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Algebraic Close Coupling Approach to Electron Hydrogen Scattering.

George Joseph Seiler

Louisiana State University and Agricultural & Mechanical College

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TO ELECTRON HYDROGEN SCATTERING

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in

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Finally, this dissertation is dedicated to my wife, Diane.
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ABSTRACT

The algebraic close coupling method is applied to slow collisions of electrons and positrons with atomic hydrogen. The wave function is assumed to be of the form appropriate for a ls-2s-2p close coupling calculation. The anomaly-free variational method proposed by Nesbet, essentially algebraic in nature, is used to calculate the appropriate phase shifts and cross sections.

Excellent agreement with previously published results of Burke, Schey, Smith, and others is obtained for scattering below the n=2 threshold. Valuable information concerning resonance structure for positrons, and for electrons in the singlet and triplet states, is also obtained. A ls-2s approximation produces results in excellent agreement with the two-state approximation of Burke, Schey, and Smith for both the elastic and the inelastic cross sections.

In the 3-state approximation above threshold, asymptotic forms of the type $j_\ell(1-e^{\gamma r})^{2\ell+1}$ and $n_\ell(1-e^{-\beta r})^{2\ell+1}$ are used, where $j_\ell$ and $n_\ell$ are spherical Bessel and Neumann functions, and $\beta$ and $\gamma$ are adjustable variational parameters. A solution is said to have converged when it is stable both with respect to variations of the parameters $\beta$ and $\gamma$, and also with respect to an increase of the basis states.
Because of the long range effect of the $1/r^2$ potential which arises from the coupling of the degenerate 2s and 2p states, the spherical Bessel and Neumann functions are not the correct asymptotic solutions for the 2p channel. This effect is brought out in the 3-state calculation above threshold, and is fully discussed in this dissertation. Finally, the correct asymptotic forms are discussed.
CHAPTER I
INTRODUCTION

The field of electron-atom scattering has been of considerable interest since the introduction of wave mechanics. In spite of great activity in this area in recent years, fundamental problems still remain in the quantum mechanics of few particle systems. One of the simplest of these is the interaction of an electron (or a positron) with a neutral hydrogen atom.

The difficulties which remain are partially numerical and partially conceptual. In an effort which began approximately ten years ago, Burke and collaborators have calculated cross sections for both elastic and inelastic scattering of electrons and positrons by hydrogen atoms. This work employed the close coupling procedure in which the wave function is expanded in eigenstates of the hydrogen atom. Complicated integro-differential equations result which must be integrated numerically. The major achievement has been the prediction of series of resonances below the various inelastic thresholds. Some of these have been observed experimentally. However, as was pointed out by Burke and Schey, the convergence of the method is slow, and only a limited number of eigenstates may be included in a practical calculation. This means that highly excited bound states and all continuum states are
excluded. Continuum states contribute 18.6% of the polarizability of the hydrogen atom in its ground state, and neglect of this contribution severely reduces the accuracy of the results at low energies. In order to improve the situation, Burke, Gallaher, and Geltman have modified the usual form of the close coupling method by including in the eigenstate expansion pseudo-states chosen in such a way as to give the ground state polarizability exactly.\(^2\)

A substantial increase in confidence in the validity of results of scattering calculations can result from the employment of variational methods. These approaches were developed by Hulthen and Kohn.\(^3\) Schwartz\(^4\) utilized the Kohn procedure to carry out an extensive calculation of the s-wave elastic scattering of electrons and positrons from atomic hydrogen using up to 50 trial functions of the type introduced by Hylleraas to describe the bound states of two-electron atoms. Armstead\(^5\) carried out a similar calculation for p-wave elastic scattering of electrons and positrons from atomic hydrogen. Because of the extensiveness of the calculations, the results of Schwartz and Armstead are considered exact below the first threshold. However, the calculations of Schwartz and Armstead were not extended to produce detail in the resonance region, and neither author considered inelastic scattering processes. Schwartz also encountered some difficulties using the Kohn method. Wild fluctuations and instability
in the phase shifts were occasionally encountered. Values ranging anywhere from \(-\infty\) to \(+\infty\) were obtained for the phase shifts which should be accurate to "second order". The algebraic source of this difficulty was pointed out by Demkov and Shepelenko.\(^6\)

Harris\(^7\) proposed an expansion method for calculating phase shifts which avoids the fluctuations encountered by Schwartz. The method was applied to low energy electron-hydrogen and electron-helium scattering by Michels and others.\(^8\) In the Harris method, the real Hamiltonian which has a continuous spectrum is approximated by an operator with a point spectrum. These points are the eigenvalues obtained from the simultaneous diagonalization of the Hamiltonian and overlap matrix on a chosen, finite basis set. We have found that the Harris eigenvalues tend to bunch near zero scattering energy and near thresholds, with only a few inbetween. The bunching near zero enables a reliable calculation of the scattering length. By adjusting the basis functions one may obtain a reasonable spectrum of scattering energies. However, in situations where there is a need to scan a narrow region of energy to study phase shifts, as encountered in resonance phenomena, the Harris method is less useful.

Nesbet\(^9\) has extended the Harris method to enable the calculation of scattering phase shifts at arbitrary energies. The Nesbet method was applied to low energy
s-wave electron-hydrogen scattering by Callaway, Oberoi, and Seiler. Resonances in both the singlet and the triplet case were uncovered and investigated in detail.

Nesbet has also developed a procedure to include inelastic processes. In an algebraic formalism which should be free of anomalies, judicious use of the Kohn or inverse Kohn formulae avoids the spurious singularities encountered by Schwartz while using the Kohn procedure. Harris and Michels have also proposed a method for inelastic processes, which is an extension of their approach to elastic scattering.

This dissertation presents calculations of low energy electron- and positron-hydrogen scattering for three partial waves below the n=2 threshold. Inelastic processes are done using both a 1s-2s and a 1s-2s-2p close coupling approximation, utilizing the procedures proposed by Nesbet. We use a close coupling expansion in hydrogen atom eigenstates, and thus are working in the same realm as Burke and collaborators. The distinct difference, however, is in the method employed to solve the resulting system of linear inhomogeneous equations. Burke et al have employed numerical integration techniques exclusively. Frequently, especially for small values of the scattering energy, the numerical iteration scheme fails to converge. The Nesbet procedure is essentially algebraic in nature. The resulting system of linear inhomogeneous equations is
solved by a matrix technique in which all of the matrix elements involve integrals which have explicit analytic expressions. The method is quite fast in terms of computer time, and is able to predict resonance structure in detail. Also, the method is quite capable of handling large numbers of closely coupled states.

In Chapter II we outline the Nesbet procedure and demonstrate how it is applied to electron- and positron-hydrogen scattering. Chapter III presents the results for electron-hydrogen scattering below the first threshold. Three partial waves were analyzed in the singlet and the triplet state. Scattering lengths and resonance structure are also included in this chapter. Chapter IV presents the results for positron-hydrogen scattering below the first threshold for three partial waves. Resonance structure was noted for all three partial waves and is described in detail. In Chapter V we report results for electron-hydrogen scattering above the n=2 threshold using both a 1s-2s and a 1s-2s-2p approximation, along with a discussion concerning asymptotic solutions. Chapter VI contains the results for positron-hydrogen scattering above the n=2 threshold. Finally, Chapter VII includes a discussion of the Nesbet procedure, along with some conclusions concerning it.

Atomic units (\(\hbar = 1\), \(m_e = \frac{1}{2}\), \(e^2 = 2\)) are used throughout this work. Energies are given in rydbergs (1 ryd. = 13.605 eV)
unless specified otherwise. Phase shifts are given in radians.
CHAPTER II

REVIEW OF THE NESBET VARIATIONAL METHOD

We are dealing with a multichannel problem so we define a channel in which a collision takes place by a complete set of quantum numbers. A convenient choice, following Burke,\textsuperscript{13} is

\[ \mathcal{V} = \rho \ell_1 S_1 \ell_2 L S M_L M_S \pi, \]

where

- \( \ell_1 S_1 \) specify the orbital angular momentum and spin of the atomic state
- \( \ell_2 \) is the orbital angular momentum of the scattered electron (positron)
- \( \rho \) specifies any further quantum numbers required to define the atomic state
- \( \pi \) is the parity of the system which is conserved in the collision.

L and S satisfy the triangular relations

\[ |\ell_1 - \ell_2| \leq L \leq \ell_1 + \ell_2 \]

\[ |S_1 - \frac{\ell}{2}| \leq S \leq S_1 + \frac{\ell}{2} \] \hspace{1cm} (II-2)
In each channel the system is represented by an atomic eigenstate compounded with the angular variables and spin of the incident electron to form an eigenstate of $L$ and $S$ multiplied by a radial wave function describing the relative motion of the electron and the atom.

We first construct a trial wave function to represent the system. Scattering phase shifts and cross sections are determined from the asymptotic form of the radial wave function. We therefore construct a variational functional $I_{\sigma \nu}$ and use the Kohn and the inverse Kohn variational principles to determine stationary values of the coefficients of the asymptotic solutions. For the single channel problem, the Hulthen and the inverse Hulthen variational principles are also used.

The $R$ matrix offers a convenient way to determine scattering cross sections. The partial cross section for a transition from channel $p$ to channel $q$ is

$$Q_{p \rightarrow q} = \left( \frac{4 \pi \hbar^2}{k_p^2} \right) \left| \left[ \frac{R}{1 - iR} \right] \right|^2.$$  \hspace{1cm} \text{(II-3)}

The Schrödinger equation for a multichannel system can be written

$$\left( \mathcal{H} - E \right) \psi(1,2) = 0,$$  \hspace{1cm} \text{(II-4)}

where
The index $v$ specifies the incident channel, $N$ the number of channels, and the sum is taken over all final channels $q$. We use the close coupling approximation to write the wave function for the scattering of an electron from a hydrogen atom in the form

$$\psi^v_{\ell, l_z} = \left(\frac{1 \pm P_{12}}{\sqrt{2}}\right) \psi^v_{g, (1)} F^{v}_{q, (2)} \psi^0_{\ell, l_z, l_z}.$$  \hspace{1cm} (II-6)

The operator $P_{12}$ is the two particle exchange operator and the function $u^q_\ell$ is the hydrogenic radial function germane to channel $q$. The angular function is defined as

$$\psi^M_{\ell, l_z} = \sum_{m, m_z} \mathcal{C}[\ell, l_z, l_z; m, m_z] \psi^m_{\ell, m} \psi^{m_z}_{l_z, m_z},$$  \hspace{1cm} (II-7)

where $\mathcal{C}$ is a Clebsch-Gordan coefficient and the $\psi^m$'s are the usual spherical harmonics.

The scattering wave function $F^v_q$ can be written as the sum of an exponentially decaying internal function $\phi^v_q$ and a free wave asymptotic solution. We write

$$F^v_q = \phi^v_q + \lambda^v_{qg} S_g + \lambda^v_{jg} C_g,$$  \hspace{1cm} (II-8)
where cross sections depend on the relative values of the \( a_{i \chi}^\nu \) \((i=0,1)\).

The asymptotic solutions are

\[
S_{g} \sim \sin \left( k_{g} r - \frac{l_{g} \pi}{2} \right) / r \, ,
\]

\[
C_{g} \sim \cos \left( k_{g} r - \frac{l_{g} \pi}{2} \right) / r \, .
\]

We can make use of the theory of the R matrix discussed earlier in this chapter by choosing

\[
\alpha_{o \chi}^\nu = S_{g} \, ,
\]

so that the wave function in Eq. (II-30) asymptotically has the same form as in the R matrix theory. The second \( \alpha \) coefficient becomes

\[
\alpha_{i \gamma}^\nu = S_{\gamma} \, ,
\]

where

\[
R_{\gamma} = \left( \frac{k_{g}}{k_{\gamma}} \right)^{1/2} S_{\gamma} \, .
\]

The Kohn variational method then determines extremum values of the elements of the R matrix.

If we choose
then we would have
\[ \alpha_{\beta} = \beta_{\gamma} \]

where
\[ R_{\beta}^{-1} = \left( \frac{\beta_{\gamma}}{\delta_{\gamma}} \right)^{1/2} \beta_{\beta} \].

The element \( R_{\beta}^{-1} \) is an element of the R-inverse matrix. We use the inverse Kohn variational method to determine extremum values of the elements of the R-inverse matrix.

We can approximate the internal function \( \psi_{\nu} \) by an expansion in a set of normalizable basis functions. If the set of basis functions could become complete, the representation of \( \psi_{\nu} \) would become exact. We write
\[ \psi_{\nu} = \sum_{q} \gamma_{q}^{\nu} \mathcal{C}_{q} \]

where \( n_{q} \) specifies the number of basis functions in channel \( q \).

The coefficients of Eq. (II-16) are determined by demanding that the trial wave function \( \psi_{\nu} \) satisfy the
Schrödinger equation in the subspace of Hilbert space spanned by the basis functions $\eta_a^q$. We demand

$$
\sum_{\beta} \langle \Theta_{\alpha}^{\gamma}(1,1) | H - E | \chi_{\beta}^{\gamma}(1,2) + \alpha_{\beta}^{\gamma} \Delta_{\alpha}^{\gamma}(1,1) + \alpha_{\beta}^{\gamma} \Delta_{\alpha}^{\gamma}(1,1) \rangle = 0
$$

\( \alpha = 1, \ldots, n_P \); \( P = 1, \ldots, N \)

(II-17)

where

$$
\chi_{\beta}^{\gamma}(1,2) = \sum_{b=1}^{n_P} \Theta_{b}^{\gamma}(1,2) \ C_{b}^{\gamma}
$$

(II-18)

$$
\Theta_{b}^{\gamma}(1,2) = \left( \frac{1 \pm P_{l_z}}{\sqrt{2}} \right) \ U_{b}^{\gamma}(1) \ \eta_{b}^{\gamma}(2) \ \mathcal{U}^{\gamma}(\hat{r}_l, \hat{r}_z)
$$

(II-19)

$$
\Delta_{\alpha}^{\gamma}(1,1) = \left( \frac{1 \pm P_{l_z}}{\sqrt{2}} \right) \ U_{\alpha}^{\gamma}(1) \ S_{\beta}^{\gamma}(2) \ \mathcal{U}^{\gamma}(\hat{r}_l, \hat{r}_z)
$$

(II-20)

$$
\Delta_{\alpha}^{\gamma}(1,1) = \left( \frac{1 \pm P_{l_z}}{\sqrt{2}} \right) \ U_{\alpha}^{\gamma}(1) \ C_{\beta}^{\gamma}(2) \ \mathcal{U}^{\gamma}(\hat{r}_l, \hat{r}_z)
$$

(II-21)

Equation (II-17) can be written

$$
\sum_{\alpha} \sum_{\beta} \langle \Theta_{\alpha}^{\gamma}(1,1) | H - E | \Theta_{\beta}^{\gamma}(1,2) \rangle \ C_{b}^{\gamma} =
-\sum_{\beta} \left[ \alpha_{\beta}^{\gamma} \langle \Theta_{\alpha}^{\gamma}(1,1) | H - E | \Delta_{\beta}^{\gamma}(1,1) \rangle + \alpha_{\beta}^{\gamma} \langle \Theta_{\alpha}^{\gamma}(1,1) | H - E | \Delta_{\beta}^{\gamma}(1,1) \rangle \right]
$$

(II-22)
Eq. (II-22) determines the coefficients $C_{b}^{S^v}$ as linear combinations of the $a$'s. We can write

$$C_{b}^{S^v} = \sum_{g} \left( a_{g}^{a} C_{b}^{a} + a_{g}^{a} C_{b}^{a} \right).$$  (II-23)

Equation (II-22) is satisfied if we choose the coefficients $C_{bi}^{S^q}$ $(i=0,1)$ of Eq. (II-23) to satisfy the equations

$$\sum_{c} \sum_{b} \left\langle \Theta_{c}^{p}(1, z) \middle| H-E \middle| \Theta_{b}^{c}(1, z) \right\rangle C_{b}^{a} = - \left\langle \Theta_{a}^{p}(1, z) \middle| H-E \middle| A_{g}^{i} \right\rangle \delta_{ij}.$$  (II-24)

It is convenient to define the functions

$$\phi_{g}^{a}(1, z) = \sum_{b} \Theta_{b}^{a}(1, z) C_{b}^{a},$$  (II-25)

so that Eqs. (II-24) can be written

$$\sum_{c} \left\langle \Theta_{c}^{p}(1, z) \middle| H-E \middle| \phi_{g}^{a}(1, z) \right\rangle = - \left\langle \Theta_{a}^{p}(1, z) \middle| H-E \middle| A_{g}^{i} \right\rangle \delta_{ij}.$$  (II-26)

It should be noted that in terms of the functions defined in Eqs. (II-25) the internal close coupling function becomes

$$\chi_{a}(1, z) = \sum_{g} \left( a_{g}^{a} \phi_{g}^{a}(1, z) + a_{g}^{a} \phi_{g}^{a}(1, z) \right).$$  (II-27)
Equation (II-26) can be written in the alternate form

\[ \sum \langle \phi^p_{i_1} \mid H-E \mid \psi^e_{i_2} \rangle = 0 \quad \text{for } i = 0, 1 \]  

(II-28)

where

\[ \psi^e_{i_2} = \phi^e_{i_2} + A^e_{i_2} \sum \phi^a \]  

(II-29)

We can use Eq. (II-29) to write the wave function for the system in the general form

\[ \psi^v_{i_1} = \sum \psi^e_{i_2} = \sum \phi^v_{i_2}, \]  

(II-30)

It should be clear that the determination of the functions \( \phi^s_{i_1} \) of Eq. (II-25) obtained by solving Eqs. (II-26) is sufficient to determine the trial wave function \( \psi^v \). It is convenient in solving Eqs. (II-26) to construct the set of eigenfunctions which satisfy the homogeneous part of Eqs. (II-24) at energy eigenvalues \( E^\alpha \) from the equations

\[ \sum \sum \left( H_{ab}^{p\alpha} - E^\alpha S_{ab}^{p\alpha} \right) C_{b\alpha} = 0 \]  

(II-31)

where
The eigenfunctions $\Psi_\alpha$ become

$$\Psi_\alpha^{(1,2)} = \sum_\alpha \Psi_\alpha^{(1,2)} = \sum_\alpha \sum_b \Theta_b^{(1,2)} C_{b\alpha}.$$  \hfill (II-33)

Since the eigenfunctions span the same subspace of Hilbert space as the basis functions we can write from Eqs. (II-26)

$$\sum_\alpha \left\langle \Psi_\alpha^{(1,2)} \middle| H - E \right\rangle \Phi_{1q}^{(1,2)} = -\left\langle \Psi_\alpha^{(1,2)} \middle| H - E \right\rangle \Phi_{1q}^{(1,2)}$$

$$\lambda = 0, 1; \lambda = 1, \ldots, N; x = 1, \ldots, N.$$ \hfill (II-34)

Moreover, since the $\Phi_{1q}^{(1)}$ have been constructed to span the same space as the eigenfunctions $\Psi_\alpha$ we can expand the internal functions in terms of the eigenfunctions. We write

$$\Phi_{1q}^{(1,2)} = \sum_{\lambda'} \Psi_{\lambda'}^{(1,2)} K_{\lambda',\lambda}.$$ \hfill (II-35)

From Eqs. (II-34) and (II-35) we find that
\[ \sum_{i} \sum_{d'} \left< \phi_{d}^{(1,2)} | H - E | \phi_{d'}^{(1,2)} \right> K_{d,i}^{\delta} = \]

\[ - \left< \phi_{d}^{(1,2)} | H - E | \phi_{d}^{(1,2)} \right> \]

\[ \delta = 0, 1; \alpha = 1, \ldots, n \times N; \quad p = 1, \ldots, N. \]  \hspace{1cm} (II-36)

Since the \( \psi_{d} \) are eigenfunctions of the Hamiltonian \( H \) at energy eigenvalues \( E \), and are themselves orthonormal we can write from Eq. (II-36)

\[ K_{d,i}^{\delta} = M_{d,i}^{\delta} \left( E - E_{\delta} \right)^{-1} \]  \hspace{1cm} (II-37)

where

\[ M_{d,i}^{\delta} = \sum_{p} \left< \phi_{d}^{p(1,2)} | H - E | \phi_{d}^{p(1,2)} \right> \cdot \]  \hspace{1cm} (II-38)

We summed both sides of Eq. (II-36) over \( p \) in deriving Eq. (II-37). The internal functions determined from Eqs. (II-35) and (II-37) become

\[ \phi_{d}^{(1,2)} = \sum_{\delta} \psi_{d}^{(1,2)} \left( E - E_{\delta} \right)^{-1} M_{d,i}^{\delta} \cdot \]  \hspace{1cm} (II-39)

The trial wave function in Eq. (II-6) is now determined except for the coefficients \( \alpha \), which are related to the
cross sections. The $\alpha$ coefficients are determined from the Kohn or inverse Kohn variational methods, properly extended to represent a multichannel system.

For a variational calculation it is necessary to define the variational functional

$$I_{\sigma, \gamma} = \left\langle \psi_{(1, z)}^{\sigma} \right| H - E \right| \psi_{(1, z)}^{\gamma} \right\rangle. \quad (II-40)$$

It is convenient to define the matrix elements

$$M_{\rho, \beta}^{\sigma, \gamma} = \sum_{I, I'} \left\langle \psi_{I, \rho}^{I, I'} \right| H - E \right| \psi_{I', \beta}^{I, I'} \right\rangle, \quad (II-41)$$

so that the variational functional can be written

$$I_{\sigma, \gamma} = \sum_{\rho, \beta} \alpha_{\rho}^{\sigma, *} M_{\rho, \beta}^{\sigma, \gamma} \alpha_{\beta}^{\gamma}. \quad (II-42)$$

We are looking for the first order variation of $I_{\sigma, \gamma}$,

$$\delta I_{\sigma, \gamma} = \sum_{I, I'} \frac{\partial I_{\sigma, \gamma}}{\partial \alpha_{I, I'}^{\sigma, *}} \delta \alpha_{I, I'}^{\sigma, *} + \sum_{\beta} \frac{\partial I_{\sigma, \gamma}}{\partial \alpha_{\beta}^{\gamma}} \delta \alpha_{\beta}^{\gamma}. \quad (II-43)$$

Equation (II-43) can be written

$$I_{\sigma, \gamma} = \sum_{I, I'} \alpha_{I, I'}^{\sigma, *} I_{I, I'}^{\rho} \delta \alpha_{I, I'}^{\rho}. \quad (II-44)$$

where
\[ I_{\nu}^p = \sum_{\delta g} M_{i, \delta}^p \alpha_{i, \delta} \]  \hspace{1cm} (II-45)

We can write from Eq. (II-44)

\[ \frac{\partial I_{\nu}^{\sigma \omega}}{\partial \alpha_{i, \alpha}^{\sigma \omega}} = I_{\nu}^p \]  \hspace{1cm} (II-46)

Since the operator \( H \) is Hermitean with respect to normalizable functions, the matrix elements \( M_{i,j}^{pq} \) can be shown to satisfy the symmetry relation

\[ M_{i,j}^{pq} = M_{j,i}^{q,p} + k_p \delta_{p,q} (\delta_{i,0} \delta_{j,1} - \delta_{i,1} \delta_{j,0}) \]

\[ i, j = 0, 1; \quad p, q = 1, \ldots, N. \]  \hspace{1cm} (II-47)

The variational functional can now be written

\[ I_{\sigma \nu} = \sum_{\delta g} \left[ I_{\sigma, \delta}^{\nu} + k_g (\delta_{j,1} \alpha_{\sigma, \delta}^{\nu} - \delta_{j,0} \alpha_{1, \delta}^{\nu})\right] \alpha_{j, \delta}^{\nu}, \]  \hspace{1cm} (II-48)

from which

\[ \frac{\partial I_{\sigma \nu}}{\partial \alpha_{j, \delta}^{\nu}} = I_{j, \sigma}^{\nu} + k_g (\delta_{j,1} \alpha_{\sigma, \delta}^{\nu} - \delta_{j,0} \alpha_{1, \delta}^{\nu}). \]  \hspace{1cm} (II-49)

From Eqs. (II-43), (II-46), and (II-49) the first order variation of the functional \( I_{\sigma \nu} \) becomes
\[ \delta I_{\sigma\nu} = \sum_p I_{1\sigma}^P \delta \alpha_{1\rho}^{\sigma \ast} + \sum_{i} I_{i\sigma}^g \delta \alpha_{i\beta}^{\nu \ast} \]

\[ + \sum_{g} k_g (\alpha_{o\bar{g}}^{\sigma \ast} \delta \alpha_{1\beta}^{-} - \alpha_{1\beta}^{\nu \ast} \delta \alpha_{o\bar{g}}^{\nu}) \]  

(II-50)

We can use Eqs. (II-11) and (II-12) to write Eq. (II-50) in the form

\[ \delta I_{\sigma\nu} = \sum_p I_{1\sigma}^P \delta \nu_{1\rho}^p + \sum_{i} I_{i\sigma}^g \delta \nu_{i\beta}^g + k_{\sigma} \delta \nu_{1\rho}^{(\nu)} \]  

(II-51)

From Eq. (II-45) we can make the integrals \( I_{1\nu}^P \) and \( I_{i\sigma}^g \) vanish simultaneously by choosing

\[ \sum_{g} M_{i1}^{P \bar{g}} \nu_{1\rho}^{(\nu)} = - M_{i1}^{P \nu} \]

\[ \nu = 1, \ldots, N ; p = 1, \ldots, N, \]  

(II-52)

where \( \nu_{1\rho}^{(\nu)} \) is the first order approximation to the \( R \) matrix element. Equation (II-51) becomes

\[ \delta \left( I_{\sigma\nu} - k_{\sigma} \nu_{1\rho}^{(\nu)} \right) = 0 \]  

(II-53)

from which the Kohn method specifies

\[ \nu_{1\rho} = \nu_{1\rho}^{(\nu)} - \frac{1}{k_{\rho}} I_{g\rho} \left( \nu_{1\rho}^{(\nu)} \right) \]  

(II-54)
From Eqs. (II-42) and (II-45) we find that

$$\delta_{\nu^*} = \delta_{\nu^*}^{(o)} - \frac{1}{k^2} \left( M_{00}^{2\omega} + \sum_{r} M_{01}^{2\omega} \beta_{r}^{(o)} \right). \tag{II-55}$$

A similar analysis using the inverse Kohn method finds that

$$\beta_{\nu^*} = \beta_{\nu^*}^{(o)} + \frac{1}{k^2} \left( M_{11}^{\omega} + \sum_{r} M_{10}^{\omega} \beta_{r}^{(o)} \right), \tag{II-56}$$

where

$$\sum_{\nu} M_{00}^{\nu^*} \beta_{\nu^*}^{(o)} = -M_{01}^{\nu^*}, \quad \nu = 1, \ldots, N; \quad p = 1, \ldots, N. \tag{II-57}$$

The R matrix elements are given by Eq. (II-12) and the inverse R matrix elements are given by Eq. (II-15). The cross sections are found from the R or the $R^{-1}$ matrix using Eq. (II-3).

For a single channel problem the R and the $R^{-1}$ matrix elements are simply related to the tangent or cotangent of the phase shifts, so that we can write for the single channel problem (p=q=1)

$$t_{k} = -\left( \frac{M_{00}}{M_{11}} \right) - \left( \frac{det \frac{M}{k_1 M_{11}}} \right), \tag{II-58}$$
where \( t_k \) is the tangent of the phase shift using the Kohn variational method, and \( c_k \) is the cotangent of the phase shift using the inverse Kohn or Rubinow methods, and

\[
C_k = - \left( \frac{M_{oo}}{M_{ko}} \right) + \left( \frac{\det M}{k^2 M_{oo}} \right) ,
\]

(II-59)

The Hulthen variational method demands that \( I_{\nu\nu} = 0 \), and for the single channel problem we find

\[
\frac{1}{2} M_{ii} = \frac{1}{2} M_{11} - \frac{1}{2} M_{00} M_{01} ,
\]

(II-60)

where \( t' \) is the tangent of the phase shift using the Hulthen method and \( c_H \) is simply the inverse of \( t_H \), which may be needed for numerical accuracy. When \( \det M \) is zero, all four methods agree exactly.

The crux of the problem involves the evaluation of the matrix elements \( M^{pq}_{ij} \) of Eq. (II-41). From Eqs. (II-29) and (II-38) we can write
\[ M_{l_{\delta}^{P}} = M_{r_{p r}, r_{\delta}^{P}} + \sum_{\ell} M_{l_{\alpha}^{P}} (E - E_{\ell}) M_{l_{\delta}^{P}} \]  

(II-63)

where

\[ M_{r_{p r}, r_{\delta}^{P}} = \langle r_{l_{p}}^{(1,2)} | H - E | r_{\delta}^{(1,2)} \rangle . \]  

(II-64)

We use as asymptotic solutions for the problem

\[ S_{p} = k_{r} j_{l_{z}} (k_{r} r) \left( 1 - \frac{\gamma_{r}}{r} \right)^{2l_{z} + 1} \]  

\[ C_{p} = k_{r} n_{l_{z}} (k_{r} r) \left( 1 - \frac{\beta_{r}}{r} \right)^{2l_{z} + 1} \]  

(II-65)

with \( j_{l} \) and \( n_{l} \) the spherical Bessel and Neumann functions. This choice has the proper asymptotic behavior dictated by Eqs. (II-9). We return to the proper choice of asymptotic solutions in Chapter V.

We call the integrals involved in Eqs. (II-32) bound-bound, in Eq. (II-38) bound-free, and in Eq. (II-64) free-free. Each integral has a direct and an exchange contribution.

We use for Eq. (II-16) the basis set

\[ \eta_{l_{\alpha}^{P}}^{P} = N_{\alpha}^{P} \int_{l_{z} \rightarrow -z_{\alpha}^{P}} \frac{r^{l_{z}}}{r} , \]  

(II-66)
where $N_a^q$ is a normalization constant and the $z_a^q$ are chosen to represent the range of the internal function. Michels and Harris$^{14}$ and Lyons and Nesbet$^{15}$ have proposed to use, instead of (II-66), functions proportional to $r^a e^{-2r}$ in which $z$ is fixed for all functions and $a$ takes integer values. Functions of the type (II-66) are easier to work with since high powers of $r$ do not occur in the integrals.

The asymptotic functions in Eqs. (II-65) have the property that they differ from the correct regular and irregular solutions of the Schrödinger equation for a free particle by terms which become exponentially small for large $r$. The asymptotic function of the $C_p$ type suggested by Armstead$^5$ and used by others

\[ j_{\ell z_{\ell 1}}(k_{\ell^*} r) - \left( \frac{(\ell+1)}{k_{\ell^*} r} \right) j_{\ell z_{\ell 2}}(k_{\ell^*} r) \]  

(II-67)

does not have this property. The functions we use might therefore be considered more suitable except that in the unique case of electron- (positron) -hydrogen scattering, the long range dipole coupling which exists between degenerate atomic levels of the same principal quantum number means that the correct solutions are not $j_{\ell^1}$ and $n_{\ell^1}$, but rather are more complicated functions. This point will be discussed further in Chapter V.

In recent papers Michels and Harris$^{14}$ and Lyons and Nesbet$^{15}$ proposed methods to solve the resulting radial
integrals involved in calculating the matrix elements. Both authors limit their methods, however, to the asymptotic forms proposed by Armstead. Moreover, numerical integration was used in evaluating the troublesome free-free exchange integrals. We believe that one of the strong points of the Nesbet procedure as adopted here, is the absence of numerical integration. We have been able to calculate the free-free exchange integrals in closed analytic form using Eqs. (II-65). Details of the evaluation of all matrix elements are found in the appendices.

Once the matrix elements are determined, one uses Eqs. (II-54) and (II-56) to determine the elements of the \( R \) and the \( R^{-1} \) matrices. For the single channel problem Eqs. (II-58), (II-59), (II-61), and (II-62) are used. For numerical accuracy it has been suggested by Nesbet\(^9,11\) to use the regular formulae when \( |M_{00}^{pq}|/|M_{11}^{pq}| < 1 \) and the inverse formulae when \( |M_{00}^{pq}|/|M_{11}^{pq}| > 1 \).
CHAPTER III

ELECTRON HYDROGEN SCATTERING BELOW THE n=2 THRESHOLD

We calculated singlet and triplet phase shifts for electron-hydrogen scattering in the energy range $k^2 = 0$ to $k^2 = 0.75$ for the total angular momentum states $L=0$ (even parity), $L=1$ (odd parity), and $L=2$ (even parity) using a $1s-2s-2p$ close coupling approximation. The $L=0$ case engenders three coupled channels while the $L=1$ and $L=2$ cases engender four coupled channels. The even parity $L=1$ and odd parity $L=2$ cases are single channel problems. However, since the single channel problems involve scattering from a hydrogen atom initially in the $2p$ state, they are not particularly interesting. The coupled channels are listed in Table I. Below the threshold at $k^2 = 0.75$ only one channel is open for any partial wave.

We used fifteen basis functions for $L=0$ and twelve basis functions for $L=1$ and $L=2$. One set of coefficients used in the exponentials of the basis set in Eq. (11-66) are given in Table II. We list the corresponding Harris eigenvalues for the three partial waves in Tables III, IV, and V. The zero of energy has been adjusted so that the values in the tables correspond to values of $k^2$, the scattering energies. The values are seen to bunch near zero and the first excitation threshold with only a few in the meaningful range between $k^2 = 0.01$ to $k^2 = 0.75$. The bunching
near $k^2=0$ enables a reliable calculation of the scattering length. Some of the eigenvalues are good approximations to the resonances. The resonance positions calculated using Eq. (III-2) are listed in the tables in parentheses.

The Nesbet procedure utilizes the variational approximations of Hulthen, Rubinow, and Kohn to derive four formulas for the calculation of scattering phase shifts below the first excitation threshold: the Kohn formula (Eq. (11-58)); the inverse Kohn or Rubinow formula (Eq. (11-59)); the Hulthen formula (Eq. (11-61)); and the inverse Hulthen formula (Eq. (11-62)). Results from the four formulas agree exactly when det M is zero, but will differ when det M is appreciable. The criteria for using the regular or the inverse formulae are discussed in Chapter II.

For scattering energies not in the resonance region det M was nearly zero ($\sim 10^{-4}$) and all four results agreed to five or six figures. In the region of resonant (and pseudoresonant) energies, however, det M became larger and the results from the Kohn formula differed from those obtained using the other three formulas. The Rubinow result agreed well with the Hulthen and the inverse Hulthen results at all energies. The Hulthen and the inverse Hulthen results were indistinguishable.

The s-wave phase shifts are the easiest to calculate since the asymptotic solutions $j_0$ and $n_0$ contain only a sine
and a cosine. These results were found to be stable with respect to variation of the parameter beta associated with \( n_0 \). The stability can be seen in Table VI where results for different values of beta are given for two energies. Singlet and triplet phase shifts at various energies are given in Table VII.

The low energy phase shifts for p and d waves should be proportional to \( k^2 \). This proportionality was apparent in our results for both the singlet and the triplet states. Since for p and d waves \( l_2 \neq 0 \) we now have two variational parameters beta and gamma in our asymptotic solutions. The results, if correct, should be independent of both parameters. The results were found to be stable with respect to variation of both parameters. This was established by a calculation in which beta was fixed and gamma was varied. Subsequently gamma was fixed and beta was varied. Further, beta and gamma were varied simultaneously. The phase shifts were stable to five figures. Results are given for \( L=1 \) in Table VIII and for \( L=2 \) in Table IX.

Scattering lengths were obtained using the modified effective range formula \(^{16}\)

\[
\tan \eta_0 = -A k - \left( \frac{1}{3a_0} \right) \alpha k^2 - \left( \frac{u}{3a_0} \right) \alpha A \ln (ka_0) + O(k^3), \quad (III-1)
\]

where \( A_0 \) is the scattering length, \( \eta_0 \) is the s-wave phase shift, and \( \alpha = 2.96 \) in this calculation since we only include
about 66% of the polarization term. We found for the singlet S state the scattering length $A^+_0=6.742$ and for the triplet state $A^-_0=1.893$. The singlet scattering length agrees exactly with Burke and Schey$^2$ while the triplet scattering length differs by one in the last figure.

We compare our results with the results of others in Tables X and XI. We compare with the results of Schwartz,$^4$ Armstead,$^5$ and Galitis$^{17}$ which are considered exact for s, p, and d waves respectively. We also compare with the results of Burke, Gallaher, and Geltman$^{20}$ who solved the close coupling equations by a numerical integration scheme. Our results agree well with those of Burke et al.$^{20}$ as they should, since we are working within the same framework. Our results differ, however, from the exact results. The discrepancy at low energies is due in large part to the fact that the 1s-2s-2p approximation includes only about 66% of the long range polarization potential. The singlet S case is most affected by correlation since the facts that the spatial part of the wave function is symmetric and the absence of the centrifugal barrier imply that, on the average, the electrons are in closer proximity than in any other state. This explains why the singlet S results differ from the exact results more than the others do. The triplet S results agree rather well with those of Schwartz implying that polarization does not play an important role in the triplet S state, and the short range
correlation present in this state is well represented by the three state approximation.

The resonance positions and widths were determined by making a non-linear least squares fit to

\[ \eta_\ell = \eta_\ell + \eta_{\text{res}} = a + b \frac{E - E_{\text{res}}}{E} \frac{\Gamma^2}{\Gamma^2} \]  \hspace{1cm} (III-2)

where \( \eta_\ell \) is the total calculated phase shift for the \( \ell \)'th partial wave, \( \eta_\ell \) is the slowly varying background phase shift for the \( \ell \)'th partial wave, and \( \eta_{\text{res}} \) is the resonance contribution to the total phase shift. The calculated resonance position is given by \( E_{\text{res}} \) and \( \Gamma \) is the corresponding width.

Since the Kohn and the Rubinow phase shifts differed in the resonance region we used both sets of data to calculate the positions and widths of the resonances. The results were the same to the number of figures given in Tables XII and XIII. This indicates that the difference between the phase shifts calculated by the different methods in the resonance region are not of great significance in the fact that when used to calculate the positions and widths of the resonances the results are in good agreement.

We give our results for the resonant energy positions in Table XII and the corresponding widths are given in Table XIII. We also compare our results with those of
others in these tables.

We compare first of all with the results of Burke et al.\textsuperscript{18} who used the same three-state approximation. The agreement is seen to be very good. We then compare with the results of Burke and Taylor\textsuperscript{19} who used correlation terms in addition to the three-state approximation. The results differ by .014 eV for the resonant energy positions, and by .00069 eV for the corresponding widths. Pseudo states were introduced into the three-state approximation to account for the ground state polarizability exactly.\textsuperscript{20} The 1S resonance position using the pseudo states is higher (in eV) than the simpler three-state approximation. However, it was shown by Galitis\textsuperscript{21} that the R matrix satisfies certain minimum principles. Since we are dealing with only one open channel, the single R-matrix element is the tangent of the phase shift. The minimum principle then states that the variational phase shift is a lower bound to the true phase shift. Moreover, if we divide Hilbert space into some P and Q space where P space designates that part of Hilbert space included in a calculation and Q space designates that part omitted, then the minimum principle demands that upon increasing the P space, the tangent of the phase shift (hence the phase shift) must increase. It can then be shown that in a resonance region, the larger the phase shift at a given energy, the lower (in eV) the resonant position. However, Burke, Gallaher, and Geltman\textsuperscript{20}
added pseudo states to the three-state approximation (thereby increasing their $P$ space) and obtained a resonant energy position for the $^1S$ state higher (in eV) than the position obtained in the simpler three-state approximation. Since such a result violates the minimum principle we can only conclude that there is some error in their calculation.

Chen$^{22}$ used an operator formalism to project out the ground state of hydrogen from the wave function for the scattering system and then solved the remaining equations for bound states which he associates with resonant states. Our results agree well with those of Chen except for the first singlet $S$ resonance, where Chen's result agrees very well with the experimental result of McGowan et al.$^{23}$

We report on three resonances for $s$-waves, both singlet and triplet, two resonances for $p$-waves, both singlet and triplet, and one resonance for the singlet $D$ state. Using twelve basis functions we did not note any resonance in the triplet $D$ state.
TABLE I

The coupled channels in the three-state approximation

<table>
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<tr>
<th>$\pi = (-1)^L$</th>
<th>$\pi = (-1)^{L+1}$</th>
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<td>$1s$, $\ell_2 = L$</td>
<td>$2p$, $\ell_2 = L$</td>
</tr>
<tr>
<td>$2s$, $\ell_2 = L$</td>
<td></td>
</tr>
<tr>
<td>$2p$, $\ell_2 = L+1$</td>
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<tr>
<td>$2p$, $\ell_2 = L-1$</td>
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</tbody>
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### TABLE II

A list of the coefficients used in the exponentials in the basis functions

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<th>$L=0$</th>
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<th>1.8</th>
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<td>.2</td>
<td>.1</td>
<td>.05</td>
<td>.03</td>
</tr>
<tr>
<td></td>
<td>.02</td>
<td>.0133</td>
<td>.01</td>
<td>.008</td>
<td>.005</td>
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<td></td>
</tr>
<tr>
<td></td>
<td>.9</td>
<td>.7</td>
<td>.52</td>
<td>.3</td>
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<td></td>
<td>.1</td>
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<td>.001</td>
<td>.0001</td>
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TABLE III

Harris eigenvalues for L=0

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<td>.00007</td>
<td>.00051</td>
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<td>.04928</td>
<td>.44715</td>
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<td>.70376</td>
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<td>(.70367)</td>
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<td>.74999</td>
<td>.75001</td>
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</tbody>
</table>

The values in parentheses are the resonant energy positions obtained using Eq. (III-2). All energies are in Rydbergs.
TABLE IV

Harris eigenvalues for L=1

<table>
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<tr>
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<td>93.791</td>
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The values in parentheses are the resonant energy positions obtained using Eq. (III-2). All energies are in Rydbergs.


<table>
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<th>Triplet</th>
</tr>
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<tbody>
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<td>0.00000</td>
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The value in parentheses is the resonant energy position obtained using Eq. (III-2). All energies are in Rydbergs.
<table>
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</table>

**TABLE VI**

Behavior of S-wave singlet phase shifts with variation of $\beta$ for two energies.
<table>
<thead>
<tr>
<th>$k^2$</th>
<th>Singlet Phase Shifts</th>
<th>Triplet Phase Shifts</th>
</tr>
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<tbody>
<tr>
<td>.01</td>
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<td>.02</td>
<td>2.259</td>
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<td>.04</td>
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<td>.09</td>
<td>1.595</td>
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<td>.40</td>
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<td>1.232</td>
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<td>3.859</td>
<td>1.557</td>
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**TABLE VII**

Electron hydrogen phase shifts for $L=0$ at various energies
TABLE VIII

Electron hydrogen phase shifts for L=1 at various energies

<table>
<thead>
<tr>
<th>$k^2$</th>
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<th>Triplet Phase Shifts</th>
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</thead>
<tbody>
<tr>
<td>.01</td>
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<td>-.0284</td>
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<tr>
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<td>3.400</td>
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TABLE IX

Electron hydrogen phase shifts for L=2 at various energies

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<th>Triplet Phase Shifts</th>
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<td>.01</td>
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<td>.09</td>
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<td>.0153</td>
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<tr>
<td>.25</td>
<td>.0204</td>
<td>.0236</td>
</tr>
<tr>
<td>.36</td>
<td>.0291</td>
<td>.0329</td>
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<tr>
<td>.49</td>
<td>.0407</td>
<td>.0430</td>
</tr>
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<td>.64</td>
<td>.0603</td>
<td>.0543</td>
</tr>
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<td>.1319</td>
<td>.0620</td>
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### TABLE X

Comparison of electron hydrogen singlet phase shifts with results of others

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</thead>
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</tr>
<tr>
<td></td>
<td>b) 2.492</td>
<td>b) .003</td>
<td>b) .001</td>
</tr>
<tr>
<td></td>
<td>c) 2.492</td>
<td>c) .004</td>
<td>c) .001</td>
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<tr>
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</tr>
<tr>
<td></td>
<td>b) 1.596</td>
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<td>b) .008</td>
</tr>
<tr>
<td></td>
<td>c) 1.595</td>
<td>c) .004</td>
<td>c) .007</td>
</tr>
<tr>
<td>.25</td>
<td>a) 1.202</td>
<td>a) -.001</td>
<td>a) .027</td>
</tr>
<tr>
<td></td>
<td>b) 1.093</td>
<td>b) -.029</td>
<td>b) .021</td>
</tr>
<tr>
<td></td>
<td>c) 1.092</td>
<td>c) -.028</td>
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<td>a) -.013</td>
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<tr>
<td></td>
<td>b) .817</td>
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</tr>
<tr>
<td></td>
<td>c) .816</td>
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<td>c) .041</td>
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<td>a) -.004</td>
<td>a) .073</td>
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<td>b) .773</td>
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<td></td>
<td>c) .772</td>
<td>c) -.058</td>
<td>c) .060</td>
</tr>
</tbody>
</table>

Row a) corresponds to variational values calculated by Schwartz for L=0, by Armstead for L=1, and by Galitis for L=2; b) corresponds to the close coupling calculation of Burke, Gallaher, and Geltman; c) corresponds to this dissertation.
TABLE XI
Comparison of electron hydrogen triplet phase shifts with results of others

<table>
<thead>
<tr>
<th>L=</th>
<th>(k^2)</th>
<th>0</th>
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</thead>
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<tr>
<td>.01</td>
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</tr>
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<td></td>
<td>b) 2.936</td>
<td>b) .007</td>
<td>b) .001</td>
<td></td>
</tr>
<tr>
<td></td>
<td>c) 2.936</td>
<td>c) .008</td>
<td>c) .001</td>
<td></td>
</tr>
<tr>
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<td>a) 2.500</td>
<td>a) .106</td>
<td>a) ----</td>
<td></td>
</tr>
<tr>
<td></td>
<td>b) 2.497</td>
<td>b) .090</td>
<td>b) .009</td>
<td></td>
</tr>
<tr>
<td></td>
<td>c) 2.497</td>
<td>c) .090</td>
<td>c) .008</td>
<td></td>
</tr>
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<td>a) .271</td>
<td>a) .030</td>
<td></td>
</tr>
<tr>
<td></td>
<td>b) 2.097</td>
<td>b) .236</td>
<td>b) .024</td>
<td></td>
</tr>
<tr>
<td></td>
<td>c) 2.096</td>
<td>c) .236</td>
<td>c) .024</td>
<td></td>
</tr>
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<td>a) .393</td>
<td>a) .051</td>
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<tr>
<td></td>
<td>b) 1.767</td>
<td>b) .353</td>
<td>b) .041</td>
<td></td>
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<tr>
<td></td>
<td>c) 1.767</td>
<td>c) .353</td>
<td>c) .043</td>
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</tr>
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<td>a) .428</td>
<td>a) .068</td>
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</tr>
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<td></td>
<td>b) 1.633</td>
<td>b) .391</td>
<td>b) .055</td>
<td></td>
</tr>
<tr>
<td></td>
<td>c) 1.631</td>
<td>c) .391</td>
<td>c) .054</td>
<td></td>
</tr>
</tbody>
</table>

Row a) corresponds to variational values calculated by Schwartz for \(L=0\), by Armstead for \(L=1\), and by Galitis for \(L=2\); b) corresponds to the close coupling calculation of Burke, Gallaher, and Geltman; c) corresponds to this dissertation.
<table>
<thead>
<tr>
<th>State</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)</th>
<th>(e)</th>
<th>(f)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1S(2)$</td>
<td>10.178</td>
<td>10.178</td>
<td>10.178</td>
<td>-----</td>
<td>10.170</td>
<td>----</td>
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<tr>
<td>$^1S(3)$</td>
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<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>10.202</td>
<td>----</td>
</tr>
<tr>
<td>$^3S(1)$</td>
<td>10.151</td>
<td>10.151</td>
<td>10.150</td>
<td>-----</td>
<td>10.149</td>
<td>----</td>
</tr>
<tr>
<td>$^3S(2)$</td>
<td>10.201</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>10.201</td>
<td>----</td>
</tr>
<tr>
<td>$^3S(3)$</td>
<td>10.204</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>10.204</td>
<td>----</td>
</tr>
<tr>
<td>$^1P(1)$</td>
<td>10.185</td>
<td>10.179</td>
<td>10.177</td>
<td>-----</td>
<td>-----</td>
<td>----</td>
</tr>
<tr>
<td>$^1P(2)$</td>
<td>10.204</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>----</td>
</tr>
<tr>
<td>$^3P(2)$</td>
<td>10.202</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>-----</td>
<td>----</td>
</tr>
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<td>$^1D$</td>
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<td>10.160</td>
<td>10.125</td>
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<td>-----</td>
<td>----</td>
</tr>
</tbody>
</table>

Row a) corresponds to this dissertation; b) corresponds to Ref. 18; c) corresponds to Ref. 19; d) corresponds to Ref. 20; e) corresponds to Ref. 22; and f) corresponds to Ref. 23.
TABLE XIII

Widths of scattering resonances for electron hydrogen scattering

<table>
<thead>
<tr>
<th>State</th>
<th>(a)</th>
<th>(b)</th>
<th>(c)</th>
<th>(d)</th>
<th>(e)</th>
<th>(f)</th>
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</thead>
<tbody>
<tr>
<td>1S(1)</td>
<td>$5.44^{-2}$</td>
<td>$5.43^{-2}$</td>
<td>$4.75^{-2}$</td>
<td>$5.01^{-2}$</td>
<td>$4.1^{-2}$</td>
<td>$4^{-2}$</td>
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<tr>
<td>1S(2)</td>
<td>$2.31^{-3}$</td>
<td>$2.41^{-3}$</td>
<td>$2.19^{-3}$</td>
<td>$--------$</td>
<td>$2.18^{-3}$</td>
<td>$--------$</td>
</tr>
<tr>
<td>1S(3)</td>
<td>$1.36^{-4}$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$1.26^{-4}$</td>
<td>$--------$</td>
</tr>
<tr>
<td>3S(1)</td>
<td>$1.90^{-5}$</td>
<td>$1.89^{-5}$</td>
<td>$2.06^{-5}$</td>
<td>$--------$</td>
<td>$2.01^{-5}$</td>
<td>$--------$</td>
</tr>
<tr>
<td>3S(2)</td>
<td>$1.36^{-6}$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$1.18^{-6}$</td>
<td>$--------$</td>
</tr>
<tr>
<td>3S(3)</td>
<td>$8.16^{-8}$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$6.81^{-8}$</td>
<td>$--------$</td>
</tr>
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<td>1P(1)</td>
<td>$2.42^{-5}$</td>
<td>$2.26^{-5}$</td>
<td>$4.50^{-5}$</td>
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<td>$--------$</td>
<td>$--------$</td>
</tr>
<tr>
<td>1P(2)</td>
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<td>$--------$</td>
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<td>3P(1)</td>
<td>$7.98^{-3}$</td>
<td>$7.97^{-3}$</td>
<td>$5.94^{-3}$</td>
<td>$5.71^{-3}$</td>
<td>$--------$</td>
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</tr>
<tr>
<td>3P(2)</td>
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<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
</tr>
<tr>
<td>1D</td>
<td>$7.74^{-3}$</td>
<td>$7.8^{-3}$</td>
<td>$8.8^{-3}$</td>
<td>$--------$</td>
<td>$--------$</td>
<td>$--------$</td>
</tr>
</tbody>
</table>

Row a) corresponds to this dissertation; b) corresponds to Ref. 18; c) corresponds to Ref. 19; d) corresponds to Ref. 20; e) corresponds to Ref. 22; and f) corresponds to Ref. 23.
Although there is, as yet, no experimental data available for positron-hydrogen scattering, the problem is of considerable theoretical interest because the relative importance of various positron effects will be different from the corresponding electron case. The mean static interaction of a positron with an atom is repulsive whereas its long-range polarization is attractive, so that the two effects tend to cancel rather than combine as is the case in electron scattering. Moreover, since the absence of exchange possibilities render the problem more accessible to computation, the positron-hydrogen system is often used as a first check for otherwise involved theoretical calculations.

We evaluated the phase shifts for positron hydrogen scattering in the energy range $k^2 = 0$ to $k^2 = 0.75$ for the first three partial waves using the $1s-2s-2p$ approximation. We present our results in Table XIV where we compare them with the results of Burke and Smith\textsuperscript{24} who used the same three-state approximation. Agreement is good except at the lowest energies. Our low energy results agree, however, with those of LaBahn\textsuperscript{25} who did a calculation similar to the one of Burke and Smith.

It is worth noting that the three-state approximation
does not predict a bound state for the positron-hydrogen system in contrast to the existence of \( \text{H}^- \) in the electron-hydrogen case.

It was predicted by Mittleman\textsuperscript{26} that a series of resonances should exist below the \( n=2 \) threshold for the positron-hydrogen scattering problem similar to the electron-hydrogen case. We have found such a series of resonances. The resonances are narrow which perhaps explains why they were overlooked in previous calculations. Since the Nesbet method is fast in terms of computer time and stable over all ranges of energy, very small regions of energy can be spanned and narrow resonances can be found.

It should be noted that for \( L=0 \) our results differ by approximately \( \pi \) from those of Burke and Smith for \( k^2=.72 \) and \( k^2=.74 \) in Table XIV. This is due to the low lying resonance at \( k^2=.719 \). For other partial waves the resonances occur above \( k^2=.74 \) so the results in Table XIII are comparable.

The resonances were calculated in the same manner as in the electron case. We report three resonances for s waves and two for p waves in Table XV.

Figure 1 gives the phase shift and the corresponding cross section for \( L=0 \) as a function of \( k^2 \). It can be seen that the resonances become narrower for higher values of \( k^2 \).
FIGURE I

POSITRON-HYDROGEN PHASE SHIFTS
AND CROSS SECTIONS IN ARBITRARY UNITS

PHASE SHIFT

CROSS SECTION

k^2

0 2 4 6 8 10 12 14 16

0 1 2 3 4 5 6

0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
TABLE XIV
Phase Shifts for positron hydrogen scattering

\[ L= \]

<table>
<thead>
<tr>
<th>( k^2 )</th>
<th>0</th>
<th>1</th>
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</thead>
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<tr>
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<td>a) -.0049</td>
<td>a) .0045</td>
<td>a) .0007</td>
</tr>
<tr>
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<td>b) .0031</td>
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<td>a) .0201</td>
<td>a) .0068</td>
</tr>
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<td>b) .0201</td>
<td>b) .0070</td>
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<td>a) .0218</td>
<td>a) .0110</td>
</tr>
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<td>a) .0180</td>
<td>a) .0149</td>
</tr>
<tr>
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<td>b) -.1990</td>
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<td>b) .0152</td>
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<td>a) .0093</td>
<td>a) .0177</td>
</tr>
<tr>
<td></td>
<td>b) -.2461</td>
<td>b) .0101</td>
<td>b) .0183</td>
</tr>
<tr>
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<td>a) -.0154</td>
<td>a) .0207</td>
</tr>
<tr>
<td></td>
<td>b) -.3225</td>
<td>b) -.0143</td>
<td>b) .0214</td>
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<tr>
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<td>a) 2.752</td>
<td>a) -.0200</td>
<td>a) .0218</td>
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<td>b) -.3867</td>
<td>b) -.0300</td>
<td>b) .0225</td>
</tr>
<tr>
<td>.74</td>
<td>a) 2.798</td>
<td>a) -.0246</td>
<td>a) .0227</td>
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<td>b) -.3414</td>
<td>b) -.0234</td>
<td>b) .0234</td>
</tr>
</tbody>
</table>

Row a) corresponds to this dissertation; b) corresponds to the three-state calculation of Burke and Smith.
<table>
<thead>
<tr>
<th>State</th>
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<th>Width</th>
</tr>
</thead>
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<td>9.7845</td>
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</tr>
<tr>
<td>$S(2)$</td>
<td>10.1783</td>
<td>$6.516^{-5}$</td>
</tr>
<tr>
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<td>$3.499^{-7}$</td>
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<td>$2.683^{-4}$</td>
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<tr>
<td>$P(2)$</td>
<td>10.2024</td>
<td>$1.638^{-6}$</td>
</tr>
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</table>
CHAPTER V

ELECTRON-HYDROGEN SCATTERING ABOVE THE n=2 THRESHOLD

We evaluated cross sections for electron-hydrogen scattering in the energy range \( k^2 = 0.81 \) to \( k^2 = 4.0 \) using a 1s-2s and a 1s-2s-2p close coupling approximation.

In the two state approximation there is no problem with the choice of asymptotic solutions since no long range potential is present. The asymptotic solutions proposed in Eqs. (II-65) were used. We present our results in Table XVI where they are compared with the results of Burke, Schey, and Smith who used the same two-state approximation. The results can be seen to agree very well for both the elastic and inelastic cross sections. We found our solutions to be stable with respect to variations of both parameters beta and gamma as discussed in Chapter III.

In the three-state approximation there is a dipole coupling between the 2s and 2p hydrogenic states which are degenerate in an approximation which ignores the Lamb shift. Since we are dealing with a coupled channel scattering problem we have to solve the equation

\[
\left[ \frac{d^2}{dr^2} - \frac{\ell (\ell + 1)}{r^2} + \vec{k}^2 + \vec{U}(r) \right] \vec{\varphi}(r) = 0, \quad (V-1)
\]

where \( \vec{k} \) and \( \vec{u} \) are diagonal matrices, \( \vec{u} \) is the square symmetric potential matrix which includes the exchange terms.
and $\hat{\psi}(r)$ is a matrix whose columns are the independent solution vectors. One important case where Eq. (V-1) can be solved exactly in the asymptotic region is the coupling of degenerate channels by a dipole interaction, considered first by Galitis and Damburg. Asymptotically the equations describing the scattering of electrons by hydrogen can be written

$$\int \frac{d^2 z}{d \xi^2} - \frac{\lambda}{l} \left( \frac{\lambda+1}{l+1} - \frac{u}{f} \right) \frac{1}{r^2} + O\left( \frac{1}{r^3} \right) \frac{1}{r^2} \int \hat{\psi}(r) = 0,$$

(V-2)

where $\hat{A}$ is the symmetric matrix which includes all dipole coupling terms. We can introduce the matrix $\hat{A}$ which diagonalizes the $1/r^2$ matrix in Eq. (V-2)

$$\hat{A}^{-1} \left[ \hat{A} (\lambda+1) + \hat{a} \right] \hat{A} = \bar{\lambda} (\lambda+1).$$

(V-3)

Provided we keep only those terms in $\hat{a}$ coupling degenerate channels then $\hat{k}^2$ and $\hat{A}$ commute. Dropping all higher multipole terms in the potential Eq. (V-2) can be written

$$\int \frac{d^2 z}{d \xi^2} - \frac{\lambda}{l} \left( \frac{\lambda+1}{l+1} - \frac{\lambda}{l} \right) + \frac{1}{r^2} \int \hat{A}^{-1} \hat{\psi}(r) = 0.$$

(V-4)

This equation can be solved in terms of the Bessel functions of order $\lambda + \frac{1}{2}$ and $-\lambda - \frac{1}{2}$.

The coupled equations for the case of the 2s-2p coupling for s-wave electron-hydrogen scattering can be
written asymptotically

\[
\left[ \frac{d^2}{dr^2} + \frac{\kappa^2}{r^2} - \frac{2}{r^2} \right] \psi_{2P} - \frac{6}{r^2} \psi_{2S} = 0,
\]

\[
\left[ \frac{d^2}{dr^2} + \kappa^2 \right] \psi_{2S} - \frac{6}{r^2} \psi_{2P} = 0.
\]  

(V-5)

The matrix of coefficients of the \(1/r^2\) potential is

\[
\begin{bmatrix}
-2 & -6 \\
-6 & 0
\end{bmatrix},
\]  

(V-6)

which can be diagonalized to yield the eigenvalues

\[
-1 \pm \sqrt{37}.
\]  

(V-7)

If we re-express this as \(-\lambda(\lambda+1)\) we have

\[
\lambda = -\frac{1}{2} + \sqrt{\sqrt{37} + \frac{5}{4}},
\]

\[
\lambda = -\frac{1}{2} + i \sqrt{\sqrt{37} - \frac{5}{4}}.
\]  

(V-8)

Thus the solutions to Eq. (V-4) are

\[
\int \frac{1}{\sqrt{\sqrt{37} + \frac{5}{4}}} (k \cdot r),
\]

\[
\int -i \frac{1}{\sqrt{\sqrt{37} - \frac{5}{4}}} (k \cdot r).
\]  

(V-9)
Although it is possible to expand these functions in inverse powers of $r$, the expansion requires many terms for convergence, especially for low values of $\frac{k^2}{2}$ (near the $n=2$ threshold).

In the course of this work many trial asymptotic solutions were tried. However, only one asymptotic solution produced results which were substantially independent of the parameters beta and gamma. As stated in Chapter II, the solutions, if correct, must be substantially independent of these parameters since they are used solely for the purpose of computational convenience.

We first tried simple sine and cosine terms for the asymptotic solutions (the first factors in $j_l$ and $n_l$). If a complete internal basis could be included, this choice would be adequate. However, fifteen basis functions is not nearly a complete set and the simple sine and cosine was found inadequate. The solutions were found to be dependent on the parameters beta and gamma and one could obtain any result he desired by a suitable change in the parameters.

We then used the full $j_l$ and $n_l$ terms but multiplied each sine and cosine term by a different cutoff factor chosen so that each term would vanish at the origin as $r^l$. This approach produced answers which were also dependent on the values of the cutoff factors.

Finally we multiplied the full $j_l$ and $n_l$ terms by a single cutoff factor (see Eqs. (II-65)). This approach
produced results which were found to be independent of the cutoff parameters. We held beta fixed and varied gamma from unity to ninety. Subsequently we held gamma fixed and varied beta from unity to ninety. Further, we varied beta and gamma simultaneously. The cross sections were stable to five figures.

It should be emphasized that stability with respect to variation of the cutoff parameters simply implies that the solutions are independent of the choice of the parameters and are numerically correct in the given approximation. The stability criteria is a necessary condition for overall correctness of the solutions, but is by no means sufficient.

The results for the cross sections in the singlet state are somewhat different than those of Burke et al., particularly for the 1s+2p cross sections. Burke used the expansion in inverse powers of r mentioned earlier in this chapter for the asymptotic solutions, so his results should be more correct. This is an example of the necessary condition for correctness being fulfilled, but the results are different from the correct results. The triplet results are in better agreement with the results of Burke as seen in Table XV, particularly for the elastic case.

As was mentioned earlier in this chapter, if a complete internal basis set could be included, only sine and cosine terms would be required in the asymptotic solutions. The calculated results showed a substantial improvement when
the basis set was increased from five to fifteen functions, and converged to the values given in Table XVI for twenty-five basis functions. The results reported in Table XVI are for twenty-five basis functions.

The Kohn and inverse Kohn results differed usually by ten to twenty percent, but the Nesbet criteria as discussed in Chapter II was reliable for choosing the best answer.
**TABLE XVI**

S-wave contributions to the elastic and inelastic cross sections for electron hydrogen scattering

<table>
<thead>
<tr>
<th>$k^2$</th>
<th>0.81</th>
<th>1.21</th>
<th>1.44</th>
<th>2.25</th>
<th>4.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>Singlet a)</td>
<td>.431</td>
<td>.186</td>
<td>.140</td>
<td>.090</td>
<td>.060</td>
</tr>
<tr>
<td>b)</td>
<td>.436</td>
<td>.186</td>
<td>.140</td>
<td>.088</td>
<td>.065</td>
</tr>
<tr>
<td>$Q_{11}$</td>
<td>Singlet c)</td>
<td>.4504</td>
<td>.1738</td>
<td>.1274</td>
<td>.0839</td>
</tr>
<tr>
<td>d)</td>
<td>.4474</td>
<td>.1722</td>
<td>.1269</td>
<td>.0836</td>
<td>.0579</td>
</tr>
<tr>
<td>Triplet c)</td>
<td>3.6863</td>
<td>2.2980</td>
<td>1.8278</td>
<td>.9639</td>
<td>.3997</td>
</tr>
<tr>
<td>d)</td>
<td>3.6866</td>
<td>2.2973</td>
<td>1.8266</td>
<td>.9657</td>
<td>.3979</td>
</tr>
<tr>
<td>Singlet a)</td>
<td>.038</td>
<td>.070</td>
<td>.0546</td>
<td>.0241</td>
<td>.0071</td>
</tr>
<tr>
<td>b)</td>
<td>.038</td>
<td>.070</td>
<td>.0547</td>
<td>.0238</td>
<td>.0073</td>
</tr>
<tr>
<td>$Q_{12}$</td>
<td>Singlet c)</td>
<td>.0499</td>
<td>.0555</td>
<td>.0367</td>
<td>.0142</td>
</tr>
<tr>
<td>d)</td>
<td>.0529</td>
<td>.0588</td>
<td>.0380</td>
<td>.0123</td>
<td>.0049</td>
</tr>
<tr>
<td>Triplet c)</td>
<td>.0015</td>
<td>.0055</td>
<td>.0049</td>
<td>.0063</td>
<td>.0040</td>
</tr>
<tr>
<td>d)</td>
<td>.0012</td>
<td>.0051</td>
<td>.0055</td>
<td>.0045</td>
<td>.0030</td>
</tr>
<tr>
<td>Singlet c)</td>
<td>.0493</td>
<td>.0391</td>
<td>.0353</td>
<td>.0169</td>
<td>.0034</td>
</tr>
<tr>
<td>d)</td>
<td>.0384</td>
<td>.0359</td>
<td>.0343</td>
<td>.0171</td>
<td>.0035</td>
</tr>
<tr>
<td>$Q_{13}$</td>
<td>Triplet c)</td>
<td>.0007</td>
<td>.0066</td>
<td>.0098</td>
<td>.0102</td>
</tr>
<tr>
<td>d)</td>
<td>.0007</td>
<td>.0068</td>
<td>.0095</td>
<td>.0106</td>
<td>.0052</td>
</tr>
</tbody>
</table>

Row a) is the $ls$-$2s$ approximation and corresponds to this dissertation; b) is the $ls$-$2s$ approximation and corresponds to Burke, Schey, and Smith; c) is the $ls$-$2s$-$2p$ approximation and corresponds to this dissertation; d) is the 3-state approximation of Burke, Schey, and Smith.
CHAPTER VI

POSITRON-HYDROGEN SCATTERING ABOVE THE $n=2$ THRESHOLD

Since the positron-hydrogen scattering problem in the Nesbet procedure is merely a subset of the more complicated electron-hydrogen case, we simply changed the sign on the potential, ignored exchange, and calculated the results. The same problem with asymptotic solutions exists as in the electron case, and we used the Bessel and Neumann functions $j_1$ and $n_1$ as asymptotic solutions. Stability was achieved as in the electron case and was established by the same procedure. Once again, however, the stability is merely a necessary and not sufficient condition for the correctness of the solutions. The results were seen to converge, however, with respect to an increase of the basis set from five to twenty-five functions. We report our results using twenty-five basis functions in Table XVII where we compare them with the results of Burke, Schey, and Smith. It can be seen that the results are in better agreement than those for the singlet electron case.
TABLE XVII

S-wave contributions to the elastic and inelastic cross sections for positron hydrogen scattering

<table>
<thead>
<tr>
<th>$k^2$</th>
<th>0.81</th>
<th>1.21</th>
<th>1.44</th>
<th>2.25</th>
<th>4.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q_{11}$</td>
<td>a)</td>
<td>0.589</td>
<td>0.496</td>
<td>0.456</td>
<td>0.343</td>
</tr>
<tr>
<td>b)</td>
<td>0.585</td>
<td>0.496</td>
<td>0.453</td>
<td>0.343</td>
<td>0.2182</td>
</tr>
<tr>
<td>$Q_{12}$</td>
<td>a)</td>
<td>0.008</td>
<td>0.009</td>
<td>0.013</td>
<td>0.018</td>
</tr>
<tr>
<td>b)</td>
<td>0.007</td>
<td>0.009</td>
<td>0.012</td>
<td>0.017</td>
<td>0.012</td>
</tr>
<tr>
<td>$Q_{13}$</td>
<td>a)</td>
<td>0.004</td>
<td>0.014</td>
<td>0.014</td>
<td>0.005</td>
</tr>
<tr>
<td>b)</td>
<td>0.005</td>
<td>0.013</td>
<td>0.012</td>
<td>0.005</td>
<td>0.001</td>
</tr>
</tbody>
</table>

Row a) is a $1s$-$2s$-$2p$ approximation and corresponds to this dissertation; b) is the $1s$-$2s$-$2p$ approximation of Burke, Schey, and Smith.
CHAPTER VII
DISCUSSIONS AND CONCLUSIONS

It is our experience that the Nesbet variational procedure works well for the scattering of electrons and positrons by hydrogen atoms below threshold. The method is free of anomalies and gives results in good agreement with previously calculated results of others. The method is quite fast in terms of computer time, and no problems of convergence exist at any energies. Since the method is stable and quite fast, small energy regions can be investigated and resonance phenomena uncovered in detail. The method is capable of handling large systems of equations since all the matrix elements can be calculated in closed form and no problems of numerical integration occur. Since the method produced excellent inelastic results for the two state problem it should work well for systems other than hydrogen which have no dipole degeneracies in the coupled states used in the calculation.

As was stated in this dissertation, stability of the phase shifts or cross sections with respect to variations of the cutoff parameters beta and gamma is not a sufficient condition for the correctness of the solutions, but a necessary one. We have found that when the solutions are indeed correct, within a given approximation, they are stable with respect to an increase of the basis states.

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We might therefore suggest that a necessary and sufficient condition for the overall correctness of the solutions would be stability with respect to variation of the cutoff parameters and convergence with respect to an increase of the basis set.
BIBLIOGRAPHY


APPENDIX I

This appendix indicates the procedures used to evaluate the integrations over angles involved in calculating the matrix elements in Eqs. (II-15) and (II-51).

The typical matrix element which must be calculated is of the form

\[ \left< \omega (i,j) \left| H - E \right| \chi (j,i) \right> \]  \hspace{1cm} (AI-1)

where we can write the Hamiltonian \( H \) in the form

\[ H = H_1 + H_2 + V_{12} \]  \hspace{1cm} (AI-2)

The operator \( H_1 \) operates only on the radial coordinate one, and the operator \( H_2 \) operates only on the radial coordinate two. We write

\[ H_1 = - \nabla_1^2 - \frac{2}{r_1} \]  \hspace{1cm} (AI-3)
\[ H_2 = - \nabla_2^2 + \frac{2}{r_2} \]

where the upper (lower) sign is for the electron (positron) scattering problem. The interaction potential is given by

\[ V_{12} = \frac{1}{r_{12}} \]  \hspace{1cm} (AI-4)
and the upper (lower) sign pertains to the electron (positron) scattering case. The coordinate \( r_{12} \) is given by

\[
\vec{r}_{12} = \left| \vec{r}_1 - \vec{r}_2 \right|. \tag{AI-5}
\]

We can now see that the integrals in Eq. (AI-1) will be of two distinct types for angular integrations. The first type includes the radial operators \( H_1 \) and \( H_2 \) only, while the second type includes only the interaction potential \( V_{12} \). Consider integrals of the type without the interaction potential \( V_{12} \). We obtain

\[
\left\langle \frac{U^{(1,2)}}{d_{L,L',M_L,M_{L'}}} \left| \frac{U^{(1,2)}}{d_{L,L',M_L,M_{L'}}} \right\rangle_{\text{angular}} = \sum_{L_R,L_C} (\sum_{M_R,M_C} ) \tag{AI-6}
\]

for the direct terms and

\[
\left\langle \frac{V^{(2,1)}}{d_{L,L',M_L,M_{L'}}} \left| \frac{V^{(2,1)}}{d_{L,L',M_L,M_{L'}}} \right\rangle_{\text{angular}} = (-1)^{M_R+L_R-L} \sum_{L_R,M_C} (\sum_{L_C,M_R} ) \tag{AI-7}
\]

for the exchange terms. The general properties of the spherical harmonics and Clebsch-Gordan coefficients were used in Eqs. (AI-6) and (AI-7).
When the interaction potential term is present we follow Percival and Seaton\textsuperscript{31} to obtain

\[
\langle \Psi_{L, L, M, 0}^{(1, 2)}(\cos \theta_a) | \frac{1}{r_{12}} | \Psi_{L, L, M, 0}^{(1, 2)}(\cos \theta_a) \rangle_{\text{angular}}
\]

\[
= \sum_{\lambda} \psi_{\lambda} \frac{P_{\lambda}(\cos \theta_a)}{r_{12}} \left[ L, R, M, L, C, M, C, L \right],
\]

(AI-8)

for the direct terms and

\[
\langle \Psi_{L, L, M, 0}^{(1, 2)}(\cos \theta_a) | \frac{1}{r_{12}} | \Psi_{L, L, M, 0}^{(1, 2)}(\cos \theta_a) \rangle_{\text{angular}}
\]

\[
= \sum_{\lambda} \psi_{\lambda} \left[ L, R, M, L, C, M, C; L \right]
\]

\[
= \sum_{\lambda} \psi_{\lambda} \left( -1 \right)^{L + M - L} \frac{P_{\lambda}(\cos \theta_a)}{r_{12}} \left[ L, R, M, L, C, M, C, L; L \right],
\]

(AI-9)

for the exchange terms where

\[
\psi_{\lambda} = \frac{\sum_{\lambda'} \lambda' \lambda}{\sum_{\lambda'} \lambda'},
\]

(AI-10)

and
\[
\tilde{f}_\lambda^{\lambda} \left[ \ell_a, \ell_b, \ell_c, \ell_d ; b ; \lambda \right] = (-1)^{\ell_a + \ell_c - b} (2 \lambda + 1)^{-1} \\
\times C \left[ \ell_a \ell_c \lambda ; 000 \right] \cdot C \left[ \ell_b \ell_d \lambda ; 000 \right] \\
\times \left[ (2 \ell_a + 1) (2 \ell_b + 1) (2 \ell_c + 1) (2 \ell_d + 1) \right]^{1/2} \\
\times W \left( \ell_a, \ell_b, \ell_c, \ell_d ; b ; \lambda \right) \quad , \quad (AI-11)
\]

with \( W \) the Racah coefficient.

We are now left with radial integrals only, and the details of calculation are found in Appendix II.
APPENDIX II

This appendix demonstrates the procedures used to evaluate the radial integrals involved in evaluating the matrix elements found in Eqs. (II-32) and (II-63).

The hydrogenic functions can be written in the general form

\[
R_{nl}^{(r)} = -R_{D1}(n, l_1) \frac{r^{ln}}{\lambda} \sum_{k=0}^{n-l-1} R_{D2}(n, l_1, k) r^k.
\]

where

\[
R_{D1}(n, l_1) = \left\{ \left( \frac{2}{n} \right) \left( \frac{n-l_1-1}{2n[(n+l_1)!]^3} \right) \right\}^{1/2} \left( \frac{2}{n} \right)^{l_1/2}.
\]

\[
R_{D2}(n, l_1, k) = \frac{(n+l_1)!}{(n-l_1-k)![(n+l_1+k)!]^k} \frac{(-1)^{k+k}}{k!}.
\]

The basis functions have already been written in the general form

\[
\eta_{l_1}^{p, r} = N_{l_1}^{p} \frac{r^2}{\lambda a^2} - \frac{2}{a} r.
\]

The spherical Bessel and Neumann functions can be written in the generalized form
\[
\begin{align*}
\hat{j}_{l, z} &= \sum_{k=0}^{l} C_{N}(l, k) \left( \frac{z - Q(l, k, J)}{k!} \right) \\
&= B_{l, z} (J)
\end{align*}
\] (AII-5)

where \( J = 0 \) (1) for the spherical Bessel (Neumann) function, and

\[
C_{N}(l, k) = \begin{cases} 
\frac{(l + k)!}{k! (l - k)!} z^{k} & \text{for } k \text{ even} \\
\frac{(-1)^{k-1}}{2^{k}} & \text{for } k \text{ odd}
\end{cases}
\] (AII-6)

\[
Q(l, k, J) = \begin{cases} 
(l_{1/2})^{2} & \text{for } k \text{ even} \\
\frac{(-1)^{k}}{2} & \text{for } k \text{ odd}
\end{cases}
\] (AII-7)

\[
Q(l, k, J) = \begin{cases} 
-(l_{1/2})^{2} & \text{for } k \text{ even} \\
-\frac{(-1)^{k+1}}{2} & \text{for } k \text{ odd}
\end{cases}
\] (AII-8)

We specify the front cutoff factors used in the spherical functions for computational convenience by

\[
\left( 1 - \frac{P(J)}{\ell} \right) M(J)
\] (AII-9)

where
\[ P(0) = \delta \quad , \quad (AII-10) \]
\[ p(1) = \beta \quad , \quad (AII-11) \]
\[ M(0) = \begin{cases} 2l_2 - l_2 = 0 \\ 2l_2 + 1 - l_2 \neq 0 \end{cases} \quad , \quad (AII-12) \]
\[ M(1) = 2l_2 + 1 \quad , \quad (AII-13) \]

Three distinct type integrals must be evaluated. These are called bound-bound, bound-free, and free-free. The bound-bound integrals occur in evaluating the matrix elements in Eqs. (II-32), the bound-free in Eq. (II-38), and the free-free in Eq. (II-64).

The most general matrix element is of the form
\[ \left\langle p_{n_l, l_a}^{(1,2)} \pm p_{n_l, l_a}^{(2,1)} \right| H - E \left| Q_{n_l, l_a}^{(1,2)} \right\rangle \quad , \quad (AII-14) \]
so that we need operate with the Hamiltonian only once. As in Appendix I we break the Hamiltonian into
\[ H = H_e + H_a + V_a \quad , \quad (AII-15) \]
It is readily seen that

\[
\hat{H}_1, \alpha_{n\ell_1, l_2}^{(1, 2)} = -\frac{i}{\hbar^2} \hat{Q}_{n\ell_1, l_2}^{(1, 2)}. \tag{AII-16}
\]

Since the energy can be written

\[
\mathcal{E} = -\frac{i}{\hbar^2} \pm \frac{2}{\hbar^2}, \tag{AII-17}
\]

we have

\[
(H - \mathcal{E}) \left\langle \alpha_{n\ell_1, l_2}^{(1, 2)} \right\rangle = (-\frac{2}{\hbar^2} + H_2 + V_{12}) \left\langle \alpha_{n\ell_1, l_2}^{(1, 2)} \right\rangle. \tag{AII-18}
\]

The \( H_2 \) and \( V_{12} \) terms are written

\[
-\frac{i}{\hbar^2} \frac{d^2}{d\tau_2^2} \tau_2 + \frac{\ell_2(\ell_2 + 1)}{\tau_2^2} \frac{1}{\hbar^2} + \frac{2}{\hbar^2} + \frac{3}{\hbar^2}, \quad \tag{AII-19}
\]

where the upper (lower) sign is for electrons (positrons). Equation (AII-18) becomes

\[
\left[ \frac{\ell_2(\ell_2 + 1)}{\tau_2^2} - \frac{2}{\hbar^2} \frac{d^2}{d\tau_2^2} \tau_2 \right] \left\langle \alpha_{n\ell_1, l_2}^{(1, 2)} \right\rangle. \tag{AII-20}
\]

Equation (AII-14) can be written in the form
The double derivative operator in Eq. (AII-21) operates only on coordinate two and in the manner presented here, this implies that it will never operate on the hydrogenic function. We need, therefore, only consider the operation on Eqs. (AII-4,5). Since this operation is elementary it will not be explicitly shown here.

It tends to become obvious that we now have two, and only two, types of integrals to evaluate. The first type is completely separable in coordinates and reduces to the product of single integrals. We have the typical general form

\[
-\hbar^2 \left\langle P_{n,l,l_2}^{(1,2)} \pm P_{n,l,l_2}^{(2,1)} \left| Q_{n,l,l_2}^{(1,2)} \right. \right. \\
+ l_2 (l_2 + 1) \left\langle P_{n,l,l_2}^{(1,2)} \right. \pm P_{n,l,l_2}^{(2,1)} \left| \frac{l_2}{l_2} \right. \right. \\
- 2 \left\langle P_{n,l,l_2}^{(1,2)} \right. \pm P_{n,l,l_2}^{(2,1)} \left| \frac{l_2}{l_2} - \frac{l_2}{l_2} \right. \right. \\
- \left\langle P_{n,l,l_2}^{(1,2)} \right. \pm P_{n,l,l_2}^{(2,1)} \left| Q_{n,l,l_2}^{(1,2)} \right. \right. \\
(AII-21)
\]

The double derivative operator in Eq. (AII-21) operates only on coordinate two and in the manner presented here, this implies that it will never operate on the hydrogenic function. We need, therefore, only consider the operation on Eqs. (AII-4,5). Since this operation is elementary it will not be explicitly shown here.

It tends to become obvious that we now have two, and only two, types of integrals to evaluate. The first type is completely separable in coordinates and reduces to the product of single integrals. We have the typical general form

\[
\int_0^\infty \frac{d^3 r}{x} \left( \frac{m_0 - b^2}{x^3} \right)^{\frac{3}{2}} \cos \left( k_x x + D \right) \frac{n}{\alpha} - \frac{a r}{\alpha} - \frac{b r}{\alpha} \sin \left( k \cdot r + c \right) \\
= \int_0^\infty \frac{d^3 r}{x} \left( \frac{m_0 - b^2}{x^3} \right)^{\frac{3}{2}} \cos \left( k_x x + D \right) d x \int_0^\infty \frac{n}{\alpha} - \frac{a r}{\alpha} - \frac{b r}{\alpha} \sin \left( k \cdot r + c \right) d r.
\]

(AII-22)
The above two integrals are most easily evaluated for \( m, n \geq 0 \). We can expand \( (1-e^{-y \tau})^L \) in a binomial series so that we have

\[
\int_0^\infty \frac{r^L}{e^{a+\gamma r}} \sin(\beta r + c) \, dr
\]

\[
= \sum_{j=0}^{L} (-1)^j \binom{L}{j} \int_0^\infty \frac{r^L}{e^{a+\gamma r}} \sin(\beta r + c) \, dr
\]

(AII-23)

which is readily evaluated (see Ref. 30). A similar analysis, of course, holds true for the cosine integral.

It should be noted how completely inclusive this approach has been thus far. For example, if we are considering free-free integrals then we choose C or D in Eq. (AII-22) to represent the proper phase as in Eq. (AII-5). If we are considering bound-free integrals we simply choose \( k_j = d = j = 0 \), so that we now have the proper form. Finally, for bound-bound integrals we set \( k_j = d = j = k = l = 0 \), \( C = \pi/2 \).

When the values of \( m, n \) in Eq. (AII-22) become negative the problem is a bit formidable, but by no means difficult. We simply write

\[
\cos(k_j x + D) = Re \, e^{i(k_j x + D)}
\]

\[
\sin(k_i r + c) = Im \, e^{i(k_i r + c)}
\]

(AII-24)
and integrate by parts until we can see the general recursion relation. Consider the cosine term. We have
\[ P_L \int_{0}^{\infty} iD \int_{0}^{\infty} \frac{\partial}{\partial x} \left( 1 - \beta \right)^{J-1} e^{i k \cdot x} \, dx, \]  \hspace{1cm} (AII-25)

where \( m \) is negative. We write Eq. (AII-25) in the form
\[ P_L \int_{0}^{\infty} iD \int_{0}^{\infty} \frac{\partial}{\partial x} \left( 1 - \beta \right)^{J-1} \frac{dx}{x^p}, \]  \hspace{1cm} (AII-26)

where \( p = -m \).

The integration by parts is simple and yields the recursion relation so that Eq. (AII-26) becomes
\[ \frac{(-1)^{P+1}}{(P-1)!} \int_{0}^{\infty} iD \int_{0}^{\infty} \frac{\partial}{\partial x} \left( \frac{-z^x}{x} \right)^{P-1} \left( 1 - \beta \right)^{J-1} \frac{dx}{x}, \]  \hspace{1cm} (AII-27)

where \( z = b - ik_j \). We use Leibnitz's rule to write the derivative as
\[ \frac{d}{dx}^{P-1} (u^v) = \sum_{g=0}^{P-1} \binom{P-1}{g} u^{(g)} v^{(P-1-g)}. \]  \hspace{1cm} (AII-28)

We are left with the elementary integral
\[ \int_{0}^{\infty} \frac{\partial}{\partial x} \left( 1 - \beta \right)^{J-1} \frac{dx}{x}, \]  \hspace{1cm} (AII-29)

where
which is readily evaluated (see Ref. 30).

The second type integrals are all that are left now since all the other integrals in Eq. (AII-21) have been evaluated. We have

$$\left\langle \mathcal{P}_{\ell, l_2}^{(1, 2), \ell_2} \pm \mathcal{P}_{\ell, l_2}^{(2, 2), \ell_2} \right| \frac{1}{x_{\ell a}} - \frac{1}{x_{\ell_2 a}} \right| \mathcal{Q}_{\ell, l_2}^{(1, 2), \ell_2}, \quad \text{(AII-30)}$$

which, after all, are the crux of the problem, particularly the formidable free-free exchange type. However, the integral in Eq. (AII-30) is in reality very simple to evaluate.

We consider the direct terms first. The most general integral is the form

$$\int_{a}^{b} \int_{c}^{d} x^m \frac{b}{a} (\frac{x}{a}) \sin(k_x x + \xi) \cos(k_z x + \zeta) \xi \chi \, dx \, dx \, \text{d}x$$

$$= \sum_{\lambda=0}^{L} \text{DRFA}(M, B, J, k_z, k_x, c, D, N, \lambda), \quad \text{(AII-31)}$$

where the functions DRFA are found in the computer programs listed in Appendix III. The procedure to evaluate Eq. (AII-31) is very straightforward. First integrate over the coordinate x and then over the coordinate y. For explicit forms of the indefinite integrals see Ref. 30. Note that the analysis includes bound-bound, bound-free, and free-free integrals. Adjustment of the parameters allows one to
calculate any type he pleases, as discussed earlier in this appendix.

As an example, let us consider the integral \( DRF_0 \).

This is

\[
\int_0^\infty \int_0^\infty x^{-b_0} (1-x^{-b_0}) \sin (k_i x + c) \cos (k_i x + D) \cos \left( \frac{1}{x} - \frac{1}{x} \right) \, dx \, dx \quad (AII-32)
\]

which after integrating over \( r \) becomes

\[
\begin{align*}
&- \frac{n!}{\alpha^{n+1}} \int_0^\infty x^{-m-1} \frac{(a+b)x}{(1-x^{-b_0})} \sin (k_i x + c) \cos (k_i x + D) \\
&+ \sum_{\lambda=0}^{n-1} \frac{1}{\alpha^{n+1}} \left[ \frac{(n-1)!}{(n-1-\lambda)!} - \frac{n!}{(n-\lambda)!} \right] \int_0^\infty x^{-m+\lambda-1} \\
& \times \frac{(a+b)x}{(1-x^{-b_0})} \sin (k_i x + c) \cos (k_i x + D) \, dx \quad (AII-33)
\end{align*}
\]

and the above single integrals have been discussed.

The exchange integrals are written in the general form

\[
\begin{align*}
&\int_0^\infty \int_0^\infty x^{-b_0} (1-x^{-b_0}) \cos (k_i x + D) \cos \left( \frac{1}{x} - \frac{1}{x} \right) \sin (k_i x + c) \\
&\times \sum_{\lambda=0}^{Q} \left[ \left( \frac{x^{\lambda}}{1-x^{-\lambda+1}} - \frac{1}{x} \delta_{\lambda0} \right) \right] \, dx \, dx \\
= \vec{EXC} \lambda (M, B, F, J, k_i, k_i, c, D, N, D, \lambda, \lambda, \lambda) \quad (AII-34)
\end{align*}
\]
where the functions EXClA are found in the computer programs listed in Appendix III. For λ=0,1 the evaluation is relatively simple and we refer to Ref. 30 for evaluation of the indefinite integrals. For example, consider EXCO which is

\[ \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{m}{x} e^{-\beta x} \cos(k_x x + \phi) \, dx \, dy \]

which is integrated to become

\[ \frac{\int (\ell t)^{-1} \eta^m}{\int Q(t) + k^2} \int_{-\infty}^{\infty} \frac{n!}{(\eta+\omega)!} \frac{(\eta^2 - \omega^2)^m}{(\eta+\omega)!} \frac{1}{Q(t) + k^2} \, d\omega \]

where

\[ \int (\ell t) = (-1)^{\ell} \left( \begin{array}{c} \ell \\ \ell \end{array} \right) \]

\[ Q(t) = a + \ell \delta \]

\[ \alpha(t) = \tan^{-1} \left[ \frac{k}{Q(t)} \right] + \frac{\pi}{2} \]
For $\lambda > 1$ the problem is more involved, but readily done. We shall consider this case in detail since it is the free-free exchange integrals which have caused some concern in the literature. Consider the integral

$$\int_{0}^{\infty} \int_{0}^{\infty} \chi \rho_{\nu} \cos(\kappa \rho + \phi) \frac{r^{n-a}}{r^3} \sin(k_{\nu} + c) \frac{r^{2}}{r^3} \; dr \; d\kappa \; \frac{d\lambda}{d\kappa} .$$

(AII-40)

Integrate over $r$ first

$$\int_{0}^{\infty} \int_{0}^{\infty} \chi \rho_{\nu} \cos(\kappa \rho + \phi) \frac{r^{n-a}}{r^3} \sin(k_{\nu} + c) \frac{r^{2}}{r^3} \; dr \; d\kappa \; \frac{d\lambda}{d\kappa}$$

(AII-41)

where

$$C \phi(t) = (-1)^{t} \left( \begin{array}{c} L \\ t \end{array} \right) ,$$

(AII-42)

$$Q(t) = a + t \phi .$$

(AII-43)

Equation (AII-41) becomes
The first part of Eq. (AII-44) is trivial and will not be considered (since \( n > 0 \)). We concentrate on the second part of Eq. (AII-44) (since \( n \leq 2 \)). We have

\[
\begin{align*}
\int_{0}^{\infty} e^{-Q(t)t} \sin \left( \frac{k_3 + c}{r} \right) \, dt
\end{align*}
\]

(AII-45)

We can write

\[
\sin \left( \frac{k_3 + c}{r} \right) = \frac{\sin \left( \frac{k_3 + c}{r} \right) - \sin \left( \frac{k_3 + c}{r} \right)}{2i}
\]

(AII-46)

so that the integral portion of Eq. (AII-45) is

\[
\frac{1}{a_i} \int_{x}^{\infty} \frac{e^{-Q(t)t} - [Q(t) - i \cdot k_3] t}{t^{3 - n}} \, dt
\]

(AII-47)

Consider the first integral in Eq. (AII-47). We have

\[
\frac{e^{-Q(t)t} - [Q(t) + i \cdot k_3] t}{t^{3 - n}}
\]

(AII-48)
where \( B(t) = Q(t) - i k_1 \). We integrate by parts \( j \) times so that \( 3-n-j = 1 \). This gives some extra front coefficients and an additional function of \( x \). We call the front coefficient \( K(t) \). The additional function of \( x \) presents no problem and will not be investigated further. Finally we arrive at

\[
\frac{e^{itc}}{2i} k(t) \int \frac{B(t)}{x} \, dx .
\]  
(AII-49)

We are left with

\[
\frac{e^{itc}}{2i} \cot(t) k(t) \chi \int \frac{e^{-y} d\gamma}{\gamma} \left[ B(\gamma) \chi \right]
\]  
(AII-50)

Equation (AII-50) is evaluated as

\[
- \frac{e^{itc}}{2i} \cot(t) k(t) \chi \int \frac{e^{-y} d\gamma}{\gamma} \left[ -B(\gamma) \chi \right] \]

\[
+ \frac{e^{itc}}{2i} \cot(t) k'(t) \chi \int \frac{e^{-y} d\gamma}{\gamma} \left[ -B'(\gamma) \chi \right] .
\]  
(AII-51)

The full integral becomes
where
\[ C_0(u) = (-1)^u \binom{J}{u} \]  \hspace{1cm} (AII-54)

\[ P(u) = b + u \beta \]  \hspace{1cm} (AII-55)

Equation (AII-53) becomes
We now evaluate the log term.
We have

\[
\frac{d}{d} \log \left[ \frac{p(u) - i k_j}{q(t) - i k_j} + 1 \right]
= \log \left[ P(u) + Q(t) - i(k_i + k_j) \right] - \log \left[ Q(t) - i k_j \right].
\]

(AII-58)

The other terms become

\[
\frac{d}{d} \log \left( \frac{Q(t) - i k_j}{P(u) - i k_j} \right)
= (-1)^{m+2} \left( \frac{\log \left( Q(t) - i k_j \right)}{\left[ P(u) - i k_j \right]^{m+2}} \right).
\]

(AII-59)

The other terms become

\[
\frac{d}{d} \log \left[ \frac{p(u) + q(t) - i(k_i + k_j)}{p(u) - i k_j} \right]
= \log \left[ P(u) + Q(t) - i k_j \right] - \log \left[ P(u) - i k_j \right].
\]

(AII-60)

and

\[
\frac{d}{d} \log \left[ \frac{p(u) + q(t) + i(k_i - k_j)}{p(u) - i k_j} \right]
= \log \left[ P(u) + Q(t) + i k_j \right] - \log \left[ P(u) - i k_j \right].
\]

(AII-61)
In general we can show that

\[
\frac{1}{b^n} \left\{ \log b \right\}^{n} \left[ \log a \right]^{\frac{1}{a}} - \sum_{k=1}^{n-1} \frac{1}{k} \left( \log a \right)^{\frac{1}{a}} x^k
\]

where

\[
\frac{d b}{d b} = 1
\]

\[
\frac{d y}{d b} = 1
\]

(AII-62)

For example consider the case where \( n=2 \). The final solution is

\[
\text{Re} \left\{ \frac{c_{0}(t)c_{0}(a)c_{m+2}!e^{i\frac{c_{0}}{2i}}}{2i} \right\}
\]

\[
\log \left[ p_{(a)} + q_{(t)} - i(k_{z} + k_{3}) \right] - \log \left[ q_{(t)} - i k_{z} \right]
\]

\[
\left[ p_{(a)} - i k_{z} \right]^{m+3}
\]

\[
- \sum_{k'=1}^{m+2} \left[ p_{(a)} - i k_{3} \right]^{m+3-i} \frac{1}{\left[ p_{(a)} + q_{(t)} - i(k_{z} + k_{3}) \right]^{2}}
\]

(AII-63)
For $n=1$ we have

$$
\sum_{t=1}^{L} \sum_{u=1}^{L} \frac{\text{Re} \left( \text{Co}(t) \cdot \text{Co}(u) \right) (m+1)! \cdot e^{-i\epsilon} e^{iD}}{2i} \left\{ \log \left[ P(u) + Q(t) - i \left( k_c + k_i \right) \right] - \log \left[ Q(t) - i k_i \right] \right\}
$$

$$
- \sum_{t=1}^{L} \sum_{u=1}^{L} \frac{\text{Re} \left( \text{Co}(t) \cdot \text{Co}(u) \right) (m+2)! \cdot e^{-i\epsilon} e^{iD}}{2i} \left\{ \log \left[ P(u) + Q(t) - i \left( k_c + k_i \right) \right] - \log \left[ Q(t) - i k_i \right] \right\}
$$

$$
- \sum_{t=1}^{L} \sum_{u=1}^{L} \frac{\text{Re} \left( \text{Co}(t) \cdot \text{Co}(u) \right) (m+3)! \cdot e^{-i\epsilon} e^{iD}}{2i} \left\{ \log \left[ P(u) + Q(t) - i \left( k_c + k_i \right) \right] - \log \left[ Q(t) - i k_i \right] \right\}
$$

$$
+ \sum_{t=1}^{L} \sum_{u=1}^{L} \frac{\text{Re} \left( \text{Co}(t) \cdot \text{Co}(u) \right) (m+4)! \cdot e^{-i\epsilon} e^{iD}}{2i} \left\{ \log \left[ P(u) + Q(t) - i \left( k_c + k_i \right) \right] - \log \left[ Q(t) - i k_i \right] \right\}
$$

(AII-64)
These functions are given in the computer program in Appendix III by EPF and EOTS. As one can readily see, the evaluation of these terms is not extensive, even though the analysis is somewhat involved and tedious.
This appendix lists the computer programs used in calculating the matrix elements involved.

The integrals referred to are the following:

\[ \int_{0}^{\infty} \int_{0}^{\infty} x^{m-1} b_x (1-x)^{y} \left( \frac{1}{x} \right)^{n+1} \sin(k_x x + c) \cos(k_x x + d) \]

\[ \times \left( \frac{r_x}{r_{x+1}} - \frac{r_{x-1}}{r_{x+1}} \right) \, dr \, dx \]

\[ = D R F L (m, b, \beta, J, k_z, k_i, c, D, n, \alpha, \Lambda) \]

\[ 0 \leq l \leq 2 \quad \alpha > 0 \quad n > l + 1 \]

(AIII-1)

\[ \int_{0}^{\infty} \int_{0}^{\infty} x^{m-1} b_x (1-x)^{y} \left( \frac{1}{x} \right)^{n+1} \sin(k_x x + c) \cos(k_x x + d) \]

\[ \times \left( \frac{1}{x} \right)^{l} \, dr \, dx \]

\[ = E X C O (m, b, \beta, J, k_z, k_i, c, D, n, \alpha, \Lambda) \]

(AIII-2)

\[ \int_{0}^{\infty} \int_{0}^{\infty} x^{m-1} b_x (1-x)^{y} \left( \frac{1}{x} \right)^{n+1} \sin(k_x x + c) \cos(k_x x + d) \]

\[ \times \left( \frac{1}{x} \right)^{l} \, dr \, dx \]

\[ = E X C I (m, b, \beta, J, k_z, D, k_i, c, n, \alpha, \Lambda, \Lambda') \]

(AIII-3)
\[
\int_0^\infty \int_0^\infty \chi \frac{e^{-b\chi}}{(1-a^2) \beta_\chi} \sin(k_i x + c) \frac{dx}{x^3} \, d\chi
\]

\[
= \text{E}_{\mathbb{R}} (m, b, \beta, J, k_i, p, n, a, \nu, k_i, c) ;
\]  \hspace{1cm} \text{(AIII-4)}

\[
\int_0^\infty \chi \frac{e^{-a\chi}}{(1-a^2) \beta_\chi} \sin(k_i x + c) \cos(k_i x + D) \, dx
\]

\[
= \text{ABN} (a, \beta, J, k_i, k_i^*, c, D, m) \quad \text{if} \quad 0 \leq m \leq \infty ; \quad J \geq |m| ;
\]  \hspace{1cm} \text{(AIII-5)}

\[
\int_0^\infty \frac{e^{-b\chi}}{1-a^2 \beta_\chi} (1-a^2 \beta^2_\chi) \sin(k_i x + c) \cos(k_i x + D) \, dx
\]

\[
= \text{BIN} (B, R, \beta, J, k_i, k_i^*, c, D, m) \quad \text{if} \quad m \geq 2
\]  \hspace{1cm} \text{(AIII-6)}

\[
\int_0^\infty \frac{e^{-b\chi}}{1-a^2 \beta_\chi} (1-a^2 \beta^2_\chi) \sin(k_i x) \frac{dx}{x^2}
\]

\[
= \text{FIN S J} (b, a, \beta, k_i, J) \quad \text{if} \quad J \geq 0
\]  \hspace{1cm} \text{(AIII-7)}
\[
\int_0^\infty e^{-b x} (1-e^{-a x}) (1-e^{-\beta x})^J \cos k_i x \frac{dx}{x^2}
= F INC J (b, a, \beta, k_i, J)
\quad \text{for } J \geq 1.
\]
(AIII-8)

\[
\int_0^\infty e^{-a x} \sin k_i x \cos k_i x \cos k_i x \frac{dx}{x}
= Q F (a, k_i, k_i)
\quad \text{for } a > 0.
\]
(AIII-9)

\[
\int_0^\infty e^{-a x} (1-e^{-\beta x})^J \cos k_i x \cos k_i x \cos k_i x \frac{dx}{x}
= Z P F J (a, \beta, k_i, k_i, J)
\quad \text{for } a > 0, \beta > 0.
\]
(AIII-10)

\[
\int_0^\infty e^{-a x} (1-e^{-\beta x})^J \sin k_i x \sin k_i x \sin k_i x \frac{dx}{x}
= Z \& J (a, \beta, k_i, k_i, J).
\]
(AIII-11)
SUBROUTINE EXC1(M,B,BETA,J,AKJ,D,A,KI,C,N,A,L,CETA)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON SN(2,2,3,3) ,ORO,OR1,DR2,ECO,EC1,EC2,DVAL,DTEX,PEST,TRGUB
COMMON POST
DIMENSION ALP(2),Q(2),CQ(2)
EC1 = 0.DO
P = N
LL = L+1
NOSE = N+2
NIP = N-1
DO 6 I=1,LL
MXT = I-I
CALL COMB(L»,MXT,MSOL)
CO(I) = (-1)**(I+1)*MSGL
Q(I) = A + MXT*BETA
ALP(I) = DATAN(AKI/QII)) + 3.141592653589700
SUM1 = 0.DO
SUM2 = 0.DO
SUM3 = 0.DO
CALL FACT(N+1,ISOL)
PAT = ISOL
CALL FACT(N-2,ISOL)
PAM = ISOL
DO 10 I=1,LL
DIV = Q(I)*Q(I) + AKI*AKI
DIV1 = DIV**((P+2.DO)/2.DO)
SUM1 = (-1)**(N+1)*PAT*CO(I)*ABN(B,CETA,J,0,AKJ,C+(P+2.DO)*ALP(I),
1D,M-2)/DIV1 + SUM1
6 DO 12JJ=1,NOSE
CALL FACT(NOSE-JJ,ISOL)
PIG = ISOL
SI = (-1)**(JJ-1)
Z = JJ
DIV2 = DIV**((Z/2.DO)
SUM2 = SUM2 + CO(I)*SI*PAT*ABN(I)+B,CETA,J,AKI,AKJ,C+JJ*ALP(I),
1D,M-2)/DIV2 + SUM2
12 CONTINUE
DO 13 K=1,NIP
CALL FACT(NIP-K,ISOL)
PEL = ISOL
SO = (-1)**(K-1)
Y = K
DIV3 = DIV**((Y/2.DO)
SUM3 = SUM3 + CO(I)*SO*ABN(I)+B,CETA,J,AKI,AKJ,C+K*ALP(I),
           ID,M+N-K)/(DIV3*PEL)
13 CONTINUE
10 CONTINUE
EC1 = SUM2 - SUM1 - SUM3
RETURN
END
DOUBLE PRECISION FUNCTION AIN1(A,BETA,J,AKI,AKJ,C,D)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON SN(2,2,3,3),DRO,DR1,DR2,EC0,EC1,EC2,DVAL,DTEX,PEST,TROUB
COMMON POST
GO TO (1,2,3,4,5),M
1 AIN = AIN1(A,BETA,J,AKI,AKJ,C,D)
RETURN
2 AIN = AIN2(A,BETA,J,AKI,AKJ,C,D)
RETURN
3 AIN = AIN3(A,BETA,J,AKI,AKJ,C,D)
RETURN
4 AIN = AIN4(A,BETA,J,AKI,AKJ,C,D)
RETURN
5 AIN = AIN5(A,BETA,J,AKI,AKJ,C,D)
RETURN
END
DOUBLE PRECISION FUNCTION AIN1(A,BETA,J,AKI,AKJ,C,D)
IMPLICIT REAL *8 (A-H,O-Z)
COMMON SN(2,2,3,3),DRO,DR1,DR2,EC0,EC1,EC2,DVAL,DTEX,PEST,TROUB
COMMON POST
ZXX = 3.1415926535897970/2.DO
Q1 = DCOS(C)
Q2 = DCCS(D)
Q3 = DSIN(C)
Q4 = DSIN(D)
QQ1 = TEXJ(A, BETA, AKI, AKJ, J)
QQ2 = ZPFJ(A, BETA, AKI, AKJ, J)
QQ3 = ZGJ(A, BETA, AKI, AKJ, J)
QQ4 = TEXJ(A, BETA, AKJ, AKI, J)
AIN1 = Q1*Q2*QQ1+Q3*Q2*QQ2-Q1*Q4*QQ3-Q3*Q4*QQ4
RETURN
END

DOUBLE PRECISION FUNCTION ABN(A, BETA, J, AKI, AKJ, C, D, M)
IMPLICIT REAL *8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), DRO, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
IF(M. GE. 0) GO TO 6
MM = -M
GO TO (1, 2, 3, 4, 5), MM
1 ABN = AINI(A, BETA, J, AKI, AKJ, C, D)
RETURN
2 ABN = AIN2(A, BETA, J, AKI, AKJ, C, D)
RETURN
3 ABN = AIN3(A, BETA, J, AKI, AKJ, C, D)
RETURN
4 ABN = AIN4(A, BETA, J, AKI, AKJ, C, D)
RETURN
5 ABN = AIN5(A, BETA, J, AKI, AKJ, C, D)
RETURN
6 ABN = FUNJ(M, A, BETA, AKI, AKJ, C, D, J)
RETURN
END

DOUBLE PRECISION FUNCTION AIN2(A, BETA, J, AKI, AKJ, C, D)
IMPLICIT REAL *8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), DRO, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
ZXX = 3.14159265358979D0/2.D0
Q1 = AIN1(A, \beta, J, AKI, AKJ, C, D)
Q2 = AIN1(A + \beta, \beta, J-1, AKI, AKJ, C, D)
Q3 = AIN1(A, \beta, J, AKI, AKJ, C + ZXX, D)
Q4 = AIN1(A, \beta, J, AKI, AKJ, C, D - ZXX)
AIN2 = -A*Q1 + \beta*J*Q2 + AKI*Q3 - AKJ*Q4
RETURN

DOUBLE PRECISION FUNCTION AIN3(A, \beta, J, AKI, AKJ, C, D)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), CR0, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
ZXX = 3.1415926535897D0/2.D0
Q1 = AIN2(A, \beta, J, AKI, AKJ, C, D)
Q2 = AIN2(A + \beta, \beta, J-1, AKI, AKJ, C, D)
Q3 = AIN2(A, \beta, J, AKI, AKJ, C + ZXX, D)
Q4 = AIN2(A, \beta, J, AKI, AKJ, C, D - ZXX)
AIN3 = .5D0*(-A*Q1 + \beta*J*Q2 + AKI*Q3 - AKJ*Q4)
RETURN

DOUBLE PRECISION FUNCTION AIN4(A, \beta, J, AKI, AKJ, C, D)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), CR0, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
ZXX = 3.1415926535897D0/2.D0
Q1 = AIN3(A, \beta, J, AKI, AKJ, C, D)
Q2 = AIN3(A + \beta, \beta, J-1, AKI, AKJ, C, D)
Q3 = AIN3(A, \beta, J, AKI, AKJ, C + ZXX, D)
Q4 = AIN3(A, \beta, J, AKI, AKJ, C, D - ZXX)
AIN4 = (1.D0/3.D0)*(-A*Q1 + \beta*J*Q2 + AKI*Q3 - AKJ*Q4)
RETURN

DOUBLE PRECISION FUNCTION BIN(B, A, \beta, J, AKI, AKJ, C, D, M)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), CR0, CR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
IF(M.GE.0) GO TO 10
IF(M.EQ.-1) GO TO 9
MB= -M
MM = MB-1
GO TO (1, 2, 3, 4), MM
1 BIN = BIN2(B,A,BETA,J,AKI,AKJ,C,D)
RETURN
2 BIN = BIN3(B,A,BETA,J,AKI,AKJ,C,D)
RETURN
3 BIN = BIN4(B,A,BETA,J,AKI,AKJ,C,D)
RETURN
4 BIN = BIN5(B,A,BETA,J,AKI,AKJ,C,D)
RETURN
10 Q1 = FUNJ(M,B,BETA,AKI,AKJ,C,D,J)
Q2 = FUNJ(M,A+B,BETA,AKI,AKJ,C,D,J)
BIN = Q1-Q2
RETURN
9 Q1 = AIN1(B,BETA,J,AKI,AKJ,C,D)
Q2 = AIN1(B+A,BETA,J,AKI,AKJ,C,D)
BIN = Q1-Q2
RETURN
END
DOUBLE PRECISION FUNCTION BIN2(B,A,BETA,J,AKI,AKJ,C,D)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2,2,3,3), DRO, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
QQ1 = DCOS(C)
QQ2 = DCOS(D)
QQ3 = DSIN(C)
QQ4 = DSIN(D)
Q1 = FINSJ(B,A,BETA,AKI-AKJ,J)
Q2 = FINSJ(B,A,BETA,AKI+AKJ,J)
Q3 = FINCJ(B,A,BETA,AKI-AKJ,J)
Q4 = FINCJ(B,A,BETA,AKI+AKJ,J)
Q5 = FINSJ(B,A,BETA,AKJ-AKI,J)
BIN2 = .5DO*(QQ1*QQ2*(Q1+Q2)+QQ3*QQ2*(Q3+Q4)-Q01*QQ4*(Q3-Q4)
1-QQ3*QQ4*(Q5+Q2))
DOUBLE PRECISION FUNCTION BIN3(B, A, BETA, J, AKI, AKJ, C, D)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), DR0, DR1, DR2, EC0, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
ZXX = 3.141592653589797D0/2.0D0
Q1 = AIN2(A+B, BETA, J, AKI, AKJ, C, D)
Q2 = BIN2(B+BETA, A, BETA, J-1, AKI, AKJ, C, D)
Q3 = BIN2(B, A, BETA, J, AKI, AKJ, C+ZXX, D)
Q4 = BIN2(B, A, BETA, J, AKI, AKJ, C, D-ZXX)
Q5 = BIN2(B, A, BETA, J, AKI, AKJ, C, D)
BIN3 = 0.5D0*(A*Q1 + J*BETA*Q2 - AKI*Q3 - AKJ*Q4 - B*Q5)
RETURN
END

DOUBLE PRECISION FUNCTION BIN4(B, A, BETA, J, AKI, AKJ, C, D)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), CRO, DR1, DR2, EC0, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
ZXX = 3.141592653589797D0/2.0D0
Q1 = AIN3(A+B, BETA, J, AKI, AKJ, C, D)
Q2 = BIN3(B+BETA, A, BETA, J-1, AK1, AKJ, C, D)
Q3 = BIN3(B, A, BETA, J, AKI, AKJ, C+ZXX, D)
Q4 = BIN3(B, A, BETA, J, AKI, AKJ, C, D-ZXX)
Q5 = BIN3(B, A, BETA, J, AKI, AKJ, C, D)
BIN4 = (1.0D0/3.0D0)*(A*Q1 + J*BETA*Q2 + AKI*Q3 - AKJ*Q4 - B*Q5)
RETURN
END

DOUBLE PRECISION FUNCTION BIN5(B, A, BETA, J, AKI, AKJ, C, D)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), DRO, DR1, DR2, EC0, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
ZXX = 3.141592653589797D0/2.0D0
Q1 = AIN4(A+B, BETA, J, AKI, AKJ, C, D)
Q2 = BIN4(B+BETA, A, BETA, J-1, AKI, AKJ, C, D)
Q3 = BIN4(B, A, BETA, J, AKI, AKJ, C+ZXX, D)
Q4 = BIN4(B, A, BETA, J, AKI, AKJ, C, D - ZXX)
Q5 = BIN4(B, A, BETA, J, AKI, AKJ, C, D)
BIN5 = 25D0*(A*Q1 + B*Q2 + AKI*Q3 - AKJ*Q4 - B*Q5)
RETURN
END

SUBROUTINE COMB(I, J, MSOL)
C THIS SUBROUTINE CALCULATES THE COMBINATION OF I THINGS TAKEN J AT A
C TIME
C
MSOL=1
IF(I .LE. J) GO TO 14
CALL FACT(I, ISOL)
INI = ISOL
CALL FACT(J, ISOL)
IN = ISOL
CALL FACT(I-J, ISOL)
INU = ISOL
MSOL = INI/(IN*INU)
14 RETURN
END

SUBROUTINE CSEC(R, Q, N, INVR)
COMPUTES CROSS SECTIONS FROM THE R MATRIX
R=R MATRIX, N = DIMENSION OF R, MAXIMUM N = 30
IF INVR.GE.1 INVERSE R MATRIX IS USED
Q = MATRIX OF PARTIAL CROSS SECTIONS EXCEPT FOR FACTOR OF 4*PI/ksq
REQUIRES SUBROUTINE GMIC
IMPLICIT REAL*8(A-H, O-Z)
COMPLEX*16 B(3, 3), Z, ZA
DIMENSION R(3, 3), Q(3, 3)
IF(INVR.GE.1) GO TO 4
DO 1 I=1, N
DO 1 J=1, N
X=0.0
IF(I .EQ. J) X=1.0
Y=-R(I, J)
1 CONTINUE
RETURN
END
1) \(B(I,J) = \text{CMPLX(SNGL(X),SNGL(Y))}\)

CALL GMIC(N,B)
DO 3 I=1,N
DO 3 J=1,N
Z=0.0
DO 2 K=1,N
ZA=R(I,K)
2) \(Z=Z+ZA*B(K,J)\)
X=REAL(Z)
Y=AIMAG(Z)
3) \(Q(I,J)=X*X+Y*Y\)
RETURN

4) DO 5 I=1,N
DO 5 J=1,N
Y=0.0
IF (I.EQ.J)Y=-1.0
X=R(I,J)
5) \(B(I,J) = \text{CMPLX(SNGL(X),SNGL(Y))}\)
CALL GMIC(N,B)
DO 6 I=1,N
DO 6 J=1,N
Z=B(I,J)
X=REAL(Z)
Y=AIMAG(Z)
6) \(Q(I,J)=X*X+Y*Y\)
RETURN
END

SUBROUTINE DETER(A,D)
C THIS SUBROUTINE IS USED TO EVALUATE A 3 BY 3 DETERMINANT
C A IS THE INPUT ELEMENTS OF THE MATRIX
C D IS THE OUTPUT EVALUATION
C
IMPLICIT REAL *8 (A-H,O-Z)
DIMENSION A(3,3)
BOY = A(1,1)*(A(2,2)*A(3,3)-A(2,3)*A(3,2)) - A(1,2)*(A(2,1)*A(3,3)-A(3,1)*A(2,3))
DOY = A(1,3)*A(2,1)*A(3,2) - A(3,1)*A(2,2)
O = BOY - COY + DOY
RETURN
END
SUBROUTINE DRFO(M,BETA,A,AKI,AKJ,C,D,N,A)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON SN(2,2,3,3),DRO,DR1,DR2,ECO,EC1,EC2,DVAL,DTEN,PEST,TROUBP
COMMON POST
DIMENSION P(5)
D RO = 0.00
IF(N.LE.0) GO TO 10
JJ = -M+1
NN = N-1
CALL FACT(N,ISOL)
PAT = ISOL
CALL FACT(N-1,ISOL)
PAM = ISOL
DIV = A**(N+1)
IF(M.GT.0) GO TO 12
GO TO (1,2,3,4,5),JJ
5 P(5) = AIN5(A+*,BETA,J,AKI,AKJ,C,D)
4 P(4) = AIN4(A,+,BETA,J,AKI,AKJ,C,D)
3 P(3) = AIN3(A+,BETA,J,AKI,AKJ,C,D)
2 P(2) = AIN2(A,+,BETA,J,AKI,AKJ,C,D)
1 P(1) = AIN1(A+,BETA,J,AKI,AKJ,C,D)
DRO = -PAT*P(JJ)/DIV
GO TO 13
12 DRO = -PAT*FUNJ(M-1,A+,BETA,AKI,AKJ,C,D,J)/DIV
13 CONTINUE
IF(NN.LE.0) GO TO 30
DO 20 I=1,NN
CALL FACT(N-1-I,ISOL)
POPS = ISOL
CALL FACT(N-I,ISOL)
TOPS = ISOL
KK = M+N-1-I
DO 20
KKK = -KK

IF(KK.LT.0) GO TO 21
Q1 = FUNJ(KK,A+B,BETA,AKI,AKJ,C,D,J)
GO TO 22

21 Q1 = P(KKK)
22 CONTINUE

DRO = DRO + (1.0D0/A**(I+1))*PAM/POPSS-PAT/TOPS)*Q1

CONTINUE

30 RETURN

WRITE(6,42)

42 FCRMAT(1H1,1X,'ERROR IS IN DPF',//)

RETURN

END

SUBROUTINE DRF1(M,B,BETA,J,AKI,AKJ,C,D,N,A)
IMPLICIT REAL*8(A-H,Q-Z)

COMMON SN(2,2,3,3),DRO,DR1,DR2,ECO,EC1,EC2,DVAL,DTEX,PEST,TROUB
COMMON POST

DR1 = 0.0D0
SUM1 = 0.0D0
SUM2 = 0.0D0
SUM3 = 0.0D0
CALL FACT(N+1,ISOL)
PEAC = ISOL
NOSE = N-2
CALL FACT(NOSE,ISOL)
PACT = ISOL
SUM1 = PEAC*BIN(B,A,BETA,J,AKI,AKJ,C,D,M-2)/A**(N+2)
DO 3 I=1,N
DIV = A**(I+1)
CALL FACT(N+I-1,ISOL)
PAM = ISOL
Q1 = ABN(A+B,BETA,J,AKI,AKJ,C,D,M+N-1-I)
SUM2 = SUM2 + PEAC*Q1/(DIV*PAM)

CONTINUE

IF(NOSE.LE.0) GO TO 7
DO 10 I=1,NOSE
CALL FACT(N-2-I, ISOL)
PAT = ISOL
DIV = A**(I+1)
Q1 = ABN(A+B, BETA, J, AKI, AKJ, C, D, M+N-1-I)
SUM3 = SUM3 + PACT*Q1/(PAT*DIV)
CONTINUE
CONTINUE
DR1 = SUM1 - SUM2 + SUM3
RETURN
END
SUBROUTINE DRF2(M, B, BETA, J, AKI, AKJ, C, D, N, A)
IMPLICIT REAL*8(A-H, O-Z)
COMMON SN(2, 2, 3, 3), DRO, OR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
DIMENSION P(5)
DR2 = 0.00
SUM1 = 0.00
SUM2 = 0.00
SUM3 = 0.00
IF(M.GT.2) GO TO 51
IF(M.LT.-2) GO TO 10
JJ = -M+3
GO TO (1, 2, 3, 4, 5), JJ
1 TRM1 = BIN(B, A, BETA, J, AKI, AKJ, C, D, -I)
GO TO 11
2 TRM1 = BIN2(B, A, BETA, J, AKI, AKJ, C, D)
GO TO 11
3 TRM1 = BIN3(B, A, BETA, J, AKI, AKJ, C, D)
GO TO 11
4 TRM1 = BIN4(B, A, BETA, J, AKI, AKJ, C, D)
GO TO 11
5 TRM1 = BIN5(B, A, BETA, J, AKI, AKJ, C, D)
GO TO 11
51 TRM1 = BIN(B, A, BETA, J, AKI, AKJ, C, D, M-3)
CONTINUE
CALL FACT(N+2, ISOL)
\( \text{PAT} = \text{ISOL} \)
\( \text{SUM1} = \text{PAT} \times \text{TRM1} / \text{A}^{\text{N}+3} \)
\( \text{LL} = -\text{M}+2 \)
\( \text{IF(} \text{LL} \leq 0 \text{)} \text{GO TO 40} \)
\( \text{GO TO } \{12, 13, 14, 15, 16\}, \text{LL} \)
16 \( \text{P(5)} = \text{AIN5(A+B,BETA,J,AKI,AKJ,C,D)} \)
15 \( \text{P(4)} = \text{AIN4(A+B,BETA,J,AKI,AKJ,C,D)} \)
14 \( \text{P(3)} = \text{AIN3(A+B,BETA,J,AKI,AKJ,C,D)} \)
13 \( \text{P(2)} = \text{AIN2(A+B,BETA,J,AKI,AKJ,C,D)} \)
12 \( \text{P(1)} = \text{AIN1(A+B,BETA,J,AKI,AKJ,C,D)} \)
40 \text{CONTINUE}

\( \text{NN} = \text{N} - 3 \)
\( \text{CALL FACT(N} - 3, \text{ISOL)} \)
\( \text{PAM} = \text{ISOL} \)
\( \text{IF(} \text{NN} \leq 0 \text{)} \text{GO TO 20} \)
\( \text{DO 21} \text{ I=1,NN} \)
\( \text{CALL FACT(N} - 3 - \text{I,ISOL)} \)
\( \text{TOPS} = \text{ISOL} \)
\( \text{DIV} = \text{A}^{\text{I}+1} \)
\( \text{KJ} = \text{M+N} - 1 - \text{I} \)
\( \text{KM} = -\text{KJ} \)
\( \text{IF(} \text{KJ} \lt 0 \text{)} \text{GO TO 22} \)
\( \text{Q1} = \text{FUNJ(KJ,A+B,BETA,AKI,AKJ,C,D,J)} \)
\( \text{GO TO 23} \)
22 \( \text{Q1} = \text{P(KM)} \)
23 \text{CONTINUE}

\( \text{SUM2} = \text{PAM} \times \text{Q1} / (\text{TOPS} \times \text{DIV}) + \text{SUM2} \)
21 \text{CONTINUE}
20 \text{CONTINUE}
\( \text{NN} = \text{N} + 1 \)
\( \text{CALL FACT(N+2,ISOL)} \)
\( \text{POPS} = \text{ISOL} \)
\( \text{IF(} \text{NN} \leq 0 \text{)} \text{GO TO 30} \)
\( \text{DO 31} \text{ I=1,NN} \)
\( \text{CALL FACT(N+2-I,ISOL)} \)
\( \text{SACK} = \text{ISOL} \)
DIV = A**(I+1)
MJ = N-1-1
MM = -MJ
IF(MJ.LT.0) GO TO 32
Q1 = FUNJ(MJ,A+B,BETA,AKI,AKJ,C,O,J)
GC TO 33
32 Q1 = P(MM)
33 CONTINUE
SUM3 = POPS*Q1/(SACK*DIV) + SUM3
31 CONTINUE
30 CONTINUE
DR2 = SUM1 + SUM2 - SUM3
200 FORMAT(10X,18.8,/) 
300 FORMAT(2X,3D18.8,/) 
RETURN
10 WRITE(6,125)
125 FORMAT(1H1,IX,'ERROR IS IN DRF2',/) 
RETURN 
END 
SUBROUTINE DSFUN(N,A,AKI,AKJ,B,C)
C
C THIS SUBROUTINE IS USED TO CALCULATE THE INTEGRAL FROM ZERO TO
C INFINITY OF THE INTEGRAL OF X TO THE POWER N TIMES THE EXPONENTIAL
C TO THE POWER MINUS A TIMES THE SIN OF KIX PLUS B TIMES THE COS
C OF KJ TIMES X PLUS C
C
IMPLICIT REAL*8(A-H,O-Z)
COMMON SN(2,2,3,3),ORD0,GR1,GR2,EC0,EC1,EC2,DVAL,DTEX,PEST,TROUB
COMMON POST
DIMENSION H(2),AIN1(2),AIN2(2)
BOWR(A,B) = (A/(A**2+B**2))**(N+1)
DO 1 I=1,2
H(I) = AKI + AKJ
H(2) = AKI - AKJ 
CALL FACT(N,ISCL)
K=N/2
NN = 1
TEMP = (N+1)*(H(I)/A)
IF(K .EQ. 0) GO TO 7
DO 2 M=1,K
   NN = -NN
   CALL COMB(N+1,2*M+1,MSOL)
   TEMP = TEMP + NN*MSOL*(H(I)/A)**(2*M+1)
2 CONTINUE
7 CONTINUE
AIN1(I) = ISOL*TEMP*BOWR(A,H(I))
1 CONTINUE
DO 10 I=1,2
   H(I) = AKI+AKJ
   H(2) = AKI-AKJ
   CALL FACT(N,ISOL)
   K=(N+1)/2
   NN=1
   TEMP = 1.000
   IF(K.EQ.0) GO TO 11
   DO 12 M=1,K
      NN = -NN
      CALL COMB(N+1,2*M,MSOL)
      TEMP = TEMP + NN*MSOL*(H(I)/A)**(2*M)
   12 CONTINUE
   11 CONTINUE
AIN2(I) = ISOL*TEMP*BOWR(A,H(I))
10 CONTINUE
DVAL = .5Cos((COS(3+C)*AIN1(I)+CCOS(B+C)*AIN1(2)+DSIN(B+C)*AIN2(1))
RETURN
END
SUBROUTINE EXCO(M,B,BETA,J,AKI,AKJ,C,D,N,A,L)
IMPLICIT REAL*8(A-H,G-Z)
COMMON SN(2,2,3,3),DRO,CR1,CR2,E0,E1,E2,DVAL,DTEN,PEST,TROUB
COMMON POST
ECO = 0.00
IF(Y.LT.1) GO TO 55
IF(N.LT.1) GO TO 55
CALL FACT(N,ISOL)
PAT = ISOL
CALL FACT(N-1,ISGL)
PAM = ISGL
FAC = (-1)**N
PP = N
PG = (PP+1.DO)/2.DO
LL = L+1
DO 20 I=1,LL
NEX = I-1
CALL CCMB(L,NEX,MSOL)
CO = (-1)**(I+1)*MSOL
Q = A + NEX*BETA
DIV = (Q*Q+AKI*AKI)**PQ
ALP = DATAN(AKI/Q) + 3.1415926535897D0
QQ1 = FUNJ(M-1,Q+B,BETA,AKI,AKJ,C+(PP+1.DO)*ALP,D,J)
ECO = ECO + CO*FAC*PAT*QQ1/DIV
DO 21 K=1,N
CALL FACT(N+1-K,ISOL)
PCPS = ISOL
CALL FACT(N-K,ISOL)
TCPS = ISOL
SI = (-1)**(K-1)
Z = K
DAV = (Q*Q + AKI*AKI)**Z/2.DO
QQ2 = FUNJ(M+N-K,Q+B,BETA,AKI,AKJ,C+K*ALP,D,J)
SUM = SI*(PAT/PCPS-PAM/TCPS)*QQ2/DAV
21 ECO = ECO + CO*SUM
20 CONTINUE
RETURN
55 WRITE(6,56)
56 FORMAT(1H1,1X,'ERROR IS IN EXC2',/) RETURN
END
SUBROUTINE FACT(I, ISGL)
C THIS SUBROUTINE CALCULATES I FACTORIAL
C
ISGL=1
IF (I.LE.0) GO TO 14
DC 10 J=1,I
10 ISGL=ISGL*J
RETURN
END

DOUBLE PRECISION FUNCTION FINSJ(B,A,C,Q,J)

IMPLICIT REAL *8(A-F,O-Z)
COMMON SN(2,2,3,3) ,DR0,DR1,DR2,EC0,EC1,EC2,DVAL,DTEX,PEST,TRGUB
COMMON POST
ZTF(A,B,C) = DATAN(C*(B-A)/(A*B+C*C))
ZPF(A,B,C) = .5D0*LOG((B*B+C*C)/(A*A+C*C))
FINS1(B,A,C,Q) = -B*ZTF(B,A+B,Q)+B*ZTF(B+C,A+B+C,Q)+A*ZTF(A+B,
1A+B+C,Q)+C*ZTF(C+B,A+B+C,Q)+Q*ZPF(B,A+B,Q)-Q*ZPF(B+C,A+B+C,Q)
FINS2(B,A,C,Q) = FINS1(B,A,C,Q) - FINS1(B+C,A,C,Q)
FINS3(B,A,C,Q) = FINS2(B,A,C,Q) - FINS2(B+C,A,C,Q)
FINS4(B,A,C,Q) = FINS3(B,A,C,Q) - FINS3(B+C,A,C,Q)
FINS5(B,A,C,Q) = FINS4(B,A,C,Q) - FINS4(B+C,A,C,Q)
FINS6(B,A,C,Q) = FINS5(B,A,C,Q) - FINS5(B+C,A,C,Q)
FINSJ = 0.DO
IF(Q.EQ.0.DO) RETURN
GO TO (1,2,3,4,5,6),J
1 FINSJ = FINS1(B,A,C,Q)
RETURN
2 FINSJ = FINS2(B,A,C,Q)
RETURN
3 FINSJ = FINS3(B,A,C,Q)
RETURN
4 FINSJ = FINS4(B,A,C,Q)
RETURN
5 FINSJ = FINS5(B,A,C,Q)
RETURN
DOUBLE PRECISION FUNCTION FUNJ(M, A, BETA, AKI, AKJ, C, D, J)
IMPLICIT REAL*8 (A-H,O-Z)
COMMON SN(2,2,3,3), CR0, CR1, CR2, ECO, EC1, EC2, CVAL, DTEX, PEST, TROUB
COMMON POST
FUNJ = 0.0
JJ = J+1
DO 6 I=1, JJ
NEX = I-1
CALL COMBIJ(NEX, MSOL)
CO = (-1)**(I+1)*MSOL
Q = A + NEX*BETA
CALL DFSUMM(M, C, AKI, AKJ, C, D)
6 FUNJ = FUNJ + CC*DVAL
RETURN
END

SUBROUTINE GNCIC(L, 3)
INVERTS A COMPLEX MATRIX OF MAXIMUM DIMENSION 30 X 30
L = DIMENSION OF ACTUAL MATRIX TO BE INVERTED
B = MATRIX TO BE INVERTED. B IS REPLACED BY ITS INVERSE.

IMPLICIT REAL*8 (A-H,O-Z)
COMPLEX*16 B(3,3), C(3,3), D(3), Q
DO 1 N=1, L
DO 1 M=1, L
1 C(N,M)=0.0
DO 5 N=1, L
DO 5 M=1, L
Q=B(N,M)
DO 2 J=1, L
2 Q=Q-C(N,J)*C(J,M)
IF(A-M)4,3,3
4 C(N,M)=Q
GO TO 5
4 \( C(N,M) = C/N(N,N) \)
5 CONTINUE
6 B(N,M) = 0.0
7 D(M) = 0.0
8 Q = Q - C(M,J) * D(J)
9 D(M) = Q / C(M,M)
10 Q = Q - C(M,J) * D(J)
11 B(M,N) = Q
RETURN

SUBROUTINE QF(A, B, C)

IMPLICIT REAL*8 (A-H, O-Z)
COMMON S(2,2,3,3), DRO, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST.
PI = 3.14159265358977D0
TERM = A**2 - B**2 + C**2
IF(A.EQ.O.DO) GC TO 10
IF(TERM) 1,2,2
1 DTEX = 0.5C0*DASIN(2.DO*A*B/(A**2-B**2+C**2)) + 3.1415926500/2.0D0
RETURN
2 DTEX = 0.5C0*DASIN(2.DO*A*B/(A**2-B**2+C**2))
RETURN
10 IF(B.EQ.C) GO TO 11
DTEX = PI/2.DO
RETURN
11 DTEX = PI/4.DO
RETURN
END

DOUBLE PRECISION FUNCTION TEXJ(A,B,C,D,J)
IMPLICIT REAL*8 (A-H,0-Z)
COMMON SN(2,2,3,3),DRO,DR1,DR2,ECO,EC1,EC2,DVAL,DTEX,PEST,TROUB
COMMON POST
TEXJ = 0.DO
JJ = J+1
DO 6 I=1,JJ
NEX = 1-1
CALL COMBIJ,NEX,MSOL)
CO = C — 1J**(I  +  I)*MSOL
Q = A  +  NEX*B
CALL QFIQ,C,D)
TEXJ = TE XJ +  CO*DTEX
RETURN
END

DOUBLE PRECISION FUNCTION AIN51A,BETA,J,AKI,AKJ,C,D)
IMPLICIT REAL*8 (A-H,0-Z)
ZXX = 3.1415926535897D0/2.D0
QI = AIN4(A,BETA,J,AKI,AKJ,C,D)
Q2 = AIN4(A+BETA,BETA,J-1,AKI,AKJ,C,D)
Q3 = AIN4(A,BETA,J,AKI,AKJ,C+ZXX,D)
Q4 = AIN4(A,BETA,J,AKI,AKJ,C,D-ZXX)
AIN5 = .25D0*(-A*Q1+BETA*J*Q2+AKI*Q3-AKJ*Q4)
RETURN
END

DOUBLE PRECISION FUNCTION FINCJ(B,A,C,Q,J)
IMPLICIT REAL*8 (A-H,0-Z)
COMMON SN(2,2,3,3),DRO,CR1,DR2,ECO,EC1,EC2,DVAL,DTEX,PEST,TROUB

CCM.vCN POST

\[ Z(A,B,C) = \text{atan}(C/(B-A)/(A*B+C*C)) \]

\[ ZPF(A,B,C) = 0.5D0*DLOG((B+C+C)/(A*A+C*C)) \]

\[ FINC1(B,A,C,Q) = -B*ZPF(B,A+Q) + B*ZPF(B+C,A+B+C,Q) + A*ZPF(A+B + 1A+B+C,Q) + C*ZPF(C+B,A+B+C,Q) - Q*ZTF(B,A+B,Q) + Q*ZTF(B+C,A+B+C,Q) \]

\[ FINC2(B,A,C,Q) = FINC1(B,A,C,Q) - FINC1(B+C,A,C,Q) \]

\[ FINC3(B,A,C,Q) = FINC2(B,A,C,Q) - FINC2(B+C,A,C,Q) \]

\[ FINC4(B,A,C,Q) = FINC3(B,A,C,Q) - FINC3(B+C,A,C,Q) \]

\[ FINC5(B,A,C,Q) = FINC4(B,A,C,Q) - FINC4(B+C,A,C,Q) \]

\[ FINC6(B,A,C,Q) = FINC5(B,A,C,Q) - FINC5(B+C,A,C,Q) \]

\[ PINC1(B,A,C,Q) = A*ZPF(A,A+C,Q) + C*ZPF(C,A+C,Q) + B \]

\[ PINC2(B,A,C,Q) = PINC1(B,A,C,Q) - FINC1(B+C,A,C,Q) \]

\[ PINC3(B,A,C,Q) = PINC1(B,A,C,Q) - 2*D0*FINC1(B+C,A,C,Q) + FINC1(B+2*D0*C,A,C,Q) \]

\[ PINC4(B,A,C,Q) = PINC3(B,A,C,Q) - 3*D0*FINC1(B+C,A,C,Q) + 3*D0*FINC1(B+2*D0*C,A,C,Q) \]

\[ PINC5(B,A,C,Q) = PINC4(B,A,C,Q) - FINC4(B+C,A,C,Q) \]

\[ PINC6(B,A,C,Q) = PINC5(B,A,C,Q) - FINC5(B+C,A,C,Q) \]

IF(\(Q.EQ.0.C0.ANC.B.EQ.0.DO\)) GO TO 5

GO TO (6,7,8,9,15,16), J

1 FINCJ = FINC1(B,A,C,Q)
RETURN

2 FINCJ = FINC2(B,A,C,Q)
RETURN

3 FINCJ = FINC3(B,A,C,Q)
RETURN

4 FINCJ = FINC4(B,A,C,Q)
RETURN

11 FINCJ = FINC5(B,A,C,Q)
RETURN

12 FINCJ = FINC6(B,A,C,Q)
RETURN

5 GO TO (6,7,8,9,15,16), J

6 FINCJ = PINC1(B,A,C,Q)
RETURN

7 FINCJ = PINC2(B,A,C,Q)
SUBROUTINE DRMA(PM,RMA,RMAIN,AK1,AK2,AK3)
C THIS SUBROUTINE CALCULATES THE ELEMENTS OF THE R MATRIX
C AND ALSO THE ELEMENTS OF THE R-INVESRE MATRIX
C
IMPLICIT REAL *8 (A-H,O-Z)
DIMENSION PM(2,2,3,3),RMA(3,3),GAMO(3,3),ABEO(3,3),GAM(3,3)
DIMENSION ABE(3,3),AC(3,3),AB(3,3),B(3),VK(3),PSUM(3,3)
DIMENSION RMAIN(3,3)
NCH = 3
DO 1 I=1,NCH
DO 1 J=I,NCH
1  A(I,J) = PM(2,2,I,J)
DO 2 I=1,NCH
DO 2 J=I,NCH
2  B(I) = -PM(2,1,I,1)
DO 3 I=1,NCH
DO 3 J=1,NCH
3  AB(I,J) = A(I,J)
CALL DETER(A,D)
DENCM = D
DO 4 M=1,NCH
DO 4 K=1,NCH
5  A(K,M) = AB(K,M)
DO 6 K=1,NCH
6  A(K,M) = B(K)
CALL DETER(A,C)
GAMO(I, M) = D/DENCM
CONTINUE
DO 7 I = 1, NCH
7 B(I) = -PM(2, I, 1, 2)
DO 8 M = 1, NCH
DO 9 I = 1, NCH
DO 9 J = 1, NCH
9 A(I, J) = AB(I, J)
DO 10 K = 1, NCH
10 A(K, M) = B(K)
CALL DETER(A, D)
GAMO(2, M) = D/DENCM
CONTINUE
DO 11 I = 1, NCH
11 B(I) = -PM(2, I, 1, 3)
DO 12 M = 1, NCH
DO 13 I = 1, NCH
DO 13 J = 1, NCH
13 A(I, J) = AB(I, J)
DO 14 K = 1, NCH
14 A(K, M) = B(K)
CALL DETER(A, D)
GAMO(3, M) = D/DENCM
CONTINUE
DO 15 I = 1, NCH
DO 15 J = 1, NCH
15 A(I, J) = PM(1, 1, I, J)
DO 16 I = 1, NCH
16 B(I) = -PM(1, 2, I, 1)
DO 17 I = 1, NCH
DO 17 J = 1, NCH
AB(I, J) = A(I, J)
CALL DETER(A, D)
DENCM = D
DO 18 M = 1, NCH
DO 19 I = 1, NCH
DO 19 J = 1, NCH
19   A(I, J) = AB(I, J)
DO 20 K = 1, NCH
20   A(K, M) = B(K)
    CALL DETER(A, C)
    ABEC(1, M) = D/DENCM
    CONTINUE
DO 21 I = 1, NCH
21   B(I) = -PM(1, 2, I, 2)
DO 22 M = 1, NCH
22   DO 23 I = 1, NCH
23      DO 24 J = 1, NCH
24         A(I, J) = A8(I, J)
25      DO 26 K = 1, NCH
26         A(K, M) = E(K)
         CALL DETER(A, D)
         ABEO(2, M) = D/DENCM
         CONTINUE
DO 29 I = 1, NCH
29   B(I) = -PM(1, 2, I, 3)
DO 27 M = 1, NCH
27   DO 25 I = 1, NCH
25      DO 26 J = 1, NCH
26         A(I, J) = A8(I, J)
27      DO 26 K = 1, NCH
26         A(K, M) = B(K)
         CALL DETER(A, D)
         ABEO(3, M) = D/DENCM
         CONTINUE
VK(1) = AK1
VK(2) = AK2
VK(3) = AK3
DO 36 IQ = 1, NCH
36      DO 30 NU = 1, NCH
30         PSUM(IQ, NU) = 0.00
DO 30 NU = 1, NCH
DO 30 IQ = 1, NCH
DO 31 IP = 1, NCH
31 PSUM(IQ, NU) = PM(1, 2, IQ, IP)*GAM(NU, IP) + PSUM(IQ, NU)
GAM(NU, IQ) = GAM(NU, IQ) - (1.DO/VKI IQ)*{PM(1, 1, IQ, NU) + PSUM(IQ, NU))
30 CONTINUE
DO 37 IQ = 1, NCH
DO 37 NU = 1, NCH
37 PSUM(IQ, NU) = 0.DO
DO 32 NU = 1, NCH
DO 32 IQ = 1, NCH
32 PSUM(IQ, NU) = PM(1, 2, IQ, IP)*ABEG(NU, IP) + PSUM(IQ, NU)
ABE(NU, IQ) = ABEG(NU, IQ) + (1.DO/VKI IQ)*{PM(1, 2, IQ, NU) + PSUM(IQ, NU))
32 CONTINUE
DO 34 IP = 1, NCH
DO 34 IQ = 1, NCH
34 RMA(IP, IQ) = DSQRT(VK(IP)/VK(IP))*GAM(IP, IQ)
DO 35 IP = 1, NCH
DO 35 IQ = 1, NCH
35 RMAIN(IP, IQ) = DSQRT(VK(IP)/VK(IP))*ABE(IP, IQ)
35 CONTINUE
RETURN
END

DOUBLE PRECISION FUNCTION ZPFJ(A, B, C, D, J)

C
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 3, 3), DR0, DR1, DR2, ECO, EC1, EC2, OVAL, DTEX, PEST, TROUB
COMMON POST
ZPF(A, B, C) = .5D0*DLG((B+B+C+C)/(A+A+C+C))
ZPF1(A, B, C, D) = .5D0*ZPF(A, A+B, C+D) + .5D0*ZPF(A, A+B, C-D)
ZPF2(A, B, C, D) = ZPF1(A, B, C, D) - ZPF1(A+B, B, C, D)
ZPF3(A, B, C, D) = ZPF2(A, B, C, D) - ZPF2(A+B, B, C, D)
ZPF4(A, B, C, D) = ZPF3(A, B, C, D) - ZPF3(A+B, B, C, D)
ZPF6(A,B,C,D) = ZPF5(A,B,C,D) - ZPF5(A+B,B,C,D)
IF(A.EQ.0.D0) GO TO 10
ZPFJ = 0.00
IF(J.EQ.0) RETURN
GO TO (1,2,3,4,5,6),J
1 ZPFJ = ZPF1(A,B,C,D)
RETURN
2 ZPFJ = ZPF2(A,B,C,D)
RETURN
3 ZPFJ = ZPF3(A,B,C,D)
RETURN
4 ZPFJ = ZPF4(A,B,C,D)
RETURN
5 ZPFJ = ZPF5(A,B,C,D)
RETURN
6 ZPFJ = ZPF6(A,B,C,D)
RETURN
10 WRITE(6,53)
53 FORMAT(1H1,1X,'ERROR IS IN ZPFJ',/) RETURN END
DOUBLE PRECISION FUNCTION ZGJ(A,B,C,D,J)
IMPLICIT REAL *8 (A-H,C-Z)
COMMON SN1,2,3,3),CROL,CR2,ECO,EC1,EC2,DVAL,DTEX,PEST,TROUB
COMMON POST
ZG(A,B,C) = .2500*DLOG((A*B+C)**2)/(A*B+C**2))
ZG1(A,B,C,D) = ZG(A,C,D) - ZG(A+B,B,C,D)
ZG2(A,B,C,D) = ZG1(A,B,C,D) - ZG1(A+B,B,C,D)
ZG3(A,B,C,D) = ZG2(A,B,C,D) - ZG2(A+B,B,C,D)
ZG4(A,B,C,D) = ZG3(A,B,C,D) - ZG3(A+B,B,C,D)
IF(A.EQ.0.D0) GO TO 10
IF(J.EQ.0) GO TO 12
GO TO (1,2,3,4,5,6),J
1  \[ ZGJ = ZG1(A, B, C, D) \]
RETURN
2  \[ ZGJ = ZG2(A, B, C, D) \]
RETURN
3  \[ ZGJ = ZG3(A, B, C, D) \]
RETURN
4  \[ ZGJ = ZG4(A, B, C, D) \]
RETURN
5  \[ ZGJ = ZG5(A, B, C, D) \]
RETURN
6  \[ ZGJ = ZG6(A, B, C, D) \]
RETURN
12 \[ ZGJ = ZG(A, C, D) \]
RETURN
10 WRITE(6,53)
53 FORMAT(1H1,1X,'ERROR IS IN ZGJ',/)
RETURN
END
SUBROUTINE EOTS IM,B,BETA,J,AKJ,D, N,A,L,AKI,C)
IMPLICIT REAL A-H,0-Z)
COMMON SN {  2  ,  2  »  3  ,3 }, DRO ,  DR 1,DR2,ECO,EC 1,EC2, DVAL ,DTEX,PEST,TRoub
COMMON POST
DIMENSION CO(A ), ALP(4), G(4)
PEST = 0.DO
LI = L+1
GO TO (1,1,2,3),LI
1  CO(1) = 1.DO
CO(2) = -1.DO
GO TO 10
2  CC(1) = 1.DO
CC(2) = -2.DO
CC(3) = 1.DO
GO TO 10
3  CC(1) = 1.DO
CO(2) = -3.DO
CC(3) = 3.DO
CC(4) = -1.0

CONTINUE
Q(1) = A
Q(2) = A + BETA
Q(3) = A + 2.0*BETA
Q(4) = A + 3.0*BETA
CALL FACT(N+2,ISOL)

PAT = ISOL
PI = 3.141592653589797D0
SIG = (-1)**(N+2)
Z = N
MM = M-3
NN = N+3
LL = L+1

DO 20 I=1,LL
ALP(I) = DATAN(AKI/Q(I)) + PI
DIV = (Q(I)*Q(I)+AKI*AKI)**((Z+3.0)/2.0)
IF(MM) 21,22,22
21 TE = AIN(B,BETA,J,0,AKJ,C+(N+3.0)*ALP(I),0,-MM)
GO TO 23
22 TE = FUNJ(MM,B,BETA,0,AKJ,C+(N+3.0)*ALP(I),D,J)
23 CONTINUE
PEST = -CG(1)*SIG*PAT*TE/DIV + PEST

DO 30 NU=1,NN
FA = (-1)**(NU-1)
CALL FACT(N+3-NU,ISOL)
PAM = ISOL
P = NU
DAV = (Q(I)*Q(I)+AKI*AKI)**(P/2.0)
K = M+N-NU
IF(K) 31,32,32
31 TP = AIN(B+Q(I),BETA,J,AKI,AKJ,C+NU*ALP(I),D,-K)
GO TO 33
32 TP = FUNJ(K,B+Q(I),BETA,AKI,AKJ,C+NU*ALP(I),D,J)
33 CONTINUE
SUM = FA*PAT*TP/(CAV*PAM)
PEST = PEST + CC(I)*SUM
30 CONTINUE
CONTINUE
RETURN
END
SUBROUTINE CPF(M, B, BETA, J, AKJ, D, N, A, L, AKI, C)
IMPLICIT REAL*8 (A-H, O-Z)
COMMON SN(2, 2, 3, 3), CRO, DR1, DR2, ECO, EC1, EC2, DVAL, DTEX, PEST, TROUB
COMMON POST
COMPLEX FALLA
COMPLEX*16 CA, DA, CAL, DAL, DEN(4), SDEN1(4, 4), SDEN2(4, 4), SDLN1(4, 4),
SDLN2(4, 4), ELG1(4), ELO2(4), ELN1(4), ELN2(4), SUM1(4, 4), SUM2(4, 4),
FR01(4, 4), FRG2(4, 4), FIN1(4, 4), FIN2(4, 4), CDAL, TIN1(4, 4),
TIN2(4, 4), TINF(4, 4), ANS, BNS
REAL*4 ZEBRA
DIMENSION CO(4), BO(4), Q(4), P(4)
TROUB = 0.00
L1 = L + 1
GO TO (1, 1, 2, 3), L1
1 CC(1) = 1.00
CO(2) = -1.00
GO TO 4
2 CC(1) = 1.00
CO(2) = -2.00
CC(3) = 1.00
GO TO 4
3 CC(1) = 1.00
CO(2) = -3.00
CC(3) = 3.00
CC(4) = 1.00
CONTINUE
GO TO (5, 6, 7), J
5 BC(1) = 1.00
BC(2) = -1.00
GO TO 9
6 BC(1) = 1.00
GO TO 9
BC(2) = -2.
BC(3) = 1.
GO TO 8
7
BC(1) = 1.
BC(2) = -3.
BC(3) = 3.
BC(4) = -1.
8
CONTINUE
DC 9 I=1,4
9
Q(I) = A + (I-1)*BETA
DO 10 I=1,4
10
P(I) = 8 + (I-1)*BETA
CALL FACT(N+2,ISOL)
PAT = ISOL
CARLB = 0.DO
CA = DCMPLX(CARLB,C)
DA = DCMPLX(CARLB,D)
CDA = DCMPLX(CARLB,-C)
CDAL = CDEXP(CDA)
CAL = CDEXP(CA)
DAL = CDEXP(DA)
J1 = J+1
MB = M+2
ANS = (0,0)
DO 13 JJ=1,J1
13
DEN(JJ) = DCMPLX(P(JJ),-AKJ)
DO 14 JJ=1,J1
14
SDEN1(JJ,LL) = DCMPLX(P(JJ)+Q(LL),-AKI+AKJ)
DO 15 JJ=1,J1
15
SDEN2(JJ,LL) = DCMPLX(P(JJ)+Q(LL),AKI-AKJ)
DO 16 JJ=1,J1
16
SDLN1(JJ,LL) = CDELGN(SDEN1(JJ,LL))
DO 17 JJ=1,J1
DO 17 LL=1,L1
17 SDLN2(JJ,LL) = CDLOG(SDEN2(JJ,LL))
DO 18 LL=1,L1
18 ELO1(LL) = COMPLEX(Q(LL),-AKI)

DO 19 LL=1,L1
19 ELO2(LL) = COMPLEX(Q(LL),AKI)

DO 20 JJ=1,J1
20 SUM1(JJ,LL) = (0,0)

DO 21 JJ=1,J1
21 SUM2(JJ,LL) = (0,0)

DO 22 MS=1,MB
22 SUM1(JJ,LL) = SUM1(JJ,LL) + (1.D0,0)/(MS*DEN(JJ)**(M+3-MS)*SDEN1(1JJ,LL)**MS)

DO 23 JJ=1,J1
23 SUM2(JJ,LL) = SUM2(JJ,LL) + (1.D0,0)/(MS*DEN(JJ)**(M+3-MS)*SDEN2(1JJ,LL)**MS)

DO 24 JJ=1,J1
24 FIN1(JJ,LL) = FRO1(JJ,LL)-SUM1(JJ,LL)

26 FIN2(JJ,LL) = FRO2(JJ,LL) - SUM2(JJ,LL)
IF(N.EQ.2) GO TO 27
GO TO 28

DO 29 JJ=1,J1
29 FIN1(JJ,LL) = FRO1(JJ,LL)-SUM1(JJ,LL)
29 FIN2(JJ,LL) = FRO2(JJ,LL) - SUM2(JJ,LL)
IF(N.EQ.2) GO TO 27
GO TO 28

DO 29 JJ=1,J1
29 FIN1(JJ,LL) = FRO1(JJ,LL)-SUM1(JJ,LL)
29 FIN2(JJ,LL) = FRO2(JJ,LL) - SUM2(JJ,LL)
IF(N.EQ.2) GO TO 27
GO TO 28

DO 29 JJ=1,J1
29 FIN1(JJ,LL) = FRO1(JJ,LL)-SUM1(JJ,LL)
29 FIN2(JJ,LL) = FRO2(JJ,LL) - SUM2(JJ,LL)
IF(N.EQ.2) GO TO 27
GO TO 28

DO 29 JJ=1,J1
TIN1(JJ, LL) = CC(LL) * BO(JJ) * CAL * DAL * PAT * FIN1(JJ, LL) /(0, 2. DO)
TIN2(JJ, LL) = CC(LL) * BO(JJ) * CDAL * DAL * PAT * FIN2(JJ, LL) /(0, 2. DO)
DO 30 JJ= 1, J1
DC 30 LL= 1, L1
30 TINF(JJ, LL) = TIN1(JJ, LL) - TIN2(JJ, LL)
DO 31 JJ= 1, J1
DO 31 LL= 1, L1
31 ANS = ANS + TINF(JJ, LL)
FALLA = ANS
ZEBRA = REAL(FALLA)
BNS = DCONJG(ANS)
ANS = (ANS+BNS)/(2. DO, 0)
IF(ZEBRA) 32, 32, 33
32 TROUB = -CDABS(ANS)
GO TO 34
33 TROUB = CCABS(ANS)
CONTINUE
GO TO 35
28 DO 36 JJ= 1, J1
DO 36 LL= 1, L1
FIN1(JJ, LL) = FIN1(JJ, LL) * ELC1(LL)
36 FIN2(JJ, LL) = FIN2(JJ, LL) * ELC2(LL)
DO 37 JJ= 1, J1
DO 37 LL= 1, L1
TIN1(JJ, LL) = CC(LL) * BO(JJ) * CAL * DAL * PAT * FIN1(JJ, LL) /(0, 2. DO)
TIN2(JJ, LL) = CC(LL) * BO(JJ) * CDAL * DAL * PAT * FIN2(JJ, LL) /(0, 2. DO)
DO 38 JJ= 1, J1
DO 38 LL= 1, L1
38 TINF(JJ, LL) = TIN2(JJ, LL) - TIN1(JJ, LL)
DO 39 JJ= 1, J1
DO 39 LL= 1, L1
39 ANS = ANS + TINF(JJ, LL)
FALLA = ANS
ZEBRA = REAL(FALLA)
BNS = DCONJG(ANS)
ANS = (ANS+BNS)/(2. DO, 0)
IF (ZEBA) 40, 40, 41
40 TROUB = -CCABS(ANS)
GO TO 42
41 TROUB = CCABS(ANS)
42 CONTINUE
BUM = 0.D0
DO 43 LL = 1, LI
TIM = FUNJ(M+1, B+Q(LL), BETA, AKI, AKJ, C, D, J)
43 BUM = BUM + CG(LLL) * TIM
TROUB = TROUB + BUM
CALL EOTS(M, B, BETA, J, AKJ, D, N, A, L, AKI, C)
TROUB = TROUB + PEST
RETURN
END
VITA

George Joseph Seiler, son of Henry and Catherine (Montalbano) Seiler Sr., was born in New Orleans, Louisiana, on January 2, 1946. He attended Our Lady of Lourdes parochial grammar school and De LaSalle High School, to which he received a four year scholarship. He graduated with honor on May 27, 1963, and entered Southeastern Louisiana College as a chemistry major. He received the freshman chemistry award in 1964, and became a member of the Sigma Tau Gamma national fraternity that same year. After changing his major to physics in the fall of 1965, he received his Bachelor of Science degree with high honor on May 27, 1967. He entered the graduate school of Auburn University in physics in September, 1967, on a NDEA Fellowship. He married Diane Theresa, daughter of Alvin and Lois (Boudreaux) Ballon on December 16, 1967. At the annual Sigma Chi banquet of 1968 he received the first year graduate award in physics. He entered Louisiana State University in September 1968 on a NDEA Fellowship and is presently a candidate for the degree of Doctor of Philosophy in the Department of Physics and Astronomy.
Candidate: George Joseph Seiler
Major Field: Physics
Title of Thesis: Algebraic Close Coupling Approach to Electron Hydrogen Scattering

Approved:

[Signature]
Major Professor and Chairman

[Signature]
Dean of the Graduate School

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Date of Examination: November 3, 1970