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ELECTRON IMPACT 2s AND 2p EXCITATIONS OF ATOMIC HYDROGEN

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CONTENTS

SUMMARY

A numerical calculation has been carried out to evaluate the 3 x 3 cross section matrix involved in the electron impact excitation of the ground state of H atom to the 2s and the 2p levels. The method of solution is that of atomic eigenstates expansion. Similar calculation has been carried out by Burke, Schey and Smith. In this paper, however, the definite integral terms in the coupled radial differential equations are eliminated through some linear transformation of the radial functions, thus avoiding iteration of these equations. As a result, the equation of reciprocity and the equation of continuity of currents are numerically satisfied with an error to value ratio less than 1 per 1000 on the average, and the maximum of this ratio, except for a few cases, has been kept below 1%. A simple perturbation theory has been developed to evaluate the effect of the long range and the centrifugal potentials. The five cross sections, 1s-2s, 1s-2p, 1s-1s, 2s-2s and 2p-2p, are tabulated.

The agreement of the 1s-2s cross sections with the experimental results are satisfactory while the calculated 1s-2p cross sections are higher than the corresponding experimental values. The 2s-2s and the 2p-2p cross sections have large values, specially at the thresholds. A Ramsauer effect in the partial cross sections of the 2s-2s elastic scattering is observed. By comparison with the eigenstate expansion calculation it is found that the Born approximation, despite its simplicity, gives meaningful results for low and close to threshold energies of the bombarding electrons. In this paper the effect of the electron spin and the exchange potentials are also investigated.

I. INTRODUCTION

The recent experimental results of Lichten and Schultz[1] on one hand, and Stebbing et al.[2] on the other, of the 1s ⟶ 2s transition cross section in the hydrogen atom by electron impact and the apparent discrepancy in these measurements, and the measurement of 1s ⟶ 2s transition by Fite et al.[3] also in hydrogen, necessitate accurate calculation for these cross sections.

Calculation of the excitation cross sections in atomic hydrogen by electron impact corresponds to the solution of the problem of three interacting bodies, one proton and two electrons. By taking the position of the proton as the center of mass, the problem will reduce to the task of finding the nonseparable wave function of the system of the two electrons with an attractive center of force. Such solution has not been found yet. However, if this wave function is expanded in terms of the eigenstates of the hydrogen atom, it is shown in this paper that through numerical integration the coefficients of the expansion, which are functions of the position vector of the free electron, can be found exactly. When an infinite number of terms are included in the expansion the solution to the problem is exact. Furthermore, the expansion has the advantage that the asymptotic form of its coefficients are automatically the asymptotic form of the free electron wave function scattered from different atomic states, which are simply related to the excitation cross sections.

In this paper atomic states 1s, 2s, 2p are included in the expansion, and by antisymmetrizing the two electron wave functions according to the exclusion principle, some contribution from the continuum in the expansion is also taken into account. The first calculation of this type was performed by Marriot[4] whose expansion consisted of the 1s and the 2s states in order to calculate the 1s ⟶ 2s transition cross section. This calculation was extended by Smith[5] to higher total orbital angular momenta of the system. Percival and Seaton[6] have formulated the eigen state expansion technique in general, and have tabulated the coefficients of the integro-differential equations for s, p and d atomic electrons. While this paper was in preparation, Burke, Smith and Shey,[7,32] using the tables of reference (6) for three states 1s, 2s, 2p, have integrated the resulting integro-differential equations. Their technique of solution is substantially different from that of this paper in more than one respect, and it is believed that the results presented here are more accurate.

The degeneracy of the 2s and the 2p levels of the hydrogen atom makes it necessary, as pointed out by Massey,[8] that any calculation concerning 1s ⟶ 2s or 1s ⟶ 2p transitions contain these two states simultaneously. In this respect the present calculation and that of reference (7) is superior to that of reference (4), where 1s and 2s states are included to calculate 1s ⟶ 2s transition, or that of Khashaba and Massey,[9] where 1s and 2p states are included to calculate 1s ⟶ 2p transition.

We treat the present problem in the following manner. In Sec. IIA we derive the integro-differential equations of the problem independent of reference (6). Sec. IIB is the derivation of the transmission matrix and the cross sections. In Sec. IIC we derive a useful relationship for numerical integration based on the symmetry of the interacting potentials. Sec. IID is the derivation of the partial wave Born approximation transmission matrix. Different parts in Sec. III deal with techniques of numerical integration and the effects of the long range potentials. The transformation of the radial wave functions presented here avoid the need for iteration of the coupled integro-differential equations, as is the case in reference (7). Finally, Sec. IV gives the results of numerical integration and their interpretation.

The numerical integrations were carried out for all partial waves, where in higher partial waves Born approximation were used. The transition between the eigenstate expansion calculation and Born approximation takes place when the results of the two calculations agree closely.

II. FORMULATION

A. Derivation of the Differential Equations

Since spin orbit interaction of the electrons are neglected, the total orbital angular momentum L, and the total spin angular momentum S, are separately conserved. We can then divide the interactions into anti-parallel spin states where $S = 0$, and parallel spin states where $S = 1$. We then deal with spatial wave functions of the electrons only and for brevity we call the orbital angular momentum the angular momentum.

Neglecting the motion of the proton of the hydrogen atom and taking its position as the origin of the coordinate system, the Schroedinger equation for the system can be written

$$[H-E]\,\psi(\mathbf{r}_1, \mathbf{r}_2) = 0, \tag{2.1}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the bound and free electrons, and in atomic units

$$H - E = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{1}{r_1} - \frac{1}{r_2} + \frac{1}{r_{12}} - E, \tag{2.2}$$

where E is the total energy of the system and r_{12} is the distance between the two electrons. We expand the total wave function $\psi(\mathbf{r}_1, \mathbf{r}_2)$ in terms of the eigenfunctions of the total angular momentum L,

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \sum_{L=0}^{\infty} \psi_L(\mathbf{r}_1, \mathbf{r}_2). \tag{2.3}$$

Since these eigenfunctions are orthogonal and distinct, substitution of Eq. (2.3) in Eq. (2.1) gives,

$$[H-E]\ \psi_L(\mathbf{r}_1, \mathbf{r}_2) = 0. \tag{2.4}$$

The explicit form of $\psi_L(\mathbf{r}_1, \mathbf{r}_2)$ is given by

$$\psi_L(\mathbf{r}_1, \mathbf{r}_2) = (1 + \beta P_{12}) \sum_{n_1 \ell_1 \ell_2} \sum_{m_1 m_2} C^{\ell_1 \ell_2 L}_{m_1 m_2 M}\ \varphi(n_1 \ell_1 m_1, \mathbf{r}_1)$$

$$\times\ r_2^{-1} u(k_{n_1} \ell_2, r_2)\, Y_{\ell_2 m_2}(\Omega_2), \tag{2.5}$$

$$\varphi(n_1 \ell_1 m_1, \mathbf{r}_1) = r_1^{-1} P(n_1 \ell_1, r_1)\, Y_{\ell_1 m_1}(\Omega_1). \tag{2.6}$$

Here $\varphi(n_1 \ell_1\, m_1, r_1)$ is the hydrogen atom wave function with radial part $r_1^{-1} P(n_1 \ell_1, r_1)$ and angular part $Y_{\ell_1 m_1}(\Omega_1)$ and quantum numbers $n\ell_1 m_1$; $r_2^{-1} u(k_{n_1} \ell_2, r_2)$ is the radial part and $Y_{\ell_2 m_2}(\Omega_2)$ is the angular part of the free electron wave function with quantum numbers $k_{n_1} \ell_2 m_2$. The relationship between the wave number k_{n_1} and n_1 is given by

$$k^2_{n_1} = 2\left(E + \frac{1}{2n_1^2}\right). \tag{2.7}$$

Finally the constants $C^{\ell_1 \ell_2 L}_{m_1 m_2 M} = (\ell_1 \ell_2 m_1 m_2 | LM)$ are vector coupling coefficients which make the linear combination of the products of the one electron wave functions in Eq. (2.5) the eigenfunction of L. In the problem under consideration $n_1 = 1, 2$; $\ell_1 = 0, 1$; $\ell_2 = |L - \ell_1|, \ldots\ldots, |L + \ell_1|$; $m_1 = -\ell_1, \ldots, \ell_1$ and $m_2 = -\ell_2, \ldots, \ell_2$. To make the total wave function symmetric for antiparallel spins or antisymmetric for parallel spins, the operator P_{12} interchanges $\mathbf{r}_1$ and $\mathbf{r}_2$ while β is $+1$ for the first case and is -1 for the second.

By taking L perpendicular to the z-axis $M = 0$ and $m_2 = -m_1$. Eq. (2.5) can then be written

$$\psi_L(\mathbf{r}_1, \mathbf{r}_2) = (1 + \beta P_{12}) \sum_{n_1 \ell_1 \ell_2} \sum_{m_1} C^{\ell_1 \ell_2 L}_{m_1 - m_1 0} \; \varphi(n_1 \ell_1 m_1, \mathbf{r}_1)$$

$$\times\, r_2^{-1}\, u(k_{n_1} \ell_2, r_2)\, Y_{\ell_2 m_2}(\Omega_2). \tag{2.8}$$

In order that $\psi_L(\mathbf{r}_1, \mathbf{r}_2)$ closely approximates the exact wave function, we minimize the expectation value of the energy operator with respect to the radial parts of the free electron wave functions,

$$\delta \int \psi_L^*(\mathbf{r}_1, \mathbf{r}_2)\, [H-E]\, \psi_L(\mathbf{r}_1, \mathbf{r}_2)\, d^3r_1\, d^3r_2 = 0. \tag{2.9}$$

It has been shown by Kohn[10] that the differences between the scattering amplitudes obtained from these equations and the exact scattering amplitudes are quadratic in the difference between $\psi_L(\mathbf{r}_1, \mathbf{r}_2)$ and the exact wave function. When the variation is carried out inside the integral we obtain

$$\sum_{m_1} C^{\ell_1 \ell_2 L}_{m_1 - m_1 0} \int \varphi^*(n_1 \ell_1 m_1, \mathbf{r}_1)\, Y^*_{\ell_2 m_2}(\Omega_2)\, [H-E]\, \psi_L(\mathbf{r}_1, \mathbf{r}_2)\, d^3r_1\, d\Omega_2 = 0. \tag{2.10}$$

By means of Eqs. (2.2), (2.8), the Schroedinger equation for the hydrogen atom,

$$\left[\nabla_1^2 + \frac{2}{r_1}\right] \varphi(n_1\ell_1 m_1, r_1) = \frac{1}{n_1^2}\, \varphi(n_1\ell_1 m_1, r_1)\,, \tag{2.11}$$

and Eq. (2.7), Eq. (2.10) reduces to

$$\sum_{m_1} \sum_{n_1'\ell_1'\ell_2'} \sum_{m_1'} C^{\ell_1\ell_2 L}_{m_1 -m_1 0}\, C^{\ell_1'\ell_2' L}_{m_1' -m_1' 0} \int \varphi^*(n_1\ell_1 m_1, r_1)\, Y^*_{\ell_2 m_2}(\Omega_2)\,(1+\beta P_{12})$$

$$\times \left[\nabla^2_{r_2} - \frac{\ell_2'(\ell_2'+1)}{r_2^2} + k^2_{n_1'} + 2\left(\frac{1}{r_2} - \frac{1}{r_{12}}\right)\right] \varphi(n_1'\ell_1' m_1', r_1)$$

$$\times\, r_2^{-1}\, u(k_{n_1'}, \ell_2', r_2)\, Y_{\ell_2' m_2'}(\Omega_2)\, d^3 r_1\, d\Omega_2 = 0\,, \tag{2.12}$$

where $\nabla^2_{r_2}$ is the radial part of ∇^2_2. By orthogonality of the hydrogen atom and spherical harmonics wave functions, the relation[11]

$$\sum_{m_1} \left[C^{\ell_1\ell_2 L}_{m_1 - m_1 0}\right]^2 = 1\,, \tag{2.13}$$

the integration by parts of the exchange terms, and the relation[12]

$$C^{\ell_2\ell_1 L}_{-m_1 m_1 0} = (-)^{L-\ell_1-\ell_2}\, C^{\ell_1\ell_2 L}_{m_1 - m_1 0}, \tag{2.14}$$

Eq. (2.12) leads to

$$\left[\nabla^2_{r_2} - \frac{\ell_2(\ell_2+1)}{r_2^2} + k^2_{n_1} + \frac{2}{r_2}\right] \frac{u(k_{n_1}\ell_2,\ r_2)}{r_2}$$

$$- 2 \sum_{m_1} \sum_{n_1'\ell_1'\ell_2'} \sum_{m_1'} C^{\ell_1\ell_2 L}_{m_1 -m_1 0}\, C^{\ell_1'\ell_2' L}_{m_1' -m_1' 0} \int \frac{\varphi^*(n_1\ell_1 m_1,\ r_1)\, Y^*_{\ell_2 m_2}(\Omega_2)}{r_{12}}$$

$$\times \left[\varphi(n_1'\ell_1' m_1',\ r_1)\, \frac{u(k_{n_1}'\ell_2',\ r_2)}{r_2} Y_{\ell_2' m_2'}(\Omega_2) + \beta\, \varphi(n_1'\ell_1' m_1',\ r_2)\right.$$

$$\left.\times \frac{u(k_{n_1}'\ell_2',\ r_1)}{r_1} Y_{\ell_2' m_2'}(\Omega_1)\right] d^3r_1\, d\Omega_2$$

$$+ \beta \sum_{n_1'\ell_1'\ell_2'} (-)^{L-\ell_1-\ell_2}\, \delta(\ell_1'\ell_2',\ \ell_2\ell_1)\left(\frac{1}{n_1^{2}} + k^{2}_{n_1'}\right) \int_0^\infty P(n_1\ell_1,\ r_1)\, r_2^{-1} P(n_1'\ell_1',\ r_2)$$

$$\times u\left(k_{n_1'},\ \ell_2',\ r_1\right) dr_1 = 0\ . \qquad (2.15)$$

If $1/r_{12}$ is expanded in terms of the Legendre polynomials and use is made of the addition theorem [13] we obtain

$$\frac{1}{r_{12}} = \sum_{\lambda=0}^{\infty} \frac{r_<^{\ \lambda}}{r_>^{\ \lambda+1}}\, P_\lambda(\cos\theta_{12})$$

$$= \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{+\lambda} \frac{4\pi}{2\lambda+1} \frac{r_<^{\ \lambda}}{r_>^{\ \lambda+1}}\, Y_{\lambda\mu}(\Omega_1)\, Y^*_{\lambda\mu}(\Omega_2)\ . \qquad (2.16)$$

In this expression θ_{12} is the angle between the position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ at the origin, and $r_<$ is the smaller and $r_>$ is the larger of $|\mathbf{r}_1|$ and $|\mathbf{r}_2|$. We also introduce

$$y_\lambda(n\ell n'\ell', r_2) = r_2^{-(\lambda+1)} \int_0^{r_2} P(n\ell, r_1)\, P(n'\ell', r_1)\, r_1^{\lambda} dr_1$$

$$+ r_2^{\lambda} \int_{r_2}^{\infty} P(n\ell, r_1)\, P(n'\ell', r_1)\, r_1^{-(\lambda+1)} dr_1 . \qquad (2.17)$$

Then it follows that

$$\int_0^{\infty} \frac{P(n\ell, r_1)\, P(n'\ell', r_1)}{r_{12}} dr_1 = \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{+\lambda} Y_{\lambda\mu}(\Omega_1) Y^*_{\lambda\mu}(\Omega_2)\, y_\lambda(n\ell n'\ell', r_2). \qquad (2.18)$$

By means of Eq. (2.18), the relation[14]

$$\int Y^*_{\ell_3 m_3}\, Y_{\ell_2 m_2}\, Y_{\ell_1 m_1}\, d\Omega = \left[\frac{(2\ell_1+1)(2\ell_2+1)}{4\pi(2\ell_3+1)}\right]^{1/2} C^{\ell_1\ell_2\ell_3}_{m_1 m_2 m_3}\, C^{\ell_1\ell_2\ell_3}_{000} , \qquad (2.19)$$

and the definition

$$(n\ell | k_{n_1}\ell') = \int_0^{\infty} P(n\ell, r)\, u(k_{n_1}\ell', r)\, dr , \qquad (2.20)$$

Eq. (2.15) when multiplied by r_2 gives

$$\left[\frac{d^2}{dr_2^2} - \frac{\ell_2(\ell_2+1)}{r_2^2} + k_{n_1}^2 + \frac{2}{r_2}\right] u(k_{n_1}\ell_2, r_2)$$

$$-2\left(\frac{2\ell_2+1}{2\ell_1+1}\right)^{\frac{1}{2}} \sum_{n_1'\ell_1'\ell_2'} \sum_{m_1 m_1'} \sum_{\lambda=0}^{\infty} \sum_{\mu=-\lambda}^{+\lambda} C^{\ell_1\ell_2 L}_{m_1\,-m_1\,0}\, C^{\ell_1'\ell_2' L}_{m_1'\,-m_1'\,0}$$

$$\times \left\{\left(\frac{2\ell_1'+1}{2\ell_2'+1}\right)^{\frac{1}{2}} C^{\lambda\ell_1'\ell_1}_{\mu m_1' m_1}\, C^{\lambda\ell_1'\ell_1}_{000}\, C^{\lambda\ell_2\ell_2'}_{\mu m_2 m_2'}, C^{\lambda\ell_2\ell_2'}_{000}\, y_\lambda(n_1\ell_1 n_1'\ell_1', r_2)\, u(k_{n_1'}\ell_2', r_2)\right.$$

$$\left. +\beta\left(\frac{2\ell_2'+1}{2\ell_1'+1}\right)^{\frac{1}{2}} C^{\lambda\ell_2'\ell_1}_{\mu m_2' m_1}\, C^{\lambda\ell_2'\ell_1}_{000}\, C^{\lambda\ell_2\ell_1'}_{\mu m_2 m_1'}\, C^{\lambda\ell_2\ell_1'}_{000}\, P(n_1'\ell_1', r_2)\, y_\lambda(n_1\ell_1 k_{n_1'}\ell_2', r_2)\right\}$$

$$+\beta \sum_{n_1'\ell_1'\ell_2'} (-)^{L-\ell_1-\ell_2}\, \delta(\ell_1'\ell_2', \ell_2\ell_1) \left(\frac{1}{n_1^2} + k_{n_1'}^2\right) P(n_1'\ell_1', r_2)\,(n_1\ell_1|k_{n_1'}\ell_2') = 0. \quad (2.21)$$

In the exchange integrals above we have defined $P(k_{n_1}\ell_2, r)$ as $u(k_{n_1}\ell_2, r)$.

The vectorial equations

$$L = \boldsymbol{\ell}_1 + \boldsymbol{\ell}_2, \quad (2.22)$$

where L is constant but $\boldsymbol{\ell}_1$ and $\boldsymbol{\ell}_2$ take the values given before, can be divided into two groups, one with $L - \ell_1 - \ell_2$ even and the other with $L - \ell_1 - \ell_2$ odd. Since the total spacial wave function has the parity of $\ell_1 + \ell_2$, in the first group the wave function has the parity of L and in the second a parity opposite to L. By conservation of parity we have two distinct groups of interactions. In this problem, where 1s, 2s and 2p states of atomic hydrogen are taken into account, it is easy to see that when $L-\ell_1-\ell_2$ is even, the set of quantum numbers $k_{n_1}\ell_2$ has 4 values; one for each of the 1s and 2s states and two for the 2p state. When $L-\ell_1-\ell_2$ is odd, $k_{n_1}\ell_2$ has one value which corresponds to the elastic scattering of electrons by the 2p state of the hydrogen atom. Eq. (2.21) is evaluated for these cases and the resulting differential equations are listed in Appendix I. In evaluating Eq. (2.21) it should be noted that the $C^{\ell_1\ell_2\ell_3}_{m_1m_2m_3}$ coefficients are subject to the condition that $\ell_1\ell_2\ell_3$ form a closed triangle and $m_3 = m_1 + m_2$.[15] This limits the summation over λ and μ considerably to few terms only. Summation over m_1, m_1', λ and μ are carried out using the numerical values of the C coefficients given by Condon and Shortley.[16]

Percival and Seaton[6] have derived the same differential equations for the scattering of free electrons by atomic s, p and d electrons in hydrogen atom using the theory of irreducible tensor operators to evaluate the interaction terms between the two electrons in the differential equations. The calculation becomes considerably simpler in this way. The results of the two methods are identical.

In the rest of the paper except Sec. IIE we discuss the solutions to the four coupled differential equations given in Appendix I and which arise when $L-\ell_1-\ell_2$ is even. The single differential equations for $L-\ell_1-\ell_2$ odd is derived in Sec. IIE. Its numerical integration can be treated as a special case of the four coupled differential equations.

When the integrals representing the direct potentials in the four differential equations are evaluated and some change is made in the limits of the exchange potential integrals, these equations can be written in the following matrix form

$$\left[\frac{d^2}{dr^2} + k_n^{\ 2} - \frac{l_n(l_n+1)}{r^2}\right] \mathbf{u}(k_n l_n, r) = 2\mathbf{V}\,\mathbf{u}(k_n l_n, r). \qquad (2.23)$$

The four components of $\mathbf{u}$ are the four radial functions of the free electron. $\mathbf{V}$ is a 4x4 symmetric matrix that is the sum of three matrices,

$$V_{ij} = D_{ij} + E_{ij},$$

$$E_{ij} = F_{ij} + \sum_{\nu=1}^{\sigma} g_{ij}^{\nu} \int_0^{\infty} h_{ij}^{\nu}\, dr, \qquad (2.24)$$

where D_{ij} is the direct and E_{ij} is the exchange potentials and both are functions of r. The matrix E_{ij} contains in addition integrals with respect to r and for the purpose of numerical integration it can be written as the sum of two matrices. The explicit forms of D_{ij}, F_{ij}, g_{ij}^{ν} and h_{ij}^{ν} are given in Appendix II. The value of σ is 2 for i=j=3 and i=j=4, and is 1 for all other values of i and j. It is understood that for the exchange terms the components of $\mathbf{u}$ on the right hand side of Eq. (2.23) are inside the integrals of the exchange terms.

B. Derivation of the Transmission Matrix From Solutions of the Differential Equations

The method is similar to that used by Bransden and McKee,[17] and by Marriot.[4] Eq. (2.23) constitutes a set of 4 coupled, second order, differential equations. Three components of **u** can be eliminated from these equations, resulting in an 8th order differential equation for the remaining component. Therefore there are 8 sets of solutions to Eq. (2.23). However, only half of these solutions are regular at the origin. Each of the four regular solutions corresponds to a definite vector **u**. The four vectors can properly be represented by a 4x4 matrix u_{nj}, $n, j = 1, 2, 3, 4$, where n corresponds to the particular component and j corresponds to the particular solution of **u**. The four solutions are carried out numerically in the next section.

From the explicit form of **V** it can be seen that **V** vanishes at infinity. The asymptotic solutions of **u** as given by Eq. (2.23) is therefore

$$u_{nj}(r) \sim a_{nj} \sin(k_n r - \frac{l_n \pi}{2} + \delta_{nj}), \qquad (2.25)$$

$$n, j = 1, 2, 3, 4,$$

where a_{nj} is the amplitude and δ_{nj} is the phase shift of the j^{th} solution of the n^{th} component of u.

Corresponding to the 4 components of u there are 4 channels open to the reaction. If the incident wave be in the m^{th} channel ($m = 1, 2, 3, 4$), the travelling wave in the n^{th} channel will be given by

$$u_n(r) \sim \exp\left[-i\left(k_n r - \frac{1}{2} l_n \pi\right)\right] \delta(m,n) - S_{mn} \exp\left[i\left(k_n r - \frac{1}{2} l_n \pi\right)\right],$$

$$n = 1,\ 2,\ 3,\ 4. \tag{2.26}$$

The constants S_{mn} are the amplitudes of the scattered waves. Since Eqs. (2.26) are also the asymptotic solutions of Eqs. (2.23), they must be equal to linear combinations of Eqs. (2.25). If we call the coefficients of the linear combinations P_j we must have

$$\sum_{j=1}^{4} P_j a_{nj} \sin\left(k_n r - \frac{l_n \pi}{2} + \delta_{nj}\right) =$$

$$(k_n)^{-1/2} \left\{\exp\left[-i\left(k_n r - \frac{1}{2} l_n \pi\right)\right] \delta(m,n) - S_{mn} \exp\left[i\left(k_n r - \frac{1}{2} l_n \pi\right)\right]\right\}, \tag{2.27}$$

$n, m = 1, 2, 3, 4.$

On the right-hand side, we have used the normalization of Blatt and Weisskopf.[18] If we equate the coefficients of $\exp\left[-i\left(k_n r - \frac{1}{2} l_n \pi\right)\right]$ and $\exp\left[i\left(k_n r - \frac{1}{2} l_n \pi\right)\right]$ in Eqs. (2.27) we obtain

$$\left.\begin{aligned} \sum_{j=1}^{4} P_j \, a_{nj} \exp -\left[i\,\delta_{nj}\right] &= \frac{-2i}{\sqrt{k_n}}\, \delta(m,n) \\ \sum_{j=1}^{4} P_j \, a_{nj} \exp \left[i\,\delta_{nj}\right] &= \frac{-2i}{\sqrt{k_n}}\, S_{mn} \end{aligned}\right\} . \tag{2.28}$$

Separation of Eqs. (2.28) into real and imaginary parts gives

$$\left.\begin{aligned} \sum_{j=1}^{4} \left[(\Re P_j)\sin \delta_{nj} - (\Im P_j)\cos \delta_{nj}\right] a_{nj} &= \frac{2}{\sqrt{k_n}}\, \delta(m,n) \\ \sum_{j=1}^{4} \left[(\Re P_j)\cos \delta_{nj} + (\Im P_j)\sin \delta_{nj}\right] a_{nj} &= 0 \\ \sum_{j=1}^{4} \left[(\Re P_j)\sin \delta_{nj} + (\Im P_j)\cos \delta_{nj}\right] a_{nj} &= \frac{-2}{\sqrt{k_n}}\, \Re S_{mn} \\ \sum_{j=1}^{4} \left[(\Re P_j)\cos \delta_{nj} - (\Im P_j)\sin \delta_{nj}\right] a_{nj} &= \frac{2}{\sqrt{k_n}}\, \Im S_{mn} \end{aligned}\right\} . \tag{2.29}$$

In the above $\Re$ or $\Im$ represent the real or the imaginary part of the quantity that follows them. Eqs. (2.29) are a set of 16 linear equations for 16 unknowns $\Re P_j$, $\Im P_j$, $\Re S_{mn}$ and $\Im S_{mn}$. Once these unknowns are found,[19] the magnitude of S_{mn} will be given by

$$|S_{mn}|^2 = (\Re S_{mn})^2 + (\Im S_{mn})^2 . \qquad (2.30)$$

The cross section is obtained by asymptotic expansion in spherical harmonics of the incident plane wave[20]

$$\exp[ikz] \sim \frac{\pi^{1/2}}{kr} \sum_{l=0}^{\infty} (2l+1)^{1/2}\, i^{l+1} \left\{ \exp\left[-i\left(kr - \frac{1}{2} l\pi\right)\right] - \exp\left[i\left(kr - \frac{1}{2} l\pi\right)\right] \right\} Y_{l,0} . \qquad (2.31)$$

The magnitude of the ingoing wave on the right hand side of Eqs. (2.27) for $n = m$ is $[k_m/\pi(2l_m + 1)]^{1/2}$ times the magnitude of the partial wave of the expansion of $r \exp[i k_m z]$.. The plane wave has a flux of v which, in atomic units, is equal to k. The ingoing flux of the right-hand side of Eqs. (2.27) is therefore $k_m^2/[\pi(2l_m + 1)]$. The outgoing flux in the channel $n \neq m$ is $|S_{mn}|^2$. The cross section is obtained when we average the ratio of the outgoing flux to the ingoing flux over the initial states, and sum over the final states. For a particular spin state of the two electrons, unpolarized electron beam and unoriented atoms, the multiplicity of the initial states is $(2l_1 + 1)(2l_2 + 1)$, where l_1 and l_2 are the angular momentum of the bound and free electrons. For a polarized beam, $m_2 = 0$, where m_2 is the magnetic quantum number of the free electron. Then $m_1 = M$, where m_1 and M are the bound electron and the total magnetic quantum numbers. Since M is constant there is only one initial state for a polarized beam. The multiplicity of the final states is 2L + 1, where L is the total orbital angular momentum. Since $\ell_m = \ell_2$, the cross section for $m \neq n$ is

$$Q_{mn} = \frac{\pi(2L+1)}{k_m^2\,(2l_1+1)}\,|S_{mn}|^2\ ,\ m \neq n. \tag{2.32}$$

The outgoing partial wave in the incident channel m consists of the scattered wave plus the outgoing wave given in the expansion of the plane wave. Then, according to Eqs. (2.27) for n = m the magnitude of the amplitude of the scattered wave is $|1 - S_{mm}|$. The elastic scattering cross section is therefore given by

$$Q_{mm} = \frac{\pi(2L+1)}{k_m^2\,(2l_1+1)}\,|1 - S_{mm}|^2 \tag{2.33}$$

If we define a matrix T by the relation

$$T = 1 - S\ , \tag{2.34}$$

Eqs. (2.32) and (2.33) can then be combined into a single equation,

$$Q_{mn} = \frac{\pi(2L+1)}{k_m^2\,(2l_1+1)}\,|T_{mn}|^2\ . \tag{2.35}$$

T_{mn} is the transmitted amplitude in the nth channel due to an incident wave in the mth channel. The elements of T_{mn} constitute the transmission matrix.

The matrix S has two properties that are useful as tests on the accuracy of numerical integration. From Eq. (2.26) it can be seen that S transforms the ingoing wave into the outgoing waves. The continuity of the electronic current requires that S be a unitary matrix

$$\sum_{n=1}^{4} |S_{mn}|^2 = 1, \; m = 1, 2, 3, 4. \qquad (2.36)$$

Furthermore, since the Hamiltonian is Hermetian, S must be symmetric,[18]

$$S_{mn} = S_{nm}. \qquad (2.37)$$

Eqs. (2.36) and (2.37) are used as tests on the accuracy of numerical integration.

C. A Useful Relationship

A relationship based on the symmetry of the interaction potentials can be derived which serves as another test on the accuracy of the solutions. The l^{th} and the k^{th} solutions of the i^{th} component of u by Eq. (2.23) are given by

$$\left.\begin{aligned}\left[\frac{d^2}{dr^2} + k_i^2 - l_i\,\frac{(l_i + 1)}{r^2}\right] u_{il} &= \sum_j V_{ij}\, u_{jl} \\[2em] \left[\frac{d^2}{dr^2} + k_i^2 - l_i\,\frac{(l_i + 1)}{r^2}\right] u_{ik} &= \sum_j V_{ij}\, u_{jk}\end{aligned}\right\} \qquad (2.38)$$

Multiplying the first by u_{ik} and the second by u_{il}, subtracting the two expressions and summing over i gives

$$\sum_i \left[u_{ik}\,\frac{d^2}{dr^2}\,u_{il} - u_{il}\,\frac{d^2}{dr^2}\,u_{ik}\right] = \sum_{i,j} V_{ij}\left[u_{ik}u_{jl} - u_{il}\,u_{jk}\right] \qquad (2.39)$$

Since $V_{ij} = V_{ji}$, the interchange of the summation indices changes the sign on the right hand side of the equation, the right hand side must therefore be zero. Integrating the left hand side from zero to infinity we obtain

$$\sum_i \int_0^\infty \left[u_{ik}\,\frac{d^2}{dr^2}\,u_{il} - u_{il}\,\frac{d^2}{dr^2}\,u_{ik}\right] dr = 0\,. \qquad (2.40)$$

Integrating the above equation by parts, and applying Eq. (2.25) we obtain

$$\left.\begin{aligned}&\sum_{i=1}^{4} k_i\, a_{ik}\, a_{il}\, \sin(\delta_{ik} - \delta_{il}) = 0 \\ &k,\ l = 1,\ 2,\ 3,\ 4,\ k \neq l\,.\end{aligned}\right. \qquad (2.41)$$

Although the terms containing the exchange potentials do not cancel out on the right hand side of Eq. (2. 39) the cancellation does take place after the integration is carried out in Eq. (2. 40).

D. Transmission Matrix According to Born Approximation

The Born approximation consists of neglecting the exchange potential terms appearing in the V matrix of Eq. (2. 23), and also of neglecting all the direct potential terms in this matrix except those terms that connect the incident channel to all other channels.[21] Eq. (2. 23), when the incident wave is in the m^th^ channel, reduces to

$$\left[\frac{d^2}{dr^2} + k_n^2 - \frac{l_n(l_n+1)}{r^2}\right] u_n = 2 D_{nm} u_m , \qquad (2.42)$$

$$n = 1, 2, 3, 4,$$

u_m and u_n are given asymptotically by

$$u_m \sim k_m^{-1/2} \sin(k_m r - l_m \pi/2) \qquad (2.43)$$

$$u_n \sim k_n^{-1/2} B_{nm} \cos(k_n r - l_n \pi/2). \qquad (2.44)$$

We have chosen the constants of proportionality of u_m and u_n such that B_{nm} is the Born approximation of the reactance matrix R.[22,23] Eq. (2. 43) shows that u_m must have the following form[24]

$$u_m = k_m^{1/2}\, r\, j_{l_m}(k_m r). \tag{2.45}$$

where $j_{l_m}(k_m r)$ are spherical Bessel functions. Furthermore, if y_n represents the homogenous solution of Eq.(2.42), it must have the following forms

$$y_n = a_n\, k_n\, r\, j_{l_n}(k_n r), \tag{2.46}$$

$$y_n \sim a_n \sin(k_n r - l_n \pi/2), \tag{2.47}$$

with a_n some unknown constant. Multiplying Eq. (2.42) on the left by y_n and integrating the result from zero to infinity we obtain by partial integration

$$2\int_0^\infty y_n D_{nm} u_m \, dr = \int_0^\infty y_n \left[\frac{d^2}{dr^2} + k_n^2 - \frac{l_n(l_n+1)}{r^2}\right] u_n \, dr$$

$$= \left[y_n \frac{d}{dr} u_n - u_n \frac{d}{dr} y_n\right]_0^\infty$$

$$= -k_n^{1/2} a_n B_{nm}.$$

The last equality has been obtained by noticing that y_n and u_n vanish at the origin, and by using their asymptotic forms as given by Eqs. (2.44) and (2.47). We therefore have

$$B_{nm} = -2(k_n k_m)^{1/2} \int_0^\infty j_{l_n}(k_n r)\, D_{nm}\, j_{l_m}(k_m r)\, r^2 \, dr. \tag{2.48}$$

This is identical to the expression given for B by Seaton.[25]

The transmission and the reactance matrices are related by $\mathbf{T} = -2i\mathbf{R}/(1-i\mathbf{R})$. Since $\mathbf{B} \ll 1$, the transmission matrix according to the Born approximation is given by

$$T_{nm}{}^{B} = 4i\,(k_n k_m)^{1/2} \int_0^\infty j_{\ell_n}(k_n r)\, D_{nm}\, j_{\ell_m}(k_m r)\, r^2\, dr . \qquad (2.49)$$

Substitution of Eq. (2. 49) is Eq. (2. 35) would give the cross section according to the Born approximation. It should be noted that the symmetry of **T** insures Eq. (2. 37) to be satisfied while Eq. (2. 36) is not satisfied anymore. If we define $\mathbf{T} = -2i\mathbf{B}/(1-i\mathbf{B})$, then $\mathbf{S} = (1+i\mathbf{B})/(1-i\mathbf{B})$ and the symmetry of **B** makes **S** unitary. Eq. (2. 36), the continuity of current, is then satisfied. This is the definition of approximation II of the Born approximation according to Seaton[23] which will be discussed later.

E. Elastic Scattering of Electrons by the 2p States of the Hydrogen Atom

The angular momentum of the free electron, l_2, in the 2p channel has the values L - 1, L , L + 1 , where L is the total angular momentum of the system. The first and the last values were considered in previous sections. The case $l_2 = L$ corresponds to a wave function in the 2p channel with a parity different from all channel wave functions considered previously. It therefore corresponds to elastic scattering. The wave function in this case is given by

$$\psi_L(r_1, r_2) = (1 + \beta P_{12}) \sum_{m_1=-1}^{+1} C^{1LL}_{m_1 - m_1 0} \varphi_{2pm_1}(r_1) \frac{u(k_2 L, r_2)}{r_2} Y_{L -m_1}(\Omega_2). \tag{2.50}$$

When Eq. (2.9) is formed with this wave function, and minimized with respect to $u(k_2L, r_2)$, treatment which led to the derivation of the four differential equations will give the following differential equation

$$\begin{aligned}
&\left[\frac{d^2}{dr^2} + k_2^2 - \frac{L(L+1)}{r^2} + \frac{2}{r}\right] u_L(r) \\
&- \beta\left(\frac{1}{4} + k_2^2\right) \delta(L, 1)\, r R_{21}(r)\, (2p|k_2L) \\
&+ 2 \left[y_0(2p2p, r) - \frac{1}{5} y_2(2p2p, r)\right] u_L(r) \\
&+ 2\beta r R_{21}(r) \left[- \frac{3y_{L-1}(2pk_2L, r)}{(2L+1)(2L-1)} + \frac{3y_{L+1}(2pk_2L, r)}{(2L+1)(2L+3)}\right] = 0
\end{aligned} \tag{2.51}$$

The asymptotic solution of this equation is given by

$$u_L \sim a_L \sin(k_2 r - L\pi/2 + \delta_L). \tag{2.52}$$

If the scattering amplitude is designated by T_{55} it can be shown from Sec. IIB that for a particular L

$$T_{55} = 1 - \exp 2i\delta = -2i \exp(i\delta) \sin\delta, \tag{2.53}$$

where for simplicity we have suppressed the subscript L. The cross section, according to Eq. (2.35), is given by

$$Q_{55} = \frac{4\pi(2L+1)}{3k_2^2} \sin^2\delta \tag{2.54}$$

The total elastic scattering cross section by the 2p states is the sum of this cross section and the cross section corresponding to $l_2 = L - 1$ and $l_2 = L + 1$ which were considered previously.

The Born amplitude, Eq. (2.48) in this case is given by

$$B_{55} = - 2k_2 \int_0^\infty j_L(k_2r) D_{55} j_L(k_2r) r^2 dr , \qquad (2.55)$$

where by Eq. (2.51),

$$D_{55} = - \frac{1}{r} + y_0(2p2p, r) - \frac{1}{5} y_2(2p2p, r) . \qquad (2.56)$$

III. NUMERICAL INTEGRATION

A. Decomposition of the Differential Equations

If it were not for the definite integrals appearing in the potential matrix $\mathbf{V}$, the set of the four coupled differential equations (2.23) could be integrated by any standard technique. The presence of these unknown constants whose integrand involve the unknown functions makes it necessary to solve these equations by iteration or by transformation of $\mathbf{u}$ into other vectors, whose differential equations do not contain definite integrals. Since the terms containing definite integrals are small as compared to the direct potentials, the iteration method can be used by assuming that the values of these integrals are zero. The differential equations are then integrated, the values of the definite integrals that are subsequently obtained are substituted in the differential equations, and the integration is repeated. The process is repeated until sufficiently consistent values of these integrals are obtained. This method is useful if the convergences of the constants are fast enough, and the cross section is not very sensitive to the values of these constants.

In the second method, the transformation of u fixes the values of the constants and thus avoids iteration, whereby the computation is reduced considerably. The description of the method will be given here.[26,27]

By making use of Eq. (2. 24), Eq. (2. 23) can be written

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2}\right]u_i = 2\sum_{j=1}^{4}\left[(D_{ij}+F_{ij})u_j + \sum_{\mu=1}^{\sigma} g_{ij}^{\mu}\, C_{ij}^{\mu}\right] \tag{3. 1}$$

where

$$C_{ij}^{\mu} = \int_0^{\infty} h_{ij}^{\mu}(r)\, u_j(r)\, dr . \tag{3. 2}$$

We introduce the functions v_i and u_i^{kl} that are solutions of the following differential equations

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2}\right] v_i = 2\sum_{j=1}^{4} \left[D_{ij} + F_{ij}\right] v_j \tag{3.3}$$

$$\left[\frac{d^2}{dr^2} + k_i^2 - \frac{l_i(l_i+1)}{r^2}\right] u_i^{kl} = 2\sum_{j=1}^{4} \left[D_{ij} + F_{ij}\right] u_j^{kl}$$

$$+ 2\,\delta\,(i,\,k)\, g_{kl}^{\nu}. \tag{3.4}$$

Then u_i is given by the following expression

$$u_i = v_i + \sum_{k=1}^{4} \sum_{l=1}^{4} \sum_{\nu=1}^{\sigma} C_{kl}^{\nu}\, u_i^{kl}\,. \tag{3.5}$$

Eq. (3.5) can be verified by multiplying Eq. (3.4) by C_{kl}^{ν}, summing over k, l and ν, and adding to Eq. (3.3), where upon Eq. (3.1) results. Substitution of Eq. (3.5) in Eq. (3.2) gives

$$\sum_{k=1}^{4} \sum_{l=1}^{4} \sum_{\nu=1}^{\sigma} \left[\delta\,(ij\mu,\, kl\nu) - A_{ij}^{\mu kl}\right] C_{kl}^{\nu} = B_{ij}^{\mu}\,, \tag{3.6}$$

i, j = 1, 2, 3, 4; $\mu = 1, 2$ for i = j = 3 and i = j = 4; $\mu = 1$ otherwise,

where $A_{ij}^{\mu kl}$ and B_{ij}^{μ} are defined by

$$\left.\begin{aligned} A_{ij}^{\mu kl} &= \int_0^{\infty} h_{ij}^{\mu}\, u_j^{kl}\, dr \\ B_{ij}^{\mu} &= \int_0^{\infty} h_{ij}^{\mu}\, v_j\, dr \end{aligned}\right\} . \tag{3.7}$$

The numerical integration is carried out by integrating Eqs. (3.3) and (3.4) by any standard method, calculating $A_{ij}^{\mu k l}$ and B_{ij}^{μ} by Eqs. (3.7) and, finally, solving the system of 18 algebraic equations given by Eqs. (3.6) to find C_{kl}^{ν}. With the known values of these constants the integration of Eqs. (3.1) is straightforward.

The determinant of Eqs. (3.6) becomes singular for L = 0 and 1. This is shown in Appendix III. To remove the singularity, some of the C_{kl}^{ν} are chosen arbitrarily, and the rest of the C_{kl}^{ν} are found in terms of the chosen ones.

B. Solution at the Origin

In order that the four soltuions of $\mathbf{u}$ be independent of each other we must have

$$\sum_{j=1}^{4} C_j \, u_{ij} \neq 0, \; i = 1, 2, 3, 4, \tag{3.8}$$

where C_j are some constants. A necessary condition for this to be satisified is that the determinant of Eq. (3.8) be nonzero,

$$|| u_{ij} || \neq 0. \tag{3.9}$$

It is not difficult to see that this also is a sufficient condition. At the origin the solution u_{ij} can be expressed as power series in r,

$$u_{ij} = \sum_{\nu=0}^{\infty} a_{ij}^{\nu} \, r^{s_i+\nu}, \tag{3.10}$$

where a^{ν}_{ij} are the coefficients of expansion, and s_i are given integers for each component of $\mathbf{u}$ and are fixed by the behavior of Eq. (2.23) at the origin. We can satisfy Eq. (3.9) at the origin by having

$$||a^{\circ}_{ij}|| \neq 0. \qquad (3.11)$$

By choosing suitable values of a°_{ij}, subject to the restriction (3.11), four independent solutions are obtained.

C. Solution at Large r

With given initial values the solution of Eq. (2.23) can be extended from origin to any desired value of r. In order to obtain the asymptotic amplitudes and the phase shifts, the presence of the centrifugal and long range potentials make it necessary to extend the solutions to infinity. This is undesirable because of the time consumption on the computer, and the accumulated error due to the long range integration. Seaton[23] has solved the problem of r^{-2} long range potentials occuring in the off diagonal terms of the potential matrix $\mathbf{V}$ by diagonalizing the asymptotic form of the differential equations (2.23) and the corresponding S matrix. By an inverse transformation the elements of the original S-matrix are found.

Instead, we develop here a perturbation theory which is based on the method described by Mott and Massey.[28] The error in the resulting solution is inversely proportional to the squared of the distance from the origin.

Eq. (2.23) for large distances of r can be written

$$\left[\frac{d^2}{dr^2} + k_n^2\right] \mathbf{u}(k_n l_n, r) = 2\mathbf{U}\mathbf{u}(k_n l_n, r), \tag{3.12}$$

where **U** is the sum of the centrifugal potential matrix and the asymptotic form of the **V** matrix. The elements of **U** are given in Appendix IV. A component of Eq. (3.12) is of the following form:

$$\left.\begin{array}{l} \left[\dfrac{d^2}{dr^2} + k^2\right] u(r) = g(r) \\ \\ \qquad g(r) \ll k^2 u(r), \qquad g(r) \to 0 \text{ as } r \to \infty \end{array}\right\}. \tag{3.13}$$

The perturbation theory is applied between some large distance R and infinity. Suppose u vanishes at R, then we have the following boundary condition

$$u(R) = 0 . \tag{3.14}$$

If we represent the solution of the homogenous equation by y(r), at infinity we must have

$$\left.\begin{array}{l} y(r) = a \sin(kr - kR) \\ u(r) = (a + \Delta a) \sin(kr - kR + \eta) \end{array}\right\}, \tag{3.15}$$

where ΔA and η are generated by g(r). Since g(r) is small, we can write

$$u = y(1 + \zeta), \tag{3.16}$$

where ζ is a small function. Substitution of Eq. (3.16) in Eq. (3.13) gives

$$\frac{d}{dr}\left(y^2 \frac{d\zeta}{dr}\right) = g(r)\, y, \tag{3.17}$$

where, upon double integration, we obtain

$$\zeta = \int_R^r \frac{dr}{y^2} \int_R^r g(r')\, y\, dr'. \tag{3.18}$$

The constants of integrations are fixed by the condition (3.14) and the fact that $u'(R) = y'(R)$.

We now integrate Eq. (3.18) by parts,

$$\zeta = \left[\int_R^r g(r)\, y\, dr\right] \left[\int_R^r \frac{dr}{y^2}\right] - \int_R^r g(r)\, y\, dr \int_R^r \frac{dr}{y^2}. \tag{3.19}$$

When the integration with respect to y is carried out, and the result is substituted in Eq. (3.17), we obtain

$$\begin{aligned} u(r) = {} & \sin(kr - kR)\left[a + \frac{1}{k}\int_R^r g(r)\cos(kr - kR)\, dr\right] \\ & + \cos(kr - kR)\left[-\frac{1}{k}\int_R^r g(r)\sin(kr - kR)\, dr\right]. \end{aligned} \tag{3.20}$$

Comparison of the second of Eqs. (3.15) and Eq. (3.20) shows that

$$\left.\begin{aligned} \Delta a &= \frac{1}{k}\int_R^{\infty} g(r)\cos(kr - kR)\,dr \\ \eta &= -\frac{1}{ak}\int_R^{\infty} g(r)\sin(kr - kR)\,dr \end{aligned}\right\}, \qquad (3.21)$$

to first order. The functions g(r) in the four differential equations (3.12) are given by

$$g_i(r) = 2\sum_j U_{ij}u_j\,. \qquad (3.22)$$

To first order this can be written by

$$g_i(r) = 2\sum_j a_j U_{ij}\sin(k_j r - k_j R_j)\,, \qquad (3.23)$$

where R_j is the last zero of u_j with positive slope. Substitution of this equation in Eq. (3.21) gives

$$\left.\begin{aligned} \Delta a_i &= -\sum_j \frac{a_j}{k_i}\int^{R_i} \cos(k_i r - k_i R_i)U_{ij}\sin(k_j r - k_j R_j)\,dr \\ \eta_i &= \sum_j \frac{a_j}{a_i k_i}\int^{R_i} \sin(k_i r - k_i R_i)U_{ij}\sin(k_j r - k_j R_j)\,dr \end{aligned}\right\}. \qquad (3.24)$$

Δa_i and η_i can easily be calculated by substituting the values of

U_{ij} from Appendix IV, integrating the resulting integrals by parts and retaining the leading terms.

The asymptotic amplitudes and phase shifts are given by

$$\left.\begin{aligned} a_i(\infty) &= a_i(R_i) + \Delta a_i \\ \delta_i(\infty) &= \delta_i(R_i) + \eta_i + [L - \delta(i,3) + \delta(i,4)]\pi/2 \end{aligned}\right\} \qquad (3.25)$$

where $a_i(R_i)$ and $\delta_i(R_i)$ are the amplitudes and total phase shifts calculated at R_i by the machine, and where $\delta(i,3)$ and $\delta(i,4)$ are the δ functions.

D. Details of the Numerical Integration

Milne's[29] method with variable mesh size and Simpson's[30] rule were used for the integration of the differential equations and evaluations of the integrals respectively. As the solution advances from the origin, the differential equations become less sensitive to the size of the increment, and the error of integration falls below certain small number ϵ. At each value of r the value of the function is found, first with the given value of the increment, and second with the value of increment divided in half. The error of integration is defined as the difference between these two solutions. When the error becomes small the increment is doubled until a maximum value is reached. At some distance R_1 all the exchange potentials and, similarly, all the direct potentials except those representing optically allowed transitions and the 2p - 2p elastic scattering potential become vanishingly small. (See Appendix IV.) At this distance the set of differential equations is replaced by the simpler set containing only these potentials. The integration is continued until some distance R_2, where the first order solution of the rest of the range of integration is obtained by the method developed in Sec. IIIC. No attempt was made to solve any set of linear equations or any matrix equations, as these equations are solvable by the computer in their original form.

The values of the constants of the numerical integration are given below. h_i and h_f are the initial and the final increment of integration. In some exceptional cases, different values were used.

Table III. 1

h_i	1×10^{-5}
h_f	0.05
ϵ	1×10^{-4}
R_1	30
R_2	200

All quantities are in units of Bohr radius except ϵ which is dimensionless.

IV. RESULTS

The four differential equations listed in Appendix I were integrated by the methods described in Sec. III. Based on the Eqs. (2.41), (2.37) and (2.36) we define the three relationships,

$$D_{mn} = \frac{\left| \sum_{i=1}^{4} k_i \, a_{im} \, a_{in} \sin(\delta_{im} - \delta_{in}) \right|}{\sum_{i=1}^{4} k_i \, a_{im} \, a_{in} \left| \sin(\delta_{im} - \delta_{in}) \right|},$$

$$m,n = 1,\ 2,\ 3,\ 4,\ m \neq n, \tag{4.1}$$

$$D'_{mn} = \frac{|S_{mn} - S_{nm}|}{|S_{mn}| + |S_{nm}|}$$

$$m,n = 1,\ 2,\ 3,\ 4,\ m \neq n, \tag{4.2}$$

$$D''_{m} = \frac{\left| \sum_{n=1}^{4} |S_{mn}|^2 - 1 \right|}{\sum_{n=1}^{4} |S_{mn}|^2 + 1},$$

$$m = 1,\ 2,\ 3,\ 4. \tag{4.3}$$

In an exact solution of the four differential equations the right-hand side of these equations should vanish, they can therefore be used to test the accuracy of the numerical integration. As an illustration the numerical values of D_{mn}, D'_{mn} and D''_{m} for the case of 1s-2s-2p eigenstates coupling, $\beta = +1$, $k_1 = 2.0$ and $L = 3$ will be given below

$$D_{12} = 1.4 \times 10^{-3}, \qquad D_{13} = 2.6 \times 10^{-4}, \qquad D_{14} = 1.3 \times 10^{-3}$$

$$D_{23} = 5.1 \times 10^{-4}, \qquad D_{24} = 2.2 \times 10^{-3}, \qquad D_{34} = 1.8 \times 10^{-3}$$

$$D'_{12} = 7.6 \times 10^{-4}, \qquad D'_{13} = 5.1 \times 10^{-3}, \qquad D'_{14} = 5.6 \times 10^{-3}$$

$$D'_{23} = 5.4 \times 10^{-3}, \qquad D'_{24} = 5.7 \times 10^{-3}, \qquad D'_{34} = 1.3 \times 10^{-3}$$

$$D''_{1} = 1.8 \times 10^{-4}, \qquad D''_{2} = 7.6 \times 10^{-5}, \qquad D''_{3} = 2.5 \times 10^{-4}, \qquad D''_{4} = 4.4 \times 10^{-6}.$$

When L is large, particularly at the threshold, the cross sections are small and the values of these cross sections are more sensitive to the errors in the numerical integration. As a result the D values become large. In the tables that follow, except for a few cases, the cross sections that are listed have maximum D values less than 1%. In the exceptional cases by combining different independent sets of solutions and different mesh sizes it has been assured that the cross sections listed are accurate to within a few units in their last significant figures.

The cross sections listed in the tables are obtained by averaging the values of cross sections from two independent sets of solutions of the four differential equations. These independent solutions are obtained by choosing two different values for the determinant (3.11). For small values of k_1 a maximum mesh size of 0.1 in Bohr radius is used while for large values of k_1 this mesh size is 0.05. It is believed that within the framework of the present formalism the cross sections are accurate within one or two units in their last significant figures.

Corresponding to the three channels 1s, 2s and 2p, the cross section matrix is a 3 × 3 matrix. By Eqs. (2.32) and (2.37) the excitation cross sections $2s \rightarrow 1s$, $2p \rightarrow 1s$ and $2p \rightarrow 2s$ can easily be found in terms of the excitation cross sections $1s \rightarrow 2s$, $1s \rightarrow 2p$ and $2s \rightarrow 2p$. The excitation cross section $2s \rightarrow 2p$ is quite large and should be calculated by taking into account the energy difference between the levels $2S_{1/2}$, $2P_{1/2}$ and $2P_{3/2}$. The summation over partial cross sections does not converge for this transition and the method of partial wave is not useful. The Born calculation of this cross section is given by Seaton.[31] In the 5 tables that follow the excitation cross sections 1s - 2s, 1s - 2p, and the elastic scattering cross sections 1s-1s, 2s-2s and 2p-2p are given. The 1s-2s, 1s-2p, and 1s-2s-2p eigenstates coupling approximations correspond respectively to the inclusion of the 1s, 2s; 1s, 2p and 1s, 2s, 2p hydrogen eigenstates in the total wave function. The case $\beta = 0$ corresponds to the neglect of the exchange terms in the 1s-2s-2p eigenstates coupling.

To find the contribution of the higher partial waves whose cross sections are difficult to calculate by the method of eigenstate expansion, we use the regular partial wave Born approximation. Although the partial wave Born approximation as defined by Seaton,[23] in which the continuity of current is satisfied, agrees better with eigenstate expansion calculation for particular elements of the cross section matrix, this is not true in general. As a result, for the sake of consistency, we calculated the contribution of higher partial waves through regular Born approximation.

The cross sections corresponding to the 5 tables are plotted in the 5 figures.

V. DISCUSSION

(i) The results of numerical integration using noniterative method agrees with the iterative numerical integration of Burke, Smith and Schey,[7,32] although the two results are different sometimes by as much as 10%. The difference between the two methods is large when the cross section is small.

(ii) 1s-2s excitation cross section. As is seen from Fig. 1, the 1s-2s and the 1s-2s-2p eigenstates calculations are in good agreement with the experimental results of Lichten and Schultz[1] although the calculations do not give the sharp peak in the cross section at the threshold as is observed experimentally. The shape of the exchange neglected 1s-2s-2p eigenstates calculation curve is in excellent agreement with the shape of the experimental curve. The two curves coincide beyond 25 ev. We notice that the Born approximation agrees with the eigenstate expansion calculations for values of bombarding energies close to the threshold. The normalization of the experimental results in reference (1) to the Born approximation at 45 ev appears therefore to be justified.

(iii) 1s-2p excitation cross section. The experimental curve[3] agrees in shape with the calculated curves but it is lower than all of them (cf. Fig. 2). It should be noted that the inclusion of the 2s state in the 1s - 2p excitation cross section calculation increases this cross section.

Since the experimental curve of Stebbings et al. in Fig. 1 is normalized according to the experimental curve in Fig. 2, if in a new measurement of the 1s-2p transition cross section higher values for the cross section is found, the two experimental curves in Fig. 1 will be brought into better agreement.

(iv) 2s-2s elastic cross section. The cross section at the threshold is large. A Ramsauer effect is evident in the L = 0 case (cf. Table IV).

(v) 2p-2p elastic cross section. The cross section at the threshold is considerably larger than 2s-2s elastic cross section. The Born approximation agrees with the eigenstate expansion calculations at higher energies. This cross section is not calculated in reference 32.

(vi) Although we have neglected the spin orbit interaction we have investigated the role that spin plays in electron atom collision. Assuming that electrons are identical but spinless particles, the total wave function should be symmetric with respect to the coordinate interchange of the two electrons. The curves 1s-2s-2p symmetric in the 5 figures correspond to such a wave function. The disagreement between theory and experiment is an indication of the important role the antisymmetry property of the total electron wave function plays in the free bound electron collisions.

(vii) A study of the 5 figures shows that the Born approximation, despite its simplicity, agrees with eigenstate expansion calculations for low and close to the thresholds bombarding electron energies. Of particular interest is the fact, yet unexplained, that the Born approximation underestimates some cross sections and overestimates others.

VI. CONCLUSION

The hydrogen eigenstate expansion of the total wave function of the system of a free electron in collision with a hydrogen atom seems to be the most natural expansion in any partial wave calculation. The formalism can easily be extended to the electron impact atomic hydrogen excitation cross section calculation higher than $n = 2$, and to the electron impact excitation cross section of any hydrogenic atom whose central potential field is given by a potential such as Hartree or Hartree Fock potentials. Where the Born approximation does not give accurate results the eigenstate expansion seems at present to be the most suitable method.

In addition the treatment of the angular momentum as described here is the same for any system of one free and two bound particles with radial interacting forces, and the formalism developed here can be applied to such problems.

We conclude that the Born approximation can be used with more reliability in electron impact atomic excitation cross sections.

Finally, it is believed that the noniterative technique employed here to solve the radial differential equations will find more applications in problems containing exchange integrals.

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APPENDIX I

The Four Differential Equations

$$\left[\frac{d^2}{dr^2} + k_1^2 - \frac{L(L+1)}{r^2} + \frac{2}{r}\right] u(k_1 L, r)$$

$$= 2y_0(1s1s, r)\,u(k_1 L, r) + 2y_0(1s\,2s, r)\,u(k_2 L, r)$$

$$+ 2\left[\frac{L}{3(2L+1)}\right]^{1/2} y_1(1s\,2p, r)\,u(k_2 L-1, r)$$

$$- 2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1(1s\,2p, r)\,u(k_2 L+1, r)$$

$$+ \frac{2\beta}{2L+1}\, rR_{10}(r)\, y_L(1s\,k_1 L, r) + \frac{2\beta}{2L+1}\, rR_{20}(r)\, y_L(1s\,k_2 L, r)$$

$$+ 2\beta\left[\frac{3L}{(2L+1)(2L-1)^2}\right]^{1/2} rR_{21}(r)\, y_{L-1}(1s\,k_2 L-1, r)$$

$$- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{21}(r)\, y_{L+1}(1s\,k_2 L+1, r)$$

$$-\beta\delta(L, 0)(1+k_1^2)(1s|k_1 L)\, rR_{10}(r)$$

$$-\beta\delta(L, 0)(1+k_2^2)(1s|k_2 L)\, rR_{20}(r)$$

$$-\beta\delta(L-1, 0)(1+k_2^2)(1s|k_2 L-1)\, rR_{21}(r). \qquad \text{(A1)}$$

$$
\begin{aligned}
&\left[\frac{d^2}{dr^2} + k_2^2 - \frac{L(L+1)}{r^2} + \frac{2}{r}\right] u(k_2 L, r) \\
&= 2y_0(1s\,2s,\, r)\, u(k_1 L,\, r) + 2y_0(2s\,2s,\, r)\, u(k_2 L,\, r) \\
&+ 2\left[\frac{L}{3(2L+1)}\right]^{1/2} y_1(2s\,2p,\, r)\, u(k_2 L-1,\, r) \\
&- 2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1(2s\,2p,\, r)\, u(k_2 L+1,\, r) \\
&+ \frac{2\beta}{2L+1}\, rR_{10}(r)\, y_L(2s\,k_1 L,\, r) + \frac{2\beta}{2L+1}\, rR_{20}(r)\, y_L(2s\,k_2 L,\, r) \\
&+ 2\beta\left[\frac{3L}{(2L+1)(2L-1)^2}\right]^{1/2} rR_{21}(r)\, y_{L-1}(2s\,k_2 L-1,\, r) \\
&- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{21}(r)\, y_{L+1}(2s\,k_2\, L+1,\, r) \\
&- \beta\delta(L,0)\left(\frac{1}{4} + k_1^2\right)(2s\,|\,k_1 L)\, rR_{10}(r) \\
&- \beta\delta(L,0)\left(\frac{1}{4} + k_2^2\right)(2s\,|\,k_2 L)\, rR_{20}(r) \\
&- \beta\delta(L-1,0)\left(\frac{1}{4} + k_2^2\right)(2s\,|\,k_2 L-1)\, rR_{21}(r)\,.
\end{aligned}
\tag{A2}
$$

$$
\begin{aligned}
&\left[\frac{d^2}{dr^2} + k_2^2 - \frac{(L-1)L}{r^2} + \frac{2}{r}\right] u(k_2 L-1, r) \\
&= 2 \left[\frac{L}{3(2L+1)}\right]^{1/2} y_1(1s\,2p, r)\, u(k_1 L, r) + 2 \left[\frac{L}{3(2L+1)}\right]^{1/2} y_1(2s\,2p, r)\, u(k_2 L, r) \\
&+ 2 \left[y_0(2p\,2p, r) + \frac{L-1}{5(2L+1)}\, y_2(2p\,2p, r)\right] u(k_2 L-1, r) \\
&- \frac{6}{5}\, \frac{\sqrt{L(L+1)}}{2L+1}\, y_2(2p\,2p, r)\, u(k_2 L+1, r) \\
&+ 2\beta \left[\frac{3L}{(2L+1)(2L-1)^2}\right]^{1/2} rR_{10}(r)\, y_{L-1}(2p k_1 L, r) \\
&+ 2\beta \left[\frac{3L}{(2L+1)(2L-1)^2}\right]^{1/2} rR_{20}(r)\, y_{L-1}(2p k_2 L, r) \\
&+ \frac{6\beta}{2L-1}\, rR_{21}(r) \left[\frac{y_L(2p k_2 L-1, r)}{(2L+1)^2} + \frac{L-1}{2L-3}\, y_{L-2}(2p k_2 L-1, r)\right] \\
&- \frac{6\beta\sqrt{L(L+1)}}{(2L+1)^2}\, y_L(2p k_2 L+1, r)\;\; rR_{21}(r) \\
&- \beta\delta(L,1) \left(\frac{1}{4} + k_1^2\right) (2p \mid k_1 L)\; rR_{10}(r) \\
&- \beta\delta(L,1) \left(\frac{1}{4} + k_2^2\right) (2p \mid k_2 L)\; rR_{20}(r) \\
&- \beta\delta(L,2) \left(\frac{1}{4} + k_2^2\right) (2p \mid k_2 L-1)\; rR_{21}(r)\,. \qquad \text{(A3)}
\end{aligned}
$$

$$\left[\frac{d^2}{dr^2} + k_2^{\,2} - \frac{(L+1)(L+2)}{r^2} + \frac{2}{r}\right] u(k_2 L+1,\, r)$$

$$= -2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1(1s\,2p,\, r)\, u(k_1 L,\, r) - 2\left[\frac{L+1}{3(2L+1)}\right]^{1/2} y_1(2s\,2p,\, r)\, u(k_2 L,\, r)$$

$$- \frac{6}{5}\,\frac{\sqrt{L(L+1)}}{2L+1}\, y_2(2p\,2p,\, r)\, u(k_2 L-1,\, r)$$

$$+ 2\left[y_0(2p\,2p,\, r) + \frac{(L+2)\, y_2(2p\,2p,\, r)}{5(2L+1)}\right] u(k_2 L+1,\, r)$$

$$- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{10}(r)\, y_{L+1}(2p\,k_1 L,\, r)$$

$$- 2\beta\left[\frac{3(L+1)}{(2L+1)(2L+3)^2}\right]^{1/2} rR_{20}(r)\, y_{L+1}(2p\,k_2 L,\, r)$$

$$- \frac{6\beta\sqrt{L(L+1)}}{(2L+1)^2}\, rR_{21}(r)\, y_L(2p\,k_2 L-1,\, r)$$

$$+ \frac{6\beta}{2L+3}\, rR_{21}(r)\left[\frac{y_L(2p\,k_2 L+1,\, r)}{(2L+1)^2} + \frac{(L+2)\, y_{L+2}(2p\,k_2 L+1,\, r)}{(2L+5)}\right]$$

$$- \beta\delta(L,0)\left(\frac{1}{4} + k_2^{\,2}\right)(2p \mid k_2 L+1)\, rR_{21}(r)\,. \qquad \textbf{(A4)}$$

APPENDIX II

Elements of the Potential Matrix
Elements of D_{ij}:

$$D_{11} = -\left(1+\frac{1}{r}\right)e^{-2r}\,,\quad D_{22} = -\left(\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{8}\right)e^{-r}$$

$$D_{33} = -\left[\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{24}\right]e^{-r}+\frac{6(L-1)}{2L+1}\left[\frac{1}{r^3}-\left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right]$$

$$D_{44} = -\left[\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{24}\right]e^{-r}+\frac{6(L+2)}{2L+1}\left[\frac{1}{r^3}-\left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right]$$

$$D_{12} = D_{21} = \frac{2\sqrt{2}}{9}\left(r+\frac{2}{3}\right)e^{-\frac{3}{2}r}$$

$$D_{13} = D_{31} = \frac{128\sqrt{2}}{243}\times\left(\frac{L}{2L+1}\right)^{1/2}\left[\frac{1}{r^2}-\left(\frac{1}{r^2}+\frac{3}{2r}+\frac{9}{8}+\frac{27r}{64}\right)e^{-\frac{3r}{2}}\right]$$

$$D_{14} = D_{41} = -\frac{128\sqrt{2}}{243}\left(\frac{L+1}{2L+1}\right)^{1/2}\left[\frac{1}{r^2}-\left(\frac{1}{r^2}+\frac{3}{2r}+\frac{9}{8}+\frac{27r}{64}\right)e^{-\frac{3r}{2}}\right]$$

$$D_{23} = D_{32} = -3\left(\frac{L}{2L+1}\right)^{1/2}\left[\frac{1}{r^2}-\left(\frac{1}{r^2}+\frac{1}{r}+\frac{1}{2}+\frac{r}{6}+\frac{r^2}{24}\right)e^{-r}\right]$$

$$D_{24} = D_{42} = 3\left(\frac{L+1}{2L+1}\right)^{1/2}\left[\frac{1}{r^2}-\left(\frac{1}{r^2}+\frac{1}{r}+\frac{1}{2}+\frac{r}{6}+\frac{r^2}{24}\right)e^{-r}\right]$$

$$D_{34} = D_{43} = -18\left[\frac{L(L+1)}{(2L+1)^2}\right]^{1/2}\left[\frac{1}{r^3}-\left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right]$$

Elements of F_{ij}:

$$F_{11} = \frac{\beta}{2L+1}\left[\frac{R_{10}}{r^L}\int_0^r R_{10}\,r'^{L+1}\,dr' - R_{10}\,r^{L+1}\int_0^r \frac{R_{10}}{r'^L}\,dr'\right]$$

$$F_{22} = \frac{\beta}{2L+1} \left[\frac{R_{20}}{r^L} \int_0^r R_{20} \; r'^{L+1} dr' - R_{20} \; r^{L+1} \int_0^r \frac{R_{20}}{r'^L} dr'\right]$$

$$F_{33} = \frac{3\beta}{2L-1} \left[\frac{1}{(2L+1)^2} \left(\frac{R_{21}}{r^L} \int_0^r R_{21} \; r'^{L+1} dr' - R_{21} \; r^{L+1} \int_0^r \frac{R_{21}}{r'^L} dr'\right)\right.$$

$$\left. + \frac{L-1}{2L-3} \left(\frac{R_{21}}{r^{L-2}} \int_0^r R_{21} \; r'^{L-1} dr' - R_{21} \; r^{L-1} \int_0^r \frac{R_{21}}{r'^{L-2}} dr'\right)\right]$$

$$F_{44} = \frac{3\beta}{2L+3} \left[\frac{1}{(2L+1)^2} \left(\frac{R_{21}}{r^L} \int_0^r R_{21} \; r'^{L+1} dr' - R_{21} \; r^{L+1} \int_0^r \frac{R_{21}}{r'^L} dr'\right)\right.$$

$$\left. + \frac{L+2}{2L+5} \left(\frac{R_{21}}{r^{L+2}} \int_0^r R_{21} \; r'^{L+3} dr' - R_{21} \; r^{L+3} \int_0^r \frac{R_{21}}{r'^{L+2}} dr'\right)\right]$$

$$F_{12} = \frac{\beta}{2L+1} \left[\frac{R_{20}}{r^L} \int_0^r R_{10} \; r'^{L+1} dr' - R_{20} \; r^{L+1} \int_0^r \frac{R_{10}}{r'^L} dr'\right]$$

$$F_{21} = F_{12} \; \left[R_{10} \rightleftharpoons R_{20}\right]$$

$$F_{13} = \sqrt{3}\beta \left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L-1}} \int_0^r R_{10} \; r'^L dr - R_{21} \; r^L \int_0^r \frac{R_{10}}{r'^{L-1}} dr'\right]$$

$$F_{31} = F_{13} \; \left[R_{10} \rightleftharpoons R_{21}\right]$$

$$F_{14} = -\sqrt{3}\,\beta \left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L+1}} \int_0^r R_{10} \; r'^{L+2} dr' - R_{21} \; r^{L+2} \int_0^r \frac{R_{10}}{r'^{L+1}} dr'\right]$$

$$F_{41} = F_{14} \; [R_{10} \rightleftharpoons R_{21}]$$

$$F_{23} = \sqrt{3}\,\beta \left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L-1}} \int_0^r R_{20} \; r'^{L} dr' - R_{21} \; r^{L} \int_0^r \frac{R_{20}}{r'^{L-1}} \, dr'\right]$$

$$F_{32} = F_{23} \; [R_{20} \rightleftharpoons R_{21}]$$

$$F_{24} = -\sqrt{3}\,\beta\left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L+1}} \int_0^r R_{20} \; r'^{L+2} dr' - R_{21} \, r^{L+2} \int_0^r \frac{R_{20}}{r'^{L+1}} \, dr'\right]$$

$$F_{42} = F_{24} \; [R_{20} \rightleftharpoons R_{21}]$$

$$F_{34} = -3\,\beta\left[\frac{L(L+1)}{(2L+1)^4}\right]^{1/2} \times \left[\frac{R_{21}}{r^{L}} \int_0^r R_{21} \, r'^{L+1} \, dr' - R_{21} \; r^{L+1} \int_0^r \frac{R_{21}}{r'^{L}} \, dr'\right]$$

$$F_{34} = F_{43}$$

Elements of g_{ij} and h_{ij} :

$$g_{11} = \frac{\beta R_{10} \; r^{L+1}}{2L+1}, \quad h_{11} = R_{10} \left[\frac{1}{r^{L}} - \frac{1 + k_1{}^2}{2} \delta\,(L,\,0)\,r\right]$$

$$g_{22} = \frac{\beta R_{20} \, r^{L+1}}{2L+1}, \quad h_{22} = R_{20} \left[\frac{1}{r^{L}} - \frac{\frac{1}{4} + k_2{}^2}{2} \delta\,(L, 0)\, r\right]$$

$$g^1_{33} = \frac{3\beta R_{21}\, r^{L+1}}{(2L-1)(2L+1)^2}\ , \quad h^1_{33} = \frac{R_{21}}{r^L}$$

$$g^2_{33} = \frac{3\beta (L-1) R_{21}\, r^{L-1}}{(2L-1)(2L-3)}\, , \quad h^2_{33} = R_{21}\left[\frac{1}{r^{L-2}} - \frac{\frac{1}{4}+k_2^2}{2}\,\delta(L,2)\, r\right]$$

$$g^1_{44} = \frac{3\beta R_{21}\, r^{L+1}}{(2L+3)(2L+1)^2}\ , \quad h^1_{44} = R_{21}\left[\frac{1}{r^L} - \frac{\frac{1}{4}+k_2^2}{2}\,\delta(L,0)\, r\right]$$

$$g^2_{44} = \frac{3\beta (L+2) R_{21}\, r^{L+3}}{(2L+3)(2L+5)}\, , \quad h^2_{44} = \frac{R_{21}}{r^{L+2}}$$

$$g_{12} = \frac{\beta}{2L+1}\, R_{20}\, r^{L+1}, \quad h_{12} = R_{10}\left[\frac{1}{r^L} - \frac{1+k_2^2}{2}\,\delta(L,0)\, r\right]$$

$$g_{21} = g_{12}\left[R_{20} \rightarrow R_{10}\right], \qquad h_{21} = k_{12}\left[R_{10} \rightarrow R_{20}\right]$$

$$g_{13} = \sqrt{3}\,\beta\left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} R_{21}\, r^L, \quad h_{13} = R_{10}\left[\frac{1}{r^{L-1}} - \frac{1+k_2^2}{2}\,\delta(L,1)\, r\right]$$

$$g_{31} = g_{13}\left[R_{21} \rightarrow R_{10}\right]\ , \quad h_{31} = h_{13}\left[R_{10} \rightarrow R_{21}\right]$$

$$g_{14} = -\sqrt{3}\,\beta\left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} R_{21}\, r^{L+2}\ , \quad h_{14} = \frac{R_{10}}{r^{L+1}}$$

$$g_{41} = g_{14}\left[R_{21} \rightarrow R_{10}\right]\ , \qquad h_{41} = h_{14}\left[R_{10} \rightarrow R_{21}\right]$$

$$g_{23} = \sqrt{3}\beta\left[\frac{L}{(2L+1)(2L-1)^2}\right]^{1/2} R_{21}\, r^L , \quad h_{23} = R_{20}\left[\frac{1}{r^{L-1}} - \frac{\frac{1}{4}+k_2^2}{2}\,\delta(L,1)\, r\right]$$

$$g_{32} = g_{23}\,[R_{21}\rightarrow R_{20}] \;. \qquad h_{32} = h_{23}\,[R_{20}\rightarrow R_{21}]$$

$$g_{24} = -\sqrt{3}\beta\left[\frac{L+1}{(2L+1)(2L+3)^2}\right]^{1/2} R_{21}\, r^{L+2} , \quad h_{24} = \frac{R_{20}}{r^{L+1}}$$

$$g_{42} = g_{24}\,[R_{21}\rightarrow R_{20}], \qquad h_{42} = h_{24}\,[R_{20}\rightarrow R_{21}]$$

$$g_{34} = -3\beta\left[\frac{L(L+1)}{(2L+1)^4}\right]^{1/2} R_{21}\, r^{L+1} , \quad h_{34} = \frac{R_{21}}{r^L}$$

$$g_{43} = g_{34}$$

In F_{ij} matrix the interchange of the functions R_{10}, R_{20} and R_{21} accompanies the interchange of their arguments too.

APPENDIX III

Singularity of the Determinant of Eq. (3.6) for L = 0 and 1

(1) L = 0 Case. By making use of the definition of D_{ij} and F_{ij} and Eq. (3.7) the following relationship can be derived from Eq. (3.3)

$$\int_0^\infty \left[rR_{20}\left(\frac{d^2}{dr^2} + k_1^2\right) v_1 - \beta r R_{10}\left(\frac{d^2}{dr^2} + k_2^2\right) v_2 \right] dr$$

$$= -\frac{2}{\sqrt{3}}\left[a_{13}\, B_{24} - \beta\, a_{23}\, B_{14}\right], \tag{A5}$$

where

$$a_{13} = \int_0^\infty R_{10}\, R_{21}\, r^3 dr = \left[2^{15} \times 3^{-9}\right]^{1/2}$$

$$a_{23} = \int_0^\infty R_{20}\, R_{21}\, r^3 dr = -\, 3\sqrt{3}$$

Integrating the left-hand side of Eq. (A5) by parts, and making use of Eqs. (2. 11) and (3. 7) we obtain

$$\int_0^\infty \left[r R_{20}\left(\frac{d^2}{dr^2} + k_1^2\right) v_1 - \beta r R_{10}\left(\frac{d^2}{dr^2} + k_2^2\right) v_2 \right] dr$$

$$= -\, 2\left[B_{21} - \beta\, B_{12}\right]. \tag{A6}$$

We conclude

$$B_{21} - \beta\, B_{12} = \frac{1}{\sqrt{3}}\left[a_{13}\, B_{24} - \beta\, a_{23}\, B_{14}\right]. \tag{A7}$$

Therefore all the elements on the right-hand side of Eqs. (3.6) are not independent. In order that these equations be consistent one of them should be a linear combination of others. By making use of the first of Eqs. (3.7) it can be shown directly that equations similar to Eq. (A7) hold among the elements of each row of the determinant of Eqs. (3.6).

(11) L = 1 Case. Similar to the previous case the following relationship can be derived from Eqs. (3.3)

$$\int_0^\infty \left[r R_{21} \left(\frac{d^2}{dr^2} + k_1^2 - \frac{2}{r^2} \right) v_1 - \beta r R_{10} \left(\frac{d^2}{dr^2} + k_2^2 \right) v_3 \right] dr$$

$$= -\frac{2}{3} \left[\beta a_{13} B_{11} + \beta a_{23} B_{12} - a_{13} B_{33}^1 + \sqrt{2} \left(a_{13} B_{34} - \frac{3}{5} \beta a_{33} B_{14} \right) \right] \quad \text{(A8)}$$

where

$$a_{33} = \int_0^\infty R_{21}^2 \; r^4 \, dr = 30$$

Integrating the left-hand side of Eq. (A8) by parts, and making use of Eqs. (2.11) and (3.7) we obtain

$$\int_0^\infty \left[r R_{21} \left(\frac{d^2}{dr^2} + k_1^2 - \frac{2}{r^2} \right) v_1 - \beta r R_{10} \left(\frac{d^2}{dr^2} + k_2^2 \right) v_3 \right] dr$$

$$= - 2 \left[B_{31} - \beta B_{13} \right] . \quad \text{(A9)}$$

Combining Eqs. (A8) and (A9) we get

$$B_{31} - \beta B_{13} = \frac{1}{3}\left[\beta a_{13} B_{11} + \beta a_{23} B_{12} - a_{13} B^1_{33} + \sqrt{2}\left(a_{13} B_{34} - \frac{3}{5}\beta a_{33} B_{14}\right)\right] \quad \text{(A10)}$$

Finally, Eqs. (3.3) give the following relationship

$$\int_0^\infty \left[r R_{21}\left(\frac{d^2}{dr^2} + k_2^2 - \frac{2}{r^2}\right) v_2 - \beta r R_{20}\left(\frac{d^2}{dr^2} + k_2^2\right) v_3\right] dr$$

$$= -\frac{2}{3}\left[\beta a_{23} B_{22} + \beta a_{13} B_{21} - a_{23} B^1_{33} + \sqrt{2}\left(a_{23} B_{34} - \frac{3}{5}\beta a_{33} B_{24}\right)\right] \quad \text{(A11)}$$

Integration by parts of the left-hand side as before gives

$$\int_0^\infty \left[r R_{21}\left(\frac{d^2}{dr^2} + k_2^2 - \frac{2}{r^2}\right) v_2 - \beta r R_{20}\left(\frac{d^2}{dr^2} + k_2^2\right) v_3\right] dr$$

$$= -2\left[B_{32} - \beta B_{23}\right] , \quad \text{(A12)}$$

whereupon we get

$$B_{32} - \beta B_{23} = \frac{1}{3}\left[\beta a_{23} B_{22} + \beta a_{13} B_{21} - a_{23} B^1_{33} + \sqrt{2}\left(a_{23} B_{34} - \frac{3}{5}\beta a_{33} B_{24}\right)\right] \quad \text{(A13)}$$

To remove the singularity in L = 0 case one of the C^{ν}_{kl} is chosen arbitrary, and a degenerate equation is removed from Eqs. (3.6). Similarly in L = 1 case two of the C^{ν}_{kl} are chosen arbitrary and two degenerate equations are removed from Eqs. (3.6).

APPENDIX IV

Elements of the Matrix of the Sum of the Asymptotic Coulomb and Centrifugal Potentials

$U_{11} = L(L+1)\, r^{-2}$, $\quad U_{22} = L(L+1)\, r^{-2}$

$U_{33} = (L-1)\, L\, r^{-2} + 12(L-1)\,(2L+1)^{-1} r^{-3}$, $U_{44} = (L+1)\,(L+2)\, r^{-2} + 12(L+2)\,(2L+1)^{-1} r^{-3}$

$U_{12} = U_{21} = 0$, $\quad U_{13} = U_{31} = \left[256\sqrt{2}/243\right] \left[L/(2L+1)\right]^{\frac{1}{2}} r^{-2}$

$U_{14} = U_{41} = -\left[256\sqrt{2}/243\right] \left[(L+1)/(2L+1)\right]^{\frac{1}{2}} r^{-2}$, $U_{23} = U_{32} = -6\left[L/(2L+1)\right]^{\frac{1}{2}} r^{-2}$

$U_{24} = U_{42} = 6\, \left[(L+1)/(2L+1)\right]^{\frac{1}{2}} r^{-2}$, $\quad U_{34} = U_{43} = -36\, [L(L+1)]^{1/2}\, (2L+1)^{-1}\, r^{-3}$

TABLES OF CROSS SECTIONS

In the following five tables the partial and the total cross sections for the processes 1s-2s, 1s-2p, 1s-1s, 2s-2s and 2p-2p in different approximations are listed. Each partial cross section corresponds to a given total orbital angular momentum L which appears at the head of each column. $\sum_S$ is the sum of the singlet and $\sum_T$ is the sum of the triplet partial cross sections within certain approximation and for a given electron energy. Q_T is the total cross section, and in the case of the eigenstates coupling, Born approximation is used to add the contribution of the partial waves beyond the maximum L which has been computed within the given eigenstates coupling approximation. This contribution can easily be obtained by using the given table of the Born approximation of the partial and the total cross sections. k_1 is the wave number of the electron beam incident on the ground state of the atom and k_2 is the wave number of the same beam when atom is in its first excited state. The energy of the beam is given in electron volt through

$$E = 13.6\, k^2,$$

where k can be k_1 or k_2. In Table V, l_1 and l_2 are the quantum numbers of the orbital angular momenta of the bound and the free electrons respectively.

TABLE I. 1s-2s Excitation Cross Sections

A. Born Approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.16376	0.00981	0.00021	0.00000	0.00000	0.00000	0.00000	0.00000	0.17378	0.17379
1.0	0.19578	0.04795	0.00428	0.00026	0.00000	0.00000	0.00000	0.00000	0.24827	0.24827
1.1	0.16272	0.07073	0.01141	0.00125	0.00011	0.00001	0.00000	0.00000	0.24622	0.24623
1.2	0.12704	0.07896	0.01858	0.00299	0.00039	0.00004	0.00000	0.00000	0.22800	0.22800
1.5	0.05872	0.06606	0.02979	0.00939	0.00242	0.00053	0.00010	0.00002	0.16703	0.16706
2.0	0.01946	0.03363	0.02521	0.01365	0.00614	0.00236	0.00081	0.00025	0.10151	0.10187
3.0	0.00388	0.00909	0.01019	0.00866	0.00628	0.00394	0.00226	0.00116	0.04546	0.04758
4.0	0.00123	0.00320	0.00420	0.00431	0.00385	0.00301	0.00216	0.00141	0.02337	0.02720

B. Exchange Neglected 1s-2s-2p Eigenstates Coupling Approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.2202	0.0749	0.3535						0.6486	0.6486
1.0	0.1685	0.1427	0.1598	0.0517					0.5227	0.5227
1.1	0.0951	0.1142	0.0298	0.0616	0.0231				0.3238	0.3238
1.2	0.0594	0.1137	0.0032	0.0360	0.0244	0.0135			0.2502	0.2502
1.5	0.0249	0.0861	0.0201	0.0068	0.0112	0.0118	0.0074		0.1683	0.1683
2.0	0.0101	0.0373	0.0255	0.0107	0.0046	0.0034	0.0033		0.0949	0.0953

C. 1s-2s Eigenstates Coupling Approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.9	0.0375	0.0017	0.0000	0.0000	0.0000	0.0000	0.0000		0.0392
1.0	0.0725	0.0583	0.0002	0.0000	0.0000	0.0000	0.0000		0.1310
1.1	0.0701	0.0525	0.0023	0.0000	0.0000	0.0000	0.0000		0.1249
1.2	0.0547	0.0534	0.0054	0.0002	0.0000	0.0000	0.0000		0.1137
1.5	0.0241	0.0384	0.0110	0.0022	0.0004	0.0001	0.0000		0.0762
2.0	0.0072	0.0157	0.0093	0.0041	0.0015	0.0005	0.0002		0.0385

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0004	0.1686	0.0060	0.0000	0.0000	0.0000	0.0000		0.1750	0.2142	0.2142
1.0	0.0021	0.1528	0.0446	0.0021	0.0001	0.0000	0.0000		0.2017	0.3327	0.3327
1.1	0.0044	0.1052	0.0568	0.0068	0.0005	0.0000	0.0000		0.1737	0.2987	0.2987
1.2	0.0061	0.0737	0.0576	0.0114	0.0015	0.0002	0.0000		0.1505	0.2642	0.2642
1.5	0.0073	0.0355	0.0406	0.0174	0.0050	0.0012	0.0002		0.1072	0.1833	0.1833
2.0	0.0049	0.0162	0.0205	0.0143	0.0074	0.0032	0.0012		0.0677	0.1062	0.1068

D. 1s-2s-2p Eigenstates Coupling Approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.9	0.0523	0.0048	0.0620						0.1191
1.0	0.0768	0.0147	0.0833	0.0092					0.1840
1.1	0.0585	0.0245	0.0647	0.0236	0.0055				0.1768
1.2	0.0382	0.0251	0.0246	0.0252	0.0081	0.0028			0.1240
1.5	0.0123	0.0308	0.0015	0.0041	0.0051	0.0034	0.0023	0.0026	0.0621
2.0	0.0049	0.0152	0.0068	0.0021	0.0010	0.0010	0.0011	0.0008	0.0329
3.0	0.0010	0.0031	0.0031	0.0023	0.0015	0.0009	0.0005	0.0006	0.0130
4.0	0.0003	0.0010	0.0012	0.0012	0.0010	0.0008			0.0055

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0013	0.0748	0.0019						0.0780	0.1971	0.1971
1.0	0.0040	0.1224	0.0195	0.0214					0.1673	0.3513	0.3513
1.1	0.0050	0.1013	0.0326	0.0077	0.0131				0.1597	0.3366	0.3366
1.2	0.0055	0.0724	0.0359	0.0036	0.0105	0.0076			0.1355	0.2596	0.2596
1.5	0.0045	0.0333	0.0309	0.0072	0.0046	0.0054	0.0049	0.0043	0.0951	0.1573	0.1573
2.0	0.0031	0.0155	0.0176	0.0101	0.0044	0.0025	0.0023	0.0019	0.0574	0.0903	0.0907
3.0	0.0013	0.0048	0.0065	0.0059	0.0044	0.0029	0.0018	0.0012	0.0288	0.0418	0.0439
4.0	0.0006	0.0019	0.0028	0.0030	0.0027	0.0022			0.0132	0.0187	0.0261

TABLE II. 1s-2p Excitation Cross Sections

A. Born Approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.00107	0.46700	0.09607	0.01025	0.00087	0.00007	0.00001	0.00000	0.56534	0.57535
1.0	0.00499	0.48867	0.35645	0.13467	0.03964	0.01032	0.00254	0.00059	1.03787	1.03851
1.1	0.00702	0.36207	0.41698	0.24992	0.11533	0.04649	0.01753	0.00624	1.22158	1.22859
1.2	0.00747	0.25540	0.38137	0.29903	0.17908	0.09269	0.04453	0.02004	1.27961	1.30741
1.5	0.00550	0.09184	0.19986	0.23775	0.21386	0.16292	0.11291	0.07232	1.09696	1.28101
2.0	0.00234	0.02222	0.05938	0.09386	0.11287	0.11376	0.10248	0.08374	0.59065	1.04055
3.0	0.00048	0.00285	0.00806	0.01537	0.02309	0.02920	0.03271	0.03273	0.14449	0.66256
4.0	0.00013	0.00066	0.00179	0.00359	0.00586	0.00816	0.01009	0.01114	0.04142	0.45252

B. Exchange Neglected 1s-2s-2p Eigenstates Coupling Approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	0.1600	0.3985	0.6497						1.2082	1.2194
1.0	0.1007	0.2917	0.8190	0.2190	0.0476	0.0224			1.5004	1.5041
1.1	0.0980	0.2008	0.6201	0.3696	0.1380	0.0586	0.0166		1.5017	1.5150
1.2	0.0822	0.1251	0.4481	0.3922	0.2044	0.1014	0.0403		1.3937	1.4416
1.5	0.0372	0.0334	0.1671	0.2568	0.2295	0.1706	0.1136		1.0082	1.2645
2.0	0.0105	0.0068	0.0394	0.0837	0.1089	0.1165	0.1042		0.4700	1.0036

C. 1s-2p Eigenstates Coupling Approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.9	0.0044	0.1216	0.1422						0.2682
1.0	0.0168	0.0655	0.3011	0.0206	0.0057	0.0059			0.4156
1.1	0.0299	0.0366	0.3948	0.0851	0.0260	0.0099	0.0060		0.5883
1.2	0.0296	0.0169	0.3088	0.1421	0.0517	0.0236	0.0103		0.5830
1.5	0.0059	0.0037	0.0821	0.0989	0.0718	0.0458	0.0304		0.3386
2.0	0.0010	0.0006	0.0131	0.0271	0.0327	0.0335	0.0296		0.1376

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0002	0.2066	0.0005						0.2073	0.4755	0.4867
1.0	0.0016	0.1078	0.0020	0.1651	0.0363	0.0187			0.3315	0.7471	0.7508
1.1	0.0037	0.0540	0.0060	0.1599	0.1002	0.0365	0.0217		0.3820	0.9703	0.9836
1.2	0.0055	0.0249	0.0098	0.1446	0.1336	0.0695	0.0341		0.4220	1.0050	1.0529
1.5	0.0059	0.0027	0.0133	0.0868	0.1231	0.1100	0.0849		0.4267	0.7652	1.0215
2.0	0.0028	0.0002	0.0073	0.0311	0.0559	0.0700	0.0772		0.2445	0.3820	0.9156

D. 1s-2s-2p Eigenstates Coupling Approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.9	0.0390	0.0745	0.1027						0.2162
1.0	0.0360	0.1123	0.2575	0.0317					0.4375
1.1	0.0358	0.1094	0.3405	0.0886	0.0308	0.0113	0.0075		0.6239
1.2	0.0345	0.0806	0.2912	0.1278	0.0506	0.0237	0.0105		0.6189
1.5	0.0172	0.0175	0.0953	0.1003	0.0693	0.0440	0.0290	0.0238	0.3964
2.0	0.0036	0.0023	0.0170	0.0303	0.0344	0.0333	0.0293	0.0229	0.1731
3.0	0.0004	0.0002	0.0015	0.0037	0.0060	0.0078	0.0094	0.0106	0.0396
4.0	0.0001	0.0001	0.0003	0.0008	0.0014	0.0020			0.0047

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	0.0007	0.0682	0.0112						0.0801	0.2963	0.3075
1.0	0.0033	0.0801	0.0500	0.1730					0.3064	0.7439	0.7976
1.1	0.0070	0.0626	0.0567	0.1841	0.1082	0.0404	0.0209		0.4799	1.1039	1.1172
1.2	0.0096	0.0418	0.0537	0.1761	0.1409	0.0729	0.0332		0.5282	1.1471	1.1950
1.5	0.0107	0.0131	0.0351	0.1081	0.1343	0.1157	0.0842	0.0596	0.5608	0.9570	1.1410
2.0	0.0053	0.0038	0.0143	0.0393	0.0625	0.0731	0.0738	0.0642	0.3363	0.5094	0.9593
3.0	0.0010	0.0006	0.0025	0.0066	0.0122	0.0175	0.0220	0.0246	0.0870	0.1266	0.6095
4.0	0.0002	0.0002	0.0006	0.0016	0.0031	0.0048			0.0105	0.0152	0.4475

TABLE III. 1s-1s Elastic Cross Sections

A. Born Approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	1.65113	0.09722	0.00379	0.00013	0.00000	0.00000	0.00000	0.00000	1.75227	1.75233
1.0	1.42354	0.11192	0.00587	0.00027	0.00001	0.00000	0.00000	0.00000	1.54161	1.54167
1.1	1.22728	0.12348	0.00835	0.00049	0.00003	0.00000	0.00000	0.00000	1.35963	1.35968
1.2	1.05936	0.13181	0.01109	0.00082	0.00006	0.00000	0.00000	0.00000	1.20314	1.20318
1.5	0.69140	0.14017	0.01955	0.00241	0.00028	0.00003	0.00000	0.00000	0.85384	0.85389
2.0	0.36283	0.12285	0.02924	0.00621	0.00124	0.00023	0.00004	0.00001	0.52265	0.52267
3.0	0.12662	0.07286	0.03013	0.01131	0.00402	0.00133	0.00042	0.00012	0.24681	0.24700
4.0	0.05565	0.04195	0.02291	0.01145	0.00546	0.00243	0.00104	0.00042	0.14131	0.14194

B. Exchange Neglected 1s-2s-2p Eigenstates Coupling Approximation

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.9	2.632	0.3300	0.1916	0.0157					3.169	3.169
1.0	2.091	0.2518	0.0890	0.0309	0.0078	0.0028			2.473	2.473
1.1	1.694	0.2302	0.0483	0.0299	0.0105	0.0038	0.0016		2.018	2.018
1.2	1.390	0.2228	0.0346	0.0248	0.0113	0.0045	0.0019		1.690	1.690
1.5	0.8181	0.2032	0.0310	0.0135	0.0091	0.0048	0.0027		1.082	1.082
2.0	0.4053	0.1742	0.0494	0.0181	0.0108	0.0036	0.0027		0.6641	0.6641

C. 1s-2s Eigenstates Coupling Approximation

Singlet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.9	0.4324	0.0382	0.0015	0.0000	0.0000	0.0000	0.0000		0.4721
1.0	0.2824	0.0338	0.0014	0.0001	0.0000	0.0000	0.0000		0.3177
1.1	0.1865	0.0199	0.0011	0.0001	0.0000	0.0000	0.0000		0.2076
1.2	0.1397	0.0111	0.0006	0.0001	0.0000	0.0000	0.0000		0.1515
1.5	0.0905	0.0012	0.0001	0.0000	0.0000	0.0000	0.0000		0.0918
2.0	0.0608	0.0083	0.0016	0.0003	0.0001	0.0000	0.0000		0.0711

Triplet

k_1	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.9	3.684	1.394	0.0477	0.0016	0.0001	0.0000	0.0000		5.127	5.599	5.599
1.0	2.903	1.162	0.0579	0.0023	0.0001	0.0000	0.0001		4.125	4.443	4.443
1.1	2.297	0.9654	0.0651	0.0036	0.0002	0.0000	0.0000		3.331	3.539	3.539
1.2	1.829	0.8085	0.0696	0.0050	0.0004	0.0000	0.0000		2.713	2.864	2.864
1.5	0.9716	0.4857	0.0727	0.0092	0.0011	0.0001	0.0000		1.5404	1.632	1.632
2.0	0.4042	0.2366	0.0627	0.0142	0.0031	0.0006	0.0001		0.7215	0.7926	0.7926

TABLE III. Continued

k_1	D. 1s-2p Eigenstates Coupling Approximation										
	Singlet										
	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S		
0.9	0.4230	0.0186	0.0442	0.0043					0.4901		
1.0	0.2984	0.0167	0.0635	0.0073	0.0017	0.0006	0.0005		0.3887		
1.1	0.2148	0.0108	0.0578	0.0104	0.0026	0.0008	0.0003		0.2975		
1.2	0.1569	0.0048	0.0338	0.0105	0.0030	0.0011	0.0005		0.2106		
1.5	0.1040	0.0008	0.0035	0.0038	0.0025	0.0012	0.0007		0.1165		
2.0	0.0698	0.0138	0.0030	0.0018	0.0018	0.0008	0.0006		0.0916		
	Triplet									$\Sigma_S + \Sigma_T$	Q_T
	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T		
0.9	3.689	1.421	0.0682	0.0136					5.192	5.682	5.682
1.0	2.914	1.236	0.0758	0.0152	0.0054	0.0019	0.0015		4.250	4.638	4.638
1.1	2.309	1.036	0.0814	0.0142	0.0066	0.0025	0.0011		3.451	3.749	3.749
1.2	1.840	0.8702	0.0850	0.0139	0.0069	0.0031	0.0015		2.821	3.031	3.031
1.5	0.9806	0.5249	0.0863	0.0152	0.0063	0.0031	0.0019		1.618	1.735	1.735
2.0	0.4184	0.2702	0.0828	0.0256	0.0111	0.0030	0.0019		0.8130	0.9045	0.9045
	E. 1s-2s-2p Eigenstates Coupling Approximation										
	Singlet										
	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S		
0.9	0.4503	0.0133	0.0457	0.0058	0.0000				0.5151		
1.0	0.2649	0.0100	0.0660	0.0076	0.0019	0.0007	0.0007		0.3518		
1.1	0.1736	0.0131	0.0582	0.0104	0.0028	0.0009	0.0004		0.2594		
1.2	0.1283	0.0102	0.0351	0.0104	0.0030	0.0012	0.0005		0.1887		
1.5	0.0854	0.0021	0.0049	0.0042	0.0025	0.0012	0.0007	0.0010	0.1020		
2.0	0.0591	0.0093	0.0016	0.0009	0.0007	0.0006	0.0004	0.0002	0.0728		
3.0	0.0266	0.0138	0.0052	0.0019	0.0008	0.0003	0.0002	0.0005	0.0493		
4.0	0.0133	0.0106	0.0061	0.0034	0.0020	0.0012			0.0366		
	Triplet									$\Sigma_S + \Sigma_T$	Q_T
	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T		
0.9	3.687	1.726	0.0875	0.0166	0.0055				5.523	6.037	6.037
1.0	2.908	1.372	0.0938	0.0174	0.0062	0.0021	0.0016		4.401	4.753	4.753
1.1	2.299	1.090	0.0949	0.0166	0.0075	0.0028	0.0012		3.512	3.772	3.772
1.2	1.828	0.8884	0.0956	0.0162	0.0076	0.0033	0.0015		2.841	3.029	3.029
1.5	0.9697	0.5228	0.0911	0.0166	0.0069	0.0033	0.0021	0.0020	1.615	1.716	1.716
2.0	0.4006	0.2433	0.0657	0.0154	0.0044	0.0020	0.0011	0.0008	0.7333	0.8061	0.8061
3.0	0.1127	0.0854	0.0388	0.0156	0.0062	0.0022	0.0009	0.0007	0.2625	0.3118	0.3120
4.0	0.0475	0.0444	0.0276	0.0160	0.0093	0.0053			0.1501	0.1867	0.1888

TABLE IV. 2s-2s Elastic Cross Sections

A. Born Approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.24	389.97	15.910	0.27680	0.00319	0.00003	0.00000	0.00000	0.00000	406.16	406.17
0.50	105.52	32.129	5.0152	0.55306	0.04846	0.00347	0.00022	0.00001	143.269	143.276
0.68	47.381	24.746	7.4981	1.7023	0.31602	0.04869	0.00658	0.00078	81.700	81.703
0.83	26.562	17.895	7.5601	2.5080	0.69820	0.16365	0.03393	0.00621	55.427	55.440
1.23	8.2461	7.6846	4.9702	2.7483	1.3500	0.57745	0.22452	0.07803	25.879	25.990
1.80	2.4331	2.7773	2.2763	1.6805	1.1541	0.71994	0.41776	0.22120	11.680	12.105
2.87	0.5245	0.71381	0.68903	0.61123	0.51876	0.41048	0.31076	0.21860	4.0011	4.8280
3.91	0.18794	0.27611	0.28658	0.27339	0.25098	0.21580	0.17946	0.14029	1.8106	2.7417

B. Exchange Neglected 1s-2s-2p Eigenstates Coupling Approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ	Q_T
0.24	32.02	8.489	42.26						82.77	82.78
0.50	2.041	7.710	23.35	9.004	9.368	7.702	5.870		65.045	65.052
0.68	2.255	8.247	15.16	5.547	4.373	3.755	2.975		42.312	42.316
0.83	1.861	8.206	10.67	4.637	2.792	2.223	1.818		32.207	32.226
1.23	1.716	4.987	5.030	3.321	1.797	1.058	0.7179		18.537	18.726
1.80	1.020	2.134	2.150	1.750	1.275	0.8320	0.5457		9.707	10.352

C. 1s-2s Eigenstates Coupling Approximation

Singlet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.24	0.3303	8.196	0.2628	0.0028					8.792
0.50	1.532	10.38	0.0275	0.0048	0.0008	0.0002	0.0249		11.97
0.68	1.115	5.536	1.502	0.1150	0.0087	0.0010	0.0017		8.279
0.83	0.8980	3.512	1.997	0.4303	0.0747	0.0129	0.0032		6.928
1.23	0.5702	1.413	1.236	0.7010	0.3129	0.1228	0.0450		4.401
1.80	0.2825	0.5370	0.5285	0.4193	0.2931	0.1863	0.1110		2.358

Triplet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.24	45.94	118.8	7.713	0.0540					172.51	181.30	181.31
0.50	0.2102	34.44	21.05	2.776	0.2521	0.0316	0.0994		58.86	70.83	70.84
0.68	1.366	18.13	12.74	4.059	0.8282	0.1463	0.0442		37.31	45.60	45.60
0.83	2.112	11.65	8.725	3.887	1.230	0.3225	0.0850		28.01	34.94	34.96
1.23	1.811	4.691	4.008	2.585	1.399	0.6637	0.2862		15.44	19.84	20.03
1.80	0.8989	1.735	1.652	1.316	0.9510	0.6359	0.4008		7.590	9.947	10.592

D. 1s-2s-2p Eigenstates Coupling Approximation

Singlet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_S
0.24	7.800	14.79	22.42						45.01
0.50	0.2858	0.6960	3.149	4.447	2.925	2.063	1.491		15.057
0.68	0.0661	1.044	2.455	1.884	1.480	1.098	0.7928		8.820
0.83	0.1675	1.088	2.105	0.9905	0.8282	0.6606	0.5071		6.347
1.23	0.3739	1.075	1.196	0.7196	0.3940	0.2496	0.1827	0.1409	4.332
1.80	0.2416	0.4974	0.5133	0.4133	0.2923	0.1928	0.1247	0.0799	2.3553
2.87	0.0847	0.1489	0.1574	0.1466	0.1280	0.1057	0.0852	0.0658	0.9223
3.91	0.0365	0.0635	0.0702	0.0698	0.0660	0.0599			0.3659

Triplet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_T	$\Sigma_S + \Sigma_T$	Q_T
0.24	16.52[a]	1.236	89.65[a]						107.41	152.42	152.43
0.50	6.172	17.19	30.69	12.90	5.559	5.373	4.257		82.14	97.206	97.213
0.68	2.346	12.88	14.52	7.937	3.046	2.459	2.090		45.28	54.099	54.103
0.83	1.709	9.166	8.976	5.367	2.365	1.514	1.246		30.343	36.686	36.705
1.23	1.391	4.199	3.880	2.681	1.585	0.9110	0.5658	0.4094	15.622	19.955	20.066
1.80	0.7898	1.656	1.603	1.291	0.9466	0.6520	0.4305	0.2786	7.648	10.002	10.427
2.87	0.2622	0.4652	0.4857	0.4479	0.3901	0.3234	0.2623	0.2045	2.8413	3.7636	4.5905
3.91	0.1113	0.1945	0.2146	0.2122	0.2000	0.1812			1.1138	1.4797	2.7306

TABLE V. 2p-2p Elastic Cross Sections

k^2	A. L-ℓ_1 - ℓ_2 Odd, Born Approximation							
	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_0
0.24	26.562	6.1961	2.1260	0.92680	0.44497	0.22694	0.08105	36.56
0.50	14.210	5.2190	2.1768	1.0526	0.55433	0.31476	0.18383	23.71
0.68	8.8346	4.0761	1.9476	1.0100	0.54983	0.31728	0.18718	16.923
0.83	6.0065	3.2062	1.6993	0.94122	0.53204	0.31331	0.18680	12.8854
1.23	2.5053	1.7048	1.1013	0.70920	0.44518	0.28212	0.17577	6.9237
1.80	0.91169	0.74615	0.56949	0.42475	0.30158	0.21122	0.14245	3.30733
2.87	0.23647	0.22647	0.20035	0.17178	0.13878	0.10926	0.08177	1.16488
	B. L-ℓ_1 -ℓ_2 Odd, Exchange Neglected 2p Eigenstates Coupling Approximations							
	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_0
0.24	61.12	8.444	2.5808	1.1408	0.6200	0.3720	0.2516	74.52
0.50	15.292	6.884	2.5436	1.1580	0.6216	0.3640	0.2352	27.10
0.68	8.008	4.940	2.2548	1.1160	0.6160	0.3640	0.2352	17.54
0.83	5.108	3.6364	1.9292	1.0380	0.5968	0.3592	0.2340	12.90
1.23	2.0484	1.7392	1.1812	0.7652	0.4972	0.3236	0.2208	6.776
1.80	0.7640	0.7220	0.5816	0.4436	0.3312	0.2400	0.1784	3.261
2.87	0.2132	0.2180	0.2004	0.1776	0.1520	0.1272	0.1064	1.195
	C. L-ℓ_1 - ℓ_2 Odd, 2p Eigenstates Coupling Approximation							
	Singlet							
	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{0S}
0.24	2.963	4.161	0.6725	0.2861	0.1552	0.0930	0.0629	8.394
0.50	3.735	3.182	0.7915	0.3066	0.1576	0.0913	0.0589	8.323
0.68	2.165	1.728	0.6851	0.3025	0.1587	0.0920	0.0590	5.190
0.83	1.371	1.107	0.5562	0.2799	0.1547	0.0913	0.0589	3.619
1.23	0.5280	0.4603	0.3115	0.1991	0.1277	0.0823	0.0558	1.7647
1.80	0.1928	0.1831	0.1475	0.1124	0.0837	0.0605	0.0449	0.8249
2.87	0.0534	0.0547	0.0503	0.0445	0.0381	0.0319	0.0267	0.2996
	Triplet							
	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{0T}
0.24	49.22	3.265	1.850	0.8528	0.4650	0.2788	0.1886	56.12
0.50	7.791	1.851	1.504	0.8193	0.4598	0.2722	0.1764	12.87
0.68	4.720	2.219	1.361	0.7700	0.4481	0.2700	0.1756	9.964
0.83	3.373	2.099	1.237	0.7198	0.4318	0.2652	0.1744	8.300
1.23	1.484	1.225	0.8376	0.5509	0.3630	0.2384	0.1639	4.863
1.80	0.5674	0.5337	0.4295	0.3283	0.2456	0.1784	0.1330	2.4159
2.87	0.1596	0.1632	0.1500	0.1328	0.1136	0.0951	0.0797	0.8940

TABLE V. (Continued)

D. $L-\ell_1-\ell_2$ Even, Born Approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_E	Q_T
0.24	12.488	230.42	4.0427	1.9014	0.30797	0.57480	0.29675	0.06128	250.09	290.69
0.50	0.1758	74.475	7.0963	0.92172	0.48094	0.45745	0.30098	0.05695	83.965	109.714
0.68	0.07386	36.478	6.5573	1.0156	0.29902	0.27895	0.23113	0.04364	44.978	63.742
0.83	0.22032	21.559	5.4143	1.1653	0.26124	0.15835	0.15225	0.02533	28.956	43.572
1.23	0.25024	7.3349	2.9703	1.1453	0.37750	0.11091	0.04377	0.03572	12.269	20.571
1.80	0.13477	2.3518	1.3155	0.74676	0.39290	0.18754	0.07731	0.02824	5.2348	9.6066
2.87	0.04395	0.55809	0.40443	0.30267	0.21866	0.15188	0.09753	0.05832	1.8355	3.8272
3.91	0.01868	0.20876	0.17048	0.14307	0.11656	0.09255	0.06896	0.04864	0.8677	2.1455

E. $L-\ell_1-\ell_2$ Even, Exchange Neglected 1s-2s-2p Eigenstates Coupling Approximation

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_E	Q_T
0.24	31.96	91.21	154.6	92.86	55.86	36.79	24.37		487.7	566.32
0.50	9.371	12.65	30.88	20.53	12.99	8.451	5.695		100.6	129.8
0.68	4.156	5.953	13.19	9.628	6.563	4.508	3.130		47.13	66.56
0.83	2.542	4.560	7.424	5.249	3.811	2.793	2.032		28.41	43.07
1.23	1.208	2.879	2.906	1.734	1.106	.8438	.6912		11.37	19.56
1.80	.5612	1.385	1.238	.8299	.5109	.3005	.2022		5.028	9.382

F. $L-\ell_1-\ell_2$ Even, 1s-2p Eigenstates Coupling Approximation

Singlet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ES}
0.24	1.964	5.238	17.34	1.260	0.4896	0.2460			26.54
0.50	0.5131	3.159	1.544	1.439	0.4063	0.1906	0.1133		7.365
0.68	0.2346	2.091	1.039	0.4944	0.2539	0.1520	0.0984		4.363
0.83	0.1227	1.252	0.9930	0.1532	0.1191	0.0990	0.0766		2.816
1.23	0.1071	0.6796	0.6167	0.2249	0.0635	0.0249	0.0217		1.7384
1.80	0.0571	0.3366	0.2926	0.1818	0.0954	0.0426	0.0172		1.0233

Triplet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ET}	Q_T
0.24	15.62	26.72	32.44	6.674	1.252	0.7359			83.44	178.89
0.50	4.844	3.384	19.97	12.52	0.8285	0.3266	0.2754		42.15	72.80
0.68	2.247	3.886	10.33	5.922	1.035	0.2270	0.1764		23.82	45.22
0.83	1.293	3.650	6.287	3.476	0.9248	0.2097	0.1162		15.957	32.45
1.23	0.4842	2.287	2.424	1.418	0.6072	0.2079	0.0717		7.500	17.28
1.80	0.1909	1.063	0.9673	0.6659	0.4001	0.2024	0.0962		3.586	8.943

G. $L-\ell_1-\ell_2$ Even, 1s-2s-2p Eigenstates Coupling Approximation

Singlet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ES}
0.24	7.852	13.45	38.56	21.41	15.44	8.610	6.432		111.75
0.50	2.470	5.026	7.433	4.900	3.201	2.101	1.417		26.548
0.68	1.344	2.283	3.025	2.683	1.756	1.166	.7903		13.047
0.83	.7424	1.316	1.579	1.518	1.079	.7580	.5313		7.524
1.23	.2813	.6752	0.6254	.3663	.2726	.2289	.1916		2.641
1.80	.1357	.3339	.2862	.1816	.1065	.0659	.0471	.0383	1.1952
2.87	.0513	.1053	.0930	.0739	.0553	.0391	.0268	.0181	0.4628
3.91	.0267	.0451	.0422	.0373	.0318	.0261	.0212	.0166	0.2470

Triplet

k_2	L = 0	L = 1	L = 2	L = 3	L = 4	L = 5	L = 6	L = 7	Σ_{ET}	Q_T
0.24	27.90	75.79	63.10	87.21	41.31	26.12	17.13		338.56	518.92
0.50	4.337	4.540	20.66	21.62	10.38	6.373	4.255		72.17	122.01
0.68	2.823	4.018	10.75	8.986	5.149	3.337	2.302		37.37	67.46
0.83	2.032	3.674	6.400	4.796	2.950	2.013	1.468		23.333	44.54
1.23	.9741	2.290	2.465	1.599	.9568	.6421	.4924		9.419	20.11
1.80	.4291	1.055	.9303	.6614	.4150	.2540	.1639	.1180	4.027	9.531
2.87	.1564	.3217	.2907	.2330	.1780	.1291	.0907	.0623	1.4619	3.945
3.91	.0805	.1366	.1285	.1143	.0982	.0810	.0655	.0524	0.7570	

LIST OF FIGURES

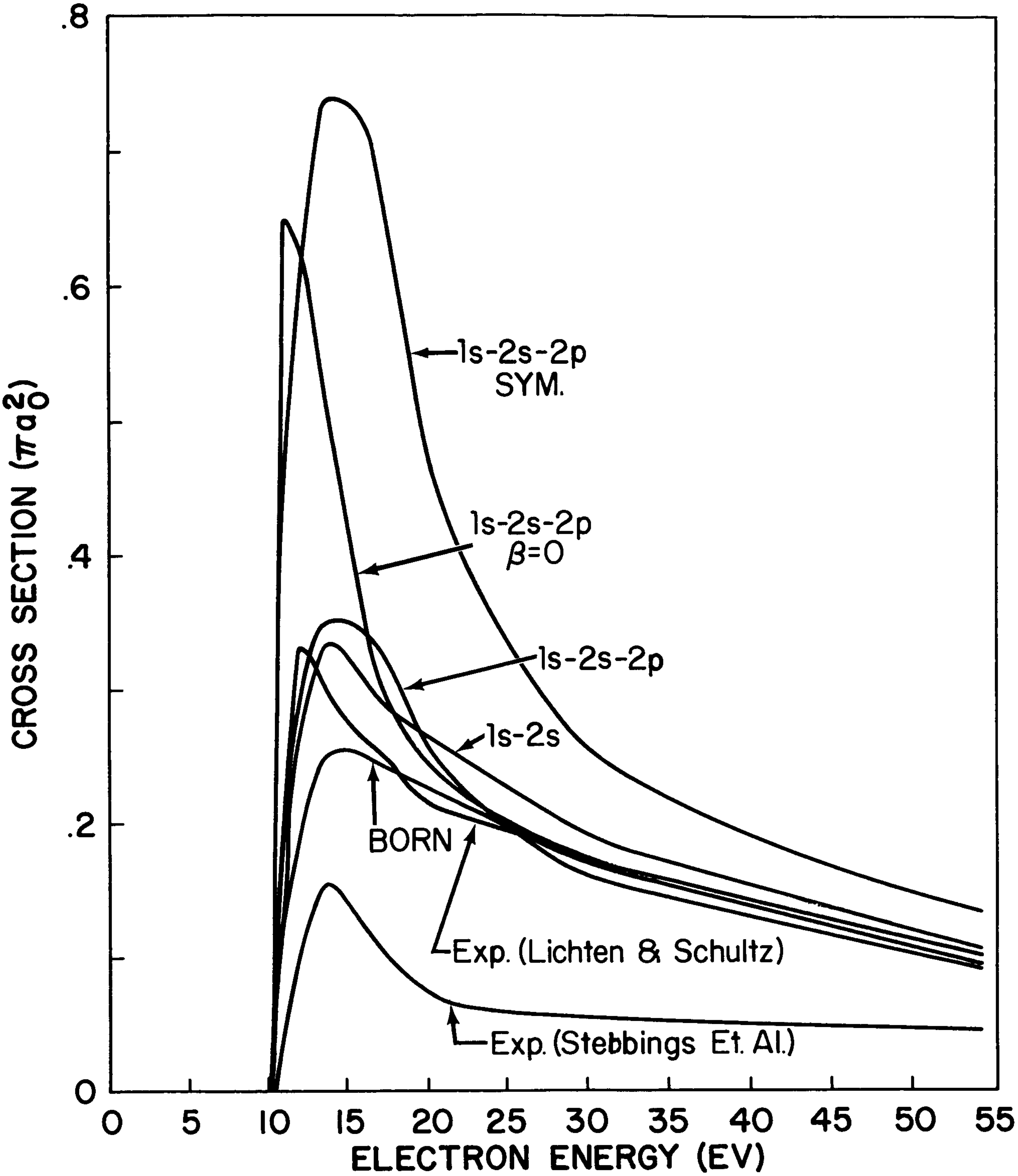

FIG. 1. 1s-2s EXCITATION CROSS SECTION

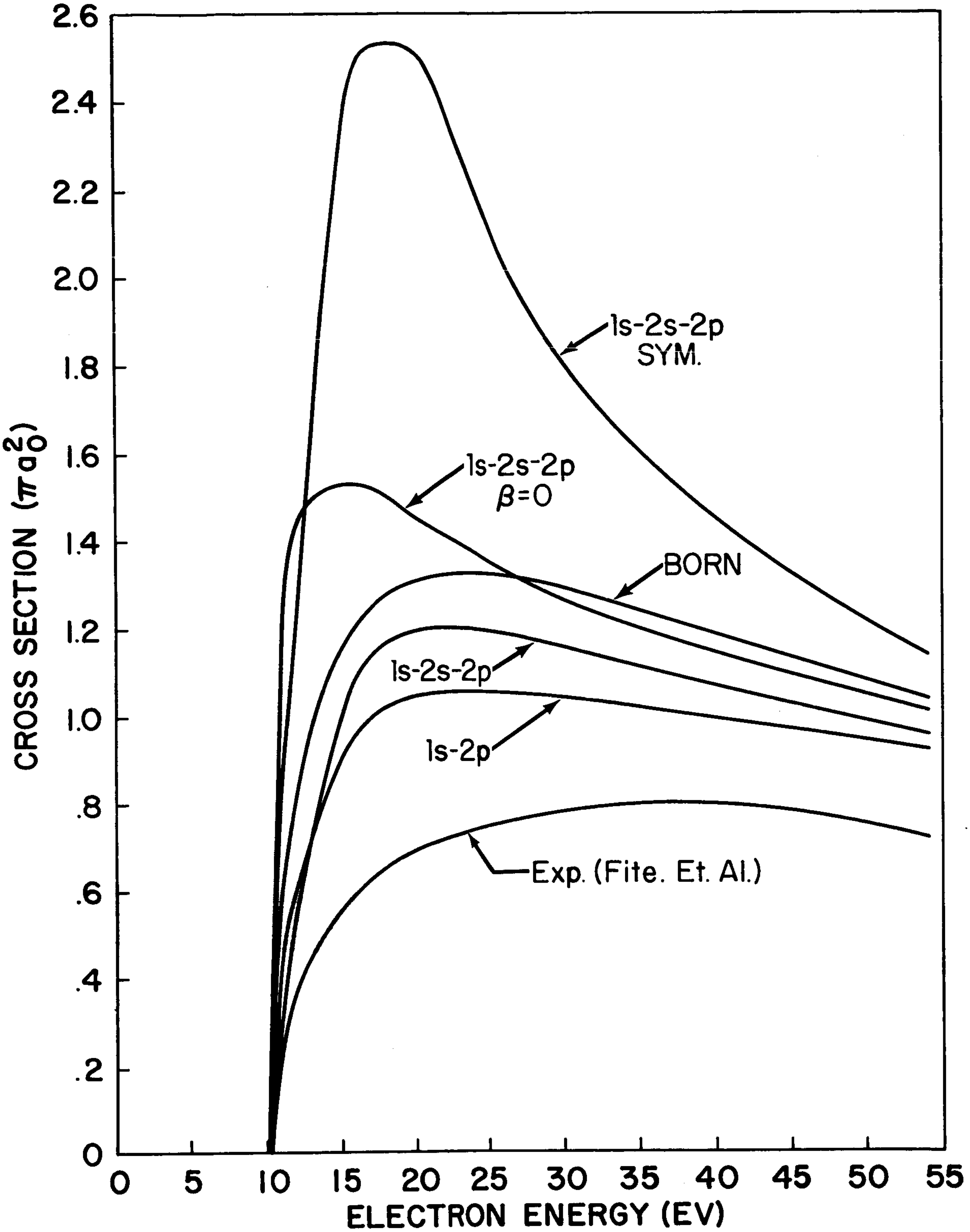

FIG. 2. 1s-2p EXCITATION CROSS SECTION

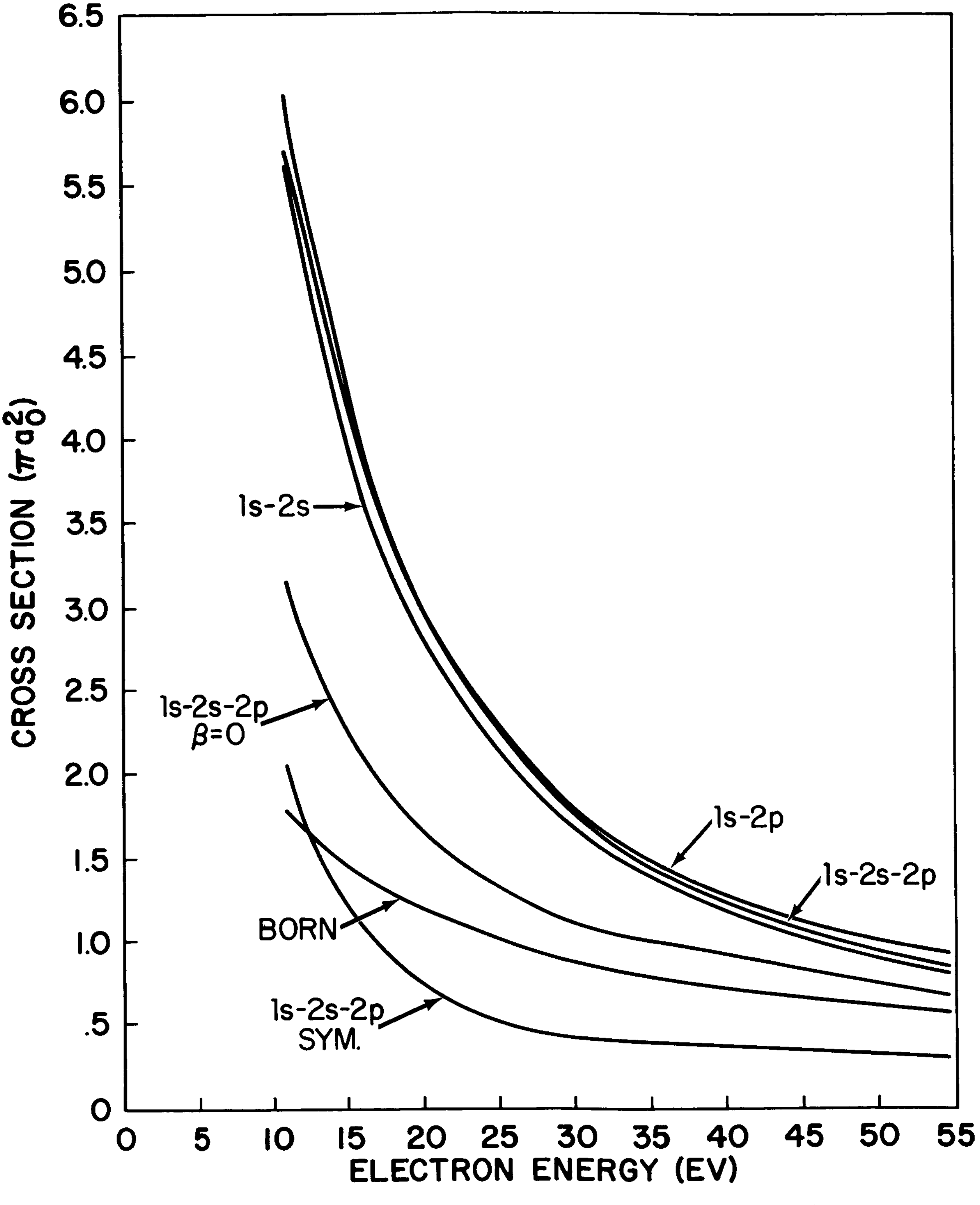

FIG. 3. 1s-1s ELASTIC CROSS SECTION

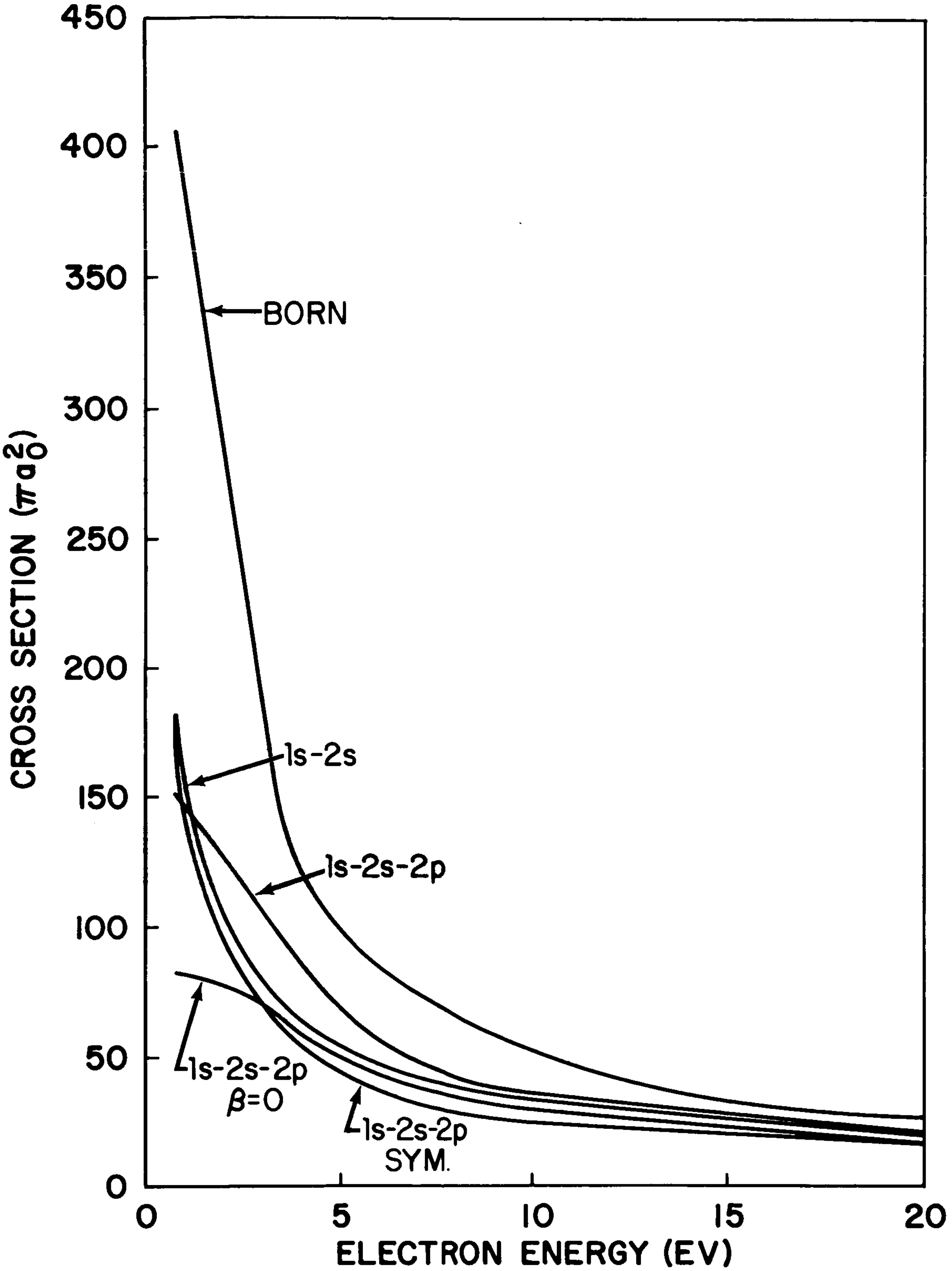

FIG. 4. 2s-2s ELASTIC CROSS SECTION

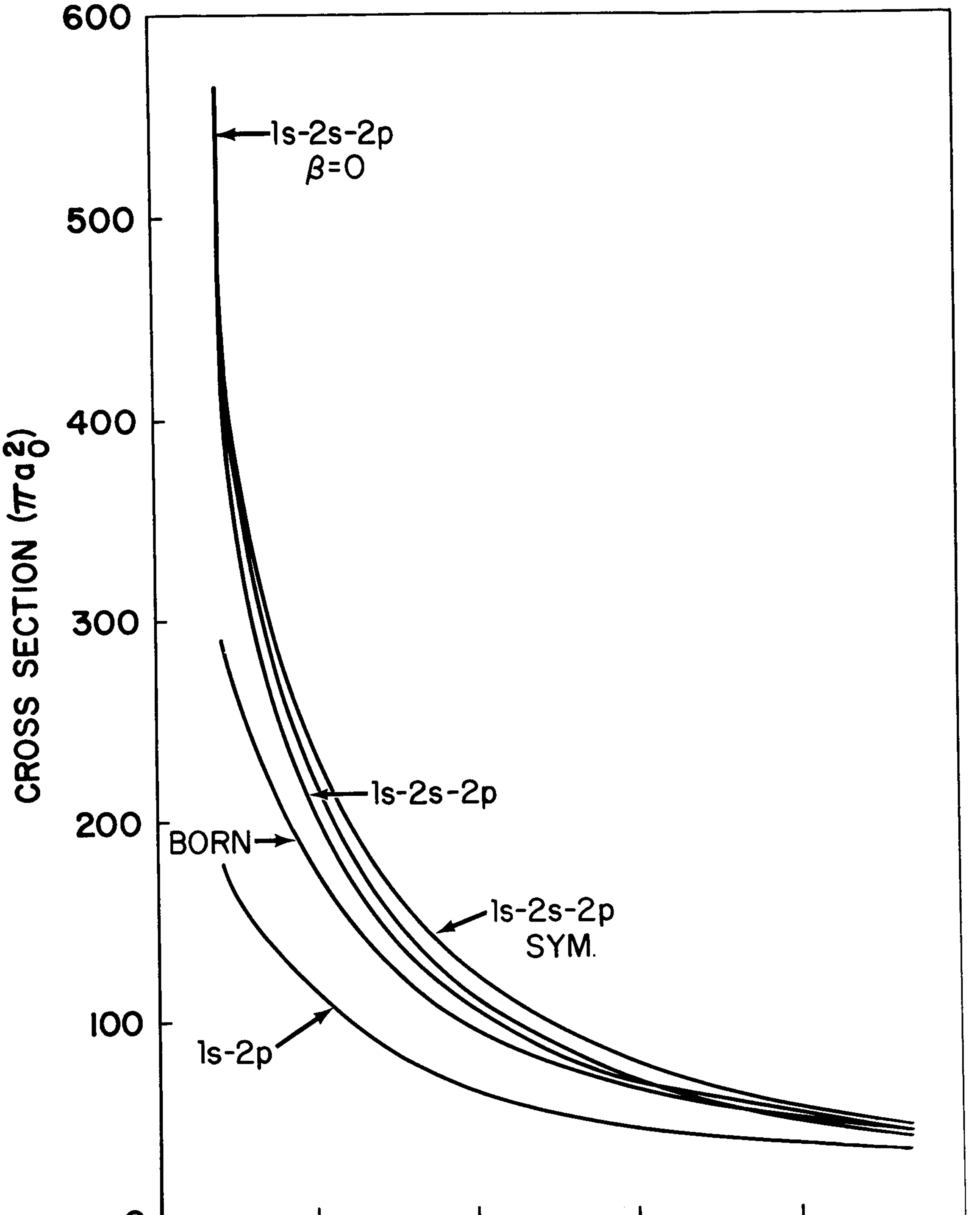

FIG. 5. 2p-2p ELASTIC CROSS SECTION

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