sqrt{8}$ | $0$ |
| $\langle d^{3/2} P^4 |$ | $0.224040$ | $0$ | $-0.010675$ |
| $0$ | $-5$ | $0$ | $\sqrt{5}$ |
| $\langle d^3 P^4 P |$ | $0.013500$ | $0.214230$ | $-0.009705$ |
| $-\sqrt{8}$ | $0$ | $-16/3$ | $4\sqrt{3}/3$ |
| $\langle p^{1/2} P^4 |$ | $-0.010675$ | $-0.009705$ | $-1740.4$ |
| $0$ | $\sqrt{5}$ | $4\sqrt{5}/3$ | $13/3$ |

Overlap: $0.957$ $0.945$ $0.998$ $0.972$
<table>
<thead>
<tr>
<th></th>
<th>$\langle d_{j}^{32}p \rangle$</th>
<th>$\langle d_{j}^{2}s_{j}^{2}p \rangle$</th>
<th>$\langle dp_{j}^{3}s_{j}^{2}p \rangle$</th>
<th>$\langle dp_{j}^{2}D_{j}^{2}p \rangle$</th>
<th>$\langle p_{j}^{2}s_{j}^{2}p \rangle$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\langle d_{j}^{32}p \rangle$</td>
<td>.25177</td>
<td>.01235</td>
<td>.00893</td>
<td>.01444</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>-8</td>
<td>0</td>
<td>$-\sqrt{14}/2$</td>
<td>$-\sqrt{14}/2$</td>
<td>0</td>
</tr>
<tr>
<td>$\langle d_{j}^{2}s_{j}^{2}p \rangle$</td>
<td>.01235</td>
<td>.237712</td>
<td>0</td>
<td>.02278</td>
<td>.010675</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>-5</td>
<td>0</td>
<td>-4</td>
<td>$\sqrt{5}$</td>
</tr>
<tr>
<td>$\langle dp_{j}^{3}s_{j}^{2}p \rangle$</td>
<td>.00893</td>
<td>0</td>
<td>.20984</td>
<td>.00992</td>
<td>-.01577</td>
</tr>
<tr>
<td></td>
<td>$-\sqrt{14}/2$</td>
<td>0</td>
<td>$-10/3$</td>
<td>-1</td>
<td>$2\sqrt{5}/3$</td>
</tr>
<tr>
<td>$\langle dp_{j}^{2}D_{j}^{2}p \rangle$</td>
<td>.01444</td>
<td>.02278</td>
<td>.00992</td>
<td>.22924</td>
<td>-.02527</td>
</tr>
<tr>
<td></td>
<td>$-\sqrt{14}/2$</td>
<td>-4</td>
<td>-1</td>
<td>-4</td>
<td>$2\sqrt{5}/3$</td>
</tr>
<tr>
<td>$\langle p_{j}^{2}s_{j}^{2}p \rangle$</td>
<td>0</td>
<td>-.010675</td>
<td>-.01577</td>
<td>-.02547</td>
<td>.21636</td>
</tr>
<tr>
<td></td>
<td>0</td>
<td>$\sqrt{5}$</td>
<td>$2\sqrt{5}/3$</td>
<td>$\sqrt{5}$</td>
<td>$-11/3$</td>
</tr>
</tbody>
</table>

Overlap: .978 .915 .832 .859 .759
\[
\begin{array}{|c|c|c|c|c|}
\hline
\text{\textit{pd}}^{21}G;2F & \text{\textit{pd}}^{21}D;2F & \text{\textit{pd}}^{23}F;2F & \text{d(sp)}^{3}p;2F & \text{d(sp)}^{1}p;2F \\
\hline
<\text{pd}^{21}G;2F> & \begin{array}{c}
.24608 \\
-13/4 \\
2\sqrt{3}/7 \\
-3\sqrt{7}/14 \\
-6\sqrt{14}/7 \\
-\sqrt{42}/3 \\
\end{array} & \begin{array}{c}
.00231 \\
.23021 \\
2/21 \\
10/21/21 \\
-2\sqrt{42}/21 \\
-2\sqrt{14}/21 \\
\end{array} & \begin{array}{c}
.00688 \\
-.01298 \\
.23228 \\
-7/6 \\
2\sqrt{2}/3 \\
-2\sqrt{6}/3 \\
\end{array} & \begin{array}{c}
.01043 \\
-.00512 \\
-.00306 \\
.21607 \\
11/3 \\
\sqrt{3} \\
\end{array} & \begin{array}{c}
.01506 \\
.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
\end{array} \\
\hline
<\text{pd}^{21}D;2F> & \begin{array}{c}
.00231 \\
2\sqrt{3}/7 \\
2/21 \\
10/21/21 \\
-2\sqrt{42}/21 \\
-2\sqrt{14}/21 \\
\end{array} & \begin{array}{c}
.01298 \\
-.01298 \\
10\sqrt{21}/21 \\
-7/6 \\
2\sqrt{2}/3 \\
-2\sqrt{6}/3 \\
\end{array} & \begin{array}{c}
.00688 \\
-.01298 \\
.23228 \\
-7/6 \\
2\sqrt{2}/3 \\
-2\sqrt{6}/3 \\
\end{array} & \begin{array}{c}
.01043 \\
-.00512 \\
-.00306 \\
.21607 \\
11/3 \\
\sqrt{3} \\
\end{array} & \begin{array}{c}
.01506 \\
.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
\end{array} \\
\hline
<\text{pd}^{23}F;2F> & \begin{array}{c}
.00688 \\
-3\sqrt{7}/14 \\
10\sqrt{21}/21 \\
-7/6 \\
2\sqrt{2}/3 \\
-2\sqrt{6}/3 \\
\end{array} & \begin{array}{c}
-.01298 \\
.23228 \\
-.00306 \\
.21607 \\
11/3 \\
\sqrt{3} \\
\end{array} & \begin{array}{c}
.01043 \\
-.00512 \\
-.00306 \\
.21607 \\
11/3 \\
\sqrt{3} \\
\end{array} & \begin{array}{c}
.01506 \\
.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
\end{array} & \begin{array}{c}
.01506 \\
.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
\end{array} \\
\hline
<d(sp)^3p;2F> & \begin{array}{c}
.01043 \\
-6\sqrt{14}/7 \\
-2\sqrt{42}/21 \\
2\sqrt{2}/3 \\
11/3 \\
\sqrt{3} \\
\end{array} & \begin{array}{c}
-.00512 \\
2\sqrt{14}/21 \\
2\sqrt{6}/3 \\
\sqrt{3} \\
1/3 \\
\end{array} & \begin{array}{c}
-.00306 \\
11/3 \\
\sqrt{3} \\
1/3 \\
\end{array} & \begin{array}{c}
.01506 \\
.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
\end{array} & \begin{array}{c}
.01506 \\
.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
\end{array} \\
\hline
<d(sp)^1p;2F> & \begin{array}{c}
.01506 \\
-\sqrt{42}/3 \\
-2\sqrt{14}/21 \\
-2\sqrt{6}/3 \\
\sqrt{3} \\
1/3 \\
\end{array} & \begin{array}{c}
.00702 \\
-2\sqrt{14}/21 \\
-2\sqrt{6}/3 \\
\sqrt{3} \\
1/3 \\
\end{array} & \begin{array}{c}
.01328 \\
1/3 \\
\sqrt{3} \\
1/3 \\
\end{array} & \begin{array}{c}
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.22576 \\
\end{array} & \begin{array}{c}
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.00702 \\
.01328 \\
-.01604 \\
.22576 \\
1/3 \\
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\]

\text{overlap:} \ 0.980 \ 0.942 \ 0.882 \ 0.753 \ 0.648
| $|pd^{23}p;^2D>$ | $|pd^{23}p;^2D>$ | $|pd^{21}D;^2D>$ | $|d(sp)^3p;^2D>$ | $|d(sp)^1p;^2D>$ | $|p^3;^2D>$ |
|---|---|---|---|---|---|
| $<pd^{23}p;^2D>$ | .24622 | .01505 | -.01129 | -.00206 | .00891 | .01300 |
| $<pd^{23}F;^2D>$ | .01505 | .23804 | .00605 | -.00514 | .02224 | 0 |
| $<pd^{21}D;^2D>$ | -.01129 | .00605 | .23528 | .01416 | .00603 | -.01444 |
| $<d(sp)^3p;^2D>$ | .00206 | -.00514 | .01416 | .19742 | .00019 | -.01973 |
| $<d(sp)^1p;^2D>$ | .00891 | .02224 | .00603 | -.00019 | .22584 | .01139 |
| $<p^3;^2D>$ | .01307 | 0 | -.01444 | -.01973 | .01139 | .20696 |

Overlap: .958 .928 .998 .748 .767 .954
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Overlap: .979 .975 .762 .721 .737 .657 .843
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Overlap: .91 .976 .802 .878 .768 .718 .819 .907
II. Comparison of \( \sum_{i<j} (L_i \cdot L_j - A_i \cdot A_j) \) and \( \sum_{i<j} \frac{1}{r_{ij}} \) configuration mixing.

We input the matrix elements of \( \sum_{i<j} (L_i \cdot L_j - A_i \cdot A_j) \) and the matrix elements of \( \sum_{i<j} \frac{1}{r_{ij}} \) (in Table 6 (I)) into the computer. We obtained the configuration mixings as well as the overlaps for each case.

For the following sections, part (1) indicates the \( \sum_{i<j} (L_i \cdot L_j - A_i \cdot A_j) \) configuration mixing and part (2) indicates the \( \sum_{i<j} \frac{1}{r_{ij}} \) configuration mixing.

1. \( \begin{pmatrix} 3 \end{pmatrix} P > \) (\( N = 2 \))

(1) \( \lambda_1 = -6 \)  \( \phi_1 = .928 |d^{23}P> + .373 |p^{23}P> \)

(2) \( \omega_1 = 0.091 \)  \( \phi_1 = .745 |d^{13}P> + .666 |p^{13}P> \)

overlap: .999 (\( \psi_1, \phi_1 \))

2. \( \begin{pmatrix} 1 \end{pmatrix} P > \) (\( N = 2 \))

(1) \( \lambda_1 = -6 \)  \( \phi_1 = .745 |d^{13}P> + .666 |p^{13}P> \)

(2) \( \omega_1 = .112 \)  \( \phi_1 = .773 |d^{13}P> + .634 |p^{13}P> \)

overlap: .999 (\( \psi_1, \phi_1 \))
3. $|3^3p\rangle \ (N = 2)$

(1) \[ \lambda_1 = -4 \quad \psi_1 = -0.913 |d_p^3p\rangle + 0.408 |p_s^3p\rangle \]
\[ \lambda_2 = 4 \quad \psi_2 = -0.408 |d_p^3p\rangle - 0.913 |p_s^3p\rangle \]

(2) \[ \omega_1 = 0.079 \quad \phi_1 = 0.931 |d_p^3p\rangle - 0.364 |p_s^3p\rangle \]
\[ \omega_2 = 0.051 \quad \phi_2 = 0.364 |d_p^3p\rangle + 0.931 |p_s^3p\rangle \]

overlap: 0.996 ($\psi_1 \phi_1$, $\psi_2 \phi_2$)

4. $|3^1d\rangle \ (N = 2)$

(1) \[ \lambda_1 = -4 \quad \psi_1 = -0.764 |d_{1s}^2d\rangle + 0.408 |d_{1s}^1d\rangle + 0.500 |p_{2s}^1d\rangle \]
\[ \lambda_2 = -2 \quad \psi_2 = -0.624 |d_{1s}^2d\rangle - 0.667 |d_{1s}^1d\rangle - 0.408 |p_{2s}^1d\rangle \]
\[ \lambda_3 = 4 \quad \psi_3 = -0.167 |d_{1s}^2d\rangle + 0.624 |d_{1s}^1d\rangle - 0.764 |p_{2s}^1d\rangle \]

(2) \[ \omega_1 = 0.105 \quad \phi_1 = 0.597 |d_{1s}^2d\rangle - 0.571 |d_{1s}^1d\rangle - 0.563 |p_{2s}^1d\rangle \]
\[ \omega_2 = 0.076 \quad \phi_2 = -0.790 |d_{1s}^2d\rangle - 0.539 |d_{1s}^1d\rangle - 0.292 |p_{2s}^1d\rangle \]
\[ \omega_3 = 0.056 \quad \phi_3 = 0.136 |d_{1s}^2d\rangle - 0.620 |d_{1s}^1d\rangle + 0.773 |p_{2s}^1d\rangle \]

overlap: 0.971 ($\psi_1 \phi_1$) overlap: 0.971 ($\psi_2 \phi_2$) overlap: 0.999 ($\psi_3 \phi_3$)

5. $|3^1s\rangle \ (N = 2)$

(1) \[ \lambda_1 = -8 \quad \psi_1 = -0.745 |d_{1s}^2s\rangle + 0.577 |p_{2s}^1s\rangle - 0.333 |s_{2s}^1s\rangle \]
\[ \lambda_2 = -4 \quad \psi_2 = 0.646 |d_{1s}^2s\rangle + 0.500 |p_{2s}^1s\rangle - 0.577 |s_{2s}^1s\rangle \]
\[ \lambda_3 = 4 \quad \psi_3 = 0.166 |d_{1s}^2s\rangle + 0.646 |p_{2s}^1s\rangle + 0.745 |s_{2s}^1s\rangle \]

(2) \[ \omega_1 = 0.132 \quad \phi_1 = -0.739 |d_{1s}^2s\rangle + 0.586 |p_{2s}^1s\rangle - 0.331 |s_{2s}^1s\rangle \]
\[ \omega_2 = 0.079 \quad \phi_2 = 0.661 |d_{1s}^2s\rangle + 0.536 |p_{2s}^1s\rangle - 0.524 |s_{2s}^1s\rangle \]
\[ \omega_3 = 0.049 \quad \phi_3 = 0.130 |d_{1s}^2s\rangle + 0.607 |p_{2s}^1s\rangle + 0.784 |s_{2s}^1s\rangle \]

overlap: 0.999 ($\psi_1 \phi_1$) overlap: 0.998 ($\psi_2 \phi_2$) overlap: 0.998 ($\psi_3 \phi_3$)
6. \( |{3^4S}\rangle \ (N = 3) \)

(1) \( \lambda_1 = -1.09 \) \( \psi_1 = -0.898|d^2p^4S\rangle + 0.440|p^3^4S\rangle \)
(2) \( \omega_1 = 0.243 \) \( \phi_1 = 0.933|d^2p^4S\rangle - 0.360|p^3^4S\rangle \)

overlap: 0.996 \( (\psi_1, \psi_2) \)

7. \( |{3^4P}\rangle \ (N = 3) \)

(1) \( \lambda_1 = 0.231 \) \( \psi_1 = 0.961|d^2^3F^4P\rangle - 0.278|d(sp)^3^4F\rangle \)
(2) \( \omega_1 = -5.464 \) \( \phi_1 = -0.888|d^2^3P^4P\rangle + 0.460|d(sp)^4^4P\rangle \)

overlap: 0.983 \( (\psi_1, \psi_2) \)

8. \( |{3^4F}\rangle \ (N = 3) \)

(1) \( \lambda_1 = -1.123 \) \( \psi_1 = -0.972|d^2p^4F\rangle + 0.235|d(sp)^4^4F\rangle \)
(2) \( \omega_1 = 0.223 \) \( \phi_1 = 0.985|d^2p^4F\rangle - 0.175|d(sp)^4^4F\rangle \)

overlap: 0.998 \( (\psi_1, \psi_2) \)
9. \( \left| 3^2G \right> \ (N = 3) \)

(1) \( \lambda = 0 \)
\[ \psi_1 = -0.791 \left| \text{pd}^2 \text{F}; 2G \right> + 0.612 \left| \text{pd}^2 \text{G}; 2G \right> \]
\[ \psi_2 = -0.612 \left| \text{pd}^2 \text{F}; 2G \right> - 0.791 \left| \text{pd}^2 \text{G}; 2G \right> \]

(2) \( \omega = 0.252 \)
\[ \phi_1 = 0.829 \left| \text{pd}^2 \text{F}; 2G \right> - 0.559 \left| \text{pd}^2 \text{G}; 2G \right> \]
\[ \phi_2 = 0.559 \left| \text{pd}^2 \text{F}; 2G \right> + 0.829 \left| \text{pd}^2 \text{G}; 2G \right> \]

Overlap: \( 0.998 \ (\psi \phi) \)

10. \( \left| 3^4F \right> \ (N = 3) \)

(1) \( \lambda = -3.464 \)
\[ \psi_1 = -0.966 \left| \text{d}^4 \text{F} \right> + 0 \left| \text{d}^2 \text{s}^4 \text{F} \right> - 0.259 \left| \text{dp}^2 \text{F} \right> \]
\[ \psi_2 = 0.259 \left| \text{d}^4 \text{F} \right> + 0 \left| \text{d}^2 \text{s}^4 \text{F} \right> - 0.966 \left| \text{dp}^2 \text{F} \right> \]
\[ \psi_3 = 0 \left| \text{d}^4 \text{F} \right> + \left| \text{d}^2 \text{s}^4 \text{F} \right> + 0 \left| \text{dp}^2 \text{F} \right> \]

(2) \( \omega = 0.241 \)
\[ \phi_1 = 0.981 \left| \text{d}^4 \text{F} \right> + 0 \left| \text{d}^2 \text{s}^4 \text{F} \right> + 0.196 \left| \text{dp}^2 \text{F} \right> \]
\[ \phi_2 = -0.196 \left| \text{d}^4 \text{F} \right> + 0 \left| \text{d}^2 \text{s}^4 \text{F} \right> + 0.901 \left| \text{dp}^2 \text{F} \right> \]
\[ \phi_3 = 0 \left| \text{d}^4 \text{F} \right> + \left| \text{d}^2 \text{s}^4 \text{F} \right> + 0 \left| \text{dp}^2 \text{F} \right> \]

Overlap: \( 0.998 \ (\psi \phi) \)

11. \( \left| 3^2S \right> \ (N = 3) \)

(1) \( \lambda = -9.252 \)
\[ \psi_1 = -0.714 \left| \text{d}^2 \text{s}^2 \text{s} \right> + 0.597 \left| \text{dp}^2 \text{S} \right> + 0.365 \left| \text{p}^2 \text{s}^2 \text{s} \right> \]
\[ \psi_2 = -3.030 \left| \text{d}^2 \text{s}^2 \text{s} \right> + 0.672 \left| \text{dp}^2 \text{S} \right> + 0.731 \left| \text{p}^2 \text{s}^2 \text{s} \right> \]
\[ \psi_3 = 2.283 \left| \text{d}^2 \text{s}^2 \text{s} \right> - 0.332 \left| \text{dp}^2 \text{S} \right> + 0.923 \left| \text{p}^2 \text{s}^2 \text{s} \right> \]

(2) \( \omega = 0.267 \)
\[ \phi_1 = 0.845 \left| \text{d}^2 \text{s}^2 \text{s} \right> - 0.359 \left| \text{dp}^2 \text{S} \right> - 0.395 \left| \text{p}^2 \text{s}^2 \text{s} \right> \]
\[ \phi_2 = 0.197 \left| \text{d}^2 \text{s}^2 \text{s} \right> + 0.458 \left| \text{dp}^2 \text{S} \right> + 0.107 \left| \text{p}^2 \text{s}^2 \text{s} \right> \]
\[ \phi_3 = 0.229 \left| \text{d}^2 \text{s}^2 \text{s} \right> + 0.927 \left| \text{dp}^2 \text{S} \right> - 0.255 \left| \text{p}^2 \text{s}^2 \text{s} \right> \]

Overlap: \( 0.963 \ (\psi \phi) \)

Overlap: \( 0.963 \ (\psi \phi) \)

Overlap: \( 0.963 \ (\psi \phi) \)
### 12. $|3^4D\rangle$ \hspace{1cm} (N = 3)

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### 13. $|3^2G\rangle$ \hspace{1cm} (N = 3)

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### Overlaps

- $\text{overlap: } \langle \psi | \phi \rangle_{11} = 0.975$
- $\text{overlap: } \langle \psi | \phi \rangle_{22} = 0.971$
- $\text{overlap: } \langle \psi | \phi \rangle_{33} = 0.992$
14. \(|^32F> (N = 3)\)

(1) \(\lambda_1 = -5.631\) 
\(\psi_1 = -0.639|^3d^2F> + 0.344|^2s^2F> - 0.489|^2p^2F> + 0.484|^2F>\)
\(\lambda_2 = 1.180\) 
\(\psi_2 = 0.487|^3d^2F> - 0.365|^2s^2F> - 0.786|^2p^2F> + 0.108|^2F>\)
\(\lambda_3 = -2.767\) 
\(\psi_3 = -0.596|^3d^2F> - 0.652|^2s^2F> - 0.128|^2p^2F> - 0.451|^2F>\)
\(\lambda_4 = 5.219\) 
\(\psi_4 = 0.016|^3d^2F> + 0.569|^2s^2F> - 0.356|^2p^2F> - 0.742|^2F>\)

(2) \(\omega_1 = 0.271\) 
\(\phi_1 = 0.824|^3d^2F> - 0.316|^2s^2F> + 0.319|^2p^2F> - 0.345|^2F>\)
\(\omega_2 = 0.242\) 
\(\phi_2 = -0.519|^3d^2F> - 0.663|^2s^2F> + 0.114|^2p^2F> - 0.527|^2F>\)
\(\omega_3 = 0.224\) 
\(\phi_3 = 0.224|^3d^2F> - 0.449|^2s^2F> - 0.850|^2p^2F> + 0.161|^2F>\)
\(\omega_4 = 0.194\) 
\(\phi_4 = -0.033|^3d^2F> - 0.509|^2s^2F> + 0.403|^2p^2F> + 0.760|^2F>\)

overlap: \(0.958 (\psi_1 \phi_1)\) overlap: \(0.959 (\psi_2 \phi_2)\) overlap: \(0.965 (\psi_3 \phi_2)\) overlap: \(0.997 (\psi_4 \phi_4)\)
15. $|3^4P> \quad (N = 3)$

(1) \[ \begin{align*}
\lambda &= -1 \quad \psi_1 = 0.808 |d^34P> + 0.057 |d^2s^4P> + 0.572 |dp^24P> - 0.128 |p^2s^4P> \\
\lambda &= -4 \quad \psi_2 = -0.527 |d^34P> - 0.373 |d^2s^4P> + 0.745 |dp^24P> - 0.167 |p^2s^4P> \\
\lambda &= 5.657 \quad \psi_3 = 0.056 |d^34P> - 0.197 |d^2s^4P> - 0.270 |dp^24P> - 0.941 |p^2s^4P> \\
\lambda &= -5.657 \quad \psi_4 = 0.256 |d^34P> - 0.905 |d^2s^4P> - 0.212 |dp^24P> + 0.266 |p^2s^4P>
\end{align*} \]

(2) \[ \begin{align*}
\omega &= 0.253 \quad \phi_1 = 0.940 |d^34P> + 0.016 |d^2s^4P> + 0.337 |dp^24P> - 0.044 |p^2s^4P> \\
\omega &= 0.211 \quad \phi_2 = 0.333 |d^34P> + 0.160 |d^2s^4P> - 0.910 |dp^24P> + 0.191 |p^2s^4P> \\
\omega &= 0.169 \quad \phi_3 = -0.378 |d^34P> + 0.188 |d^2s^4P> + 0.220 |dp^24P> + 0.956 |p^2s^4P> \\
\omega &= 0.226 \quad \phi_4 = 0.0633 |d^34P> - 0.969 |d^2s^4P> - 0.102 |dp^24P> + 0.216 |p^2s^4P>
\end{align*} \]

overlap: \(0.957 (\psi_1 \phi_1)\) overlap: \(0.945 (\psi_2 \phi_2)\) overlap: \(0.998 (\psi_3 \phi_3)\) overlap: \(0.972 (\psi_4 \phi_4)\)
16. $|3^2p\rangle \quad (N = 3)$

(1) $\lambda_1 = -1.22 \quad \psi_1 = .363|d^3s^2p\rangle + .479|d^2s^2p\rangle + .224|dp^{22}p\rangle + .600|dp^{22}p\rangle - .477|p^2s^2p\rangle$

$\lambda_2 = -8.19 \quad \psi_2 = -.865|d^3s^2p\rangle + .347|d^2s^2p\rangle - .231|dp^{22}p\rangle + .144|dp^{22}p\rangle - .238|p^2s^2p\rangle$

$\lambda_3 = 1.25 \quad \psi_3 = -.170|d^3s^2p\rangle - .266|d^2s^2p\rangle + .097|dp^{22}p\rangle + .742|dp^{22}p\rangle + .583|p^2s^2p\rangle$

$\lambda_4 = -3.38 \quad \psi_4 = -.284|d^3s^2p\rangle - .487|d^2s^2p\rangle + .725|dp^{22}p\rangle - .024|dp^{22}p\rangle - .395|p^2s^2p\rangle$

$\lambda_5 = -1.44 \quad \psi_5 = .097|d^3s^2p\rangle - .585|d^2s^2p\rangle - .601|dp^{22}p\rangle + .259|dp^{22}p\rangle - .468|p^2s^2p\rangle$

(2) $\omega_1 = .283 \quad \phi_1 = -.520|d^3s^2p\rangle - .507|d^2s^2p\rangle - .215|dp^{22}p\rangle - .557|dp^{22}p\rangle + .347|p^2s^2p\rangle$

$\omega_2 = .243 \quad \phi_2 = -.830|d^3s^2p\rangle + .203|d^2s^2p\rangle + .063|dp^{22}p\rangle + .306|dp^{22}p\rangle - .411|p^2s^2p\rangle$

$\omega_3 = .191 \quad \phi_3 = -.175|d^3s^2p\rangle + .005|d^2s^2p\rangle + .482|dp^{22}p\rangle + .432|dp^{22}p\rangle + .743|p^2s^2p\rangle$

$\omega_4 = .226 \quad \phi_4 = -.043|d^3s^2p\rangle + .389|d^2s^2p\rangle + .670|dp^{22}p\rangle - .625|dp^{22}p\rangle - .0841|p^2s^2p\rangle$

$\omega_5 = .202 \quad \phi_5 = .102|d^3s^2p\rangle - .742|d^2s^2p\rangle + .518|dp^{22}p\rangle + .140|dp^{22}p\rangle - .389|p^2s^2p\rangle$

overlap: $0.978 (\psi_1 \phi_1); 0.915 (\psi_2 \phi_2); 0.832 (\psi_3 \phi_3); 0.759 (\psi_4 \phi_5); 0.859 (\psi_5 \phi_4)$
17. $|3^2 F> (N = 3)$

(1) $\lambda_1 = 6.51$  
$\psi_1 = -0.461|pd^{21}G;^2 F> - 0.129|pd^{21}D;^2 F> + 0.012|pd^{23}F;^2 F> + 0.788|d(sp)^3 P;^2 F> + 0.387|d(sp)^1 P;^2 F> 

$\lambda_2 = -4.01$  
$\psi_2 = 0.493|pd^{21}G;^2 F> - 0.362|pd^{21}D;^2 F> + 0.643|pd^{23}F;^2 F> + 0.006|d(sp)^3 P;^2 F> + 0.460|d(sp)^1 P;^2 F> 

$\lambda_3 = -2.58$  
$\psi_3 = -0.720|pd^{21}G;^2 F> - 0.322|pd^{21}D;^2 F> + 0.419|pd^{23}F;^2 F> - 0.442|d(sp)^3 P;^2 F> - 0.074|d(sp)^1 P;^2 F> 

$\lambda_4 = -0.233$  
$\psi_4 = -0.159|pd^{21}G;^2 F> + 0.611|pd^{21}D;^2 F> - 0.037|pd^{23}F;^2 F> - 0.335|d(sp)^3 P;^2 F> + 0.699|d(sp)^1 P;^2 F> 

$\lambda_5 = 2.31$  
$\psi_5 = -0.025|pd^{21}G;^2 F> + 0.613|pd^{21}D;^2 F> + 0.639|pd^{23}F;^2 F> + 0.263|d(sp)^3 P;^2 F> - 0.381|d(sp)^1 P;^2 F> 

(2) $\omega = 0.260$  
$\phi_1 = 0.739|pd^{21}G;^2 F> - 0.005|pd^{21}D;^2 F> + 0.436|pd^{23}F;^2 F> - 0.042|d(sp)^3 P;^2 F> + 0.513|d(sp)^1 P;^2 F> 

$\omega = 0.197$  
$\phi_2 = 0.320|pd^{21}G;^2 F> + 0.064|pd^{21}D;^2 F> + 0.143|pd^{23}F;^2 F> - 0.683|d(sp)^3 P;^2 F> - 0.638|d(sp)^1 P;^2 F> 

$\omega = 0.240$  
$\phi_3 = 0.517|pd^{21}G;^2 F> - 0.217|pd^{21}D;^2 F> - 0.249|pd^{23}F;^2 F> + 0.623|d(sp)^3 P;^2 F> - 0.485|d(sp)^1 P;^2 F> 

$\omega = 0.210$  
$\phi_4 = 0.152|pd^{21}G;^2 F> - 0.612|pd^{21}D;^2 F> - 0.623|pd^{23}F;^2 F> - 0.373|d(sp)^3 P;^2 F> + 0.275|d(sp)^1 P;^2 F> 

$\omega = 0.243$  
$\phi_5 = -0.248|pd^{21}G;^2 F> - 0.758|pd^{21}D;^2 F> + 0.583|pd^{23}F;^2 F> + 0.066|d(sp)^3 P;^2 F> - 0.140|d(sp)^1 P;^2 F> 

overlap: 0.882 ($\psi_1 \phi_2$); 0.942 ($\psi_2 \phi_1$); 0.648 ($\psi_3 \phi_2$); 0.753 ($\psi_4 \phi_3$); 0.980 ($\psi_5 \phi_4$)
18. $|3^2D\rangle$ (N = 3)

(1)

\[
\begin{align*}
\lambda_1 &= -9.146 & \psi_1 &= -0.624 |pd^{23}p_{2D}\rangle - 0.323 |pd^{23}p_{1D}\rangle + 0.357 |pd^{21}d_{2D}\rangle + 0.235 |d(sp)^3p_{2D}\rangle - 0.355 |d(sp)^1p_{1D}\rangle - 0.434 |p^3_{2D}\rangle \\
\lambda_2 &= 5.591 & \psi_2 &= -0.110 |pd^{23}p_{2D}\rangle + 0.199 |pd^{23}p_{1D}\rangle - 0.063 |pd^{21}d_{2D}\rangle + 0.750 |d(sp)^3p_{2D}\rangle - 0.220 |d(sp)^1p_{1D}\rangle + 0.576 |p^3_{2D}\rangle \\
\lambda_3 &= -6.924 & \psi_3 &= -0.186 |pd^{23}p_{2D}\rangle + 0.505 |pd^{23}p_{1D}\rangle + 0.524 |pd^{21}d_{2D}\rangle + 0.151 |d(sp)^3p_{2D}\rangle + 0.633 |d(sp)^1p_{1D}\rangle - 0.108 |p^3_{2D}\rangle \\
\lambda_4 &= -1.128 & \psi_4 &= -0.562 |pd^{23}p_{2D}\rangle + 0.420 |pd^{23}p_{1D}\rangle + 0.279 |pd^{21}d_{2D}\rangle + 0.148 |d(sp)^3p_{2D}\rangle - 0.504 |d(sp)^1p_{1D}\rangle - 0.393 |p^3_{2D}\rangle \\
\lambda_5 &= -2.699 & \psi_5 &= -0.497 |pd^{23}p_{2D}\rangle - 0.650 |pd^{23}p_{1D}\rangle + 0.365 |pd^{21}d_{2D}\rangle + 0.336 |d(sp)^3p_{2D}\rangle + 0.287 |d(sp)^1p_{1D}\rangle + 0.032 |p^3_{2D}\rangle \\
\lambda_6 &= -0.458 & \psi_6 &= -0.041 |pd^{23}p_{2D}\rangle - 0.027 |pd^{23}p_{1D}\rangle + 0.618 |pd^{21}d_{2D}\rangle - 0.463 |d(sp)^3p_{2D}\rangle - 0.297 |d(sp)^1p_{1D}\rangle + 0.559 |p^3_{2D}\rangle
\end{align*}
\]

(2)

\[
\begin{align*}
\omega_1 &= 0.274 & \phi_1 &= -0.649 |pd^{23}p_{2D}\rangle - 0.509 |pd^{23}p_{1D}\rangle + 0.219 |pd^{21}d_{2D}\rangle + 0.166 |d(sp)^3p_{2D}\rangle - 0.398 |d(sp)^1p_{1D}\rangle - 0.292 |p^3_{2D}\rangle \\
\omega_2 &= 0.255 & \phi_2 &= -0.174 |pd^{23}p_{2D}\rangle + 0.478 |pd^{23}p_{1D}\rangle + 0.703 |pd^{21}d_{2D}\rangle + 0.228 |d(sp)^3p_{2D}\rangle + 0.351 |d(sp)^1p_{1D}\rangle - 0.268 |p^3_{2D}\rangle \\
\omega_3 &= 0.179 & \phi_3 &= -0.177 |pd^{23}p_{2D}\rangle + 0.175 |pd^{23}p_{1D}\rangle - 0.042 |pd^{21}d_{2D}\rangle + 0.724 |d(sp)^3p_{2D}\rangle - 0.208 |d(sp)^1p_{1D}\rangle + 0.622 |p^3_{2D}\rangle \\
\omega_4 &= 0.226 & \phi_4 &= -0.724 |pd^{23}p_{2D}\rangle + 0.224 |pd^{23}p_{1D}\rangle - 0.295 |pd^{21}d_{2D}\rangle - 0.336 |d(sp)^3p_{2D}\rangle + 0.371 |d(sp)^1p_{1D}\rangle + 0.297 |p^3_{2D}\rangle \\
\omega_5 &= 0.213 & \phi_5 &= -0.104 |pd^{23}p_{2D}\rangle + 0.643 |pd^{23}p_{1D}\rangle + 0.338 |pd^{21}d_{2D}\rangle - 0.008 |d(sp)^3p_{2D}\rangle - 0.550 |d(sp)^1p_{1D}\rangle - 0.398 |p^3_{2D}\rangle \\
\omega_6 &= 0.103 & \phi_6 &= -0.022 |pd^{23}p_{2D}\rangle + 0.131 |pd^{23}p_{1D}\rangle + 0.505 |pd^{21}d_{2D}\rangle - 0.532 |d(sp)^3p_{2D}\rangle - 0.484 |d(sp)^1p_{1D}\rangle + 0.459 |p^3_{2D}\rangle
\end{align*}
\]

Overlap: 0.958 ($\psi \phi$); 0.928 ($\psi \phi$); 0.998 ($\psi \phi$); 0.748 ($\psi \phi$); 0.767 ($\psi \phi$); 0.954 ($\psi \phi$)
19. $|3^2p\rangle$ (N = 3)

(1)

\[
\begin{align*}
\lambda_1 &= .121 \\
\lambda_2 &= 6.19 \\
\lambda_3 &= -8.76 \\
\lambda_4 &= -1.22 \\
\lambda_5 &= -5.48 \\
\lambda_6 &= -3.93 \\
\lambda_7 &= 1.65 \\
\end{align*}
\]

\[
\begin{align*}
\gamma_1 &= .267|p^2d^2s^2p\rangle - .617|p^2d^2p^2p\rangle - .096|d(s)p^1p\rangle - .479|d(s)p^1p^2p\rangle - .452|p^3^2p\rangle + .252|p^3^2s^2p\rangle \\
\gamma_2 &= .022|p^2d^2s^2p\rangle - .120|p^2d^2p^2p\rangle - .114|d(s)p^1p\rangle + .201|d(s)p^1p^2p\rangle + .274|d(s)p^1p^2p\rangle + .450|p^3^2p\rangle + .808|p^3^2s^2p\rangle \\
\gamma_3 &= -.516|p^2d^2s^2p\rangle - .167|p^2d^2p^2p\rangle - .646|p^2d^2p^2p\rangle - .280|d(s)p^1p\rangle - .432|d(s)p^1p^2p\rangle + .023|p^3^2p\rangle + .152|p^3^2s^2p\rangle \\
\gamma_4 &= .544|p^2d^2s^2p\rangle -.0277|p^2d^2p^2p\rangle - .397|d(s)p^1p\rangle - .437|d(s)p^1p^2p\rangle + .568|p^3^2p\rangle - .096|p^3^2s^2p\rangle \\
\gamma_5 &= -.464|p^2d^2s^2p\rangle + .0479|p^2d^2p^2p\rangle + .707|p^2d^2p^2p\rangle + .087|d(s)p^1p\rangle - .471|d(s)p^1p^2p\rangle + .146|p^3^2p\rangle + .176|p^3^2s^2p\rangle \\
\gamma_6 &= -.387|p^2d^2s^2p\rangle - .752|p^2d^2p^2p\rangle - .029|p^2d^2p^2p\rangle - .146|d(s)p^1p\rangle + .214|d(s)p^1p^2p\rangle + .331|p^3^2p\rangle - .326|p^3^2s^2p\rangle \\
\gamma_7 &= .003|p^2d^2s^2p\rangle - .087|p^2d^2p^2p\rangle + .243|p^2d^2p^2p\rangle - .809|d(s)p^1p\rangle + .224|d(s)p^1p^2p\rangle - .341|p^3^2p\rangle + .337|p^3^2s^2p\rangle \\
\end{align*}
\]

(2)

\[
\begin{align*}
\omega_1 &= .286 \\
\omega_2 &= .166 \\
\omega_3 &= .263 \\
\omega_4 &= -.203 \\
\omega_5 &= .241 \\
\omega_6 &= .210 \\
\omega_7 &= .223 \\
\end{align*}
\]

\[
\begin{align*}
\phi_1 &= .395|p^2d^2s^2p\rangle - .636|p^2d^2p^2p\rangle - .209|p^2d^2p^2p\rangle + .172|d(s)p^1p\rangle - .408|d(s)p^1p^2p\rangle - .404|p^3^2p\rangle + .189|p^3^2s^2p\rangle \\
\phi_2 &= .043|p^2d^2s^2p\rangle + .100|p^2d^2p^2p\rangle + .115|p^2d^2p^2p\rangle - .402|d(s)p^1p\rangle + .286|d(s)p^1p^2p\rangle - .409|p^3^2p\rangle - .751|p^3^2s^2p\rangle \\
\phi_3 &= .796|p^2d^2s^2p\rangle + .224|p^2d^2p^2p\rangle + .311|p^2d^2p^2p\rangle + .003|d(s)p^1p\rangle - .439|d(s)p^1p^2p\rangle - .159|p^3^2p\rangle + .040|p^3^2s^2p\rangle \\
\phi_4 &= -.398|p^2d^2s^2p\rangle - .069|p^2d^2p^2p\rangle + .109|p^2d^2p^2p\rangle - .262|d(s)p^1p\rangle + .399|d(s)p^1p^2p\rangle - .689|p^3^2p\rangle + .349|p^3^2s^2p\rangle \\
\phi_5 &= -.109|p^2d^2s^2p\rangle - .664|p^2d^2p^2p\rangle + .615|p^2d^2p^2p\rangle - .067|d(s)p^1p\rangle + .219|d(s)p^1p^2p\rangle + .276|p^3^2p\rangle - .199|p^3^2s^2p\rangle \\
\phi_6 &= .179|p^2d^2s^2p\rangle - .036|p^2d^2p^2p\rangle - .028|p^2d^2p^2p\rangle - .837|d(s)p^1p\rangle - .212|d(s)p^1p^2p\rangle + .282|p^3^2p\rangle + .376|p^3^2s^2p\rangle \\
\phi_7 &= .081|p^2d^2s^2p\rangle - .297|p^2d^2p^2p\rangle - .675|p^2d^2p^2p\rangle - .189|d(s)p^1p\rangle + .553|d(s)p^1p^2p\rangle + .120|p^3^2p\rangle - .309|p^3^2s^2p\rangle \\
\end{align*}
\]

Overlap: 

\[
\begin{align*}
\text{overlap: .979 (} \psi_1 \phi_1 \text{); .975 (} \psi_2 \phi_2 \text{); .762 (} \psi_3 \phi_3 \text{); .721 (} \psi_4 \phi_4 \text{); .737 (} \psi_5 \phi_5 \text{); .657 (} \psi_6 \phi_6 \text{); .843 (} \psi_7 \phi_7 \text{)}
\end{align*}
\]
(1)

$$\lambda_1 = 6.495 \quad \psi_1 = 0.004 |d^{3}_{1/2} > + 0.079 |d^{3}_{j} > - 0.345 |p^{2}_{3/2} > - 0.159 |p^{2}_{j} > + 0.134 |s^{1}_{1/2} > - 0.098 |s^{1}_{j} > - 0.013 |s^{2}_{1/2} > - 0.402 |s^{2}_{j} >$$

$$\lambda_2 = -9.412 \quad \psi_2 = 0.515 |d^{3}_{1/2} > + 0.360 |d^{3}_{j} > + 0.503 |p^{2}_{3/2} > - 0.451 |p^{1}_{1/2} > - 0.051 |p^{1}_{j} > + 0.076 |s^{2}_{1/2} > - 0.245 |s^{2}_{j} > + 0.201 |s^{2}_{j} >$$

$$\lambda_3 = 3.949 \quad \psi_3 = 0.153 |d^{3}_{1/2} > + 0.045 |d^{3}_{j} > - 0.057 |p^{2}_{3/2} > + 0.682 |p^{1}_{1/2} > + 0.181 |p^{1}_{j} > - 0.019 |s^{2}_{1/2} > - 0.362 |s^{2}_{j} > + 0.506 |s^{2}_{j} >$$

$$\lambda_4 = -7.564 \quad \psi_4 = -0.443 |d^{3}_{1/2} > + 0.654 |d^{3}_{j} > + 0.158 |p^{2}_{3/2} > + 0.257 |p^{1}_{1/2} > - 0.441 |p^{1}_{j} > + 0.255 |s^{1}_{1/2} > - 0.096 |s^{2}_{1/2} > - 0.128 |s^{2}_{j} >$$

$$\lambda_5 = -0.179 \quad \psi_5 = 0.115 |d^{3}_{1/2} > + 0.103 |d^{3}_{j} > + 0.006 |p^{2}_{3/2} > - 0.049 |p^{1}_{1/2} > + 0.728 |p^{1}_{j} > + 0.637 |s^{2}_{1/2} > + 0.101 |s^{2}_{j} > - 0.067 |s^{2}_{j} >$$

$$\lambda_6 = -5.185 \quad \psi_6 = -0.243 |d^{3}_{1/2} > - 0.491 |d^{3}_{j} > - 0.060 |p^{2}_{3/2} > - 0.243 |p^{1}_{1/2} > - 0.358 |p^{1}_{j} > + 0.567 |s^{1}_{1/2} > - 0.270 |s^{2}_{1/2} > + 0.337 |s^{2}_{j} >$$

$$\lambda_7 = -1.962 \quad \psi_7 = -1.64 |d^{3}_{1/2} > - 0.307 |d^{3}_{j} > + 0.765 |p^{2}_{3/2} > + 0.251 |p^{1}_{1/2} > + 0.126 |p^{1}_{j} > - 0.050 |s^{2}_{1/2} > - 0.224 |s^{2}_{1/2} > - 0.327 |s^{2}_{j} >$$

$$\lambda_8 = -4.204 \quad \psi_8 = -0.644 |d^{3}_{1/2} > + 0.099 |d^{3}_{j} > + 0.105 |p^{2}_{3/2} > - 0.341 |p^{1}_{1/2} > + 0.279 |p^{1}_{j} > - 0.434 |s^{2}_{1/2} > - 0.079 |s^{2}_{1/2} > + 0.418 |s^{2}_{j} >$$

(2)

$$\omega_1 = 0.291 \quad \phi_1 = -0.772 |d^{3}_{1/2} > - 0.253 |d^{3}_{j} > - 0.257 |p^{2}_{3/2} > + 0.454 |p^{1}_{1/2} > - 0.059 |p^{1}_{j} > - 0.014 |s^{1}_{1/2} > + 0.093 |s^{2}_{1/2} > - 0.236 |s^{2}_{j} >$$

$$\omega_2 = 0.178 \quad \phi_2 = 0.002 |d^{3}_{1/2} > + 0.051 |d^{3}_{j} > - 0.303 |p^{2}_{3/2} > - 0.257 |p^{2}_{1/2} > - 0.0004 |p^{2}_{j} > - 0.124 |s^{1}_{1/2} > + 0.748 |s^{2}_{1/2} > - 0.514 |s^{2}_{j} >$$

$$\omega_3 = 0.265 \quad \phi_3 = 0.213 |d^{3}_{1/2} > - 0.080 |d^{3}_{j} > - 0.234 |p^{2}_{3/2} > - 0.176 |p^{1}_{1/2} > + 0.344 |p^{1}_{j} > - 0.285 |s^{2}_{1/2} > + 0.111 |s^{2}_{j} > + 0.056 |s^{2}_{j} >$$

$$\omega_4 = 0.198 \quad \phi_4 = 0.068 |d^{3}_{1/2} > + 0.045 |d^{3}_{j} > - 0.168 |p^{2}_{3/2} > + 0.458 |p^{2}_{1/2} > + 0.051 |p^{2}_{j} > - 0.343 |s^{2}_{1/2} > - 0.471 |s^{2}_{j} > + 0.643 |s^{2}_{j} >$$

$$\omega_5 = 0.244 \quad \phi_5 = 3.84 |d^{3}_{1/2} > + 0.348 |d^{3}_{j} > - 0.459 |p^{2}_{3/2} > + 0.328 |p^{2}_{1/2} > + 0.045 |p^{2}_{j} > - 0.383 |s^{2}_{1/2} > + 0.391 |s^{2}_{j} > - 0.333 |s^{2}_{j} >$$

$$\omega_6 = 0.226 \quad \phi_6 = 0.442 |d^{3}_{1/2} > - 0.337 |d^{3}_{j} > + 0.240 |p^{2}_{3/2} > + 0.571 |p^{1}_{1/2} > + 0.173 |p^{1}_{j} > - 0.397 |s^{2}_{1/2} > - 0.176 |s^{2}_{j} > - 0.297 |s^{2}_{j} >$$

$$\omega_7 = 0.238 \quad \phi_7 = -0.103 |d^{3}_{1/2} > + 0.076 |d^{3}_{j} > + 0.668 |p^{2}_{3/2} > + 0.110 |p^{1}_{1/2} > + 0.433 |p^{1}_{j} > - 0.505 |s^{2}_{1/2} > - 0.078 |s^{2}_{j} > - 0.239 |s^{2}_{j} >$$

$$\omega_8 = 0.211 \quad \phi_8 = -0.015 |d^{3}_{1/2} > + 0.195 |d^{3}_{j} > - 0.210 |p^{2}_{3/2} > + 0.147 |p^{2}_{1/2} > + 0.810 |p^{2}_{j} > + 0.475 |s^{1}_{1/2} > - 0.088 |s^{2}_{1/2} > + 0.082 |s^{2}_{j} >$$

overlap: 0.910 (ψ1 ψ2), 0.976 (ψ3 ψ4), 0.802 (ψ1 ψ6), 0.878 (ψ1 ψ1), 0.768 (ψ2 ψ2), 0.819 (ψ2 ψ4), 0.718 (ψ2 ψ6), 0.907 (ψ2 ψ8)
3. Explorations

If we look at the comparison of exact and approximate configuration mixing carefully, we find that the sum of $O(4)$ Casimir operators $\sum_{ij}(L_i \cdot L_j - A_i \cdot A_j)$ is a good approximate constant of motion within the $3s$-$3p$-$3d$ shell in all cases when $N = 2$. When $N = 3$ we notice that for some cases which have higher orbital and spin angular momenta $L$ and $S$, $\sum_{ij}(L_i \cdot L_j - A_i \cdot A_j)$ is still a good approximate constant of motion. Examples are $|3^4P>$, $|4^F>$, $|5^G>$, $|4^S>$. In some cases which have lower orbital and spin angular momenta $L$ and $S$, for example $|3^6S>$, $|3^5P>$, $|3^5D>\sum_{ij}(L_i \cdot L_j - A_i \cdot A_j)$ is no longer a good approximate constant of motion. This result is not an unexpected result because the introduction of $d$ electrons makes the Coulomb interaction between the electrons more complicated. We need to find a new constant of motion. Doing this will be simplified if we can find an expression for the in-shell Coulomb interaction in terms of $O(4)$ single-particle operators.

(IV) The expression for the Coulomb interaction between two electrons in the $n = 3$ shell in terms of $O(4)$ operators

We have developed some new methods for finding an expression for $v = 1/r_{ij}$ in terms of $A$ and $L$. Applying this expression to the $n = 2$ case, we get the
same results as those obtained by other methods, for example the $U(4) \mathcal{O}(4)$ analysis of Moshinsky, et al (14).

1. An expression for the Coulomb interaction in terms of $\mathcal{A}_2$ and $\xi_2$.

For $n = 3$ we have:

$$v_{12} = \sum_{k} 4 \pi / (2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}(\xi, r_{2})$$

$$= 4 \pi (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k} + 4 \pi / 3 \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}$$

$$+ 4 \pi / 5 \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k} + 4 \pi / 7 \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}$$

$$+ 4 \pi / 9 \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}$$

Here $f_{k} = \frac{e^{-k}}{k!}$, so the matrix element of $v_{12}$ is

$$<n, l, m, n, l, m | v_{12} | n', l', m', n', l' > = \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}$$

$$x \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}$$

$$x (-) \sum_{k} (1/2k+1) \frac{\bar{g}}{g} (-1)^{k} Y_{k}^{T}(\xi) Y_{k-n}^{T}(\xi) f_{k}$$

Here $R^{(n, l, n', l')}$ are the Slater integrals.

$$R^{(n, l, n', l')} = \int R_{n, l, n, l'}(r, r_{1}, r_{2}) f_{k}(r, r_{1}) R_{n, l, n', l'}(r, r_{2}) n_{1}^{2} n_{2}^{2} dr_{1} dr_{2}$$

Now multiply the right side of (III-1-2) by a factor:

$$\frac{<n, l, Y_{k}(\mathcal{A}_{2}) | n', l'> <n, l, Y_{k}(\mathcal{A}_{2}) | n', l'>}{<n, l, Y_{k}(\mathcal{A}_{2}) | n', l'> <n, l, Y_{k}(\mathcal{A}_{2}) | n', l'>}$$

This doesn't change the value at all so we have:
\[ <n, \ell, m; n, \ell', m' | V_{12} | n', \ell', m' ; n', \ell', m'> = \]

\[ \sum_k (4\pi/2k+1) R^k(n,\ell, n, \ell, n', \ell, n', \ell') \frac{\hat{\delta} + \delta}{\delta} (1/2k+1) <\ell, m, \ell, m | \ell', k | q> \]

\[ \frac{<n, \ell, \ell' | Y_k(A_0) | n', \ell', l'}{<n, \ell, \ell' | Y_k(A_1) | n, \ell, l'>} \]

\[ = \sum_k (4\pi/2k+1) R^k(n,\ell, n, \ell, n', \ell, n', \ell') \frac{\hat{\delta} + \delta}{\delta} Y_k(A_0) Y_k(A_1) \]

\[ \times \frac{<n, \ell, \ell' | Y_k(A_0) | n, \ell, l'> <n, \ell, \ell' | Y_k(A_1) | n', \ell', l'>}{<n, \ell, \ell' | Y_k(A_0) | n, \ell, l'> <n, \ell, \ell' | Y_k(A_1) | n', \ell', l'>} \]

(1) Evaluation of the ratio of reduced matrix elements for the \( n = 2 \) and \( n = 3 \) shells.

In order to make the expression (I-1-3) more explicit, we have evaluated the \( C^k(n, \ell, n, \ell, n', \ell, n', \ell') \) in both the \( n = 2 \) and \( n = 3 \) cases and assumed that \( n, n' = n_2 = n_2' \). We have for \( n = 2 \):

\[ <2 \ell, m, 2 \ell, m | V_{12} | 2 \ell', m', 2 \ell', m'> = R^0(2s2s;2s2s) \]
\[ + \left[ \frac{4\pi R(2p2p;2s2s)}{9} \right] \langle p2p \rangle \sum_{\delta} (-1)^{\frac{9}{2}} \frac{Y_{\delta}}{Y_{1,\delta}} (A_{1}, A_{1}) \left| 2s2s \right> \]
\[ + \left( 4 \pi/5 \right) \left( 4/25 \right) R^2(2p2p;2p2p) \langle p2p \rangle \sum_{\delta} (-1)^{\frac{9}{2}} \frac{Y_{\delta}}{Y_{2,\delta}} (A_{2}, A_{2}) \left| 2p2p \right> \]

We find:

\[ \sum_{\delta} (-1)^{\frac{9}{2}} \frac{Y_{\delta}}{Y_{1,\delta}} (A_{1}) \left| Y_{2,\delta} (A_{2}) \right> = \left( 3/4\pi \right) A_{1,1} A_{2,2} \]
\[ \sum_{\delta} (-1)^{\frac{9}{2}} \frac{Y_{\delta}}{Y_{2,\delta}} (A_{1}) \left| Y_{2,\delta} (A_{2}) \right> = \left( 15/32\pi \right) \left\{ 4(A_{1,1} A_{2,2}) + 2L_{\xi} L_{\xi} - (4/3) A_{1,2} A_{2,2} \right\} \]

\[ <2 l, m, 2 l', m'> = R^0(2s2s;2s2s) \]
\[ + (1/3) R^1(2p2p;2s2s) <2p2p | A_{1,1} A_{2,2} > 2s2s > + (3/50) \]
\[ xR^1(2p2p;2p2p) <2p2p | 4 (A_{1,1} A_{2,2}) + 2L_{\xi} L_{\xi} - (4/3) A_{1,2} A_{2,2} > 2s2s > \]
\[ + R^0(2p2p;2p2p) + R^0(2p2s;2p2s) \]

We mention here for \( n = 2 \) \( N = 2 \) \( k = 2 \):

Our form is:

\[ \langle 2p2p | V' | 2p2p > = R^2(2p2p)(3/50) \]
\[ x(2p2p | 4 A_{1,1} A_{2,2} + 2L_{\xi} L_{\xi} - (4/3) A_{1,2} A_{2,2} | 2p2p > \]

Moshinsky's form is:

\[ \langle 2p2p | V' | 2p2p > = (1/5) R^2(2p2p) \]
\[ x<2p2p | 2N_{p} - (1/2) N_{p}^2 - (6/5) S_{z} - (3/10) L_{z} | 2p2p > \]

We have calculated the matrix elements by this two forms.

The results are the same.

\( n = 3 \) we find:

\[ <3p,3l | 1/r_{12} | 3l'3l' > = R^0(3s3s;3s3s) + R^0(3s3p;3s3p) \]
\[ + R^0 (3d3s;3d3s) + \left( \frac{1}{8} \right) R^0 (3p3p;3s3s) < 3p3p|A_x A_x|3s3s > \\
+ R^0 (3p3p;3p3p) + R^0 (3d3d;3d3d) + R^0 (3d3p;3d3p) . \]

\[ + (\sqrt{10}/20) R^0 (3p3d;3s3p) < 3p3d|A_x A_x|3s3p > \]

\[ + (1/5) R^0 (3p3d;3d3p) < 3p3d|A_x A_x|3d3p > \]

\[ + (3/320) R^2 (3s3d;3d3s) < 3s3d|4(A_x A_x) + 2L_x L_x -(4/3) A_x A_x|3d3s > \]

\[ + (\sqrt{10}/400) R^2 (3p3s;3p3d) < 3p3s|4(A_x A_x) + 2L_x L_x -(4/3) A_x A_x|3p3d > \]

\[ + (1/70) R^2 (3p3d;3p3d) < 3p3d|4(A_x A_x) + 2L_x L_x -(4/3) A_x A_x|3p3d > \]

\[ + (1/150) R^2 (3p3p;3p3p) < 3p3p|4(A_x A_x) + 2L_x L_x -(4/3) A_x A_x|3p3p > \]

\[ + (3/98) R^2 (3d3d;3d3d) < 3d3d|4(A_x A_x) + 2L_x L_x -(4/3) A_x A_x|3d3d > \]

\[ + (\sqrt{10}/176) R^2 (3d3d;3d3d) < 3d3d|4(A_x A_x) + 2L_x L_x -(4/3) A_x A_x|3d3d > \]

\[ + (4 \pi/1715) R^4 (3d3p;3d3p) < 3d3p \left| \sum_{\delta} (-)^{\delta} Y_{3.8} \frac{1}{2} (A_x) Y_{3.8} (A_x) \right| 3p3d > \]

\[ + (16 \pi/35721) R^4 (3d3d;3d3d) < 3d3d \left| \sum_{\delta} (-)^{\delta} Y_{4.9} \frac{1}{2} (A_x) Y_{4.9} (A_x) \right| 3d3d > \]

\[ \text{Here:} \]

\[ C^0 (3d3s;3d3s) = 1 \quad , \quad C^0 (3p3p;3p3p) = 1 \]

\[ C^0 (3p3s;3p3s) = 1 \quad , \quad C^0 (3d3p;3d3p) = 1 \]

\[ C^0 (3d3d;3d3d) = 1 \quad , \quad C^0 (3s3s;3s3s) = 1 \]

\[ C^4 (3d3d;3d3d) = 4/49 \quad , \quad C^4 (3p3p;3s3s) = 1/8 \]

\[ C^4 (3s3d;3d3d) = \sqrt{10}/70 \quad , \quad C^4 (3p3d;3d3p) = 1/5 \]

\[ C^4 (3s3d;3d3s) = 1/40 \quad , \quad C^4 (3d3p;3p3s) = \sqrt{10}/20 \]
We used three different methods to calculate the 
\( C^k(n_1, l_1, n_2, l_2; n_1', l_1', n_2', l_2') \) and they all gave the same result. 
(We have given examples in appendix 2.)

(2) The symmetrized form for \( Y_{Kz}(\mathbf{A}) \) that satisfies

\[
[Y_{Kz}(\mathbf{A})]^+ = (-1)^k Y_{Kz}(\mathbf{A})
\]

In order to express \( \sum_{k' z} Y_{Kz}(\mathbf{A}) Y_{Kz}(\mathbf{A}_z) \) in terms of scalar products of \( \mathbf{A} \) and \( L_z \), we have found the symmetrized form for \( Y_{Kz}(\mathbf{A}) \) by using:

\[
[L_z, T(k, q)] = T(k, q+1) \hbar [(k+q)(k+q+1)]^{1/2},
\]

\[
[L_\ell, T(k, q)] = T(k, q) \hbar q.
\]

Here \( L_z = L_x + iL_y \) and \( T(k, q) \) is the component of an irreducible tensor operator of rank \( k \).

We have found:

\[ k = 1 \quad Y_{10}(\mathbf{A}) = (3/4\pi) A^z, \]
\[ Y_{1z}(\mathbf{A}) = -(3/8\pi)^{1/2} (A_x \pm iA_y). \]

\[ k = 2 \quad Y_{20}(\mathbf{A}) = -(5/16\pi)^{1/2} \frac{z}{2} A^z \pm A^x, \quad Y_{2z}(\mathbf{A}) = -(5/16\pi)^{1/2} \frac{z}{2} A^z \pm A^y, \]
\[ Y_{2 \pm 1}(A) = \pm \left( \frac{15}{32\pi} \right)^{\frac{3}{2}} \left[ A_y^2 (A_x \pm iA_y) + (A_x \pm iA_y)A^x_y \right] \]
\[ Y_{2 \pm 2}(A) = \left( \frac{15}{32\pi} \right)^{\frac{3}{2}} (A_x \pm iA_y)^{\frac{3}{2}} \]

\[ k = 3 \]

\[ Y_{30}(A) = \left( \frac{7}{64\pi} \right)^{\frac{15}{2}} \left[ A_y^2 (2A^2_y - A_x^2 - A_y^2) + (2A^2_y - A_x^2 - A_y^2)A^y_x \right] \]
\[- (A_x - iA_y)A^2_y (A_x + iA_y) - (A_x + iA_y)A^2_y (A_x - iA_y), \]
\[ Y_{3 \pm 1}(A) = \mp \left( \frac{1}{24} \right)(21/\pi)^{\frac{15}{2}} \left[ A^2_y (A_x \pm iA_y) + 4(A_x \pm iA_y)A^x_y \right] \]
\[ + 4A^2_y (A_x \pm iA_y)A^2_y - (A_x \pm iA_y)(A_x \pm iA_y)(A_x \pm iA_y) \]
\[- (A_x \mp iA_y)(A_x \mp iA_y) - (A_x \pm iA_y)(A_x \mp iA_y), \]
\[ Y_{3 \pm 2}(A) = \left( \frac{1}{12} \right)(105/2\pi)^{\frac{15}{2}} \left[ (A_x \pm iA_y)^2 \right] \]
\[ + (A_x \pm iA_y)^2 A^2_y + (A_x \pm iA_y)A^2_y (A_x \pm iA_y), \]
\[ Y_{3 \pm 3}(A) = \pm \left( \frac{35}{64\pi} \right)^{\frac{15}{2}} (A_x \pm iA_y)^{\frac{3}{2}} \]

\[ k = 4 \]

\[ Y_{40}(A) = \left( \frac{1}{64\pi} \right)^{\frac{15}{2}} \left\{ (A^2_x + A^2_y - 4A^2_y)(2A^2_y - A^2_x - A^2_y) \right\} \]
\[ + (2A^2_y - A^2_x - A^2_y)(A^2_x + A^2_y - 4A^2_y) \]
\[ + 4(A_x + iA_y)A^2_y (A_x - iA_y) + 4(A_x - iA_y)A^2_y (A_x + iA_y) \]
\[ + 4(A_x + iA_y)A^2_y (A_x - iA_y)A^2_y + 4A^2_y (A_x + iA_y)A^2_y (A_x - iA_y) \]
\[ + 4A^2_y (A_x + iA_y)A^2_y (A_x - iA_y) + 4A^2_y (A_x + iA_y) (A_x - iA_y)A^2_y \]
\[ + 4A^2_y (A_x - iA_y) (A_x + iA_y)A^2_y + 4(A_x - iA_y)A^2_y (A_x + iA_y)A^2_y \]
\[-(Ax + iAy)(Ax - iAy) - (Ax - iAy)(Ax + iAy)^2\] ,

\[Y_{\pm 1}(\vec{A}) = \frac{(5/64\pi)^{1/2}}{2}\{ (Ax \pm iAy)A_{\pm}^2 (Ax \pm iAy) + (Ax \pm iAy)(Ax \mp iAy)A_{\pm}^2 \]

\[+ A_{\pm}^2 (Ax \mp iAy)(Ax \pm iAy)^2 - (4A_{\pm}^4 - 2Ax - 2Ay)A_{\pm}^2 (Ax \pm iAy) \]

\[- (Ax \pm iAy)A_{\pm}^2 (4A_{\pm}^2 - 2Ax - 2Ay) - (4A_{\pm}^2 - 2Ax - 2Ay)(Ax \pm iAy)A_{\pm}^2 \]

\[- A_{\pm}^2 (Ax \pm iAy)(4A_{\pm}^2 - 2Ax - 2Ay) \]

\[Y_{\pm 2}(\vec{A}) = (3/32)(5/2\pi)^{1/2}\{ (Ax \mp iAy)(Ax \pm iAy)^3 \]

\[+ (Ax \pm iAy)(Ax \mp iAy)^3 - 4A_{\pm}^4 (Ax \pm iAy)^2 \]

\[- 4(Ax \pm iAy)A_{\pm}^2 (4A_{\pm}^2 - 4Ax \pm iAy)A_{\pm}^2 (Ax \pm iAy) \]

\[- 4(Ax \pm iAy)A_{\pm}^2 (Ax \pm iAy)(Ax \mp iAy)A_{\pm}^2 \]

\[- 4(Ax \pm iAy)A_{\pm}^2 (Ax \mp iAy)^2 + (Ax \pm iAy)(Ax \mp iAy)A_{\pm}^2 \]

\[+ (Ax \pm iAy)(Ax \mp iAy)A_{\pm}^2 \}

\[Y_{\pm 3}(\vec{A}) = \frac{(3/32)(35/3\pi)^{1/2}}{2}A_{\pm}(Ax \pm iAy)^3 \]

\[+ (Ax \pm iAy)A_{\pm}^2 (Ax \pm iAy)A_{\pm}^2 \]

\[+ (Ax \pm iAy)A_{\pm}^2 (Ax \pm iAy) \}

\[Y_{\pm 4}(\vec{A}) = (3/16)(35/3\pi)^{1/2} (Ax \pm iAy)^4 \]

(3) Discussion

The first work in which in-shell Coulomb
interactions are expressed as a function of \( A \), \( L \) and radial integrals is that of Moshinsky, et al (14). In this work the Coulomb interaction was first expressed in terms of products of Slater integrals and unit tensor operators of the unitary group \( U(M) \) where \( M = n^2 \) is the number of orbitals in the hydrogenic shell with principal quantum number \( n \). Then the matrix elements of \( A \), \( A \cdot A \) etc. were expressed as products of a reduced matrix element and a unit tensor of \( U(M) \). Comparing the two expressions it proved possible to obtain a simple expression for the in-shell Coulomb interaction as a product of Slater integrals and functions of \( A \), \( L \). This \( U(n^2) \to O(4) \) analysis is no longer practical when one considers the s,p,d orbitals of the third hydrogenic shell. We therefore developed an alternative, direct method for expressing the in-shell Coulomb interaction as a function of radial integrals and the \( O(4) \) generators \( A \), \( L \). This method gives the known \( n = 2 \) results by simpler means and enables us to rather easily obtain corresponding results for \( n = 3 \). We also thought it might be helpful to express the Coulomb interaction as a product of radial integrals and the \( O(4,1) \) generators \( A \) and \( B \).

2. An expression for the Coulomb interaction potential in terms of \( A \) and \( B \).

Using the notation of Bednar (13) a two-electron repulsion integral can be written:
Here $\chi_{n\ell m}(\xi)$ are Bednar hydrogenic wave functions defined by:

$$\chi_{n\ell m}(2\xi) = \frac{2}{\sqrt{(n-\ell-1)!(n+\ell)!}} (2\pi)^{\ell+1} e^{-r} L_{n-\ell-1}^{2\ell+1}(2\pi r) Y_{\ell m}(\theta, \phi).$$

The $L_{n-\ell-1}^{2\ell+1}(2\pi r)$ are Laguerre polynomials, defined by:

$$L_{n-\ell-1}^{2\ell+1}(2\pi r) = \frac{d^{2\ell+1}}{d(2\pi r)^{2\ell+1}} \left( L_{n-\ell-1}(2\pi r) \right).$$

and $\bar{r} = e^{-\frac{T_0 T_2}{2}} r e^{\frac{T_0 T_2}{2}} = \left( \frac{n}{Z} \right) r$, $\theta_n = \theta(n/Z)$ so:

$$I = \frac{Z \pi}{n^3} \int \int \chi_{n_1 \ell_1 m_1}(\xi_1) \chi_{n_2 \ell_2 m_2}(\xi_2) \Sigma_{k} \frac{\gamma_k}{2^{k+1}} 4\pi \int \int \delta(r_2) Y_{\ell_1}(\theta_2) Y_{\ell_1}(\theta_2)$$

$$\times \chi_{n_1 \ell_1 m_1}(\xi_1) \chi_{n_2 \ell_2 m_2}(\xi_2) r_1 r_2 d\Omega_1 d\Omega_2 d\omega_1 d\omega_2.$$

Because $\bar{r} = \frac{r}{r}$

$$I = \frac{Z \pi}{n^3} \int \int \chi_{n_1 \ell_1 m_1}(\xi_1) \chi_{n_2 \ell_2 m_2}(\xi_2) \Sigma_{k} \frac{\gamma_k}{r_1 r_2} 4\pi \int \int \Sigma(-1)^{l_1} Y_{\ell_1}(\theta_1) Y_{\ell_1}(\theta_1)$$

$$\times \chi_{n_1 \ell_1 m_1}(\xi_1) \chi_{n_2 \ell_2 m_2}(\xi_2) r_1 r_2 d\Omega_1 d\Omega_2 d\omega_1 d\omega_2.$$

In Bednar's space we have $\xi = A - B$, $r = T_2 - T_1$

where $A = (1/2)(Lx \bar{z} - px \bar{z} + \bar{r})$

$B = (1/2)(Lx \bar{z} - px \bar{z} - \bar{r})$
\( L = \exp \). Substituting these into (IV-2-1) we have:

\[
I = \frac{2}{n^3} \sqrt{\frac{4\pi}{\gamma}} \sum_{\gamma \kappa \lambda} \sum_{\kappa \lambda \nu} \frac{4\pi}{\gamma} \frac{f_{\kappa \lambda}^{(\gamma \nu)}}{\gamma} \sum_{\kappa \lambda \nu} \delta(\gamma \nu \kappa \lambda) \gamma_k \gamma_{\kappa \lambda} (x-y)
\]

\[
\times \sum_{\kappa \lambda \nu} \frac{4\pi}{\gamma} \frac{f_{\kappa \lambda}^{(\gamma \nu)}}{\gamma} \sum_{\kappa \lambda \nu} \delta(\gamma \nu \kappa \lambda) \gamma_k \gamma_{\kappa \lambda} (x-y)
\]

\[
\text{(IV-2-2)}
\]

We have expressed \( \sum_{\kappa \lambda \nu} \delta(\gamma \nu \kappa \lambda) \gamma_k \gamma_{\kappa \lambda} (x-y) \) in terms of products of \( \gamma \) and \( \gamma^* \).

(1) Expressing \( \sum_{\kappa \lambda \nu} \delta(\gamma \nu \kappa \lambda) \gamma_k \gamma_{\kappa \lambda} (x-y) \) in terms of products of \( \gamma \) and \( \gamma^* \), we obtain:

for \( k = 1 \):

\[
Y_{10}(\gamma) = \left( \frac{3}{4\pi} \right)^{1/2}
\]

\[
Y_{11}(\gamma) = \frac{3}{8\pi} \left( x + i y \right)
\]

so we have: \( \sum_{\kappa \lambda \nu} \delta(\gamma \nu \kappa \lambda) \gamma_k \gamma_{\kappa \lambda} (x-y) = \left( \frac{3}{4\pi} \right) \gamma \gamma^* \).

For \( k = 2 \):

\[
Y_{20}(\gamma) = \left( \frac{5}{16\pi} \right)^{1/2} \left( 2z^2 - x^2 - y^2 \right)
\]

\[
Y_{21}(\gamma) = \left( -\frac{15}{8\pi} \right)^{1/2} \left( x + iy \right)
\]

\[
Y_{22}(\gamma) = \left( \frac{15}{32\pi} \right)^{1/2} \left( x + iy \right)^2
\]

we have: \( \sum_{\kappa \lambda \nu} \delta(\gamma \nu \kappa \lambda) \gamma_k \gamma_{\kappa \lambda} (x-y) = \frac{15}{8\pi} \left( \gamma \gamma^* \right) - \frac{5}{8\pi} \gamma \gamma^* \).

For \( k = 3 \):

\[
Y_{30}(\gamma) = \left( \frac{7}{16\pi} \right) \left( 2z^2 - 3x^2 - 3y^2 \right) \gamma
\]
\[
Y_{3t1}(\xi) = \frac{1}{2}(7/64 \pi)^{1/2}(4z^2 - x^2 - y^2)(x \pm iy),
\]
\[
Y_{3t2}(\xi) = (105/32 \pi)^{1/2}z(x \pm iy)^2,
\]
\[
Y_{3t3}(\xi) = \frac{1}{2}(35/64 \pi)^{1/2}(x \pm iy)^3,
\]

so we have:

\[
\sum_{\theta} (-1)^{\theta} y_{32}^{\theta}(\xi_1) y_{32}^{\theta}(\xi_2) = \frac{35}{8 \pi} (r_1, r_2)^2 - \frac{2}{8 \pi} r_1^2 r_2^2 (r_1, r_2).
\]

For \( k = 4 \):

\[
Y_{4t0}(\xi) = (3/16)(1/\pi)^{1/2}[8z^4 - 24(x^4 + y^4)z^2 + 3(x^2 + y^2)^2]
\]
\[
Y_{4t1}(\xi) = \pm(3/8)(5/\pi)^{1/2}(x \pm iy)z(4z^2 - 3x^2 - 3y^2)
\]
\[
Y_{4t2}(\xi) = (3/8)(5/2 \pi)^{1/2}(x \pm iy)(6z^2 - x^2 - y^2)
\]
\[
Y_{4t3}(\xi) = \frac{1}{2}(3/8)(35/\pi)z(x \pm iy)^3
\]
\[
Y_{4t4}(\xi) = (3/16)(35/2 \pi)^{1/2}(x \pm iy)^4
\]

so we have:

\[
\sum_{\theta} (-1)^{\theta} y_{4k}^{\theta}(r_1) y_{4k}^{\theta}(r_2) = (27/32 \pi)r_1^4 r_2^4
\]
\[
+ (315/32 \pi)(r_1, r_2)^4 - (135/16 \pi)r_1^2 r_2^2 (r_1, r_2)^2
\]

Because \( \xi = B - A \) we finally obtain:

\[
\frac{1}{r_{12}} = \frac{f_0}{r_1 r_2} + \frac{f_1}{r_1 r_2} (A_1 - B_1)(A_2 - B_2) + \frac{f_2}{r_1^2 r_2} \left\{ \frac{3}{2} \left[ (A_1 - B_1)(A_2 - B_2) \right] - \frac{1}{2} (\xi, A_1, B_1, A_2, B_2)^2 \right\}
\]
\[
+ \frac{f_3}{r_1^2 r_2^2} \left\{ \frac{3}{2} \left[ (A_1 - B_1)(A_2 - B_2) \right] - \frac{3}{2} (\xi, A_1, B_1, A_2, B_2)^2 \right\}
\]
Looking at this result we see we have expressed $1/r_{12}$ partly in terms of $A, B$ but the problem is that we haven't a good way to express the term $f_k/r_{12}^k$ in terms of the group generators.

(2) A method for evaluating the matrix elements

We have evaluated the matrix elements (IV-2-1) for some cases (see appendix 3) by using the method we have found, (IV-2-3), and have obtained the same results as those evaluated by the earlier methods. Because $A$ acting on $\mathcal{X}_{n\ell m}$ will change $\ell$ and $B$ acting on $\mathcal{X}_{n\ell m}$ will change $n$ and $\ell$ it follows that $\sum_{\ell} (-1)^\ell Y_{k\ell} (A, B) Y_{k\ell}(A, B)$ acting on $\mathcal{X}_{n'\ell' m'}$ should be a linear combination of $\mathcal{X}_{n m}$ with different $n, \ell, m$. e.g.

$$Y_{k\ell} (A, B) \mathcal{X}_{n m} = \sum_{\ell=\ell-k, m=m-\ell} Y_{k\ell} (n, m, \ell, m) \mathcal{X}_{n, \ell, m}$$

Here

$$Y_{k\ell} (n, m, \ell, m) = \int \mathcal{X}_{n, \ell, m} (y) Y_{k\ell} (x) \mathcal{X}_{n, m} (x) r^2 d\omega$$

$$= \int R_{n, \ell} (y) r^2 R_{n, m} (y) \int Y_{k\ell} (y) Y_{k\ell} (x) r^2 d\omega.$$
\[ I = \frac{2}{n^3} \int \chi_{n, l, m, \lambda} \chi_{n_x, l_x, m_x, \lambda_x} \sum_{k, k_1, k_2} \frac{4\pi}{k^{2k+1}} \left( \frac{f_{k, k_1, k_2}}{\gamma_{k, k_1, k_2}} \right) \sum_{\rho, \rho_1, \rho_2} \delta_{\rho, \rho_1} \delta_{\rho_2, \rho} y_{k, \rho, \rho_1, \rho_2} (n, l, m, \lambda, n_x, l_x, m_x, \lambda_x, n, l, m, \lambda, n_x, l_x, m_x, \lambda_x) \]

\[ \chi \sum_{k, k_1, k_2} \sum_{\rho, \rho_1, \rho_2} \delta_{\rho, \rho_1} \delta_{\rho_2, \rho} y_{k, \rho, \rho_1, \rho_2} (n, l, m, \lambda, n_x, l_x, m_x, \lambda_x, n, l, m, \lambda, n_x, l_x, m_x, \lambda_x) \]

(IV-2-3)

We give the evaluation of (IV-2-1) for some cases in appendix 3.
Appendix 1: Example calculation of the matrix elements

of \( \sum_{ij} (L_i \cdot L_j - A_i A_j) \)

By using

\[
<\ell'_{s1\ell 1} \ell'_{s2\ell 2} S L | \sum_{ij} \ell_{s1\ell 1} \ell_{s2\ell 2} S L | \ell'_{s1\ell 1} \ell'_{s2\ell 2} S L > = \\
\frac{1}{2} [L(L+1) - NL(l+1) - k\ell(\ell'+1)]
\]

we have \( <pd^3 p^4 D | \sum_{ij} A_i A_j | pd^3 p^4 D> = \frac{1}{2} \left\{ 2 \times (2+1) - 1 \times (1+1) - 2 \times 2 \times (2+1) \right\} = -4 \).

(2) \( <pd^3 p^4 D | \sum_{ij} A_i A_j | pd^3 p^4 D> = <d^2 p | A_i A_j | d^2 p> + 2 \sum_{\sigma} <pd^3 p^4 D | (pd)_{\sigma \lambda} d^\sigma D | <pd_{\sigma \lambda} A_i A_j | pd_{\sigma \lambda}> \)

From table 1 and table 3 we have:

\( <d^2 p | A_i A_j | d^2 p> = 0 \), \( <pd^3 p | A_i A_j | pd^3 p> = -1/3 \)

\( <pd^3 D | A_i A_j | pd^3 D> = 1 \), \( <pd^3 F | A_i A_j | pd^3 F> = -2 \)

\( <pd^3 p^4 D | (pd)^3 p^4 D> = 3/10 \)

\( <pd^3 p^4 D | (pd)^3 D d^4 D> = -\sqrt{35}/10 \)

\( <pd^3 p^4 D | (pd)^3 d^4 D> = \sqrt{14}/5 \)

so \( <pd^2 p^4 D | \sum_{ij} A_i A_j | pd^2 p^4 D> = 0 + 2 \times (9/100) \times (-1/3) + 2 \times (35/100) \times (1) + (14/25) \times (-2) = -8/5 \)
Appendix 2: Example of a calculation of the ratio of reduced matrix elements

(1) We calculate the reduced matrix elements of the solid spherical harmonics by using vector-coupling methods.

For example consider \( k = 2, \ell = \ell' = \ell'' = 2 \) and use Moshinsky's notation (14) for reduced matrix elements of \( A \). We have:

\[
\frac{4\pi \langle \ell''|Y_{\ell''}(A)|\ell\rangle}{2\ell + 1} = \left\{ \frac{(2\ell'' + 1)(2\ell + 1)}{(2\ell + 1)(2\ell + 1)} \right\}^{1/2} \langle \ell''|k\ 00|\ell\ 0\rangle
\]

If \( k = 2, \ell = \ell' = \ell'' = 2 \), then:

\[
(4\pi/5)\langle 32|Y_{32}(A)|32\rangle = \left\{ \frac{(2x2 + 1)(2x2 + 1)}{(2x2 + 1)(2x2 + 1)} \right\}^{1/2} \langle 32|2200\rangle = \frac{2}{7} \cdot 5x(2/7x5) = 2/7 .
\]

and

\[
<3\ell'|T^k(A)|3\ell> = \sum_{LM \bar{q}_1 \bar{q}_2} <\ell m|Y_{\ell''}(A)|LM> <LM|Y_{\ell''}(A)|\ell' m'> <\ell' k m q|l m>
\]

Let \( k = k = 1, K = 2, q_1 = q_2 = 1, q = 2, \) and \( \ell' = \ell = 2 \),

we have \( L = 1 \) then:
\[ \langle 32 \parallel T_2(\mathcal{A}) \parallel 32 \rangle = \frac{\langle 1 \parallel Y, (\mathcal{A}) \parallel 2 \rangle < 2 \parallel Y, (\mathcal{A}) \parallel 1 \rangle \langle 1 \parallel 1 \parallel m-1 \parallel 1 \rangle 2 m \rangle}{\langle 2 \parallel 2 \parallel m-2 \parallel 2 \parallel 2 \rangle m \rangle}. \]

\[ x < 2 \parallel 1 \parallel m-2 \parallel 1 \parallel m-1 \rangle \langle 1 \parallel 1 \parallel 1 \rangle 2 2 \rangle \]

\[ = -\sqrt{21}/4 \pi. \]

But \[ T_{2g}(\mathcal{A}) = \left( \frac{(2 \ell + 1)(2 \ell + 1)}{4\pi(2 \ell + 1)} \right) \langle \ell, 0 \parallel 0 \rangle \langle 0, 0 \parallel 0 \rangle \langle \ell, \ell \rangle - \ell \langle \mathcal{A} \rangle \]

\[ \ell_1 = \ell_2 = 1, \quad \ell = 2 \quad \text{so:} \]

\[ T_{2g}(\mathcal{A}) = \left( \frac{(2\times1 + 1)(2\times1 + 1)}{4\pi(2\times2 + 1)} \right) \langle 1 \parallel 0 \parallel 1 \parallel 1 \parallel 2 \parallel 0 \rangle \langle \mathcal{A} \rangle \]

\[ = \sqrt{3/10\pi} \langle Y, (\mathcal{A}) \rangle. \]

\[ \langle 32 \parallel T_2(\mathcal{A}) \parallel 32 \rangle = \langle 32 \parallel \sqrt{3/10\pi} \parallel Y, (\mathcal{A}) \parallel 32 \rangle = -\sqrt{21}/4 \pi \]

hence \[ \langle 32 \parallel Y, (\mathcal{A}) \parallel 32 \rangle = -\left( \frac{\sqrt{21}/4\pi}{10\pi/3} \right) \ell^2 = -\sqrt{70/16} \pi \]

\[ C^2(3d3d; 3d3d) = \frac{\langle 3 \parallel 2 \parallel Y, (\mathcal{A}) \parallel 3 \parallel 2 \rangle \langle 3 \parallel 2 \parallel Y, (\mathcal{A}) \parallel 3 \parallel 2 \rangle}{\langle 3 \parallel 2 \parallel Y, (\mathcal{A}) \parallel 3 \parallel 2 \rangle \langle 3 \parallel 2 \parallel Y, (\mathcal{A}) \parallel 3 \parallel 2 \rangle} \]

\[ = 4/49. \]

(2) We use Adman's notation:

\[ \langle \ell' \parallel Y, (r) \parallel \ell \rangle = (-1)^{\ell'} \left( \frac{(2 \ell' + 1)(2 \ell + 1)(2k + 1)}{4} \right) \ell' \ell k \ell \]

Let \[ \ell' = \ell = 2, \quad k = 2, \quad \text{so:} \]
\[
\langle 2 \mid Y_2(A) \mid 2 \rangle = (-)^{2(2x2 + 1)1(2x2 + 1)1(2x2 + 1)} \left[ \frac{2 \ 2 \ 2}{4 \pi} \right]^{\frac{1}{2}} (0 \ 0 \ 0)
\]

\[
= (-5/14) \sqrt{14/\pi},
\]

and \[
\langle 3d_0 \mid Y_{20}(A) \mid 3d_0 \rangle = \langle 3d_0 \mid \sqrt{5/16} (3A_0^3 - A) \mid 3d_0 \rangle
\]

\[
= \frac{\sqrt{3}}{4A \pi} \langle 3d_0 \mid \left[ \left( -\frac{3}{\sqrt{3}} \right) (-\sqrt{3/3}) 3s_0 \left( -\frac{3}{\sqrt{3}} \right) 3d_0 \right] - 2 \mid 3d_0 \rangle
\]

\[
= \frac{\sqrt{3}}{4A \pi} \times 2 = \frac{\sqrt{3}}{2 \pi},
\]

Here \[
\begin{align*}
|A_0 3d > &= -2/\sqrt{3} |3p > \\
|A^2 3p > &= -\frac{\sqrt{8/3}}{3} |3s > - 4/\sqrt{3} |3d_0 > \\
|A^2 3d_0 > &= 2 |3d_0 >
\end{align*}
\]

so, \[
\langle 32 \mid Y_{20}(A) \mid 32 \rangle = \frac{\sqrt{3}}{4A \pi} (-)^2 \left( \begin{array}{ccc} 2 & 2 & 2 \\ 0 & 0 & 0 \end{array} \right) = -\frac{5}{4} \sqrt{\frac{14}{\pi}}
\]

Then:

\[
C^2(3d3d;3d3d) = \frac{\left( -\frac{5}{4} \sqrt{\frac{14}{\pi}} \right)^2}{\left( -\frac{5}{4} \sqrt{\frac{14}{\pi}} \right)^2} = \frac{4}{49}.
\]

This result agrees with the result from (1). Also we can express:

\[
\sum_{\beta} (-1)^{\frac{\beta}{2}} Y_{\beta}(n_1 l_1, n_2 l_2) Y_{\beta}^*(n'_1 l'_1, n'_2 l'_2),
\]

and \[
\sum_{\beta} (-1)^{\frac{\beta}{2}} Y_{\beta}(n_1 l_1, n_2 l_2) Y_{\beta}(n'_1 l'_1, n'_2 l'_2)
\]

in second quantized form. Comparing the two expressions we can find \[
C^k(n_1 l_1, n_2 l_2; n'_1 l'_1, n'_2 l'_2).
\]
Appendix 3: Example calculation of Coulomb integrals:

$$I = \frac{Z}{n^3} \iint \chi_n^* \chi_m (r) \chi_{n'}^* \chi_{m'} (r') \frac{4\pi}{\ell \ell'} \frac{(\ell \ell')}{n(n') \ell \ell'} \frac{1}{r_{nm}} \left( \frac{\ell}{\ell'} \right) \sum_{\ell = \ell - \ell'} \frac{1}{y_{\ell} y_{\ell'}}$$

$$\times \chi_{n', m'} (r') \chi_{n''} (r) \chi_{m''} (r) r_{12} d\omega_1 d\omega_2 ,$$

where

$$y_{\ell} (n \ell m \pi \ell m') = \int \chi \bar{\chi} \bar{\chi} \bar{\chi} (r) \chi_{n \ell m \pi \ell m'} r \ d r \ d \omega$$

$$= \int R_{\ell m} r^\ell R_{\ell m'} r \ d r \int \chi \bar{\chi} \bar{\chi} \bar{\chi} (r') \ y_{\ell} (r') y_{\ell'} (r') \ d \omega .$$

We consider a simple case that to calculate the matrix element: $$\langle 2s^1 l \ 1/| r_{12} | 2s^2 ' s \rangle$$, where $$n_1 = n_2 = 2$$, $$l_1 = l_2 = 0$$, $$s_1 = s_2 = 1/2$$, $$k = 0$$, and:

$$\langle 2s^1 ' s \rangle = \sum_{m} \langle 0m0m | 0m \rangle | 2s_m \rangle | 2s_m \rangle$$

$$= \langle 0000 | 00 | 2s_m | 2s_m \rangle = \langle 2s \rangle | 2s \rangle$$

so $$\langle 2s^1 ' s | 1/| r_{12} | 2s^2 ' s \rangle = \frac{2}{n^3} \iint \chi_{200}^* (x_1) \chi_{200} (x_2) \frac{4\pi}{r_1 r_2}$$

$$\times y_{00} (200, 200) y_{00} (200, 200) \chi_{200} (x_1) \chi_{200} (x_2)$$

$$\times r_1 r_2 d r_1 d r_2 d \omega_1 d \omega_2 .$$

Here $$y_{00} = \int R_{20} r^0 R_{20} r \ d r \int \chi_{00} \chi_{00} \ Y_{00} \ Y_{00} \ d \omega .$$

Finally

$$\langle 2s^1 ' s | 1/| r_{12} | 2s^2 ' s \rangle = \frac{2}{2^3} \iint \chi_{200}^* \chi_{200} \ r_1 r_2 f_0 \chi_{200} \chi_{200} \ r_1 r_2 d r_1 d r_2 d \omega_1 d \omega_2$$
We have calculated the integral by computer. We find:

\[ \frac{2}{r_1^3} \int \int \chi_2^* \chi_2^* \frac{1}{r_1} \chi_2 \chi_2 \frac{1}{r_2} \chi_2 \chi_2 \frac{1}{r_1} \chi_2 \chi_2 \frac{1}{r_2} \chi_2 \chi_2 d\omega_1 d\omega_2 d\omega_3 d\omega_4 \]

\[ + \frac{2}{2^3} \int \int \chi_2^* \chi_2^* \frac{1}{r_1} \chi_2 \chi_2 \frac{1}{r_2} \chi_2 \chi_2 \frac{1}{r_1} \chi_2 \chi_2 \frac{1}{r_2} \chi_2 \chi_2 d\omega_1 d\omega_2 . \]

Let \( Z = 1 \) So:

\[ \langle 2s^1 ' S' | 1/r_{1a} | 2s^2 ' S' \rangle = \frac{1}{8} \times 2 \times \frac{17}{128} = .150390625. \]

This agrees with Moshinsky's result (14).

\[ \langle 2s^1 ' S' 1/r_{1a} 2s^2 ' S' \rangle = F = 0.1503906 \]

Also we have calculated the matrix element of:

\[ \langle 2p^1 ' S' | 1/r_{1a} | 2s^2 ' S' \rangle = -.05074512 \]

It agrees with Moshinsky's result for \(-(1/\sqrt{3})G \) (14).
Appendix 4: The Slater integrals with effective nuclear charges in \((\Pi - 2 - 7)\). (Calculated by Nacsyma.)

\[
F_{ssss}(Z_a, Z_b, 0) = \left( Z_a^8 Z_b^8 + 8 Z_a^8 Z_b^7 - 14 Z_a^8 Z_b^6 + 160 Z_a^4 Z_b^5 - 106 Z_a^5 Z_b^4 
+ 28 Z_a^6 Z_b^3 \right) / (4 Z_a^8 + 32 Z_a Z_b^8 + 112 Z_a^2 Z_b^6 + 224 Z_a^3 Z_b^5 
+ 280 Z_a^4 Z_b^4 + 224 Z_a^5 Z_b^3 + 112 Z_a^6 Z_b^2 + 32 Z_a^7 Z_b + 4 Z_a^8) 
+ (28 Z_a^3 Z_b^6 - 106 Z_a^4 Z_b^5 + 160 Z_a^5 Z_b^4 - 14 Z_a^6 Z_b^3 
- 14 Z_a^6 Z_b^3 - 8 Z_a^7 Z_b^2 + 4 Z_a^8) / (4 Z_a^8 + 32 Z_a Z_b^8 
+ 112 Z_a^2 Z_b^6 + 224 Z_a^3 Z_b^5 + 280 Z_a^4 Z_b^4 + 224 Z_a^5 Z_b^3 
+ 112 Z_a^6 Z_b^2 + 32 Z_a^7 Z_b + 4 Z_a^8) 
\]

\[
F_{pppp}(Z_a, Z_b, 0) = Z_a^5 Z_b^5 \left( 8064 Z_b^3 + 4032 Z_a Z_b^2 + 1152 Z_a^2 Z_b + 144 Z_a^3 \right) 
/ (576 \left( Z_b^8 + 8 Z_a Z_b^7 + 28 Z_a^2 Z_b^6 + 56 Z_a^3 Z_b^5 \right) 
+ 70 Z_a^4 Z_b^8 + 56 Z_a^5 Z_b^7 + 28 Z_a^6 Z_b^6 + 8 Z_a^7 Z_b^5 + 4 Z_a^8) 
+ Z_a^5 Z_b^5 \left( 144 Z_b^3 + 1152 Z_a Z_b^2 + 4032 Z_a^2 Z_b + 8064 Z_a^3 \right) 
/ (576 \left( Z_a^8 + 8 Z_a Z_b^7 + 28 Z_a^2 Z_b^6 + 56 Z_a^3 Z_b^5 \right) 
+ 70 Z_a^4 Z_b^8 + 56 Z_a^5 Z_b^7 + 28 Z_a^6 Z_b^6 + 8 Z_a^7 Z_b^5 + 12) 
\]
F_{pppp}(Z_a, Z_b, 2) = Z_a^5 Z_b^5 (5760 Z_b + 720 Z_a) / (576 (Z_b^{10} + 8 Z_a Z_b^9 \\
+ 28 Z_a^2 Z_b^8 + 56 Z_a^3 Z_b^7 + 70 Z_a^4 Z_b^6 + 56 Z_a^5 Z_b^5 \\
+ 28 Z_a^6 Z_b^4 + 8 Z_a^7 Z_b^3 + Z_a^8 Z_b^2)) + Z_a^5 Z_b (720 Z_b \\
+ 5760 Z_a) / (576 (Z_a^2 Z_b^8 + 8 Z_a^3 Z_b^7 + 28 Z_a^4 Z_b^6 \\
+ 56 Z_a^5 Z_b^5 + 70 Z_a^6 Z_b^4 + 56 Z_a^7 Z_b^3 + 28 Z_a^8 Z_b^2 \\
+ 8 Z_a^9 Z_b + Z_a^{10}))

F_{SSSSE}(Z_a, Z_b, 0) = Z_a Z_b (832 Z_a^2 Z_b^6 - 6080 Z_a^3 Z_b^5 + 12960 Z_a^4 Z_b^4 \\
- 6080 Z_a^5 Z_b^4 + 832 Z_a^6 Z_b^2) / (32 (Z_b^9 + 9 Z_a Z_b^8 \\
+ 36 Z_a^2 Z_b^7 + 84 Z_a^3 Z_b^6 + 126 Z_a^4 Z_b^5 + 126 Z_a^5 Z_b^4 \\
+ 84 Z_a^6 Z_b^3 + 36 Z_a^7 Z_b^2 + 9 Z_a^8 Z_b + Z_a^{10}))

F_{PPPPE}(Z_a, Z_b, 0) = 93 Z_a^5 Z_b^5 / (Z_b^9 + 9 Z_a Z_b^8 + 36 Z_a^2 Z_b^7 + 84 Z_a^3 Z_b^6 \\
+ 126 Z_a^4 Z_b^5 + 126 Z_a^5 Z_b^4 + 84 Z_a^6 Z_b^3 + 36 Z_a^7 Z_b^2 \\
+ 9 Z_a^8 Z_b + Z_a^{10})
\[ F_{PPPPE}(Z_a, Z_b, 2) = 45 Z_a^5 Z_b^5 / \left( Z_b^9 + 9 Z_a Z_b^8 + 36 Z_a^2 Z_b^7 + 84 Z_a^3 Z_b^6 + 126 Z_a^4 Z_b^5 + 126 Z_a^5 Z_b^4 + 84 Z_a^6 Z_b^3 + 36 Z_a^7 Z_b^2 + 9 Z_a^8 Z_b + Z_a^9 \right) \]

\[ F_{PSPE}(Z_a, Z_b, 1) = \frac{(3600 Z_a^4 Z_b^5 - 1440 Z_a^5 Z_b^4)}{(192 (Z_b^8 + 8 Z_a Z_b^7 + 28 Z_a^2 Z_b^6 + 56 Z_a^3 Z_b^5 + 70 Z_a^4 Z_b^4 + 56 Z_a^5 Z_b^3 + 28 Z_a^6 Z_b^2 + 8 Z_a^7 Z_b + Z_a^8)) - (1440 Z_a^4 Z_b^5 - 3600 Z_a^5 Z_b^4)} / (192 (Z_b^8 + 8 Z_a Z_b^7 + 28 Z_a^2 Z_b^6 + 56 Z_a^3 Z_b^5 + 70 Z_a^4 Z_b^4 + 56 Z_a^5 Z_b^3 + 28 Z_a^6 Z_b^2 + 8 Z_a^7 Z_b + Z_a^8)) \]

\[ D_{SE}(Z_a, Z_b) = Z_a Z_b (128 Z_a Z_b^3 - 512 Z_a Z_b^2 + 128 Z_a Z_b) / (64 (Z_b^5 + 5 Z_a Z_b^4 + 10 Z_a Z_b^3 + 10 Z_a Z_b^2 + 5 Z_a^4 Z_b + Z_a^5))^2 \]

\[ D_{PPE}(Z_a, Z_b) = (Z_a Z_b^5) / (Z_b / 2 + Z_a / 2)^{10} \]

\[ F_{PSPE}(Z_a, Z_b, 1) = -Z_a Z_b (4224 Z_a^3 Z_b^5 - 11040 Z_a^4 Z_b^4 + 2496 Z_a^5 Z_b^3) / \left( (192 (Z_b^9 + 9 Z_a Z_b^8 + 36 Z_a Z_b^7 + 84 Z_a Z_b^6 + 126 Z_a Z_b^5 + 126 Z_a Z_b^4 + 84 Z_a Z_b^3 + 36 Z_a Z_b^2 + 9 Z_a Z_b + Z_a^2) - Z_a Z_b (2496 Z_a Z_b^3 - 11040 Z_a Z_b^2) \right) \]
\[ + 4224 z_a^5 z_b^7 \] / \( 192 (z_b^9 + 9 z_a z_b^8 + 36 z_a^2 z_b^7 \]

\[ + 84 z_a^3 z_b^6 + 126 z_a^4 z_b^5 + 126 z_a^5 z_b^4 + 84 z_a^6 z_b^3 \]

\[ + 36 z_a^7 z_b^2 + 9 z_a^8 z_b + z_a^9 \)
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