Electron-Impact Excitation Cross-Sections for Atomic Oxygen.

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Finally, the author dedicates this thesis to his parents and wife.
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ABSTRACT

The angular momentum recoupling coefficients which arise in the close-coupling treatment of electron-atom scattering are classified and evaluated. The electron-impact excitation cross sections for \( \text{OI} ({}^3\text{P}-{}^3\text{s}^3\text{S}^0) \) are calculated in the unitarized Born, nonexchange, and close-coupling approximations. The close-coupling cross sections have the same energy dependence as measurements by Stone and Zipf, but are lower in magnitude by a factor of 4. Two autodetaching levels, \( 0^- {}^2\text{p}^3({}^4\text{S}){}^3\text{s}^2({}^4\text{S}^0) \) and \( 0^- {}^2\text{p}^3({}^4\text{S}){}^3\text{s}{}^3\text{p}^2({}^2\text{P}) \), are found at 10.61 and 9.66 eV, respectively. In comparison with other works, the energies of these autodetaching levels are too high. This is as expected and the sources of error are indicated. Finally, suggestions are given for improvement of electron-atom scattering calculations in future work.
CHAPTER I
INTRODUCTION

The Quantum Mechanical treatment of electron-atom scattering has been a subject of continued interest since the discovery of Quantum Mechanics. Atomic physicists and chemists are interested in details of atomic structure that can be inferred from scattering cross sections. From a more practical point of view, information obtainable from the solution of electron-atom scattering problems is of interest in plasma physics, aeronomy, astrophysics, and radiation physics.

The close-coupling approximation is one of the most successful methods used to calculate atomic scattering cross sections. The wave function of projectile plus target is approximated by

$$\psi = A \sum_{i=1}^{N} \phi_i F_i(\vec{x})$$

(1)

where the $\phi_i$ are the eigenfunctions of the target, the $F_i(\vec{x})$ are the expansion coefficients, $\vec{x}$ is the spatial and spin coordinate of the projectile electron, $N$ is the number of states included in the expansion, and $A$ is the antisymmetrization operator. When more than one target configuration is included in the expansion, it is referred to as a multi-configuration close-coupling (MCCC) expansion.
Smith and Morgan\textsuperscript{1} used techniques developed by Fano\textsuperscript{2} to derive expressions for the potentials that arise in the MCCC approximation. These expressions are completely general, i.e., no restrictions are placed on the configurations which are included in the close-coupling expansion except that the orbitals used in the representation of these configurations must be mutually orthogonal. The potentials involve rather complicated angular momentum recoupling coefficients which have not been evaluated previously. Smith and Morgan\textsuperscript{2} give expressions for two of the spin recoupling coefficients and make a few statements about the algebra of recoupling, but make no attempt to classify and evaluate the complete set of recoupling coefficients that arise in the evaluation of the close-coupling potentials. In this work, the recoupling coefficients that are involved in the MCCC approximation are classified and evaluated. To investigate the utility of the MCCC approximation, we calculate the cross section for excitation of oxygen from the $^3P$ ground state to the $3s^3S_0$ excited state (the notation for this process is $\text{OI}(^3P-3s^3S_0)$). Although there are many similar problems which are good tests of the MCCC approximation, the $\text{OI}(^3P-3s^3S_0)$ cross section is of particular interest in the atmospheric physics of Earth\textsuperscript{3} and Mars.\textsuperscript{4} Fast photoelectrons, produced in the upper atmosphere of the Earth by the absorption of solar ultraviolet radiation by the
neutral constituents, lose energy in collision processes. The excitation of the neutral particles produces a substantial component of the dayglow luminosity of the upper atmosphere. The resonance triplet of atomic oxygen

\[ \text{OI}(2p^3 3s^3 S^o) \rightarrow \text{OI}(2p^4 3P) + h\nu \quad (2) \]

is one of the prominent features. Thus, a knowledge of the electron impact excitation cross section is of particular importance.

Prior to the start of this work, no experimental determination of the \( \text{OI}(^3P-3s^3 S^o) \) cross section had been made, and the only previous theoretical calculation for this process is based on a semi-classical impact-parameter method developed by Seaton. In Seaton's method, the cross section for transition from an initial target state \( i \) to a final target state \( j \) is given by

\[ Q(i\rightarrow j) = 2\pi \int_0^\infty P_{ji}(\beta) \beta d\beta \quad (3) \]

where \( P_{ji}(\beta) \), the transition probability, is a function of the impact parameter, \( \beta \). The parameter \( \beta_0 \) is discussed below. From first order time-dependent perturbation theory, the transition probability is

\[ P_{ji} = \frac{1}{\mathcal{H}} \frac{1}{\omega_i} \left| \int_{-\infty}^{+} e^{i\Delta Et/\mathcal{H}} v_{ji}(t) dt \right|^2, \quad (4) \]
where \( \omega_i \) is the statistical weight of the initial level, and \( \Delta E \) is the energy difference between the initial and final states. The potential that is used in the calculation of \( V_{ji}(t) \) is the coulomb interaction of the projectile with the nucleus and bound electrons of the target. In the calculation of \( V_{ji}(t) \), it is assumed that the projectile electron moves in a rectilinear orbit with the distance of closest approach being \( \beta \). As \( \beta \to 0 \), \( P_{ji}(\beta) \) diverges and the cutoff at \( \beta_0 \) is introduced to eliminate this divergence. The justification for this method is that the major contribution to the total cross section for an allowed transition comes from large impact parameters; moreover, procedures can be given for making a reasonable estimate of the cutoff parameter. For example, \( \beta_0 \) may be adjusted so that agreement with a first Born approximation is obtained at high energies.

The impact parameter calculation of the \( \text{OI}(^3P-3s^3S^0) \) cross section was carried out by Stauffer and McDowell. They used a 3s orbital in the representation of the \( 3s^3S^0 \) state which was generated by Percival in an approximation that neglected exchange effects. This gives rise to a 3s orbital which is spatially too extended and results in an overestimate of the cross sections at high energies. At low energies, where small impact parameters dominate total cross sections, their results probably give only an order-of-magnitude estimate of the cross section.
Stone and Zipf have very recently measured the electron excitation function for OI(3s\(^3\)S\(^0\)). In their experiment, electrons are inelastically scattered by oxygen atoms in the \(^3\)P ground state. These atoms, being in excited states, make radiative transitions to lower states. The experimentalists monitor the intensity of the radiation that corresponds to a transition from 3s\(^3\)S\(^0\) to \(^3\)P (The wavelength is 1304 Å). Thus, their results are a measure of the population of the 3s\(^3\)S\(^0\) state and include a component which is due to other excited states cascading down to the 3s\(^3\)S\(^0\) state. One of the primary difficulties in this experiment is the determination of the density of OI(\(^3\)P).

Sawada and Ganas calculated this excitation cross section in a distorted wave independent-particle model (IPM) approximation. The excited electron is assumed to be in the IPM potential of the form

\[
U_B(r) = -\frac{2}{r} \left\{ \frac{Z-1}{H(e^{-r/d}-1)+1} + 1 \right\}
\]

where \(Z=8\). The parameters \(d\) and \(H\) are chosen so as to reproduce the single particle levels of atomic oxygen. The 2p and 3s orbitals, which are used in the cross-section calculation, are obtained from the solution of

\[
\left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} - U_B(r) + E_n \lambda \right] P_{n\lambda}(r) = 0,
\]
where \( n^l=2p,3s \).

The scattering electron moves in an IPM potential of the form

\[
U(r) = -\frac{2}{r}\left\{\frac{Z}{H'(e^{-r/d'}-1)+1}\right\}
\]

(7)

where \( d' \) and \( H' \) are chosen so as to reproduce the total cross section, \( \sigma_T \), as measured by Sunshine et al.\(^{10} \) Once these parameters have been determined, they then use this potential to calculate the \( \text{OI}(^3P-3s^3S^0) \) cross section. They make a partial wave expansion of the total wave function and approximate the direct contribution to the transition matrix by

\[
T_{ij}^D = \sqrt{k_i k_j} \int_0^\infty f_{\ell_i}(r)V_{ij}(r)f_{\ell_j}(r)dr .
\]

(8)

The distorted wave \( f_{\ell_i}(r) \) is obtained from the regular solution of

\[
\left[ \frac{d^2}{dr^2} - \frac{\ell_i(\ell_i+1)}{r^2} - U(r) + k_i^2 \right] f_{\ell_i}(r) = 0 ,
\]

(9)

where \( k_i^2 \) and \( \ell_i \) are, respectively, the energy and orbital angular momentum of the projectile in channel \( i \). The interaction matrix is

\[
V_{ij} = \langle \psi_i | V | \psi_j \rangle
\]

(10)
where $V$ is the coulomb interaction of the projectile with the nucleus and bound electrons of the target. The IPM 2p and 3s functions are used in the representation of the target states $\psi_i$ and $\psi_j$. The exchange contribution to the transition matrix is calculated in a similar manner.

In this work, the OI(\,^3P-3s^3S) cross section is calculated in an unitarized Born, nonexchange (MCCC approximation with exchange terms in MCCC equations left out), and MCCC approximations.

In the unitarized Born approximation,\textsuperscript{11} the $R$-matrix, which is related to the $T$-matrix by

$$T = -2i \frac{R}{(1-iR)},$$

is approximated by

$$R_{ij}^B = \sqrt{k_i k_j} \int_0^\infty j_{\ell_i}(r) V_{ij}(r) j_{\ell_j}(r) dr,$$

where $j_{\ell_i}(r)$ and $j_{\ell_j}(r)$ are spherical bessel functions, and $V_{ij}$ is the interaction matrix as defined in the discussion of the IPM distorted wave approximation with the exception that the Hartree-Fock functions are used in the calculation of $V_{ij}(r)$.

In the nonexchange and MCCC approximations the $R$-matrix is obtained from the numerical solution of the
appropriate set of equations. The procedures for the solution of these equations were developed by Smith, Henry, and Burke\textsuperscript{12} and details of the method are given in Ref. 13.

The organization of the rest of this work is as follows: in Chapter II, the MCCC theory is reviewed; in Chapter III, techniques used in the evaluation of the recoupling coefficients are reviewed and three of the angular momentum recoupling coefficients that arise in the MCCC theory are evaluated; in Chapter IV, the calculated results for the OI($^3P$-$^3S$) cross section are presented, discrepancies between experiment and theory discussed, and suggestions for improved cross-section calculation are given.
CHAPTER II
REVIEW OF MULTI-CONFIGURATION CLOSE-COUPLING

In this chapter, the derivation of the MCCC equations is reviewed. In the first section, the form of the trial wave function is discussed. In the second section, the derivation of the MCCC is outlined and expressions for the MCCC potentials are recorded.

The Trial Wave Function

In this work, it is assumed that the Hamiltonian is spin-independent; consequently, the conserved quantum numbers are $L, m_L, S, m_S,$ and $\pi$, where $L$ is the total orbital angular momentum, $m_L$ is the azimuthal projection of $L$, $S$ is the total spin angular momentum, $m_S$ is the azimuthal projection of $S$, and $\pi$ is the parity. In order to take advantage of this, the representation used is diagonal in $L^2, m_L, S^2, m_S,$ and $\pi$.

Consider the collision of an electron with an atomic system of N electrons and nuclear charge $Z$. Let the totally antisymmetric $N+1$ electron wave function be

$$\psi(\Gamma_1, \hat{x}_1 \ldots \hat{x}_{N+1}) = (N+1)^{-1/2} \sum_{p=1}^{N+1} (-1)^{N+1-p}$$

$$\sum_j \psi(\Gamma_j \hat{x}_j \hat{r}_p \sigma_p) F_{ji}(r_p)/r_p \quad (13)$$
where

$$\psi(\Gamma_j, \hat{x}_p, \sigma_p) = [\psi(\gamma_j, \hat{x}) \times \langle p | k_j \ell_j \ell_{1/2} \rangle^\Gamma_j]$$

(14)

and

$$\psi(\gamma_j, \hat{x}) = (N_\lambda)^{-1/2} \sum (-1)^q \prod \pi_\lambda \langle q_\lambda | n_\lambda \ell_\lambda \alpha_\lambda L_\lambda S_\lambda \rangle^\gamma_j$$

(15)

is an eigenstate of the target. The notation used here, which is summarized in Appendix I, is due to Fano. The space and spin coordinates of the N-electron target are denoted by \( \hat{x} \). The \( \hat{r}_p \) and \( \sigma_p \) denote the angular and spin coordinates, respectively, of the projectile. The quantum number \( \gamma_j \) denotes the complete set of quantum numbers required to specify the target state. The wave function for each subshell \( \lambda \), of principle quantum number \( n_\lambda \) and orbital quantum number \( l_\lambda \), with resultant quantum numbers \( \alpha_\lambda L_\lambda S_\lambda \), is antisymmetrized. The shell angular momenta are coupled together to give \( \alpha_j L_j S_j \). The \( \alpha_j \) specify the way in which the \( L_\lambda \) and \( S_\lambda \) are coupled together, and \( L_j \) and \( S_j \) specify the total orbital and spin angular momenta, respectively, of the target in channel \( j \). The \( \chi \) denotes the vector coupling of the N-electron function and the single-electron spin-angle function \( \langle p | k_j \ell_j \ell_{1/2} \rangle \). The
projectile energy in channel \( j \) is \( k_j^2 \) and the angular momentum is \( \lambda_j \). The complete set of quantum numbers required to specify the state of the atomic system (projectile plus target) in channel \( j \) is \( \Gamma_j = \gamma_j k_j \lambda_j L S M_L M_S \). The function \( F_{ji}^j(r_p) \) describes the radial motion of the outgoing electron in channel \( j \) when the system was initially in channel \( i \). In principle, the summation over \( j \), occurring in Eq. (13), includes all eigenstates of the \( N \)-electron target and all \( \lambda_j \) which satisfy the triangular rules

\[
\mathbf{L} = \mathbf{L}_j + \mathbf{L}_j
\]  

and

\[
\mathbf{S} = \mathbf{S}_j + \frac{1}{2}
\]

and which are not parity forbidden; however, in practice, it is necessary to truncate the summation.

Within the formalism developed by Fano\textsuperscript{2} to calculate atomic matrix elements, the one-electron orbitals with the same angular momentum are required to be mutually orthogonal; for example, the radial part of the \( 1s, 2s, 3s, \ldots \) orbital must be mutually orthogonal. This presents no difficulty in the case of those orbitals used in the representation of the target. However, the scattering
orbitals, $F'_{ji}(r_p)\hat{Y}_j^l(r_p)$, are not in general orthogonal to those orbitals used in the representation of the target. In order to circumvent this problem, the orbital $F'_{ji}(r_p)$ is written

$$F'_{ji} = F_{ji} + \sum_k \alpha_k p_{nl}^k$$  \hspace{1cm} (18)

where

$$\alpha_k = \langle F'_{ji}|p_{nl}^k \rangle \delta_{k}^{l} \delta_{j}^{l'}$$  \hspace{1cm} (19)

$$\langle F_{ji}|p_{nl}^k \rangle \delta_{k}^{l} \delta_{j}^{l'} = 0 \hspace{0.5cm} \forall \ k,$$  \hspace{1cm} (20)

and $k$ ranges over all the one-electron orbitals included in the representation of the target. Equation (18) is substituted into Eq. (13) to give

$$\psi(\Gamma_j, \hat{x}_1, \ldots, \hat{x}_{N+1}) = (N+1)^{-1/2} \sum_{p=1}^{N+1} (-1)^{N+1-p} \sum \psi(\Gamma_j, \hat{x}_{i}, \hat{r}_p \sigma_p)$$

$$F_{ji}(r_p)/r_p + \sum \phi_{i}^{\mu}(LS\pi, \hat{x}_1, \ldots, \hat{x}_{N+1})$$  \hspace{1cm} (21)

where $\psi(\Gamma_j, \hat{x}_{i}, \hat{r}_p \sigma_p)$ is defined by Eq. (14) and

$$\phi_{i}^{\mu}(LS\pi, \hat{x}_1, \ldots, \hat{x}_{N+1}) = \sum_{q} (-1)^{q} \phi_{i}^{q}(q_{\mu}LS\pi, \hat{x}_1, \ldots, \hat{x}_{N+1}).$$  \hspace{1cm} (22)
The coefficients, $c^j_\mu$, are constants which are determined from the variational principle given in the next section. The sum over $\mu$ runs over all the incomplete subshells included in the eigenfunction expansion and $\phi_\mu$ is an unsymmetrized wave function given by

$$
\phi_\mu(q_\mu LS\pi, x_1 \ldots x_{N+1}) = [\pi_\lambda(q_\lambda | n_\lambda S_{\lambda} \alpha_\lambda L_{\lambda} S_{\lambda})]^{LS\pi}.
$$

(23)

For example, consider the $^1S$ partial wave of the e-H scattering problem where only the $1s$ state is retained in the close-coupling expansion. The orbital angular momentum of the projectile is zero and the radial part of the scattering function is constrained to be orthogonal to the $1s$ orbital. To relax this orthogonality constraint, the expansion for the wave function includes the bound state term $\phi(1s^2 1S)$.

Equation (21) can be interpreted as a configuration interaction expansion: In the first term one of the electrons is in a continuum orbital, while all of the electrons are in bound orbitals in the second term. This expansion satisfies the requirement that all orbitals with the same angular momentum be mutually orthogonal. Equation (21) defines the trial wave function.
In the next section, it is shown that the functions, $F_{ji}(r_p)$, and coefficients, $c^i$, satisfy coupled systems of second order ordinary integro-differential equations. The scattering boundary conditions are

\[ F_{ji}(r_p) \sim r^{j+1} r_p \to 0 \quad (24) \]

\[ F_{ji}(r_p) \sim k_{ji}^{-1/2} (\delta_{ji} \sin \theta_j + R_{ji} \cos \theta_j) \quad k_{ji}^2 > 0 \quad (25) \]

\[ \sim e^{-|k_{ji}|r - |\eta_j| \ln 2k_{ji}} r_p \quad k_{ji}^2 < 0 \quad (26) \]

where

\[ \theta_j = k_{ji} r_p - \lambda_j \pi/2 - \eta_j \ln 2k_{ji} + \sigma_{\lambda_j} \quad (27) \]

\[ \eta_j = - (Z-N)/k_{ji} \quad (28) \]

\[ \sigma_{\lambda_j} = \arg \Gamma(\lambda_j + 1 + i\eta_j) \quad (29) \]

and

\[ k_{ji}^2 = 2(E-E_j) \quad (30) \]
Here $E$ is the total energy, $E_j$ is the energy of the target in channel $j$, and the $R_{ij}$ are the elements of the $R$-matrix.

For notational purposes, it is convenient to establish the following definition:

$$
\psi(\Gamma_i, x_1, \ldots, x_{N+1}) \equiv \sum_j \psi_{ji} + \phi^i(\Gamma, x_1, \ldots, x_{N+1})
$$

where

$$
\psi_{ji} = (N+1)^{-1/2} \sum_{p=1}^{N+1} (-1)^{N+1-p} \psi(\Gamma_j, x_p, \sigma_p) F_{ji}(r_p)/r_p
$$

and

$$
\phi^i(\Gamma, x_1, \ldots, x_{N+1}) \equiv \sum_\mu c_\mu^i \phi(\Gamma, x_1, \ldots, x_{N+1})
$$

**Variational Principle**

The close-coupling equations are derived from the variational principle

$$
\delta [L_{kl} - 1/2 R_{kl}] = 0
$$
where $\delta$ denotes variations with respect to $F_{kl}$ and $c_{\mu}^i$. The variations in the scattering function are such that

$$\delta F_{kl} \sim k^{-1/2} \delta R_{kl} \cos \theta_k$$  \hspace{1cm} (35)$$

subject to the orthogonality constraint, Eq. (19), and the variations $\delta c_{\mu}^i$ are arbitrary. In Eq. (34), the elements of the real and symmetric $R$-matrix $R_{kl}$ are defined by Eq. (6) in terms of the open-channel ($k_j^2 > 0$) wave functions, and

$$I_{kl} = \langle \psi_t^k | H_{N+1} - E | \psi_t^1 \rangle$$  \hspace{1cm} (36)$$

with the Hamiltonian of the full system being

$$H_{N+1} = H_N + H_1(\bar{X}_{N+1}) + \sum_\alpha \frac{1}{r_{N+1,\alpha}}$$  \hspace{1cm} (37)$$

where $H_N$ is the Hamiltonian of the target, $H_1$ is the kinetic energy plus the coulomb interaction of the projectile with the nucleus, and $\sum_\alpha 1/r_{N+1,\alpha}$ is the coulomb interaction between the bound electrons of the target and the projectile electron. The trial $\psi_t^k$ is defined by Eq. (21) or alternatively by Eq. (31).

Substitution of $\psi_t^k$ into Eq. (35) along with the application of Green's theorem gives
\[ L_{k1} = \sum_{i,j} L_{ik,jl} + \sum_{i} (L_{ik,l}^c + L_{il,k}^c) + \sum_{\mu,\nu} A_{\mu,\nu} \]  

(38)

where

\[ L_{ik,jl} \equiv \langle \psi_{ik} | H-E | \psi_{jl} \rangle , \]  

(39)

\[ L_{il,k}^c \equiv \langle \psi_{ik} | H-E | \phi^i (L_k S_k \pi_k) \rangle , \]  

(40)

and

\[ A_{\mu,\nu} \equiv \langle \phi^\mu (L_k S_k \pi_k) | H-E | \phi^\nu (L_j S_j \pi_j) \rangle . \]  

(41)

Techniques for the evaluation of the matrix elements defined by Eqs. (39), (40), and (41) have been developed by Fano. The matrix elements have been evaluated by Smith and Morgan. In the reduction of Eq. (24), they assume that \( \psi(\gamma_1 \bar{x}) \) is an exact eigenfunction of the \( N \)-electron atom with eigenenergy \( \epsilon_i \); i.e.,

\[ \langle \psi(\gamma_1 \bar{x}) | H_{N-\epsilon_i} | \psi(\gamma_j \bar{x}) \rangle = \delta_{ij} . \]  

(42)

Equations (32) and (42) are substituted into Eq. (39) and reduced to
\[ L_{ik,jl} = \int F_{ik} L_{ij} F_{jk} \, dr \]  
\[ (43) \]

where

\[ L_{ij} = -\frac{1}{2} \left[ \frac{d^2}{dr^2} - \frac{\ell_i (\ell_i + 1)}{r^2} + \frac{2z}{r} + 2(E - \varepsilon_i) \right] \delta_{ij} \]

\[ + V_{ij} + W_{ij}, \]  
\[ (44) \]

\[ V_{ij}(r) = \sum \left( \left[ \pi^2 \delta \left(N_i^2 + N_j^2 + \delta \lambda \rho_i - \delta \lambda \rho_j \right) \right] \left[ N_{ij} \lambda \right]^{1/2} \]

\[ (-1)^{\lambda+\rho_i+\rho_j} \sum \left( \left[ \pi^2 \delta \left(N_i^2 + N_j^2 + \delta \lambda \rho_i - \delta \lambda \rho_j \right) \right] \left[ N_{ij} \lambda \right]^{1/2} \]

\[ \sum \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \frac{1}{\rho_i \rho_j} \]

\[ \left( \ell_i \ell_j \ell_i \ell_j \ell_i \ell_j \ell_i \ell_j \right) \]

\[ (45) \]
\[ W_{ij} F_{j1}(r) = \sum_{\lambda} \left\{ [\pi_\lambda \delta(N^i_{\lambda}, N^j_{\lambda} + \delta \rho_i \delta \rho_j)] [N_{\rho_i} N_{\rho_j}] \right\}^{1/2} \]

\[ (-1)^{\lambda + 1} \left( 2^\lambda + 1 \right) \left( 2^{\rho_i + 1} \right) \left( 2^{\rho_j + 1} \right)^{-1/2} \sum \bar{a}_i \ldots L_{\rho_j} \]

\[ \left( \rho_i \rho_j \bar{a}_i \bar{L}_i \rho_i \rho_j \bar{a}_j \bar{L}_j \right) \left( \rho_j \rho_j \bar{a}_j \bar{L}_j \rho_j \rho_j \bar{a}_j \bar{L}_j \right) \]

\[ \left( \rho_i \rho_j \bar{a}_i \bar{L}_i \rho_i \rho_j \bar{a}_j \bar{L}_j \right) \left( \rho_j \rho_j \bar{a}_j \bar{L}_j \rho_j \rho_j \bar{a}_j \bar{L}_j \right) \]

The sum over \( \bar{c} \) is defined by

\[ \Sigma \] \[ \begin{cases} b_i b_j & \text{if } \pi_\lambda \delta(N^i_{\lambda}, N^j_{\lambda}) = 1 \\ 0 & \text{if } \pi_\lambda \delta(N^i_{\lambda}, N^j_{\lambda}) = 0 \end{cases} \]
The reduced matrix element, \( (\ell | c^{k}| \ell') \), is non-zero for \( |\ell-\ell'| k \leq \ell+\ell' \) and \( t+\ell+\ell' \) even. The range of the sum over \( t \) is restricted to those values of \( t \) for which the reduced matrix elements appearing under the summation are non-zero. For example, in the expression for \( V_{ij} \) the lower limit on \( t \) is given by

\[
\text{Max}(|\ell_i-\ell_j|,|\rho_i-\rho_j|) \tag{48}
\]

and the upper limit is given by

\[
\text{Min}(\ell_i+\ell_j,\rho_i+\rho_j) \tag{49}
\]

If \( t+\ell_i+\ell_j \) is even and

\[
(-1)^{\ell_i+\ell_j} = (-1)^{\rho_i+\rho_j} \tag{50}
\]

then there is a non-zero contribution from the sum over \( t \).

The sum over \( \tilde{\alpha}_i \tilde{S}_i \tilde{L}_i \) arises from the fractional parentage expansion of the \( \rho_i \)th shell wave of \( \psi_{ik} \); i.e.,

\[
(q_{\rho_i} | \eta_{\rho_i}^{\ell} \tilde{\alpha}_i \tilde{S}_i \tilde{L}_i) = \sum_{\rho_i} \frac{N_{\rho_i}^{\ell} - 1}{\rho_i \rho_i \rho_i} (\rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_i \rho_
where $x$ denotes the vector coupling of $\bar{S}_{\rho_i}$ with $1/2$ to give $S_{\rho_i}^\lambda$ and $\bar{L}_{\rho_i}$ with $l_{\rho_i}$ to give $L_{\rho_i}^\lambda$. The wave function for the $\rho_j$th shell of $\psi_j \phi \lambda$ is expanded in a similar manner and this expansion gives rise to a sum over $\bar{\alpha}_{\rho_j \rho_i \rho_i}$. The other barred quantum numbers are defined for each subshell, $\lambda$, by

\[
\bar{L}_\lambda = L_{\lambda}^i = L_{\lambda}^j,
\]

\[
\bar{S}_\lambda = S_{\lambda}^i = S_{\lambda}^j,
\]

and

\[
\bar{\alpha}_\lambda = \alpha_{\lambda}^i = \alpha_{\lambda}^j.
\]

The barred quantum numbers are referred to as spectator quantum numbers. The spin and angular parts of the matrix elements are diagonal in the spectator quantum numbers. The overlap of the two spin functions is a recoupling coefficient,

\[
\langle S_1 \ldots (\bar{S}_{\rho_i} \frac{1}{2}(N)) S_{\rho_i} \ldots \bar{S}_{b_j} \frac{1}{2}(N+1), \alpha_j S_j | \bar{S}_1 \ldots
\]

\[
(\bar{S}_{\rho_j} \frac{1}{2}(N)) S_{\rho_j} \ldots \bar{S}_{b_j} \frac{1}{2}(N+1), \alpha_j S_j \rangle. \quad (55a)
\]

On the left, $\alpha_j$ specifies the way
\begin{equation}
\bar{S}_1, \bar{S}_2, \ldots, \bar{S}_{\rho_i-1}, \bar{S}_{\rho_i}, \bar{S}_{\rho_i+1}, \ldots, \frac{1}{2} (N+1) \tag{55b}
\end{equation}

are coupled together to give a total spin of $S_i$. An angular momentum of $\frac{1}{2}$ is coupled to $\bar{S}_{\rho_i}^i$ to give $S_{\rho_i}^i$; the notation for this is $(\bar{S}_{\rho_i}^i \frac{1}{2} (N)) S_{\rho_i}^i$. The $N$ and $N+1$ are used to distinguish between the two angular momentum of $1/2$. On the right, $\alpha_j$ specifies the way

\begin{equation}
\bar{S}_1, \bar{S}_2, \ldots, \bar{S}_{\rho_j-1}, \bar{S}_{\rho_j}, \bar{S}_{\rho_j+1}, \ldots, \frac{1}{2} (N+1-\varepsilon) \tag{56}
\end{equation}

are coupled together to give a total spin of $S_j$. An angular momentum of $\frac{1}{2}$ is coupled to $\bar{S}_{\rho_j}^j$ to give $S_{\rho_j}^j$; the notation for this is $(\bar{S}_{\rho_j}^j \frac{1}{2} (N+\varepsilon)) S_{\rho_j}^j$. For the direct potential, $V_{ij}$, the value of $\varepsilon$ is 0. For the exchange potential, $W_{ij}$, the value of $\varepsilon$ is 1. The definition of the orbital recoupling coefficients is analogous to that of the spin recoupling coefficient. The notation

$$[\bar{L}_{\rho_i}^j (\lambda \rho_j \lambda) \rho_i \rho_j] \tag{57}$$

means $\lambda \rho_j^j$ is coupled with $\lambda \rho_i^i$ to give $\lambda \rho_i^i$ and then $\lambda \rho_i^i$ is coupled with $\bar{L}_{\rho_i}^i$ to give $L_{\rho_i}^i$. Chapter III is devoted to the evaluation of these recoupling coefficients. The spectator occupation numbers, $\bar{N}_\lambda$, are defined by
\[
\tilde{N}_\lambda = \begin{cases} 
N_\lambda & \lambda \neq \rho_i \text{ or } \lambda \neq \rho_j \\
N_{i-1} & \lambda = \rho_i \\
N_{j-1} & \lambda = \rho_j 
\end{cases}
\] (58)

Substitution of Eqs. (32) and (33) into Eq. (40) gives

\[
L_{i l, k} = \sum_v c_v^1 \int v_{i, v} F_{i k} \, dr
\] (59)

where

\[
v_{i, v}(r) = \sum_{\rho_v} \frac{b_v}{\rho_v+1} \sum_{\lambda} \frac{N_{\lambda}^{1/2}(-1)^{1/2}}{N_{\rho_v}^{1/2}(-1)^{1/2}} \langle \ldots \tilde{S}_{\rho_v} \ldots \tilde{S}_{\rho_v} \ldots \alpha_1 S_1 \ldots (\tilde{S}_{\rho_v} \frac{1}{2} S_{\rho_v} \ldots \tilde{S}_{\rho_v} \alpha_v S_v) \rangle \\
\langle \ldots \tilde{L}_{\rho_v} \ldots \tilde{L}_{\rho_v} \alpha_1 L_1 \ldots (\tilde{L}_{\rho_v} \frac{1}{2} L_{\rho_v} \ldots \tilde{L}_{\rho_v} \alpha_v L_v) \rangle \\
\left[ -\frac{1}{2} \left( \frac{d^2}{dr^2} - \frac{\ell \rho_v (\ell \rho_v + 1)}{r^2} + \frac{2\ell}{r} \right) \right] + \sum_c
\]

\[
\frac{1}{\pi} \delta(N_{\lambda}^{1/2}, N_{\rho_v}^{1/2} + \delta \lambda \rho_i - \delta \lambda \rho_v - \delta \lambda \rho_v) \right) \right] \frac{N_{\rho_v}}{N_{\rho_i}} \frac{N_{\rho_i}}{N_{\rho_v}} \\
n(\alpha_{\rho_i} \ldots \tilde{L}_{\rho_i} \ldots \alpha_{\rho_i} \ldots \tilde{L}_{\rho_i})^{1/2}(-1)^{\Delta \rho_i} \sum_{\rho_i} \frac{(l \rho_i N_{\rho_i} + \alpha_{\rho_i} S \ldots L_{\rho_i}) \{ \alpha_{\rho_i} \ldots \tilde{L}_{\rho_i} \}}{
\tilde{L}_{\rho_i} \ldots \tilde{L}_{\rho_i} \ldots \alpha_{\rho_i} \ldots \tilde{L}_{\rho_i}}
\] (60)
\[ \langle \sigma_v \mid c^t \mid \rho_i \rangle = \theta_{i} \theta_{j}^{\varepsilon = 0} \psi_t (P_{\rho_i}, P_{\rho_v}, r) \]

\[ + (1 - \delta_{\rho_i \sigma_v}) \langle S_i \mid S_v \rangle^{\varepsilon = 1} \psi_t (P_{\rho_i}, P_{\rho_v}, r) \]
and

\[ <\theta_i|\theta_v> = <\bar{L}_1\cdots(\bar{L}_{\rho_i}\rho_i)L^i_{\rho_i}\cdots\bar{L}_{\rho_{i+1}}(\bar{L}_{\rho_{i+1}}\rho_{i+1})L^i_{\rho_{i+1}}\cdots L_{M-i,L_i}| \]

\[ \bar{L}_1\cdots(\bar{L}_{\rho_{i+1}}\rho_{i+1})L^v_{\rho_{i+1}}\cdots[\bar{L}_{\rho_{i+1}}(\bar{L}_{\rho_{i+1}}\rho_{i+1})L^v_{\rho_{i+1}}\cdots L_v> . \]

(64)

The definition of the sum over \( \bar{c} \) in the expression for \( V_{i,v} \) in dependent on the occupation numbers \( N^i_\lambda \) and \( N^j_\lambda \). If

\[ b_v \sum_{\lambda=1}^\infty |N^i_\lambda - N^j_\lambda| = 1 , \] (65)

then \( \sigma_v \) is defined to be that value of \( \lambda \) for which

\[ |N^i_\lambda - N^j_\lambda| = 1 \] (66)

and

\[ \sum_{c} \frac{b_i b_v}{\rho_i \rho_v} \delta(\rho_i \rho_j) \] (67)

If

\[ b_v \sum_{\lambda=1}^\infty |N^i_\lambda - N^j_\lambda| = 3 , \] (68)
then

$$
\Sigma = \sum_{\sigma} \rho_{i,\sigma,\sigma}^{\nu} \rho_{\nu > \sigma}^{\nu}
$$

(69)

If

$$
\sum_{\lambda=1}^{b_{\nu}} |N_{\lambda}^{i} - N_{\lambda}^{j}|
$$

(70)

is not equal to 1 or 3, then the contribution from the sum over $\bar{c}$ is zero. All other summations and notation have been discussed previously in connection with the evaluation of the direct potential $V_{ij}$ and the exchange potential $W_{ij}$. Substitution of Eq. (22) into Eq. (41) gives

$$
A_{\mu,\nu} = \sum_{\rho > \rho} \sum_{\lambda=\rho_{<}+1}^{\rho_{>} - \rho_{<}} \{ (\ldots N_{\lambda}^{i}, N_{\lambda}^{j} \ldots ) \} \left( \sum_{\alpha} \alpha_{\mu} \ldots \bar{N}_{\nu} \right) \left( \sum_{\beta} \beta_{\nu} \right) \left( \sum_{\gamma} \gamma_{\nu} \right)
$$

(71)
\[ <\bar{s}_1 \ldots (\bar{s}_\rho \frac{1}{x^2}) s_\rho \ldots s_\mu | \bar{L}_1 \ldots (\bar{L}_\rho \& \rho) L_\rho \ldots s_\mu s_\nu > \]

\[ <\bar{L}_1 \ldots (\bar{L}_\rho \& \rho) L_\rho \ldots s_\mu | \bar{L}_1 \ldots (\bar{L}_\rho \& \rho) L_\rho \ldots s_\mu s_\nu > \]

\[ (-\frac{1}{2}) \int dr \left[ \frac{d^2}{dr^2} - \frac{\ell_\rho (\ell_\rho + 1)}{r^2} + \frac{2z}{r} \right] p_{nl} (r) \]

\[ + \phi_i | \sum_{i,j} 1/\rho_i \phi_i > - \delta_{\mu,\nu} \]

where the two-body matrix element has been evaluated by Fano. The notation and summation ranges have been discussed in connection with the evaluation of \( V_{ij} \) and \( W_{ij} \). Substituting Eqs. (43), (60), and (71) into Eq. (34) gives

\[ \delta \left[ \sum_{i,j} F_{ik} L_{ij} F_{jl} dr + \sum_{j,\mu} c_{\mu}^k | V_{\nu}, j F_{jl} dr \right] \]

\[ + \sum_{i,\nu} c_{\nu}^l | V_{\nu}, i F_{ik} dr + \sum_{\mu,\nu} c_{\mu}^k c_{\nu}^l A_{\mu,\nu} - \frac{1}{2} R_{kl} \right] = 0 . \]

(72)

Variations of Eq. (72) with respect to \( F_{mn} \) gives

\[ \sum_{i,j} L_{ij} F_{jl} + \sum_{\mu} c_{\mu}^1 V_{\mu,i} = 0 . \]

(73)

Variations of Eq. (72) with respect to \( c_{\lambda}^m \) leads to
\[ \sum \mathcal{V} \mu \mathcal{v} + \sum \int \mathcal{v} \mu, j \mathcal{F} \mathcal{j} \mathcal{l} \, dr = 0 \quad \text{(74)} \]

Introducing the orthogonality requirement into Eq. (73) using Lagrange multipliers, \( M_\lambda \), gives

\[ \sum \mathcal{L} \mathcal{i} \mathcal{j} \mathcal{F} \mathcal{j} \mathcal{l} + \sum \mathcal{C} \mu \mathcal{v}, \mu, i + \sum M_\lambda \mathcal{P} n_\lambda \delta_\lambda \mathcal{L} \mathcal{i} \mathcal{L} \mathcal{\lambda} = 0 \quad \text{(75)} \]
CHAPTER III

CLASSIFICATION AND EVALUATION OF
ATOMIC RECOUPLING COEFFICIENTS

In Chapter II, the integro-differential equations for the scattering function were expressed in terms of potentials which involved angular momentum recoupling coefficients. In this chapter, all of the possible recoupling coefficients that can arise in the evaluations of these potentials are given and classified. After a review of basic recoupling theory, three of the recoupling coefficients are evaluated to illustrate the recoupling techniques used here. The complete evaluation of the recoupling coefficients is given in Appendix II.

Classification of Recoupling Coefficients

The general form of the orbital recoupling coefficients is

\[ <\overline{L}_1 \overline{L}_2 \cdots \overline{L}_{\rho_i-1} [\overline{\rho}_i (k \rho_j) \rho_i ] \overline{L}_i \overline{L}_j \cdots (\overline{\sigma}_i \sigma_i) \cdots, \]

\[ \overline{L}_i | \overline{L}_1 \overline{L}_2 \cdots (\overline{\rho}_j \rho_j) \cdots \overline{L}_{\sigma_j-1} [\overline{\sigma}_j (k \sigma_j) \sigma_j ] \overline{L}_j \overline{L}_j \cdots, \overline{L}_j > \]

(76)

and that of the spin is
\[
<\tilde{s}_1 \tilde{s}_2 \ldots \tilde{s}_{\rho_i - 1} (\tilde{s}_i \frac{1}{2}(N)) s_i \tilde{s}_i \ldots (\tilde{s}_i \frac{1}{2}(N+1)) \ldots,
\]
\[
S_i |\tilde{s}_1 \tilde{s}_2 \ldots (\tilde{s}_j \frac{1}{2}(N)) s_j \ldots (\tilde{s}_j \frac{1}{2}(N+1)) s_j \ldots , s_j
\]

(77)

where \(\rho_i\) and \(\sigma_j\) always locate the shell containing the angular momentum \(k\), and the \(L^\alpha_\lambda\) and \(S^\alpha_\lambda\) are the results of coupling the \(\lambda\)th shell to the previous coupling; i.e.,

\[
| \ldots ((\tilde{l}_1 \tilde{l}_2) L_3 \ldots L_{\rho_i - 1} L_{\rho_i - 1}) L_i \rangle. \quad (78)
\]

If \(\rho_i = \sigma_i\), then the left-hand side of Eq. (76) and (77) is replaced by

\[
<\tilde{l}_1 \tilde{l}_2 \ldots [(\tilde{l}_i \tilde{l}_j) \tilde{l}_i \ldots \tilde{l}_i \tilde{l}_i \ldots L_i \rangle \quad (79)
\]

and

\[
<\tilde{s}_1 \tilde{s}_2 \ldots [(\tilde{s}_i \frac{1}{2}(N)) \tilde{s}_i \frac{1}{2}(N+1)] s_i \ldots , s_i \rangle, \quad (80)
\]

respectively.

For \(\rho_j = \sigma_j\), the right-hand side of Eqs. (76) and (77) is replaced by

\[
| \tilde{l}_1 \tilde{l}_2 \ldots [(\tilde{l}_j \tilde{l}_j) \tilde{l}_j \ldots \tilde{l}_j \tilde{l}_j \ldots L_j \rangle. \quad (81)
\]
and

\[ |\hat{S}_1\hat{S}_2\ldots[(\hat{S}_\rho)^{1/2}(N)\hat{S}\hat{S}_\rho^{1/2}(N+1)]\hat{S}_j\ldots,\hat{S}_j> \quad (82) \]

respectively.

Except for the presence of the angular momentum \( k \), the spin and orbital recoupling coefficients are of the same form. In fact, if \( k \) is set equal to zero and \( \{L_\lambda,\overline{L}_\lambda,L_\lambda\ldots\} \) is replaced by \( \{S_\lambda,\overline{S}_\lambda,S_\lambda\ldots\} \), then it is seen that they are exactly the same. Since the spin recoupling coefficients are a special case of the orbital recoupling coefficients, only the latter are to be considered.

For no two elements of \( \{\rho_i,\sigma_i,\rho_j,\sigma_j\} \) equal, diagramatic representations of the \( 4! \) recoupling coefficients that can occur are given in Figs. 1a, 1b, and 1c.\(^1\) The left and right sides of these recoupling coefficients are represented, respectively, by the top and bottom portions of these recoupling diagrams. Those recoupling coefficients which satisfy the criteria \( \text{Max}(\rho_i,\rho_j) < \text{Min}(\sigma_i,\sigma_j) \) or \( \text{Max}(\sigma_i,\sigma_j) < \text{Min}(\rho_i,\rho_j) \) are referred to as direct recoupling coefficients, and are shown in Fig. 1a. The diagrams shown in Fig. 1b satisfy the criteria \( \text{Max}(\rho_i,\sigma_j) < \text{Min}(\rho_j,\sigma_i) \) or \( \text{Max}(\rho_j,\sigma_i) < \text{Min}(\rho_i,\sigma_j) \), and there are lines crossing in each of these diagrams. Finally, the translational coefficients shown
in Fig. 1c are defined by \( \text{Max}(\rho_i, \sigma_i) < \text{Min}(\rho_j, \sigma_j) \) or \( \text{Max}(\rho_j, \sigma_j) < \text{Min}(\rho_i, \sigma_i) \). Some of these translational coefficients do have lines crossing, but this does not introduce any additional complexity into the evaluation of these coefficients.

Since these recoupling coefficients are Hermitian, the diagrams on the right of Figs. 1a, 1b, and 1c are equal to those on the left. Thus, for no two elements of \( \{\rho_i, \sigma_i, \rho_j, \sigma_j\} \) equal, there are 12 recoupling coefficients to be evaluated: 4 direct, 4 exchange, and 4 translational.

For \( \rho_i = \sigma_i \) or \( \rho_j = \sigma_j \), these recoupling diagrams reduce to two lines, and all the possible two-line recoupling diagrams are shown in Figs. 2a and 2b. These recoupling coefficients are degenerate forms of those shown in Figs. 1a, 1b, and 1c, and their evaluation presents no additional difficulties.

Recoupling Theory

Consider the coupling of three angular momenta \( j_1 \), \( j_2 \), and \( j_3 \) to give a resultant \( J \). There are three possible intermediate angular momenta \( j_{12} \), \( j_{23} \), and \( j_{13} \) with corresponding representations

\[
| j_{12} j_{23} j_{13}; JM \rangle ,
\]

(83)
\[ |j_1(j_2j_3)j_{23};JM> , \] (84)

and

\[ |j_2(j_1j_3)j_{13};JM> . \] (85)

Since these three representations span the same subspace, they are connected by a linear transformation. The transformation connecting the first two representations is

\[ |(j_1j_2)j_{12}j_3;JM> = \sum_{j_{23}} |j_1(j_2j_3)j_{23};J>(j_1j_2)j_{12}j_{23};J> |j_1(j_2j_3)j_{23};JM> \] (86)

where the transformation coefficient is defined in terms of the Racah W-coefficient \( ^{15B} \); i.e.,

\[ |j_1(j_2j_3)j_{23};J>(j_1j_3)j_{12}j_3;j> = \]

\[ [(2j_{12}+1)(2j_{23}+1)]^{1/2} W(j_1j_2j_3;j_{12}j_{23}) . \] (87)

In a similar manner, all the other transformation coefficients relating these three representations can be expressed in terms of Racah W-coefficients.

Now, consider the coupling of four angular momenta where a possible transformation coefficient that may arise
Although this coefficient can be related directly to a Wigner 9-j symbol, which in turn can be related to a sum over Racah W-coefficients, this is not done here. Instead, for the purpose of illustrating a couple of points, this coefficient is evaluated directly in terms of a sum over Racah W-coefficients.

The technique used here is to perform successive recoupling operations until the recoupling coefficient has been expressed as a sum over a product of Racah W-coefficients. The first operation is to uncouple \( j_1 \) and \( j_2 \):

\[
\langle j_{12} j_{34}^J | j_{13} j_{24}^J \rangle = \sum_{\alpha} \langle j_{1j_2} | j_{12} j_{34}^J | (j_{1j_3})_{\alpha j_2}^J \rangle \langle [j_{1} (j_{3} j_{4})_{j_{34}}]_{\alpha j_2}^J | (j_{1} j_{3})_{j_{13}} (j_{2} j_{4})_{j_{24}}^J \rangle
\] (89)

Next, \( j_1 \) and \( j_3 \) are coupled together to give

\[
\langle j_{12} j_{34}^J | j_{13} j_{24}^J \rangle = \sum_{\alpha, \beta} \langle j_{1j_3} | j_{12} j_{34}^J | (j_{1} j_{3})_{\alpha j_2}^J \rangle \langle (j_{1j_3})_{\alpha j_3}^J | (j_{1} j_{3})_{\alpha j_2}^J \rangle
\]
Finally, $j_2$ is coupled with $j_4$ to give

\[
\langle j_1 (j_3 j_4) j_{34}^\alpha | (j_1 j_3) \beta j_4^\alpha \rangle
\]

\[
\langle [ (j_1 j_3) \beta j_4^\alpha ] j_2^J | (j_1 j_3) j_{13} (j_2 j_4) j_{24}^J \rangle . \quad (90)
\]

\[
\langle j_1 j_2 j_{34}^J | j_{13} j_{24}^J \rangle = \sum_{\alpha, \beta, \gamma} \langle j_1 j_2 j_{12} j_{34}^J | (j_1 j_{34}^J) \alpha j_2^J \rangle
\]

\[
\langle j_1 (j_3 j_4) j_{34}^\alpha | (j_1 j_3) \beta j_4^J \rangle
\]

\[
\langle (\beta j_4^\alpha) \alpha j_2^J | \beta (j_2 j_4^\gamma) \gamma J \rangle
\]

\[
\langle (j_1 j_3) \alpha (j_2 j_4)^\gamma J | (j_1 j_2) j_{12} (j_3 j_4) j_{34}^J \rangle . \quad (91)
\]

On the right, the last term in the sum is

\[
\langle (j_1 j_3) \alpha (j_3 j_4) \gamma J | (j_1 j_3) j_{13} (j_2 j_4) J \rangle = \delta_{\beta, j_{13}} \delta_{\gamma, j_{24}}
\]

\[
(92)
\]

Thus, the evaluation of the recoupling reduces to

\[
\langle j_1 j_2 j_{34}^J | j_{13} j_{24}^J \rangle = \sum_{\alpha} \langle j_1 j_2 j_{12} j_{34}^J | (j_1 j_{34}^J) \alpha j_2^J \rangle
\]

\[
\langle (j_1 (j_3 j_4) j_{34}^\alpha | (j_1 j_3) j_{13} j_{4}^\alpha \rangle
\]
where each of the terms in the sum can now be expressed as a product of three Racah W-coefficients.

Note that it is necessary to introduce a sum into the recoupling only when that particular composite angular momentum does not already appear. For example, the composite of $j_1$ and $j_{34}$ does not appear and the sum over $\alpha$ is introduced, but the composite of $j_1$ and $j_3$ appears on the right-hand side of the recoupling coefficient and therefore, the sum over $\beta$ is eliminated. Similarly, the sum over $\gamma$ is eliminated since the composite of $j_2$ and $j_4$ appears.

The second point to be made is that every recoupling coefficient, regardless of complexity, can be reduced to a series of sums over products of recoupling coefficients which involve only three angular momenta. With these two points established, the orbital recoupling coefficients are now evaluated.

Consider the recoupling coefficients

\[
\langle \theta_i | \theta_j \rangle = \langle \bar{L}_1 \bar{L}_2 \rangle L_2^{\alpha_i} \ldots [\bar{L} \rho_i \rho_j \rho_i \rho_i \sigma_i \sigma_i ] L_i \ldots (\bar{L} \rho_i \rho_i \rho_i \sigma_i \sigma_i )
\]

\[
L_i \ldots , L_i | (\bar{L}_1 \bar{L}_2 \rangle L_2^{\alpha_j} \ldots (\bar{L} \rho_j \rho_j \rho_j \rho_j \rho_j \sigma_j \sigma_j ) L_i \ldots [\bar{L} \rho_j \rho_j \rho_j \rho_j \sigma_j \sigma_j ]
\]
which is represented by the first diagram in Fig. 1a.

This recoupling coefficient is evaluated as follows:

1) $\ell_{\rho_i}$ is uncoupled from the $\rho_i$th shell.

2) $\ell_{\rho_i}$ is coupled down to the $\rho_j$th shell.

3) $\ell_{\rho_j}$ is uncoupled from $k$ and recoupled to $\rho_j$th shell.

4) $k$ is coupled down to the $\sigma_i$th shell.

5) $\ell_{\sigma_i}$ is uncoupled from the $\sigma_i$th shell and coupled with $k$ to give $\ell_{\sigma_j}$.

6) $\ell_{\sigma_j}$ is coupled down to the $\sigma_j$th shell.

7) $\ell_{\sigma_j}$ is coupled to the $\sigma_i$th shell.

After each step, the results are as follows:

1) $\langle \theta_i | \theta_j \rangle = D_1 \ldots [L_{\rho_j} L_{\rho_i} \ldots L_{\rho_i}] \ldots (L_{\sigma_j})_{\sigma_i} \ldots (L_{\sigma_i})_{\sigma_i}$
\[ \ldots L_i | \ldots [L_{\rho_j-1} (\tilde{L}_{\rho_j} \rho_{\rho_j}) L_{\rho_j}^\alpha_j] L_{\rho_j} \ldots (\tilde{L}_{\sigma_j} \rho_{\sigma_j}) L_{\sigma_j}^\alpha_j \ldots L_j > \]

(95)

where

\[ D_1 = <L_{\rho_i-1} (\tilde{L}_{\rho_i} \rho_{\rho_i}) L_{\rho_i}^\alpha_i|L_{\rho_i-1} (\tilde{L}_{\rho_i} \rho_{\rho_i}) L_{\rho_i}^\alpha_i >. \]

(96)

2) \[ <\theta_i | \theta_j > = D_1 D_2 <\ldots (L_{\rho_i-1} \rho_{\rho_i}) L_{\rho_j-1} \ldots L_i | \ldots \]

\[ [L_{\rho_j-1} (\tilde{L}_{\rho_j} \rho_{\rho_j}) L_{\rho_j}^\alpha_j L_{\rho_j} \ldots L_j > \] (97)

where

\[ D_2 = \prod_{\lambda = \rho_i + 1}^{\rho_j-1} <L_{\rho_i}^\alpha_i \tilde{L}_{\lambda-1} \lambda \lambda |L_{\lambda-1} \lambda \lambda |L_{\lambda-1} \lambda \lambda |L_{\lambda-1} \lambda \lambda >. \] (98)

3) \[ <\theta_i | \theta_j > = D_1 D_2 D_3 <\ldots (L_{\rho_j-1} (\tilde{L}_{\rho_j} \rho_{\rho_j}) L_{\rho_j}^\alpha_j L_{\rho_j} \ldots L_j > \]

\[ \ldots L_i | \ldots [L_{\rho_j-1} (\tilde{L}_{\rho_j} \rho_{\rho_j}) L_{\rho_j}^\alpha_j L_{\rho_j} \ldots L_j > \] (99)
where

\[ D_3 = \langle [L_{\rho j-1}p^j_{\rho j}]L_{\rho j-1}L_{\rho j} \rangle \]

\[ \langle [L_{\rho j-1}p^j_{\rho j}]L_{\rho j-1}L_{\rho j} \rangle \]

\[ \langle L^{\alpha_j}_{\rho j-1}\alpha_i^{\rho_j}L^{\alpha_i}_{\rho j} \rangle \] (100)

4) \[ <\theta_i|\theta_j> = D_1D_2D_3D_4<\ldots\langle (L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i}) \rangle \ldots \rangle \]

\[ \langle (L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i}) \rangle \ldots \rangle \]

\[ \langle L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i} \rangle \ldots \rangle \] (101)

where

\[ D_4 = \prod_{\lambda=\rho_j+1}^{\sigma_j-1} \langle L^{\alpha_j}_{\lambda-1}L^{\alpha_i}_{\lambda-1}L^{\alpha_i}_{\lambda} \rangle \]

\[ \langle L^{\alpha_j}_{\lambda-1}L^{\alpha_i}_{\lambda-1}L^{\alpha_i}_{\lambda} \rangle \]

\[ \langle L^{\alpha_j}_{\lambda-1}L^{\alpha_i}_{\lambda-1}L^{\alpha_i}_{\lambda} \rangle \ldots \rangle \] (102)

5) \[ <\theta_i|\theta_j> = D_1D_2D_3D_4D_5<\ldots\langle (L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i}) \rangle \ldots \rangle \]

\[ \langle (L^{\alpha_i}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i}) \rangle \ldots \rangle \]

\[ \langle L^{\alpha_j}_{\sigma_i-1}L^{\alpha_i}_{\sigma_i+1} \rangle \ldots \rangle \] (103)

where
\[
D_5 = \langle \sigma_{i-1}^j k \rangle \sigma_{i-1}^j \langle \varphi_{i-1}^j \rangle \sigma_{i-1}^j \sigma_{i-1}^j \mid \left( \langle \sigma_{i-1}^j \rangle \sigma_{i-1}^j \sigma_{i-1}^j \right) \rangle
\]

(104)

\[
\langle \theta_i \mid \theta_j \rangle = D_1 D_2 D_3 D_4 D_5 D_6 \langle \langle \sigma_{i-1}^j \rangle \sigma_{i-1}^j \sigma_{i-1}^j \rangle L_{i-1}^j \mid \left( \langle \sigma_{i-1}^j \rangle \right) \rangle \sigma_{i-1}^j \sigma_{i-1}^j \sigma_{i-1}^j \rangle
\]

(105)

where

\[
D_6 = \prod_{\lambda = \sigma_{i-1}^j + 1}^{} \langle \langle \sigma_{i-1}^j \rangle \sigma_{i-1}^j \sigma_{i-1}^j \rangle L_{\lambda}^j \sigma_{\lambda}^j \rangle \sigma_{\lambda}^j \sigma_{\lambda}^j \rangle \sigma_{\lambda}^j \rangle
\]

(106)

7) \[
\langle \theta_i \mid \theta_j \rangle = D_1 D_2 D_3 D_4 D_5 D_6 D_7
\]

\[
\langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \rangle \rangle
\]

\[
\langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \rangle \rangle
\]

\[
\langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \langle \langle \tilde{L}_{1}^j \rangle \rangle L_{2}^i \rangle \rangle
\]

(107)
\[
L^j_{\sigma j} \ldots L^i_{\sigma i} \ldots L^i_{\rho i} = (L_{\rho i} L_{\rho i}) L^j_{\sigma j} \ldots (L_{\rho i} L_{\rho i})
\]

\[
\alpha_j \ldots [L_{\rho i} (L_{\rho i} L_{\rho i}) L^j_{\sigma j} L^i_{\rho i}] L_{\rho i} \ldots
\]

\[
(L_{\sigma i} L_{\sigma i} L_{\sigma j} \ldots L_{\sigma j} - 1) (L_{\sigma j} L_{\sigma j}) L^j_{\sigma j} \ldots L^j_{\sigma j} >
\]

(107)

where

\[
D_7 = \langle (L_{\sigma j} L_{\sigma j} - 1) L^i_{\rho i} \rangle L^i_{\rho i} \langle L^i_{\sigma i} L^i_{\sigma i} \rangle L^i_{\sigma i} - 1 (L_{\sigma j} L_{\sigma j}) L^j_{\sigma j} L^j_{\sigma j} \rangle.
\]

(108)

The trivial evaluation of the last term on the right side of Eq. (69) gives

\[
\langle \theta_i | \theta_j \rangle = D_1 D_2 D_3 D_4 D_5 D_6 D_7 \delta (b_i b_j) \delta (L_i L_j)
\]

\[
\rho_i \pi \delta (L_{\lambda i} L_{\lambda j}) \pi \delta (L_{\lambda i} L_{\lambda j}) \delta (L_{\lambda i} L_{\lambda j}) \delta (L_{\lambda i} L_{\lambda j}).
\]

(109)

Consider the recoupling coefficient

\[
\langle \theta_i | \theta_j \rangle = \langle \tilde{L}_i L^i_{\rho i} \alpha_i \ldots L^i_{\rho i} \rangle \alpha_i \ldots \alpha_i \rangle
\]

(109)
which is represented by the first diagram in Fig. 1b.
This recoupling coefficient is evaluated as follows:

1) $\ell_{\rho_i}$ is uncoupled from the $\rho_i$th shell.

2) $\ell_{\rho_i}$ is coupled down to the $\sigma_j$th shell.

3) $k$ is uncoupled from $\ell_{\rho_j}$ and coupled with $L_{\sigma_j}$ to give $L'$; then $L'$ is coupled with $L_{\sigma_j-1}^{\alpha_j}$ to give $L''_{\sigma_j}$. Since the composite of $k$ and $L_{\sigma_j}$ does not appear anywhere, $L'$ is summed over. Similarly, it is necessary to sum over $L''_{\sigma_j}$.

4) $\ell_{\rho_j}$ is coupled down to the $\rho_j$th shell. At each shell it is necessary to introduce a $L_{\lambda}$ which must be summed over.

5) $\ell_{\rho_j}$ is coupled with $L_{\rho_j}$ to give $L^j_{\rho_j}$.

6) $k$ is uncoupled from $\ell_{\sigma_i}$ and coupled with $L_{\sigma_i}$ to give $L'$. 

\[ \ldots \{L_{\sigma_j}^{\rho_i} \ell_{\sigma_j} \} L_{\sigma_j}^j \ldots \{L_{\rho_j}^{\rho_j} \ell_{\rho_j} \} L_{\rho_j}^j \ldots , L_j >, \]

(110)
7) \( l_{\sigma_i} \) is coupled down to the \( \rho_j \)th where the successive couplings are equal to \( L_\lambda^i \).

8) \( l_{\sigma_i} \) is coupled through the \( \rho_j \)th node.

9) \( l_{\sigma_i} \) is coupled from the \( \rho_j \)th shell down to the \( \sigma_i \)th shell.

10) \( l_{\sigma_i} \) is coupled with \( L_{\sigma_i} \) to give \( L_{\sigma_i}^i \).

After each step, the results are as follows:

1) \( \langle \theta_1 | \theta_j \rangle = E_1 \cdots [L_{\rho_i}^{\alpha_i} L_{\rho_i}^{\alpha_j} L_{\rho_j}^{\alpha_i} \cdots (L_{\sigma_i}^{\alpha_i} L_{\sigma_i}^{\alpha_j}) L_{\sigma_i}^{\alpha_i} \cdots L_i \cdots L_j \rangle \)

\( \cdots L_i \cdots [L_{\rho_j}^{\alpha_j} L_{\rho_j}^{\alpha_j} \cdots (L_{\sigma_j}^{\alpha_j} L_{\sigma_j}^{\alpha_j}) L_{\sigma_j}^{\alpha_j} \cdots L_j \rangle \)

(111)

where

\[ E_1 = L_{\rho_i}^{\alpha_i} L_{\rho_i}^{\alpha_j} L_{\rho_j}^{\alpha_i} \cdots (L_{\sigma_i}^{\alpha_i} L_{\sigma_i}^{\alpha_j}) L_{\sigma_i}^{\alpha_i} \cdots L_i \cdots L_j \]

(112)

2) \( \langle \theta_1 | \theta_j \rangle = E_1 E_2 \cdots [L_{\sigma_j}^{\alpha_j} L_{\sigma_i}^{\alpha_i} \cdots L_i \cdots L_j \rangle \cdots \)
\[ [L_{\sigma_j}^{\alpha_j} (\bar{L}_{\sigma_j}^{\alpha_j}) L_{\sigma_j}^{\alpha_j} \cdots L_{\sigma_j}^{\alpha_j}] L_{\sigma_j}^{\alpha_j} \cdots L_{\sigma_j}^{\alpha_j} \]  

(113)

where

\[ E_2 = \prod_{\lambda=\rho_i+1}^{\sigma_j-1} <(L_{\lambda-1}^{\alpha_j} \rho_i^{\alpha_j}) L_{\lambda-1}^{\alpha_i} \bar{L}_{\lambda}^{\alpha_i} L_{\lambda}^{\alpha_i} | (L_{\lambda-1}^{\alpha_j} \rho_i^{\alpha_j}) L_{\lambda}^{\alpha_j} \rho_i^{\alpha_i} L_{\lambda}^{\alpha_i}> . \]

(114)

3) \[ <\theta_i | \theta_j> = E_1 E_2 L', L'_{\sigma_j} \Sigma E_3 (L', L'_{\sigma_j}) \]

\[ <\cdots [L_{\sigma_j}^{\alpha_j} (\bar{L}_{\sigma_j}^{\alpha_j}) L'] L_{\sigma_j}^{\alpha_j} \rho_j^{\alpha_i} L_{\sigma_j}^{\alpha_i} \cdots L_i | \cdots L_{\sigma_j}^{\alpha_j} \cdots L_j> \]

(115)

where

\[ E_3 = <[L_{\sigma_j}^{\alpha_j} (\rho_j^{\alpha_j}) L_{\sigma_j}^{\alpha_i} \bar{L}_{\sigma_j}^{\alpha_i} L_{\sigma_j}^{\alpha_i}] \]

\[ [L_{\sigma_j}^{\alpha_j} (\bar{L}_{\sigma_j}^{\alpha_j}) L'] L_{\sigma_j}^{\alpha_j} \rho_j^{\alpha_i} L_{\sigma_j}^{\alpha_i}> . \]

(116)

4) \[ <\theta_i | \theta_j> = E_1 E_2 L', L'_{\sigma_j} \Sigma E_3 (L', L'_{\sigma_j}) \]

\[ E_4 (L_{\sigma_j}^{\alpha_j} L_{\sigma_j}^{\alpha_j+1}) \cdots L_{\sigma_j}^{\alpha_i} \rho_j \Sigma E_4 (L_{\lambda-1}^{\alpha_j} L_{\lambda}^{\alpha_i}) \cdots \]

(117)
\[ E_4(L_{j-1}^i, L_{j-2}^i) \ldots (L_{j-1}^i \cdot L_{j}^i) \cdot L_{j}^i \cdot \ldots \cdot L_i \]

\[ \ldots [L_{j-1}^i (L_{j}^i \cdot L_{j}^i)]^a_j \ldots \]

where

\[ E_4(L_{\lambda-1}^i, L_{\lambda}^i) = \langle (L_{\lambda-1}^i \cdot L_{\lambda}^i) \cdot L_{\lambda}^i \cdot L_{\lambda}^i \rangle_{L_{\sigma}^i} \ldots \]

(118)

5) \[ \langle \theta_i | \theta_j \rangle = E_1 E_2 L_{\sigma}^i L_{\sigma}^j E_3 (L_{\lambda}^i \cdot L_{\lambda}^i) \cdot L_{\sigma}^i \cdot \ldots \]

\[ E_4(L_{\sigma}^i \cdot L_{\sigma}^i) \ldots E_4(L_{\lambda}^i \cdot L_{\lambda}^i) \ldots E_4(L_{\rho}^i \cdot L_{\rho}^i) \ldots E_4(L_{\rho}^i \cdot L_{\rho}^i) \ldots E_4(L_{\rho}^i \cdot L_{\rho}^i) \ldots E_4(L_{\rho}^i \cdot L_{\rho}^i) \]

(119)

where

\[ E_5(L_{\rho}^i \cdot L_{\rho}^i) = \langle (L_{\rho}^i \cdot L_{\rho}^i) \cdot L_{\rho}^i \cdot L_{\rho}^i \cdot (L_{\rho}^i \cdot L_{\rho}^i) \rangle_{L_{\rho}^i \cdot L_{\rho}^i} \]

(120)
6) \[ <\theta_i | \theta_j> = E_1 E_2 \Sigma_{L', L'_{\sigma_j}} E_3 (L', L'_{\sigma_j}) E_6 (L', L'_{\sigma_j}) \]
\[ \Sigma_{L'_{\sigma_j} + 1} E_4 (L'_{\sigma_j}, L'_{\sigma_j} + 1) \ldots \Sigma_{L'_{\lambda-1}} E_4 (L'_{\lambda}, L'_{\lambda}) \ldots \]
\[ \Sigma_{L'_{\rho_j-1}} E_4 (L'_{\rho_j-2}, L'_{\rho_j-1}) E_5 (L'_{\rho_j-1}) \]
\[ (121) \]

\[ < \ldots [L'_{\sigma_j} (\bar{L} \sigma_j k) L'_{\sigma_j}] L'_{\sigma_j} \ldots L_i | \ldots \]

\[ [L'_{\sigma_j-1} (\bar{L} \sigma_j k) L'_{\sigma_j}] L'_{\sigma_j} \ldots L_j > \]

where

\[ E_6 (L', L'_{\sigma_j}) = <L'_{\sigma_j} (k L'_{\sigma_j} L'_{\sigma_j}) | (\bar{L} \sigma_j k) L'_{\sigma_j} L'_{\sigma_j}> \]

\[ <L'_{\sigma_j} L'_{\sigma_j} L'_{\sigma_j} \ldots L'_{\sigma_j} | (L'_{\sigma_j-1}) (L'_{\sigma_j}) (L'_{\sigma_j}) L'_{\sigma_j} L'_{\sigma_j}> . \]  

(122)

7) \[ <\theta_i | \theta_j> = E_1 E_2 \Sigma_{L', L'_{\sigma_j}} E_3 (L', L'_{\sigma_j}) E_6 (L', L'_{\sigma_j}) \]
\[ \Sigma_{L'_{\sigma_j} + 1} E_4 (L'_{\sigma_j}, L'_{\sigma_j} + 1) E_7 (L'_{\sigma_j}, L'_{\sigma_j} + 1) \ldots \]
\[ \Sigma_{L'_{\lambda-1}} E_4 (L'_{\lambda-1}, L'_{\lambda}) E_7 (L'_{\lambda-1}, L'_{\lambda}) \ldots \]
\[ E^E_7(L_{\rho_j-2}^s L_{\rho_j-1}^s) \]
\[ E_7(L_{\rho_j-2}^s L_{\rho_j-1}^s) E_5(L_{\rho_j-1}^s) \]
\[ \langle \ldots [L_{\rho_j-1}^s \bar{L}_{\rho_j} \bar{L}_{\rho_j}^j] L_i^i \ldots L_i | \ldots \]
\[ (L_{\rho_j-1}^s \bar{L}_{\rho_j} \bar{L}_{\rho_j}^j L_{\rho_j-1}^s \ldots L_j \rangle \]

where

\[ E_7(L_{\lambda-1}^s, L_{\lambda}^s) = \langle (L_{\lambda-1}^s \bar{L}_{\lambda} \bar{L}_{\lambda}^j) L_{\lambda-1}^s \bar{L}_{\lambda} \bar{L}_{\lambda}^j | (L_{\lambda-1}^s \bar{L}_{\lambda} \bar{L}_{\lambda}^j) L_{\lambda}^s \bar{L}_{\lambda} \bar{L}_{\lambda}^j \rangle \]

(124)

8) \[ \langle \theta_i | \theta_j \rangle = E_1 E_2 \sum_{L_i^s, L_j^s} E_3 (L_i^s L_j^s) E_6 (L_i^s, L_j^s) \ldots \]
\[ \sum_{L_{\sigma_j+1}^s} E_4 (L_{\sigma_j+1}^s L_{\sigma_j+1}^s) E_7 (L_{\sigma_j+1}^s L_{\sigma_j+1}^s) \ldots \]
\[ \sum_{L_{\lambda}^s} E_4 (L_{\lambda-1}^s L_{\lambda}^s) E_7 (L_{\lambda-1}^s L_{\lambda}^s) \ldots \]
\[ \sum_{L_{\rho_j-1}^s} E_4 (L_{\rho_j-2}^s L_{\rho_j-1}^s) E_7 (L_{\rho_j-2}^s L_{\rho_j-1}^s) \]
\[ E_5 (L_{\rho_j-1}^s) E_8 (L_{\rho_j-1}^s) \]
\[ \langle \ldots (L_{\rho_j-1}^s L_j^j) L_{\rho_j} \rho_j \ldots L_i | \ldots (L_{\rho_j-1}^s L_j^j) L_{\rho_j} \rho_j \ldots L_j \rangle \]

(125)
where

\[ E_8(L_{\rho_j}^j - 1) = \langle (L_{\rho_j}^j - 1 \cdot \sigma_i) L_{\rho_j}^j \cdot L_{\rho_j}^j | (L_{\rho_j}^j - 1 \cdot L_{\rho_j}^j) L_{\rho_j}^j \cdot L_{\rho_j}^j \rangle. \]

(126)

9) \[ \langle \theta_i | \theta_j \rangle = E_1 E_2 E_9 \Sigma \ldots \Sigma \ldots \Sigma \ldots \]

\[ \langle \ldots [L_{\sigma_i} - 1] (\overline{L}_{\sigma_i} \cdot \sigma_i) L_{\sigma_i} \sigma_i \ldots L_i | \ldots \]

\[ (L_{\sigma_i} - 1 \cdot \sigma_i) L_{\sigma_i} \sigma_i \ldots L_j \rangle \]

(127)

where

\[ E_9 = \prod_{\lambda=\rho_j + 1}^{\sigma_i - 1} \langle (L_{\lambda - 1} \cdot \sigma_i) L_{\lambda} \cdot L_{\lambda} | (L_{\lambda - 1} \cdot L_{\lambda}) L_{\lambda} \cdot L_{\lambda} \rangle. \]

(128)

10) \[ \langle \theta_i | \theta_j \rangle = E_1 E_2 E_9 E_10 L_1 \Sigma L_1 \ldots L_1 \]

\[ \ldots E_8(L_{\rho_j}^j - 1) \langle L_{\rho_j}^j \cdot L_{\rho_j}^j \rangle L_{\rho_j}^j \ldots \]

\[ \ldots (L_{\rho_j}^j - 1 \cdot L_{\rho_j}^j) L_{\rho_j}^j \ldots \]

\[ \langle \ldots [L_{\sigma_j} - 1] (\overline{L}_{\sigma_j} \cdot \sigma_j) L_{\sigma_j} \ldots [L_{\rho_j}^j - 1] (\overline{L}_{\rho_j}^j \cdot \sigma_j) L_{\rho_j}^j \rangle \]

\[ \langle \ldots [L_{\sigma_i} - 1] (\overline{L}_{\sigma_i} \cdot \sigma_i) L_{\sigma_i} \ldots L_{\sigma_i}^i \rangle \]

\[ \langle \ldots [L_{\sigma_i} - 1] (\overline{L}_{\sigma_i} \cdot \sigma_i) L_{\sigma_i} \ldots L_{\sigma_i}^i \rangle \]
The last term on the right side of Eq. (129) is now evaluated to give

\[ \langle \theta_i | \theta_i \rangle = E_1 E_2 E_9 E_{10} \sum L' \ldots L'_{j-1} L_i \cdot L'_{j-1} \cdot L_i \cdot L'_{j} \cdot L_i \cdot L'_{j} \ldots \]

(131)

Consider the recoupling coefficient
\[
<\theta_i | \theta_j > = \langle \tilde{L}_1 \tilde{L}_2 \rangle L_2^{a_1} \ldots [\tilde{L}_{\rho_i} (\ell_{\rho_j} k) \ell_{\rho_i}] L_i^i \ldots
\]

\[
(\tilde{L}_{\sigma_i} \ell_{\sigma_i}) L_i^i \ldots \tilde{L}_{\rho_j} \ldots \tilde{L}_{\sigma_j} \ldots, L_i | \ldots \tilde{L}_{\rho_i} \ldots \tilde{L}_{\sigma_i} \ldots
\]

\[
[\tilde{L}_{\sigma_j} (\ell_{\sigma_i} k) \ell_{\sigma_j}] L_j^j \ldots (\tilde{L}_{\rho_j} \ell_{\rho_j}) L_j^j \ldots, L_j > ,
\]  

(132)

which is represented by the top left diagram in Fig. 1c. This recoupling coefficient is evaluated as follows:

1) \(\ell_{\rho_i}\) is uncoupled from the \(\rho_i\)th shell.

2) \(\ell_{\rho_i}\) is coupled down to the \(\sigma_i\)th shell.

3) \(\ell_{\rho_i}\) is coupled with \(\ell_{\sigma_i}\) to give \(L'\) where it is necessary to sum over \(L'\). Then \(K\) is uncoupled from \(\ell_{\rho_j}\) and recoupled with \(\ell_{\sigma_i}\) to give \(\ell_{\sigma_j}\).

4) \(L'\) is coupled down to the \(\rho_j\)th shell.

5) \(\ell_{\rho_j}\) is coupled with \(\tilde{L}_{\rho_j}\) to give \(L_j^j\).

6) \(\ell_{\sigma_j}\) is coupled down to \(\sigma_j\)th shell.

7) \(\ell_{\sigma_j}\) is coupled with \(\tilde{L}_{\sigma_j}\) to give \(L_j^j\).
After each step, the results are as follows:

1) \[ <\theta_i | \theta_j> = T_1 \cdots (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \]

\[ (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \cdots L_j > \quad (133) \]

where

\[ T_1 = \frac{\alpha_i}{\alpha_i} (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \]

\[ \frac{\alpha_i}{\alpha_i} (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \cdots L_j > \quad (134) \]

2) \[ <\theta_i | \theta_j> = T_1 T_2 \cdots (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \]

\[ \frac{\alpha_j}{\alpha_j} (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \cdots L_j > \quad (135) \]

where

\[ T_2 = \frac{\sigma_i}{\sigma_i} \frac{\alpha_j}{\alpha_j} \frac{\alpha_i}{\alpha_i} (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \]

\[ \frac{\alpha_j}{\alpha_j} (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \cdots L_j > \quad (136) \]

3) \[ <\theta_i | \theta_j> = T_1 T_2 \sum_{L_i} T_3 (L') \]

\[ \cdots (L_{\rho_i} L_{\rho_i} L_{\rho_i} \cdots L_i) \cdots L_j > \]
\[ \ldots (L^{\alpha_j}_{\sigma_i - 1} L^{\tau_i}_{\sigma_i}) L^{\alpha_j}_{\sigma_i} \ldots L_j > \] (137)

where

\[ T_3(L') = \langle L^{\alpha_j}_{\sigma_i - 1} \ell \rho_i \rangle L^{\alpha_i}_{\sigma_i} (\tilde{L}^{\alpha_i}_{\sigma_i} \ell \rho_i) L^i_{\sigma_i} L^{\alpha_i}_{\sigma_i} \]

\[ (L^{\alpha_j}_{\sigma_i - 1} L^{\tau_i}_{\sigma_i}) L^{\alpha_j}_{\sigma_i} (\ell \rho_i \ell \sigma_i) L^i_{\sigma_i} L^{\alpha_i}_{\sigma_i} \]

\[ \langle (\ell \rho_j \kappa) \ell \rho_i \ell \sigma_i L' \rangle \langle (k \ell \sigma_i) \ell \rho_j L' \rangle . \] (138)

4) \[ \langle \theta_i | \theta_j \rangle = T_1 T_2 \sum L' T_3(L') T_4(L') \ldots \]

\[ [L^{\alpha_j}_{\rho_j - 1} (\ell \rho_j \ell \sigma_i) L'] L^{\alpha_i}_{\rho_j - 1} \tilde{L}^{\alpha_i}_{\rho_j} L^{\alpha_i}_{\rho_j} \ldots L_i | \ldots \]

\[ [L^{\alpha_j}_{\rho_j - 1} (\tilde{L}^{\alpha_j}_{\rho_j \rho_j}) L^j_{\rho_j \rho_j} L^{\alpha_j}_{\rho_j} \ldots L_j > \] (139)

where

\[ T_4(L') = \prod_{\lambda = \sigma_i + 1}^{\rho_j - 1} \langle L^{\alpha_j}_{\lambda - 1} L' \rangle L^{\alpha_i}_{\lambda - 1} \tilde{L}^{\alpha_i}_{\lambda} L^i_{\lambda} \langle L^{\alpha_j}_{\lambda - 1} L^i_{\lambda} \rangle \]

\[ L^{\alpha_j}_{\lambda} L^{\alpha_i}_{\lambda} \langle (\ell \rho_j \kappa) \ell \rho_i \ell \sigma_i L' \rangle \langle (k \ell \sigma_i) \ell \rho_j L' \rangle . \] (140)

5) \[ \langle \theta_i | \theta_j \rangle = T_1 T_2 \sum L' T_3(L') T_4(L') T_5(L') \]
\[ \langle \ldots [L_{\rho_{j-1}}^{\alpha_j} (\tilde{L}_{\rho_{j}} \rho_{j} L_{\rho_{j}}^{\alpha_j}) L_{\rho_{j}}^{\alpha_j} ] L_{\rho_{j}}^{\alpha_j} \rangle \ldots [L_{\rho_{j-1}}^{\alpha_j} (\tilde{L}_{\rho_{j}} \rho_{j} L_{\rho_{j}}^{\alpha_j}) L_{\rho_{j}}^{\alpha_j} ] \ldots \]

\[ L_{\rho_{j}}^{\alpha_j} L_{\rho_{j-1}}^{\alpha_j} L_{\rho_{j}}^{\alpha_j} \ldots \]

(141)

where

\[ T_5 (L') = \langle [L_{\rho_{j-1}}^{\alpha_j} (\tilde{L}_{\rho_{j}} \rho_{j} L_{\rho_{j}}^{\alpha_j}) L_{\rho_{j}}^{\alpha_j} ] L_{\rho_{j}}^{\alpha_j} L_{\rho_{j}}^{\alpha_i} \rangle \]

(142)

\[ \langle [L_{\rho_{j-1}}^{\alpha_j} (\tilde{L}_{\rho_{j}} \rho_{j} L_{\rho_{j}}^{\alpha_j}) L_{\rho_{j}}^{\alpha_j} ] L_{\rho_{j}}^{\alpha_j} L_{\rho_{j}}^{\alpha_i} \rangle . \]

(143)

where

\[ T_6 = \prod_{\lambda = \sigma_{j} + 1}^{\rho_{j} - 1} \langle [L_{\lambda-1}^{\alpha_j} (\tilde{L}_{\lambda} \rho_{j} L_{\lambda}^{\alpha_j}) L_{\lambda}^{\alpha_j} \tilde{L}_{\lambda} L_{\lambda}^{\alpha_j} ] (L_{\lambda}^{\alpha_j} (\tilde{L}_{\lambda} \rho_{j} L_{\lambda}^{\alpha_j}) L_{\lambda}^{\alpha_j} \rho_{j} L_{\lambda}^{\alpha_i} \rangle . \]

(144)
7) \[ <\theta_i | \theta_j> = T_1 T_2 T_6 T_7 \sum_{L'} T_3 (L') T_4 (L') T_5 (L') \]

\[ <\ldots L_{\rho_j}^{\alpha_j} - 1 (L'_{\rho_j} \rho_j) L_j^{\alpha_j} \ldots L_i^{\alpha_i} > \]

where

\[ T_7 = \sum_{L_{\rho_j}^{\alpha_j} - 1 (L'_{\rho_j} \rho_j)} L_j^{\alpha_j} L_{\rho_j}^{\alpha_j} \]

The last term on the right side of Eq. (145) is now evaluated to give

\[ <\theta_i | \theta_j> = T_1 T_2 T_6 T_7 \sum_{L'} T_3 (L') T_4 (L') T_5 (L') . \] (147)

The remaining recoupling coefficients can be evaluated in a manner similar to that described above. The evaluation of all of the recoupling coefficients represented in Figs. 1a, 1b, 1c, 2a, and 2b is given in Appendix II.
CHAPTER IV
OI\(^{(3P-3s^3S^0)}\) EXCITATION CROSS SECTION

In this chapter, results for the OI\(^{(3P-3s^3S)}\) cross section calculated within the unitarized Born, non-exchange, and MCCC approximations are presented and compared with the results of other works.

The total wave function of the system (target + projectile) is expanded in terms of the ground \(1s^22s^22p^4(3p)\) state and the excited \(1s^22s^22p^3(4S^0)3s(3S^0)\) state of oxygen. The differential equations that describe the scattering functions, Eqs. (74) and (75), are solved numerically using a computer code developed by Smith, Henry, and Burke.\(^{12}\) The procedures used to solve these equations are discussed in detail in Ref. 13. The input to the SHB computer code is \(P_\lambda(r), V_{ij}(r), W_{ij}(r), V_{\mu,i}(r), A_{\mu,\nu}\) and the channel quantum numbers. These quantities are defined in Chapter II. The exchange potential, \(W_{ij}(r)\), is a function of the unknown scattering functions and must be evaluated in the process of solving the differential equation. All quantities pertinent to the evaluation of \(W_{ij}(r)\) are read into the SHB programs. The quantities \(P_\lambda(r), V_{ij}(r),\) and \(V_{\mu,i}(r)\) are input into the SHB program in tabulated form. The output of this program in the R-matrix and the cross sections. The stability of the R-matrix and cross sections is
investigated by changing the integration step size, retabulating all of the potentials, and again solving the equations.

In the collision problem, the wave functions of the target are assumed to be known. The $1s$, $2s$, and $2p$ one-electron orbitals for $\text{OI}(^3\text{P})$, as given by Clementi,$^{16}$ are used in the representation of the $1s^22s^22p_4(^3\text{P})$ state and the $1s^22s^22p_3(^4\text{S}^0)$ core of the $3s^3\text{S}^0$ excited state. Two different representations are used for the $3s$ function. Kelly$^{17}$ has presented self-consistent-field (SCF) functions in analytical form for oxygen in the configuration $1s^22s^22p_3(^4\text{S}^0)3s(^3\text{S}^0)$ and this is the source of one of the $3s$ functions used in this work. Kelly's $3s$ orbital will be referred to by $3sK$. An alternative representation of the $3s$ orbital has been generated by Hibbert$^{18}$ in the frozen core approximation. The $1s^22s^22p_3(^4\text{S}^0)$ core is represented by the oxygen-ion wave functions of Clementi.$^{16}$ The exponents in the expansion

$$p_{3s}(r) = \sum_{i=1}^{3} c_i r e^{-\alpha_i r}$$

are determined variationally and the coefficients are obtained from the orthonormality conditions. This orbital will be referred to by $3sH$ and the parameters describing it are given in Table I.
Figure 3 gives the reduced 3s orbital for oxygen versus radial distance. Curves K and H represent the orbitals obtained by Kelly\textsuperscript{17} and Hibbert\textsuperscript{18} respectively. Curve P gives a function generated by Percival\textsuperscript{7} in an approximation in which exchange of electrons is neglected. This function was used by Stauffer and McDowell\textsuperscript{6} in their calculation of the OI(3P-3s\textsuperscript{3}S\textsuperscript{0}) cross sections. Since exchange is neglected, the spatial extent of the orbital is too large and hence cross sections calculated with this function will be overestimated.

"Spot check" calculations were made using two independent computer programs, and identical results were obtained. One of these programs was written in connection with this work, while the other is a modified version of a program supplied by Hibbert\textsuperscript{18}.

The sensitivity of the OI(3P-3s\textsuperscript{3}S) cross section to the representation of the 3s orbital is investigated in the unitarized Born approximation. Figure 4 presents the cross section as a function of energy for incident electron energies up to 70 eV. Curves K and H represent calculations using 3sK and 3sH functions, respectively. The results agree to within 10%. Since facilities are available to extend these calculations to other excited states, the orbitals of which are not currently available in the literature, the 3sH orbital is used in the MCCC calculation of the OI(3P-3s\textsuperscript{3}S\textsuperscript{0}) cross section. The
excitation energy has been taken to be the experimental value\textsuperscript{19} of 9.52 eV.

The unitarized-Born-approximation cross section increases slowly from threshold and has a broad peak at incident electron energies of 25-40 eV. The nonexchange results (Curve N) peak at a lower energy and more closely follow the energy dependence of the close-coupling calculations except at low energies. Partial cross sections calculated in the nonexchange approximation are within 10\% of those obtained in the close-coupling approximation for \( l > 3 \) and 5, respectively, for incident energies of 1 and 2 Ry. At the highest energies, where all approximations are in good agreement, 40 partial waves are included in order to ensure convergence of the partial-wave expansion.

Near the threshold, the close-coupling results are dominated by resonances which occur for the \( ^4S^0 \) and \( ^2P \) partial waves. An open-channel resonance can occur when centrifugal-barrier, direct, and exchange-interaction potential effects combine to trap temporarily the incident electron in a quasibound state of the system. An analysis of the partial cross sections indicate that the \( ^2P \) contribution to this resonance feature is due to the trapping of an outgoing p wave:

\[
e^{-}(l=0) + OI(3p) \rightarrow O^{-**}[2P^3(^4S^0)3s3p(^2P)]
\]

\[
\rightarrow e^{-}(l=1) + OI(3s^3S).
\]
The approximate resonance position is 9.66 eV. The resonance position in the $^4S^o$ partial wave is at 10.61 eV and is due to the inclusion of the configuration

$$\text{O}^{-**} [2P^3 (^4S^o) 3s^2 (^4S)]$$

in the trial wave function; i.e., this is the contribution to the trial wave function which is included to take into account the fact that the incident s-wave in the $3s^3S^o$ channel is constrained to be orthogonal to the $3s$ orbital.

Recent experimental\(^{21,22}\) and theoretical\(^{23}\) work indicates that the position of the resonance in the $^2P$ partial wave is 9.50 eV, which is in reasonably good agreement with this work. The difference of .16 eV can be explained in terms of the neglected states; i.e., truncation of the close-coupling expansion. The effect of neglected states is that of an attractive potential and so it is reasonable to expect that the resonance positions will be shifted to lower energies if these states are included.\(^{20}\)

The resonance position in the $^4S^o$ partial wave can be obtained theoretically using the procedure of Ref. 23. The resonance state is assumed to be a superposition of states of the type

$$\text{O}^{-**} [2P (^4S^o) n\ell n'\ell' (^4S^o)]$$
where n and \( n' \) take on the values 3s, 3p, 3d, and 4s. The \( 1s^22s^22p^3(4S^0) \) core is represented by the \( 0^+(4S^0) \) wave functions of Clementi, and the 3s, 3p, 3d, and 4s orbitals, which were generated in the frozen-core approximation, are given in Table I. The associated eigenvalue problem is solved for the minimum energy state which is dominated by the

\[
0^{-**}[2p^3(4S^0)3s^2(4S^0)]
\]

corresponding energy is denoted by \( E^- \). It is assumed that a good value for the resonance energy is given by

\[
9.52 \text{ eV} - \Delta E
\]

where \( \Delta E \) is defined to be the difference in eV between the \( 3s^3S^0 \) energy given in Table I and \( E^- \). The resonance in the \( 4S^0 \) partial wave is predicted to be 8.73 eV.

Assuming that the \( 4S^0 \) resonance energy is indeed 8.73, the position of the resonance predicted by the scattering calculation is in error by approximately 2 eV and such a discrepancy is not explainable solely in terms of neglected states. The discrepancy is due to the poor representation of the
excited state. Denote the energy of this state by $E_{N+1}$ and let $E$ be the energy of the system. The scattering equations contain a term which is proportional to $(E_{N+1} - E)^{-1}$ and the $4s^0$ resonance occurs just before this term changes sign; i.e., the resonance occurs at 10.61 eV and $E_{N+1} = 10.74$. In this particular treatment only one set of orbitals can be used, and as has already been mentioned, the $1s$, $2s$, and $2p$ orbitals of $\text{OII}(^3\text{P})$ are used to represent the ground state and the $1s^2 2s^2 2p^3(4s^0)$ core of the excited states. The cores of the excited states are better represented by the $1s$, $2s$, and $2p$ wave functions of $\text{OII}(^4\text{S})$ and a value of $E_{N+1}$ obtained with this representation of the core is about 2 eV lower. This implies that the $4s^0$ resonance should be below threshold at an energy of about 8.61 eV.

Figure 5 presents the $\text{OII}(^3\text{P}-3s^3\text{S}^0)$ cross sections as a function of energy for energies less than 300 eV. Experimental results of Stone and Zipf\textsuperscript{8} are given by circles. Their measurements are normalized by comparing the optical signal for the atomic excitation with the signal for pure dissociative excitation of $\text{O}_2$. Absolute cross sections for dissociative excitations by Mumma and Zipf\textsuperscript{24} and Lawrence\textsuperscript{25} were used as standards. The energy resolution of Stone and Zipf's experiment is $\pm 1$ eV.
Curve S is the IPM results of Sawada and Ganaz. Since the resonance feature in the close-coupling results is too narrow to be detected by the Stone and Zipf experiment, the close-coupling results in Fig. 4 are averaged over 2 eV and are presented as Curve C in Fig. 5.

For energies $E > 60$ eV, all the cross sections exhibit the anticipated behavior of an optically allowed excitation process; i.e.,

$$Q(3P-3s^3S) \propto \frac{\ln k^2}{k^2}$$

where $k^2$ is the energy in Ry.

Although the two theoretical cross sections are smaller than the measured values, the close-coupling results have an energy dependence very similar to that of the experimental results. Part of the discrepancy is due to cascade contributions. The experiment measures the population of the excited $3s^3S^0$ by all mechanisms, whereas the theoretical results assume that only direct excitation of the $3P$ ground state by electron impact populates the $3s^3S^0$ excited state.

In an effort to get some idea of the magnitude of the cascade contribution, excitation cross sections for $OI(3P-n\ell^3\ell)$ have been calculated for $n\ell=3s,3p,4s,3d$. These cross sections, which were calculated in a two-
state unitarized Born approximation using wave functions generated in the frozen-core approximation\textsuperscript{18} (Table I), are given in Table III. The cascade scheme for these states is shown in Figure 6. Transition probabilities given in Table IV were used to determine the fractional cascade contributions to each level. Under the assumption that allowed radiative transitions to occur before any collisional deexcitation process, the population of the $3s^3S^0$ level is proportional to

$$Q(3s)+Q(3p)+.17Q(4s)+.44Q(3d)+...,$$

where $Q(n\ell)$ is the OI($^3P-n\ell^3S^0$) excitation cross section. Using the cross sections given in Table III, a cascade contribution of 30% at 5 Ry is estimated. At this energy the excitation cross sections calculated in the two-state close-coupling and the unitarized Born approximation agree to within 3% for the same set of orbital functions. Though not all of the cascade contributions to the $3s^3S^0$ are included in this treatment, it seems unlikely that this is the explanation of the factor of 4 discrepancy between the experimental and our theoretical estimates of the OI($^3P-3s^3S^0$) cross sections.

Except for the work done on He, the present calculation represents one of the first attempts to compute excitation cross sections in the close-coupling approxi-
mation for atomic systems in which there is more than one open shell. One difficulty with this approach is the failure to accurately represent the core states of the target; i.e., only one set of discrete orbitals can be used to represent both the ground and excited configurations. This difficulty manifests itself in the fact that the \( 0^- (4s^0) \) autodetaching level is in error by about 2 eV.

A second difficulty, which again pertains to the representation of the target state and may well explain some of the discrepancy between the theoretical and experimental predictions of the \( OI(3P-3s^3S) \) cross section, is the convergence of the asymptotic part of the direct potentials. It is well known that properties of atomic systems calculated using only HF wave functions are not in good agreement with experiment. Therefore, it is likely that the cross sections calculated here are in error. However, it is expected that the error in these cross sections is no more than 40-50%. This is based on the assumption that at high energies the excitation cross sections for allowed transitions are proportional to the corresponding oscillator strengths (Bethe approximation) and the fact that HF oscillator strengths are in error by no more than 40-50%.

Though it is quite evident that the present treatment has some serious difficulties, there is every reason to believe that these difficulties can be overcome.
Atomic physicists have had a great deal of success with the configuration interaction (CI) method in the calculation of energy levels, autodetaching levels, oscillator strengths, etc. Therefore, it is obvious that the next step in the calculation of electron-atom scattering cross sections is to include CI representations of the target states. This should improve considerably the values of the cross sections in the high energy region (above 30 eV); however, the resonance structure will still be erroneous. The resonance structure can be improved by relaxing the constraint that only one set of orbitals be used in the representation of all target states; i.e., let the one-electron orbitals fluctuate from one target state to the next. Pseudo state techniques, which are used to improve the convergence of the close-coupling expansion, are receiving a lot of attention and should be incorporated wherever possible. From this vantage point, the ultimate goal should be to incorporate pseudo states, fluctuating orbitals, and configuration interactions. Such an ambitious goal will possibly be realizable with the next generation of computers and it should give cross sections which are accurate to within a few per cent.
8. E. J. Stone and E. C. Zipf, Phys. Rev. A 4, 610 (1971); and private communication. The experimental cross sections given in Fig. 5 represent revisions of the published values.


18. A. Hibbert, private communication.


Figure 1a
Figure 1b
Figure 1c
Figure 2a
Figure 2b
Figure 3

3s FUNCTION

Figure 3

RADIUS (a₀)
CROSS SECTION \((10^{-17} \text{ cm}^2)\)

Figure 4
Figure 5
Figure 6
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<td>10.34</td>
<td>0.084</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.7800</td>
<td>10.61</td>
<td>0.140</td>
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<tr>
<td>0.8000</td>
<td>10.88</td>
<td>0.115</td>
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<tr>
<td>0.8400</td>
<td>11.43</td>
<td>0.086</td>
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<tr>
<td>0.8800</td>
<td>11.97</td>
<td>0.083</td>
<td></td>
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<tr>
<td>0.9200</td>
<td>12.52</td>
<td>0.084</td>
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<tr>
<td>1.0000</td>
<td>13.61</td>
<td>0.088</td>
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<tr>
<td>1.2500</td>
<td>17.01</td>
<td>0.097</td>
<td></td>
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<tr>
<td>1.5000</td>
<td>20.41</td>
<td>0.097</td>
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<tr>
<td>1.7500</td>
<td>23.81</td>
<td>0.094</td>
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<tr>
<td>2.0000</td>
<td>27.21</td>
<td>0.091</td>
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<td>3.0000</td>
<td>40.82</td>
<td>0.080</td>
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<td>4.0000</td>
<td>54.42</td>
<td>0.072</td>
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<tr>
<td>5.0000</td>
<td>68.03</td>
<td>0.064</td>
<td></td>
<td></td>
</tr>
<tr>
<td>( Q(\pi a_0^2) )</td>
<td>( E(\text{Ry}) )</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>-----------------</td>
<td>-----------------</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
</tr>
<tr>
<td>( \text{OI}(^3P-3s^3S) )</td>
<td>0.03968</td>
<td>0.07297</td>
<td>0.07253</td>
<td>0.06741</td>
</tr>
<tr>
<td>( \text{OI}(^3P-3p^3P) )</td>
<td>0.00795</td>
<td>0.01633</td>
<td>0.01584</td>
<td>0.01413</td>
</tr>
<tr>
<td>( \text{OI}(^3P-4s^3S) )</td>
<td>0.00061</td>
<td>0.00507</td>
<td>0.00669</td>
<td>0.00696</td>
</tr>
<tr>
<td>( \text{OI}(^3P-3d^3D) )</td>
<td>0.00137</td>
<td>0.00971</td>
<td>0.01250</td>
<td>0.01298</td>
</tr>
</tbody>
</table>
TABLE IV

$A_{ki} (10^8 s^{-1})$

<table>
<thead>
<tr>
<th>Transition</th>
<th>$A_{ki}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^3P-3s^3S$</td>
<td>2.910</td>
</tr>
<tr>
<td>$^3P-4s^3S$</td>
<td>0.996</td>
</tr>
<tr>
<td>$^3P-3d^3D$</td>
<td>0.376</td>
</tr>
<tr>
<td>$3s^3S-3p^3P$</td>
<td>0.319</td>
</tr>
<tr>
<td>$3p^3P-4s^3S$</td>
<td>0.199</td>
</tr>
<tr>
<td>$3p^3P-3d^3D$</td>
<td>0.300</td>
</tr>
</tbody>
</table>
### APPENDIX I

### GLOSSARY OF NOTATION

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\lambda$</td>
<td>A numerical running index used to label the successive atomic subshells $1s$, $2s$, $2p$, ... There are $b$ such subshells.</td>
</tr>
<tr>
<td>$n_\lambda$</td>
<td>Principle and orbital quantum numbers, respectively, of the $\lambda$th subshell.</td>
</tr>
<tr>
<td>$N_\lambda$</td>
<td>Occupation number of $\lambda$th subshell.</td>
</tr>
<tr>
<td>$N = \sum_\lambda N_\lambda$</td>
<td>Number of electrons in atom.</td>
</tr>
<tr>
<td>$q_\lambda = {s_i^r_i}$</td>
<td>Set of $N_\lambda$ pairs of spin and spatial variables of a subshell function which are ordered in the sequence of increasing $i$.</td>
</tr>
<tr>
<td>$q = {q_\lambda}$</td>
<td>A distribution of $N$ electrons in mutually exclusive sets $q_\lambda$.</td>
</tr>
<tr>
<td>$N(N_\lambda) = N! / \prod_\lambda N_\lambda!$</td>
<td>Number of different $q$.</td>
</tr>
<tr>
<td>$P_q$</td>
<td>Parity of distribution $q$, relative to the ordered set $(1,2,...,i,...N)$.</td>
</tr>
<tr>
<td>$\alpha_\lambda S_\lambda L_\lambda$</td>
<td>$\alpha_\lambda$, seniority number, as defined in Ref. (26); $S_\lambda$, total spin angular momentum; $L_\lambda$, total orbital angular momentum.</td>
</tr>
<tr>
<td>$(q_\lambda</td>
<td>n_\lambda {\lambda \alpha_\lambda S_\lambda L_\lambda M_\lambda M_{\lambda\lambda}}^N$</td>
</tr>
<tr>
<td>$(q_\lambda</td>
<td>n_\lambda {\lambda \alpha_\lambda S_\lambda L_\lambda}^N$</td>
</tr>
</tbody>
</table>
\[ \psi_u(q, \alpha_{SL} M_{SML}) = \{ \pi_{\lambda} (q | n_{\lambda} \alpha_{S}, L_{\lambda}) \} (\alpha_{SL})_{M_{SML}} \]

Unsymmetrized LS-coupled product of antisymmetrized subshell wave functions.

Quantum number that distinguishes different ways of adding the \( S_{\lambda} \) and \( L_{\lambda} \) vectorially to yield \( S \) and \( L \).

\[ \psi(\alpha_{SLM,L_S}) = N(\lambda)^{-1/2} \]

Antisymmetrized and normalized superposition of all \( \psi_u \) with different \( q \).

\[ \Sigma_q (-1)^q \psi_u(q, \alpha_{LSM,L_S}) \]

Coefficient of fractional parentage as defined in Ref. 26.

\[ (\lambda^N-1 N_{\lambda}^S \lambda S_{\lambda}) \]

Analogs of \( N_{\lambda}, q, q_{\lambda}, \alpha_{\lambda}, S_{\lambda}, \) and \( L_{\lambda} \) for spectator electrons.

Intermediate quantum numbers in two-step parentage expansion.

Intermediate matrix element as defined in Ref. (1).

\[ p_{n_{\lambda}} \equiv p_{\lambda} \]

Reduced radial wave function of the \( \lambda \)th subshell.

\[ \chi_k(\rho, \rho', r) = \frac{1}{r^{k+1}} \int_0^r r' P_{\rho}(r') p_{\rho}(r') dr' + r^k \]

\[ \int_0^\infty \frac{1}{r^{k+1}} P_{\rho}(r') p_{\rho}(r') dr' \]
\[ R_k(\rho, \rho', \sigma, \sigma') = \int_0^\infty \int_0^\infty \frac{r^k}{r^{k+1}} P_\rho(r) P_\rho(r') P_\sigma(r) P_\sigma(r') \, dr \, dr' \]

\[ < \bar{L}_1 \ldots [ \bar{L}_{\rho_i} (t \rho_j \bar{L}_{\rho_i} \bar{L}_{\rho_i} \ldots [ \bar{L}_{\sigma_i} (t \sigma_i \bar{L}_{\sigma_i} \bar{L}_{\sigma_i} \ldots, \alpha_i \bar{L}_i] \]

\[ \bar{L}_1 \ldots (\bar{L}_{\rho_j} \bar{L}_{\rho_j} \bar{L}_{\rho_j} \ldots [ \bar{L}_{\sigma_j} (t \sigma_j \bar{L}_{\sigma_j} \bar{L}_{\sigma_j} \ldots, \alpha_j \bar{L}_j] \]

Orbital recoupling coefficient

\[ < \bar{S}_1 \ldots (\bar{S}_{\rho_i} \frac{1}{2}(N)) S_{\rho_i} \ldots (\bar{S}_{\sigma_i} \frac{1}{2}(N+1)) S_{\sigma_i} \ldots, \alpha_i S_i] \]

\[ \bar{S}_1 \ldots (\bar{S}_{\rho_j} \frac{1}{2}(N)) S_{\sigma_j} \ldots (\bar{S}_{\sigma_j} \frac{1}{2}(N+1)) S_{\sigma_j} \ldots, \alpha_j S_j] \]

Spin recoupling coefficient
APPENDIX II
EVALUATION OF ATOMIC RECOUPLING

COEFFICIENTS

The nodes in the recoupling diagrams are labeled from left to right A, B, C, and D, where shells containing two interacting electrons in the same shell receive two labels. The evaluation of the recoupling encountered in atomic theory can be expressed as

\[ \langle \theta_i | \theta_j \rangle = R(A\rightarrow B) R(B\rightarrow C) R(C\rightarrow D) \]

\[ \prod_{\lambda=1}^{A} \delta(L_{\lambda}^a, L_{\lambda}^a) \prod_{\lambda=D}^{B-1} \delta(L_{\lambda}^b, L_{\lambda}^b) \delta(b_i, b_j) . \]

The recoupling of \( \lambda_A \) from node A to node B is given by

\[ R(A\rightarrow B) = \delta(A, B) + \left[ (1-\delta(A, B)) \prod_{\lambda=A}^{B-1} \alpha_{L_{\lambda}^A L_{\lambda}^A} \alpha_{L_{\lambda}^B L_{\lambda}^B} \right] \]

where

\[ \begin{cases} o = I \text{ and } N = J & \text{if } A \in \{\rho_i, \sigma_i\} \\ o = J \text{ and } N = I & \text{if } A \in \{\rho_j, \sigma_j\} \end{cases} \]

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and the recoupling of $\ell_D$ from $C$ to $D$ is given by

$$R(C\rightarrow D) = \delta(C,D) + \sum_{\lambda=C+1}^{D} \delta(C,D) \frac{\ell_D}{\ell_{\lambda-1} \ell_{\lambda} \ell_{\lambda}} L_{\lambda-1} L_{\lambda} L_{\lambda} \langle L_{\lambda-1} \ell_D \ell_{\lambda} \ell_{\lambda} \ell_D \rangle$$

$$\sum_{\lambda=C+1}^{D} \delta(C,D) \frac{\ell_D}{\ell_{\lambda-1} \ell_{\lambda} \ell_{\lambda}} L_{\lambda-1} L_{\lambda} L_{\lambda} \langle L_{\lambda-1} \ell_D \ell_{\lambda} \ell_{\lambda} \ell_D \rangle$$

$$L_{\lambda-1} L_{\lambda} L_{\lambda} \langle L_{\lambda-1} \ell_D \ell_{\lambda} \ell_{\lambda} \ell_D \rangle$$

where

$$\begin{cases} o' = I \text{ and } N' = J & \text{if } A \in \{\rho_i, \sigma_i\} \\ o' = J \text{ and } N' = I & \text{if } A \in \{\rho_j, \sigma_j\} \end{cases}$$

The recoupling from node $B$ to $C$, $R(B\rightarrow C)$, is rather complicated and is very much dependent on the particular coefficient to be evaluated. Below, $R(B\rightarrow C)$ is given for those diagrams on the left in Figs. 1a, 1b, 1c, and 2a. Those coefficients on the right in Figs. 1a, 1b, 1c, and 2a can be evaluated by first taking the Hermitian conjugate of the recoupling coefficient and then relabeling. The relabeling is as follows:

$$i^+_j, j^+_i, \rho_i^+ \sigma_j, \rho_j^+ \sigma_i, \sigma_i^+ \rho_j, \sigma_j^+ \rho_i$$
In the event that $\sigma_j = \rho_j$, then it is also necessary to introduce the phase factor

$$(-1)^{\ell_A + \ell_B - L'}$$

where $L'$ is a summation index defined in the expressions for $R(B \rightarrow C)$. All coefficients represented in Fig. 2b are explicitly evaluated.

For those coefficients represented in Fig. 1a

$$R(B \rightarrow C) = \prod_{\lambda=B+1}^{C-1} \langle L_{\lambda-1}^{\lambda} kL_{\lambda} \rangle L_{\lambda} \bar{L}_{\lambda} L_{\lambda} ^{\alpha} \bar{L}_{\lambda} ^{\alpha} \alpha_{\lambda} ^{\alpha} \alpha_{\lambda} ^{\alpha} \alpha_{\lambda} ^{\alpha} \alpha_{\lambda} ^{\alpha}$$

\[
\begin{cases}
\langle L_{\rho_j-1}^{\rho_j} (\ell, \rho) \rangle L_{\rho_j} \bar{L}_{\rho_j} L_{\rho_j} \alpha_{\rho_j} \alpha_{\rho_j} \alpha_{\rho_j} \alpha_{\rho_j} \alpha_{\rho_j} \rangle \\
\langle \bar{L}_{\rho_i}^{\rho_i} (\ell, \rho) \rangle L_{\rho_i} \bar{L}_{\rho_i} \alpha_{\rho_i} \alpha_{\rho_i} \rangle \\
\langle L_{\rho_i-1}^{\rho_i} (\ell, \rho) \rangle L_{\rho_i} \bar{L}_{\rho_i} \alpha_{\rho_i} \alpha_{\rho_i} \rangle \\
\langle \bar{L}_{\rho_j}^{\rho_j} (\ell, \rho) \rangle L_{\rho_j} \bar{L}_{\rho_j} \alpha_{\rho_j} \alpha_{\rho_j} \rangle \\
\end{cases}
\]
The evaluation of $R(C \rightarrow B)$ for those recoupling coefficients in Fig. 1b is

\[
R(B \rightarrow C) = \sum_{L_B'} R_{L_B'}^{E}(L_B')
\]

\[
\sum_{L_B'} \langle L_B' \& l \rangle \frac{\alpha_i}{L_B'} L_B L_B+l \frac{\alpha_i}{L_B'} \mid \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \rangle
\]

\[
\langle L_B' \& l \rangle \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \mid \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \rangle
\]

\[
\langle L_B' \& l \rangle \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \mid \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \rangle
\]

\[
\langle L_B' \& l \rangle \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \mid \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \rangle
\]

\[
\langle L_B' \& l \rangle \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \mid \frac{\alpha_j}{L_B'} L_B L_B+l \frac{\alpha_j}{L_B'} \rangle
\]
\[
\sum_{i} <(L'_{C-2} \ell_{1})L_{C-2}L_{C-1} | (L'_{C-2} \bar{L}_{C-1})L_{C-1} \ell_{1} L_{C-1}^{\alpha_{i}} > \\
\sum_{j} \frac{\alpha_{j}}{\alpha_{j}} <(L'_{C-2} \ell_{2})L_{C-2}L_{C-1}L_{C-1} | (L'_{C-2} \bar{L}_{C-2}) \ell_{2} L_{C-1}^{\alpha_{j}} > \\
\hat{R}_{2}^{E}(L'_{C-1}) .
\]

In the case of the evaluation of the first and second exchange recoupling coefficient

\[
\ell_{1} = \ell \rho_{j} , \\
\ell_{2} = \ell \sigma_{i} , \\
\hat{R}_{1}^{E}(L'_{B}) = \sum_{i,j} \frac{\alpha_{j}}{\alpha_{j}} <(L'_{\sigma_{j}} \ell_{\rho_{i}}) L_{B} L_{j} \ell_{\rho_{i}} L_{\sigma_{j}} | (L'_{\sigma_{i}} \ell_{\rho_{i}}) L_{B} L_{j} \ell_{\sigma_{j}} > \\
\ell_{1} = \ell \rho_{j} , \\
\ell_{2} = \ell \sigma_{i} , \\
\hat{R}_{2}^{E}(L'_{B}) = \sum_{i,j} \frac{\alpha_{j}}{\alpha_{j}} <(L'_{\sigma_{j}} \ell_{\rho_{i}}) L_{B} L_{j} \ell_{\rho_{i}} L_{\sigma_{j}} | (L'_{\sigma_{i}} \ell_{\rho_{i}}) L_{B} L_{j} \ell_{\sigma_{j}} > \\
\ell_{1} = \ell \rho_{j} , \\
\ell_{2} = \ell \sigma_{i} .
\]

[Equations and expressions follow, with indices and coefficients specified.]
and

\[ R_2^E (L_{C-1}) = \]

\[
\begin{cases}
\langle L_{C-1}^l L_{C}^\alpha C \mid L_{C-1}^l (L_{C}^\alpha C)^* \rangle \\
\langle L_{C-1}^l L_{C}^\alpha C \mid L_{C-1}^l L_{C}^\alpha C \rangle ,
\end{cases}
\]

\[
\begin{cases}
o = J, N = I \text{ for } \#1 & \rho_j \neq \sigma_i \\
o = I, N = J \text{ for } \#2 &
\end{cases}
\]

\[
\begin{cases}
\langle L_{\sigma_i-1}^l \rangle L_{\sigma_i-1}^\alpha_i (L_{\sigma_i}^l L_{\sigma_i}^* L_{\sigma_i}^\alpha_i) \langle L_{\sigma_i-1}^l \rangle \\
L_{\sigma_i-1}^\alpha_j (L_{\sigma_i}^l L_{\sigma_i}^* L_{\sigma_i}^\alpha_i)
\end{cases}
\]

\[
\begin{cases}
\rho_j = \sigma_i &
\end{cases}
\]

In the case of the evaluation of the third and fourth exchange recoupling coefficient

\[ \ell_1 = \ell_{\sigma_i} , \]

\[ \ell_2 = \ell_{\rho_j} , \]

\[ R_1^E (L_{B}^l ) = \]
\[
\begin{align*}
\langle L_{B-1} \ell_A \rangle_{B-1} & \langle L_B \rangle_{B} \langle L_B \rangle_{B} | (L_{B-1} \ell_B)_{B} L_B L_B \rangle \\
\langle L_{B-1} \ell_B \rangle_{B} L_B \langle L_B \rangle_{B} & | (L_{B-1} \ell_B)_{B} L_B L_B \rangle \\
\end{align*}
\]

\[
\begin{cases}
o = I, N = J \text{ for } \# 3 \\
o = J, N = I \text{ for } \# 4
\end{cases}
\]

\[
\begin{align*}
\alpha_i & \langle L_{\sigma_i-1} \ell_{\sigma_i} \rangle_{\sigma_i} L_{\sigma_i} \ell_{\sigma_i} | (L_{\sigma_i-1} \ell_{\sigma_i})_{\sigma_i} L_{\sigma_i} \ell_{\sigma_i} \rangle \\
\alpha_j & \langle L_{\sigma_i-1} \ell_{\sigma_i} \rangle_{\sigma_i} L_{\sigma_i} \ell_{\sigma_i} | (L_{\sigma_i-1} \ell_{\sigma_i})_{\sigma_i} L_{\sigma_i} \ell_{\sigma_i} \rangle
\end{align*}
\]

and

\[
\mathcal{R}_2^E(L_{C-1}) = \\
\sum_{\rho_i, \rho_j} \{ \langle L'_{\ell - \ell} \rangle_{\rho_i} L_{\rho_i} L_{\rho_i} | L'_{\rho_i} L_{\rho_i} \rangle \\
\langle L'_{\rho_i} \ell_{\rho_j} \rangle_{\rho_i} L_{\rho_i} \ell_{\rho_i} | (L'_{\rho_i} \ell_{\rho_j})_{\rho_i} L_{\rho_i} \ell_{\rho_i} \rangle \\
\langle L'_{\rho_i-1} \ell_{\rho_i} \rangle_{\rho_i} L_{\rho_i-1} | (L'_{\rho_i-1} \ell_{\rho_i})_{\rho_i} L_{\rho_i-1} \rangle \\
\langle (k \ell_{\sigma_i})_{\rho_i} L_{\rho_i} \ell_{\rho_i} \rangle_{\rho_i} \}
\]

\[
\rho_i \neq \alpha_j
\]
The evaluation which follows is for those recoupling coefficients represented diagramatically in Figs. 1c and 2a. For $B \neq C$,

$$R(B \rightarrow C) = \sum_{L'} \left\{ \prod_{\pi=\lambda}^{C-1} \langle (L'_{\rho_i-1} \sigma_i L_i)_{\rho_i}^{\alpha_i} \rangle_{L'_{\rho_j}-1} \langle L'_{\rho_i-1} \sigma_i L_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$

$$= \sum_{\sigma_i} \left\{ \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \langle L'_{\rho_i-1} \sigma_i \rangle_{L'_{\rho_j}} \right\}_{L}$$
For $B=C$,

$R(B+C) =$

\[\begin{align*}
\{ \begin{array}{c}
\ell_{\sigma_i} + \ell \rho_i - L_i \\
(\ell \rho_i) \\
\ell_{\sigma_j} + \ell \rho_j - L_j \\
(\ell \rho_j)
\end{array} \begin{array}{c}
\rho_i < \sigma_i \text{ & } \rho_j > \sigma_j \\
\rho_i > \sigma_i \text{ & } \rho_j < \sigma_j
\end{array}
\]
$$\langle [L^{\alpha_j}_{\sigma_1-1} (\ell \cdot k) \cdot \rho_j \cdot \rho_i] L^{\alpha_i}_{\sigma_1} - L^{\alpha_i}_{\sigma_1} L^{\alpha_i}_{\sigma_1} | [L^{\alpha_j}_{\sigma_1-1} (L^j L^i)$$

$$L^{\alpha_j}_{\sigma_1} \cdot \rho_j \cdot \sigma_i \sigma_i$$

$$\langle (\sum_{\sigma_i} L^i L^j L^j) L^i L^j | (k \cdot \rho_j) \cdot \sigma_i \cdot \rho_j \cdot \rho_i \cdot \sigma_i \rangle$$

$$\sigma_i = \sigma_j$$

$$\langle (L^i L^j L^j) L^i L^j | (L^i L^j) L^i L^j \rangle$$

$$\rho_i = \rho_j$$

or

$$R(B \cdot C) = \sum_{L_i} \langle (L^i L^j L^j) L^i L^j L^i L^j | (L^i L^j) L^i L^j \rangle$$

$$\langle (k \cdot \rho_j) \cdot \sigma_i \cdot \rho_j \rangle$$

$$\sigma_i = \rho_j$$

$$\langle L^{\alpha_i}_{\sigma_1} (\ell \cdot k) \cdot \rho_j \cdot \rho_j \cdot \sigma_i \sigma_j \sigma_j \rangle$$

$$L^{\alpha_i}_{\sigma_1} L^{\alpha_i}_{\sigma_1} | [L^{\alpha_j}_{\sigma_1} (k \cdot \rho_j) \sigma_i \sigma_j \sigma_j$$

$$\langle L^{\alpha_i}_{\sigma_1} L^{\alpha_i}_{\sigma_1} L^j L^j | (k \cdot \rho_j) \sigma_i \sigma_j \sigma_j \rangle$$

$$\rho_i = \sigma_j$$
The recoupling function $R(B\rightarrow C)$ for those coefficients in Fig. 2c which satisfy the criterion

$$\text{Min}(\rho_j, \sigma_j) < \rho_i = \sigma_i < \text{Max}(\rho_j, \sigma_j)$$

or

$$\text{Min}(\rho_i, \sigma_i) < \rho_j = \sigma_j < \text{Max}(\rho_i, \sigma_i)$$

is

$$R(B\rightarrow C) = \sum \left\langle \frac{\alpha_N}{L B-1} (L' D) L' B \mid \frac{\alpha_i}{L B-1} L B \right\rangle \left\langle \frac{\alpha_j}{L B-1} (L' D) L' B \mid \frac{\alpha_i}{L B-1} L B \right\rangle \left\langle \frac{\alpha_j}{L B-1} (L' D) L' B \mid \frac{\alpha_j}{L B-1} L B \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \right\rangle \r..
For those coefficients which satisfy the criterion

\[ \min(\rho_j, \sigma_j) = \rho_i = \sigma_i < \max(\rho_j, \sigma_j) \]

or

\[ \min(\rho_i, \sigma_i) = \rho_j = \sigma_j < \max(\rho_i, \sigma_i) \]
\[ R(B \rightarrow C) = \left< L_{\alpha_i}^{i} (L_{\alpha_j}^{j}) L_{\alpha_k}^{\beta} \right| L_{\alpha_i}^{i} L_{\alpha_j}^{j} \right>^{R'} \]

where

\[
\begin{align*}
(0 & = I \text{ and } N = J \text{ if } \rho_i = \sigma_i \\
(0 & = J \text{ and } N = I \text{ if } \rho_j = \sigma_j ,
\end{align*}
\]

and

\[
R' = \left< L_{\alpha_i}^{i} (k \ell_{\sigma_i}) \ell_{\sigma_j}^{j} \right| L_{\alpha_i}^{i} L_{\alpha_j}^{j} \right>^{R'} \cdot \rho_i = \sigma_j = \rho_j < \sigma_i
\]

\[
\left< L_{\alpha_j}^{j} (k \ell_{\sigma_j}) \ell_{\sigma_i}^{i} \right| L_{\alpha_j}^{j} \right>^{R'} \cdot \left< L_{\alpha_i}^{i} (k \ell_{\sigma_i}) \ell_{\sigma_j}^{j} \right| L_{\alpha_i}^{i} \right>^{R'} \cdot \sigma_i = \sigma_j = \rho_j < \rho_i
\]

\[
\left< L_{\alpha_i}^{i} (k \ell_{\sigma_i}) \ell_{\sigma_j}^{j} \right| L_{\alpha_i}^{i} L_{\alpha_j}^{j} \right>^{R'} \cdot \sigma_j = \rho_i = \sigma_i < \rho_j
\]

\[
\left< L_{\alpha_j}^{j} (k \ell_{\sigma_j}) \ell_{\sigma_i}^{i} \right| L_{\alpha_j}^{j} \right>^{R'} \cdot \left< L_{\alpha_i}^{i} (k \ell_{\sigma_i}) \ell_{\sigma_j}^{j} \right| L_{\alpha_i}^{i} \right>^{R'} \cdot \rho_j = \rho_i = \sigma_i < \sigma_j
\]
For those coefficients which satisfy the criterion

\[ \min(p_j, \sigma_j) < \rho_i = \sigma_i = \max(p_j, \sigma_j) \]

or

\[ \min(p_i, \sigma_i) < \rho_j = \sigma_j = \max(p_i, \sigma_i) \]

\[ R(B \to C) = \langle \frac{\alpha}{L_D - L_{D'}} \frac{\alpha}{L_D - L_{D'}} \frac{\alpha}{L_D - L_{D'}} \frac{\alpha}{L_D - L_{D'}} \frac{\alpha}{L_D - L_{D'}} \frac{\alpha}{L_D - L_{D'}} > R' \]

where

\[
\begin{cases}
\emptyset = I \text{ and } N = J \text{ if } \rho = \sigma \\
\emptyset = J \text{ and } N = I \text{ if } \rho = \sigma 
\end{cases}
\]

and

\[
R' = \left\{ \begin{array}{ll}
\langle \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \rangle & \rho_i < \sigma_i = \sigma_j = \rho_j \\
\langle \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \frac{\alpha}{L_{D - L_{D'}}} \rangle & c_i < \rho_i = \sigma_j = \rho_j 
\end{array} \right. 
\]
The evaluation of $R(B \rightarrow C)$ for $A=B=C=D$ is

\[ R(B \rightarrow C) = \langle \tilde{L}_i k \tilde{L}_j l \tilde{L}_i l \mid \tilde{L}_i k \tilde{L}_j l \tilde{L}_i l \rangle \]

\[ \langle \tilde{L}_i k \tilde{L}_j l \tilde{L}_i l \rangle = \langle \tilde{L}_i k \tilde{L}_j l \tilde{L}_i l \rangle \]
VITA

Steven Prescott Rountree was born on February 12, 1946 in Lafayette, Louisiana. He graduated from Hackberry High School in 1964. He received the degree of Bachelor of Science in Electrical Engineering from Louisiana State University in 1969. Continuing his education, he received his degree of Masters of Science in Physics from Louisiana State University in 1971. He is now a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy.
EXAMINATION AND THESIS REPORT

Candidate: Steven Prescott Rountree

Major Field: Physics

Title of Thesis: Electron-Impact Excitation Cross Sections for Atomic Oxygen

Approved:

[Signatures]

Major Professor and Chairman
Dean of the Graduate School

EXAMINING COMMITTEE:

[Signatures]

Date of Examination:

5/24/73