TABLE XIV. Same as caption for Table XIII except copper is replaced by gold.

			Z=79			
		T=200 keV			T=100 keV	
θ (deg)	$d\sigma/d\Omega_{DS}$	$d\sigma/d\Omega_{S}$	$d\sigma/d\Omega_{C}$	$d\sigma/d\Omega_{DS}$	$d\sigma/d\Omega_{S}$	$d\sigma/d\Omega_{C}$
30	7.493×10^{4}	6.236×10^{4}	6.996×10^{4}	2.611×10^{5}	1.787×10^{5}	2.250×10^{5}
60	5.351×10^{3}	6.653×10^{3}	6.738×10^{3}	1.910×10^{4}	1.970×10^{4}	2.059×10^{4}
90	1.148×10^{3}	1.965×10^{3}	1.940×10^{3}	4.339×10^{3}	6.381×10^{3}	6.267×10^{3}
120	3.961×10^{2}	8.504×10^{2}	8.241×10^{2}	1.649×10^{3}	3.236×19^{3}	3.032×10^{3}
150	1.953×10^{2}	4.886×10^{2}	4.653×10^{2}	9.144×10^{2}	2.227×10^{3}	2.016×10^{3}

S would not change more than 10% even if we changed the potential from the one-term exponential to the three-term exponential potential or to the Hartree potential.

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2s and 2p Electron Impact Excitation in Atomic Hydrogen

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A numerical calculation has been carried out to evaluate the 3×3 cross-section matrix involved in the electron impact excitation of the ground state of H atom to the 2s and 2p levels. The method of solution is that of atomic eigenstates expansion. In this paper, instead of the iterative technique used by other authors, 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. The accuracy of the numerical integration is tested by satisfying the equation of reciprocity and the equation of continuity of currents 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 5%. The results are in agreement with the results of an iterative technique. To evaluate the effect of the long range and the centrifugal potential, a simple perturbation theory is developed. The six cross sections $1s \rightarrow 2s$, $1s \rightarrow 2p$, $1s \rightarrow 1s$, $2s \rightarrow 2s$, $2s \rightarrow 2p$, and $2p \rightarrow 2p$ are tabulated elsewhere, only the $2s \rightarrow 2p$ and the $2p \rightarrow 2p$ cross sections are reported here. The $2p \rightarrow 2p$ cross section requires the solution of the sets of differential equations with different parities. Assuming the validity of the eigenstates expansion, it is found by comparison with the eigenstates expansion calculation that the Born approximation, despite its simplicity, gives meaningful results for low and close-to-the-threshold energies of the bombarding electrons. The effect of the exchange potentials on the cross sections is also investigated. Finally, an interesting structure of the $1s \rightarrow 2s$ excitation cross section above threshold is found.

I. INTRODUCTION

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. However, if this wave function is expanded in terms of the eigenstates of the hydrogen atom, the coefficients of the expansion, which are functions of the position vector of the free electron, can be found through numerical integration. 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,[1] whose expansion consisted of the $1s$ and the $2s$ states in order to calculate the $1s \rightarrow 2s$ transition cross section. This calculation was extended by Smith[2] to higher total orbital angular momenta of the system. Percival and Seaton[3] have formulated the eigenstate expansion technique in general, and have tabulated the coefficients of the integrodifferential equations for s, p, and d atomic electrons. Burke, Smith, and Schey,[4] using the equations of Percival and Seaton for the three states $1s$, $2s$, $2p$, have integrated the resulting integrodifferential equations. In this paper we solve the same differential equations by a linear transformation of the differential equations in order to avoid the need for iteration of these equations.[5]

The numerical integrations were carried out for all partial waves, while in higher partial waves the Born approximation were used. The transition between the eigenstates expansion calculation and the 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 antiparallel spin states, where $S=0$, and parallel spin states, where $S=1$. In this way we 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 and taking its position as the origin of the coordinate system, the Schrödinger 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 the free electrons and, in atomic units,

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

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 $\mathbf{L}$,

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

Since these eigenfunctions are orthogonal, 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

$$\psi_L(\mathbf{r}_1,\mathbf{r}_2)=(1+\beta P_{12})\sum_{n_1l_1l_2}\sum_{m_1m_2}C_{m_1m_2M}^{l_1l_2L}\varphi(n_1l_1m_1,\mathbf{r}_1)\times r_2^{-1}u(k_{n_1}l_2,r_2)Y_{l_2m_2}(\Omega_2), \tag{2.5}$$

$$\varphi(n_1l_1m_1,\mathbf{r}_1)=r_1^{-1}P(n_1l_1,\mathbf{r}_1)Y_{l_1m_1}(\Omega_1). \tag{2.6}$$

Here $\varphi(n_1l_1m_1r_1)$ is the hydrogen atom wave function with radial part $r_1^{-1}P(n_1l_1,r_1)$ and angular part $Y_{l_1m_1}(\Omega_1)$ and quantum numbers nl_1m_1; $r_2^{-1}u(k_{n_1}l_2,r_2)$ is the radial part, and $Y_{l_2m_2}(\Omega_2)$ is the angular part of the free-electron wave function with quantum numbers $k_{n_1}l_2m_2$. The relation between the wave number k_{n_1} and n_1 is given by

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

Finally the constants $C_{m_1m_2M}^{l_1l_2L}=(l_1l_2m_1m_2|LM)$, with M representing the total magnetic quantum number, 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 the total angular momentum L. In the problem under consideration $n_1=1,\ 2;\ l_1=0,\ 1;\ l_2=|L-l_1|,\ \cdots,\ |L+l_1|$; $m_1=-l_1,\ \cdots,\ l_1$ and $m_2=-l_2,\ \cdots,\ l_2$. 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 $\mathbf{L}$ perpendicular to the z axis $M=0$ and $m_2=-m_1$, Eq. (2.5) can then be written

$$\psi_L(\mathbf{r}_1,\mathbf{r}_2)=(1+\beta P_{12})\sum_{n_1l_1l_2}\sum_{m_1}C_{m_1-m_10}^{l_1l_2L}\varphi(n_1l_1m_1,\mathbf{r}_1)\times r_2^{-l}u(k_{n_1}l_2,r_2)Y_{l_2m_2}(\Omega_2). \tag{2.8}$$

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

$$\delta\int\psi_L^*(\mathbf{r}_1,\mathbf{r}_2)[H-E]\psi_L(\mathbf{r}_1,\mathbf{r}_2)d^3\mathbf{r}_1d^3\mathbf{r}_2=0. \tag{2.9}$$

Percival and Seaton[3] have evaluated Eq. (2.9) and have derived the differential equations for the scattering

[1] R. Marriott, Proc. Phys. Soc. (London) **72**, 121 (1958).
[2] K. Smith, Phys. Rev. **120**, 845 (1960).
[3] I. C. Percival and M. J. Seaton, Proc. Cambridge Phil. Soc. **53**, 654 (1957).
[4] (a) P. G. Burke and K. Smith, Rev. Mod. Phys. **34**, 458 (1962). (b) P. G. Burke, H. M. Schey, and K. Smith, Phys. Rev. **129**, 1258 (1963).
[5] Similar calculation has been carried out by R. Damburg and R. Peterkop, Proc. Phys. Soc. (London) **80**, 563 and 1073 (1962). Here the $L=0$, 1 cases have been solved by noniterative, and all other cases by iterative, methods.

of free electrons by atomic s, p, and d electrons in hydrogen atom, using the theory of the irreducible tensor operators in order to evaluate the interaction terms between the two electrons. The result is a set of coupled second-order differential equations which are functions of the radial coordinate of the free electron. We have evaluated Eq. (2.9) independently using ordinary methods, and have verified the results of Percival and Seaton.[6]

When the integrals representing the direct potentials in the coupled set of 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:

$$\left[\frac{d^2}{dr^2}+k_n^2-\frac{l_n(l_n+1)}{r^2}\right]\mathbf{u}(k_nl_n,r)=2\mathbf{V}\mathbf{u}(k_nl_n,r). \quad (2.10)$$

The components of $\mathbf{u}$ are the radial functions of the free electron, and $\mathbf{V}$ is the potential matrix. $\mathbf{u}$ has four components when $L-l_1-l_2$ is even and one component when this is odd. Similarly $\mathbf{V}$ is a 4×4 matrix when $L-l_1-l_2$ is even and it has one component when this quantity is odd. The case $L=0$ is an exception. Here when $L-l_1-l_2$ is even $\mathbf{u}$ has three components and $\mathbf{V}$ is a 3×3 matrix, and the case $L-l_1-l_2$ odd does not occur. $\mathbf{V}$ can be written as the sum of three matrices,

$$\begin{aligned} V_{ij}&=D_{ij}+E_{ij},\\ E_{ij}&=F_{ij}+\sum_{\nu=1}^{\sigma} g_{ij}{}^{\nu}\int_0^{\infty} h_{ij}{}^{\nu}dr, \end{aligned} \quad (2.11)$$

where D_{ij} is the direct potential and E_{ij} is the exchange potential 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}, $g_{ij}{}^{\nu}$, and $h_{ij}{}^{\nu}$ are given in Appendix I. 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. (2.10) are inside the integrals of the exchange terms.

Below we discuss the general solution of Eq. (2.10) when it has four components.

B. 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 (2.10) 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 with 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 $\mathbf{u}$ fixes the values of the constants and thus avoids iteration, whereby the computation is reduced considerably. We have used the second method and the description of the method will be given here.[7,8]

By making use of Eq. (2.11), Eq. (2.10) can be written

$$\left[\frac{d^2}{dr^2}+k_i^2-\frac{l_i(l_i+1)}{r^2}\right]u_i = 2\sum_{j=1}^{4}\left[(D_{ij}+F_{ij})u_j+\sum_{\mu=1}^{\sigma} g_{ij}{}^{\mu}C_{ij}{}^{\mu}\right], \quad (2.12)$$

where

$$C_{ij}{}^{\mu}=\int_0^{\infty} h_{ij}{}^{\mu}(r)u_j(r)dr. \quad (2.13)$$

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

$$\left[\frac{d^2}{dr^2}+k_i^2-\frac{l_i(l_i+1)}{r^2}\right]v_i=2\sum_{j=1}^{4}[D_{ij}+F_{ij}]v_j, \quad (2.14)$$

$$\left[\frac{d^2}{dr^2}+k_i^2-\frac{l_i(l_i+1)}{r^2}\right]u_i{}^{kl}=2\sum_{j=1}^{4}[D_{ij}+F_{ij}]u_j{}^{kl} +2\delta(i,k)g_{kl}{}^{\nu}. \quad (2.15)$$

Then u_i is given by the following expression:

$$u_i=v_i+\sum_{k=1}^{4}\sum_{l=1}^{4}\sum_{\nu=1}^{\sigma} C_{kl}{}^{\nu}u_i{}^{kl}. \quad (2.16)$$

Equation (2.16) can be verified by multiplying Eq. (2.15) by $C_{kl}{}^{\nu}$, summing over k, l and ν, and adding to Eq. (2.14), whereupon Eq. (2.12) results. Substitution

[6] K. Omidvar, Technical Note G-419, Goddard Space Flight Center, National Aeronautics and Space Administration, 1963 (unpublished).

[7] K. Omidvar, Research Report No. Cx-37, p. 22, Inst. Math. Sci., New York University, 1959 (unpublished).

[8] See Ref. 1. This description differs from the description of Ref. 7 and the present paper. In Ref. 1, v_i in Eq. (2.16) is set to zero; this makes $B_{ij}{}^{\mu}=0$. Eq. (2.17) then reduces to a set of homogeneous equations whose determinant must be zero. Since the amplitude of any of the 4 components of $\mathbf{u}$ can be left arbitrary, one of the $C_{kl}{}^{\nu}$ is set to 1 and the rest of the constants are found subsequently.

of Eq. (2.16) in Eq. (2.13) gives

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

$i, j=1, 2, 3, 4;$

$$\mu=1, 2 \quad \text{for} \quad i=j=3 \quad \text{and} \quad i=j=4; \quad \mu=1 \quad \text{otherwise}, \tag{2.17}$$

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

$$A_{ij}{}^{\mu kl}=\int_0^{\infty} h_{ij}{}^{\mu}u_j{}^{kl}dr,$$
$$B_{ij}{}^{\mu}=\int_0^{\infty} h_{ij}{}^{\mu}v_j dr. \tag{2.18}$$

The numerical integration is carried out by integrating Eqs. (2.14) and (2.15) by any standard method, calculating $A_{ij}{}^{\mu kl}$ and $B_{ij}{}^{\mu}$ by Eqs. (2.18) and, finally, solving the system of 18 algebraic equations given by Eqs. (2.17) to find $C_{kl}{}^{\nu}$. With the known values of these constants the integration of Eqs. (2.12) is straightforward.

The determinant of Eqs. (2.17) becomes singular for $L=0$ and 1. To remove the singularity, some of the $C_{kl}{}^{\nu}$ are chosen arbitrarily, and the rest of the $C_{kl}{}^{\nu}$ are found in terms of the chosen ones (cf. Appendix II).

III. NUMERICAL INTEGRATION

A. Solution at the Origin

Equation (2.10) or its equivalent, Eqs. (2.14) and (2.15), constitute a set of four 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 eight sets of solutions to Eq. (2.10). 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 4×4 matrix u_{ij}, $i, j=1, 2, 3, 4$, where i corresponds to a particular component and j corresponds to a particular solution of **u**. In order that the four solutions of **u** be independent of each other, we must have

$$\sum_{j=1}^{4} C_j u_{ij}\neq 0, \quad i=1, 2, 3, 4, \tag{3.1}$$

where C_j are some constants. A necessary condition for this to be satisfied is that the determinant of Eq. (3.1) be nonzero,

$$\|u_{ij}\|\neq 0. \tag{3.2}$$

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,

$$u_{ij}=\sum_{\nu=0}^{\infty} a_{ij}{}^{\nu}r^{s_i+\nu}, \tag{3.3}$$

where $a_{ij}{}^{\nu}$ are the coefficients of the expansion and s_i are given integers for each component of **u** and are fixed by the behavior of Eq. (2.10) at the origin. Equation (3.2) is satisfied near the origin if

$$\|a_{ij}{}^{0}\|\neq 0. \tag{3.4}$$

By choosing suitable values of $a_{ij}{}^{0}$, subject to the restriction (3.4), four independent solutions are obtained.

B. Solution at Larger r

With the solution found at the origin, the solution of Eq. (2.10) or its equivalent, Eqs. (2.14) and (2.15), can be extended from origin through numerical integration to any desired value of r. In order to obtain the asymptotic amplitudes and the phase shifts, the presence of the centrifugal and the long-range potentials, which fall off as r^{-2}, make it necessary to extend the solution to infinity. This is undesirable because of the time consumption on the computer, and the accumulated errors due to the long-range integration. Seaton[9] has solved the problem of r^{-2} long-range potentials occuring in the off-diagonal elements of the potential matrix **V** by diagonalizing the asymptotic form of the differential equations (2.10) and the corresponding S matrix. By an inverse transformation the elements of the original S matrix are found. Burke, Schey, and Smith have used a different method.[10]

Instead, we develop here a perturbation theory which is based on the method described by Mott and Massey.[11] The error in the resulting solution is inversely proportional to the square of the distance from the origin.

Equation (2.10) for large distances of r can be written

$$\left[\frac{d^2}{dr^2}+k_n{}^2\right]\mathbf{u}(k_n l_n,r)=2\mathbf{U}\mathbf{u}(k_n l_n,r), \tag{3.5}$$

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 III. A component of Eq. (3.5) is of the following form:

$$\left[\frac{d^2}{dr^2}+k^2\right]u(r)=g(r),$$
$$g(r)\ll k^2u(r), \quad g(r)\to 0 \quad \text{as} \quad r\to\infty. \tag{3.6}$$

The perturbation theory is applied between some large distance R and infinity. Let u vanish at R; then we have

[9] M. J. Seaton, Proc. Phys. Soc. (London) **77**, 174 (1961).
[10] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962); see also Ref. 4(a).
[11] N. F. Mott and H. S. W. Massey, *The Theory of Atomic Collisions* (Oxford Press, Oxford, England, 1949), 2nd ed., Chap. II.

the following boundary condition:

$$u(R)=0. \tag{3.7}$$

If we represent the homogeneous solution of Eq. (3.6) by $y(r)$, at infinity we must have

$$\begin{aligned} y(r)&=a\sin(kr-kR)\,,\\ u(r)&=(a+\Delta a)\sin(kr-kR+\eta)\,, \end{aligned} \tag{3.8}$$

where a is the amplitude of $u(r)$ if $g(r)$ were identically zero and Δa and η are generated by $g(r)$. Since $g(r)$ is small, we can write

$$u=y(1+\zeta)\,, \tag{3.9}$$

where ζ is a small function. Substitution of Eq. (3.9) in Eq. (3.6) gives

$$\frac{d}{dr}\left(y^2\frac{d\zeta}{dr}\right)=g(r)y, \tag{3.10}$$

where, upon double integration, we obtain

$$\zeta=\int_R^r\frac{dr}{y^2}\int_R^r g(r')y\,dr'. \tag{3.11}$$

The constants of integrations are fixed by the condition (3.7) and the fact that $u'(R)=y'(R)$.

We now integrate Eq. (3.11) by parts,

$$\zeta=\left[\int_R^r g(r)y\,dr\right]\left[\int_R^r\frac{dr}{y^2}\right]-\int_R^r g(r)y\,dr\int_R^r\frac{dr}{y^2}. \tag{3.12}$$

When the integration with respect to y is carried out, and the result is substituted in Eq. (3.9), we obtain

$$\begin{aligned} u(r)=&\sin(kr-kR)\left[a+\frac{1}{k}\int_R^r g(r)\cos(kr-kR)dr\right]\\ &+\cos(kr-kR)\left[-\frac{1}{k}\int_R^r g(r)\sin(kr-kR)dr\right]. \end{aligned} \tag{3.13}$$

Comparison of the second of Eqs. (3.8) and Eq. (3.13) shows that

$$\begin{aligned} \Delta a&=\frac{1}{k}\int_R^\infty g(r)\cos(kr-kR)dr,\\ \eta&=-\frac{1}{ak}\int_R^\infty g(r)\sin(kr-kR)dr, \end{aligned} \tag{3.14}$$

to first order. The functions $g(r)$ in the four differential equations (3.5) are given by

$$g_i(r)=2\sum_j U_{ij}u_j. \tag{3.15}$$

To first order this can be written by

$$g_i(r)=2\sum_j a_jU_{ij}\sin(k_jr-k_jR_j)\,, \tag{3.16}$$

where R_j is where u_j has become zero for the last time with positive slope. Substitution of this equation in Eq. (3.14) gives

$$\begin{aligned} \Delta a_i&=-\sum_j\frac{a_j}{k_i}\int^{R_i}\cos(k_ir-k_iR_i)U_{ij}\sin(k_jr-k_jR_j)dr,\\ \eta_i&=\sum_j\frac{a_j}{a_ik_i}\int^{R_i}\sin(k_ir-k_iR_i)U_{ij}\sin(k_jr-k_jR_j)dr. \end{aligned} \tag{3.17}$$

Δa_i and η_i can easily be calculated by substituting the values of U_{ij} from Appendix III, integrating the resulting integrals by parts and retaining the leading terms.

The asymptotic amplitudes and phase shifts are given by

$$\begin{aligned} a_i(\infty)&=a_i(R_i)+\Delta a_i\,,\\ \delta_i(\infty)&=\delta_i(R_i)+\eta_i+[L-\delta(i,3)+\delta(i,4)]\pi/2\,, \end{aligned} \tag{3.18}$$

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.

C. Derivation of the Cross Section

When contribution of the long-range potentials to the amplitudes and the phase shifts are added to these values calculated by the numerical integration, we find the asymptotic form of u_{ij},

$$u_{ij}(r)\sim a_{ij}\sin\left(k_ir-\frac{l_i\pi}{2}+\delta_{ij}\right). \tag{3.19}$$

The elements of the scattering matrix S_{mn} are related to a_{ij} and δ_{ij} through linear relations.[12] The cross section for the $m\rightarrow n$ transition is then given by[12]

$$Q_{mn}=\frac{\pi(2L+1)}{k_m^2(2l_1+1)}|T_{mn}|^2, \tag{3.20}$$

$$T_{mn}=\delta_{mn}-S_{mn}\,, \tag{3.21}$$

where k_m is the wave number in the initial channel m and l_1 is the angular momentum quantum number of the atom in the initial state m.

D. A Useful Relation

A relation based on the symmetry of the interaction potentials, which serves as a test on the accuracy of the solutions, can be derived. The lth and the kth solutions of the ith component of **u** by Eq. (2.10) are given by

$$\begin{aligned} \left[\frac{d^2}{dr^2}+k_i^2-l_i\frac{(l_i+1)}{r^2}\right]u_{il}&=\sum_j V_{ij}u_{jl}\,,\\ \left[\frac{d^2}{dr^2}+k_i^2-l_i\frac{(l_i+1)}{r^2}\right]u_{ik}&=\sum_j V_{ij}u_{jk}\,. \end{aligned} \tag{3.22}$$

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

[12] See Ref. 6, Sec. IIB. See also Refs. 4.

gives

$$\sum_i \left[u_{ik}\frac{d^2}{dr^2}u_{il} - u_{il}\frac{d^2}{dr^2}u_{ik} \right] = \sum_{i,j} V_{ij}[u_{ik}u_{jl} - u_{il}u_{jk}]. \quad (3.23)$$

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. By integrating the left-hand side from zero to infinity, we obtain

$$\sum_i \int_0^\infty \left[u_{ik}\frac{d^2}{dr^2}u_{il} - u_{il}\frac{d^2}{dr^2}u_{ik} \right] dr = 0. \quad (3.24)$$

By integrating the above equation by parts and applying Eq. (3.19), we obtain

$$\sum_{i=1}^{4} k_i a_{ik} a_{il} \sin(\delta_{ik}-\delta_{il}) = 0, \quad k, l = 1, 2, 3, 4, \quad k \neq l. \quad (3.25)$$

Although the terms containing the exchange potentials do not cancel out on the right-hand side of Eq. (3.23), the cancellation does take place after the integration is carried out in Eq. (3.24).

E. Details of the Numerical Integration

Milne's[13] method with variable mesh size and Simpson's[14] 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 the 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 $2p \rightarrow 2p$ elastic scattering potential become vanishingly small (see Appendix III). At this distance the set of the 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. IIIB. 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.

$$h_i = 1\times10^{-5},$$
$$h_f = 0.05,$$
$$\epsilon = 1\times10^{-4},$$
$$R_1 = 30,$$
$$R_2 = 200.$$

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

[13] W. E. Milne, *Numerical Calculus* (Princeton University Press, Princeton, New Jersey, 1949), Sec. 40.
[14] See Ref. 13, Sec. 33.

IV. RESULTS AND DISCUSSION

The four differential equations listed in Appendix I were integrated numerically by the methods described in Sec. III. By choosing different values for the determinant (3.4) different sets of independent solutions can be generated. The cross sections reported in this paper have been obtained by averaging the cross sections obtained from two independent sets of solutions. To test the accuracy of the numerical integration we define the three quantities D_{mn}, D_{mn}' and D_m'' given by

$$D_{mn} = \left| \sum_{i=1}^{4} k_i a_{im} a_{in} \sin(\delta_{im}-\delta_{in}) \right| \Big/ \sum_{i=1}^{4} k_i a_{im} a_{in} \left| \sin(\delta_{im}-\delta_{in}) \right|, \quad m, n = 1, 2, 3, 4, \quad m \neq n, \quad (4.1)$$

$$D_{mn}' = \frac{|S_{mn}-S_{nm}|}{|S_{mn}|+|S_{nm}|}, \quad m, n = 1, 2, 3, 4, \quad m \neq n, \quad (4.2)$$

$$D_m'' = \left| \sum_{n=1}^{4} |S_{mn}|^2 - 1 \right| \Big/ \sum_{n=1}^{4} |S_{mn}|^2 + 1, \quad m = 1, 2, 3, 4. \quad (4.3)$$

Based on Eqs. (3.25), the symmetry, and the unitary property of the S matrix, in an exact solution of the four differential equations the right-hand side of these equations would 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 $1s-2s-2p$ coupling, $\beta=+1$, $k_1=2.0$, and $L=3$ are given below:

$$D_{12}=1.4\times10^{-3}, \quad D_{13}=2.6\times10^{-4}, \quad D_{14}=1.3\times10^{-3},$$
$$D_{23}=5.1\times10^{-4}, \quad D_{24}=2.2\times10^{-3}, \quad D_{34}=1.8\times10^{-3},$$
$$D_{12}'=7.6\times10^{-4}, \quad D_{13}'=5.1\times10^{-3}, \quad D_{14}'=5.6\times10^{-3},$$
$$D_{23}'=5.4\times10^{-3}, \quad D_{24}'=5.7\times10^{-3}, \quad D_{34}'=1.3\times10^{-3},$$
$$D_1''=1.8\times10^{-4}, \quad D_2''=7.6\times10^{-5},$$
$$D_3''=2.5\times10^{-4}, \quad D_4''=4.4\times10^{-6}.$$

To compare the results of the numerical integration by noniterative method as we have carried out here with those of iterative method of Refs. 2 and 4 we have

TABLE I. Comparison of the iterative and the noniterative results for the singlet, $L=0, 1$; $k_1=0.9, 1.0$, $1s \rightarrow 2s$ excitation cross section. I and II refer to interative and noniterative methods, respectively. D_{max} is the maximum of the error to value ratios in the reciprocity relationships.

		A. $1s-2s$ coupling			
		$Q_{1s\rightarrow 2s}$		D_{max} (percent)	
k_1	L	I[a]	II	I	II
0.90	0	0.0384	0.0375	7.1	0.72
1.00	0	0.0714	0.0725	unknown	0.53
0.90	1	0.008	0.0017	386	0.91
1.00	1	0.051	0.0583	55	0.75
		B. $1s-2s-2p$ coupling			
		$Q_{1s\rightarrow 2s}$		D_{max} (percent)	
		I[b]	II	I	II
0.90	0	0.0529	0.523	0.40	0.40
1.00	0	0.0766	0.0768	0.12	0.60
0.90	1	0.0045	0.0048	2.3	10
1.00	1	0.0145	0.0147	0.33	1.3

[a] See Ref. 2.
[b] See Refs. 4(a), 4(b).

provided Table I.[15] The $1s \rightarrow 2s$ excitation cross section is given by the two methods. Methods I and II refer to the iterative and noniterative methods, respectively, and D_{max} is the maximum of the error to value ratios in the reciprocity relations (4.2). In the $1s-2s$ eigenstates coupling approximation the noniterative method is far more accurate than the iterative method, and as is seen the cross sections by the two methods differ from each other sometimes in their first significant figure. In the $1s-2s-2p$ eigenstates coupling approximation, on the other hand, the results by the iterative method seems to be somewhat more accurate. The reason is contributed to the effect of the r^{-2} long-range potential which appear in the differential equations when in the eigenstates coupling approximation the $2p$ state is included. Two different methods are used in Refs. 4 and the present paper to estimate the effect of this potential for large distances, and it may be that in Refs. 4 this effect is better accounted for. Nevertheless the cross sections are the same in their first three decimal places.

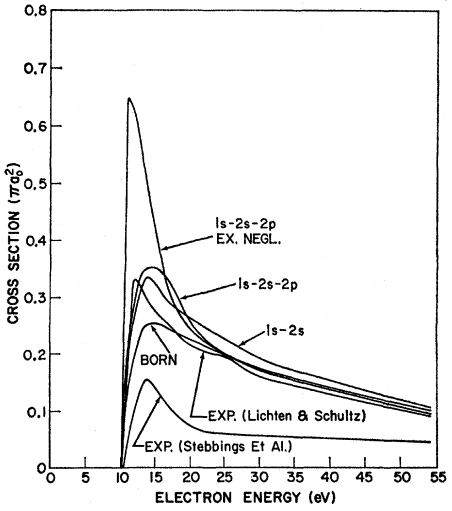

FIG. 1. $1s \rightarrow 2s$ total excitation cross section. $1s-2s$ refers to $1s-2s$ eigenstates coupling approximation. $1s-2s-2p$ has similar meaning. EX. NEGL. refers to exchange neglected case. BORN is the Born approximation. EXP. refers to experiment.

[15] I am indebted to Dr. K. Smith for sending me some of the data in this table.

In Fig. 1 we present the theoretical and the experimental estimate of the $1s \rightarrow 2s$ excitation cross section. The calculated curves are Born, $1s-2s$ coupling, $1s-2s-2p$ coupling exchange neglected, and $1s-2s-2p$ coupling exchange included, approximation. The first three of these curves are the same as Refs. 4(a) and 4(b). The experimental curves are those of Lichten and Schultz,[16] and Stebbings, Fite, and Hummer.[17] The various calculated results agrees better with the results of Lichten and Schultz. However, recent calculations of Taylor and Burke[18] have shown that, in an eigenstates expansion calculation where $1s$, $2s$, $2p$, $3s$, and $3p$ are included, the cross section at the peak of the $1s-2s-2p$ curve is reduced by 30%. This suggests that, within eigenstates expansion approximation, more states should be included to insure that the convergence has been achieved; and the discrepancy between the two experimental results is still an unresolved problem. As another theoretical approach to the problem, H. L. Kyle and A. Temkin[19] have extended the nonadiabatic theory of scattering developed by A. Temkin[20] to the $L=0$, $1s \rightarrow 2s$ inelastic scattering of electrons by the hydrogen atom. They find a 30% decrease in the $1s \rightarrow 2s$ cross section as calculated by the $1s-2s$ close coupling approximation.

Comparison of the exchange neglected and exchange included $1s-2s-2p$ coupling shows that exchange is mostly important at threshold, and its effect does not extend beyond 20 eV.

The $1s \rightarrow 2s$ excitation cross section in the singlet state has an interesting behavior immediately above threshold. In Fig. 2 this cross section for a range of 600 meV above threshold is plotted. In the $1s-2s$ coupling approximation a maximum appears at 34 meV while in the $1s-2s-2p$ coupling approximation there are three maxima of approximately the same magnitudes at 17, 34, and 87 meV, respectively. In the singlet case the cross section rises sharply within a range of 17 meV above threshold to a value of about $0.04\pi a_0^2$. It then rises with an approximately constant and small slope. The contribution of the triplet case is seen to be almost

[16] W. Lichten and S. Schultz, Phys. Rev. **116**, 1132 (1959).
[17] R. F. Stebbings, Wade L. Fite, David G. Hummer, and R. T. Brackmann, Phys. Rev. **119**, 1939 (1960).
[18] A. J. Taylor and P. G. Burke, in Bulletin of the Third International Conference on the Physics of Electronic and Atomic Collisions, University College, London, July 1963 (unpublished).
[19] H. L. Kyle and A. Temkin, in Bulletin of the Third International Conference on the Physics of Electronic and Atomic Collisions, University College, London, July 1963 (unpublished).
[20] A. Temkin, Phys. Rev. **126**, 130 (1962).

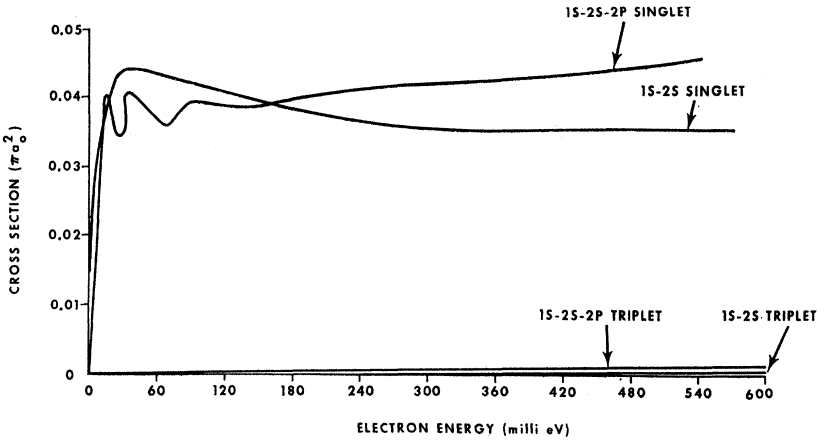

FIG. 2. $L=0$, $1s \rightarrow 2s$ excitation cross section above threshold. The cross sections are given for the two spin states singlet and triplet, and for the two approximations $1s-2s$ and $1s-2s-2p$. The total cross section is the sum of the singlet and the triplet cross sections.

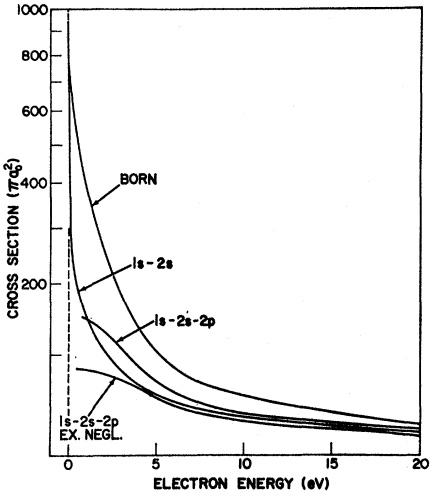

FIG. 3. $2s \rightarrow 2s$ total elastic cross section. Curves are designated as in Fig. 1.

negligible at the threshold, and it has no maximum in this region (see Table II). It should be noted that the principal maximum in the $1s \rightarrow 2s$ excitation cross section appears at about 3 eV with a value of about 0.35, and has contribution from higher angular momentum than $L=0$. Although no study has been made to relate the existence of the maxima above threshold to any physical phenomena, it may be said that, similar to resonances below threshold in the elastic scattering of electrons by the hydrogen atom, these maxima are due to formation of some unstable states of the negative hydrogen ion. Damburg and Peterkop,[5] and Gailitis and Damburg[21] have made an extensive study of the behavior of different cross sections near threshold in the $1s-2s$, and the $1s-2s-2p$ eigenstates coupling approximations.

In Fig. 3 we have shown the $2s \rightarrow 2s$ elastic cross

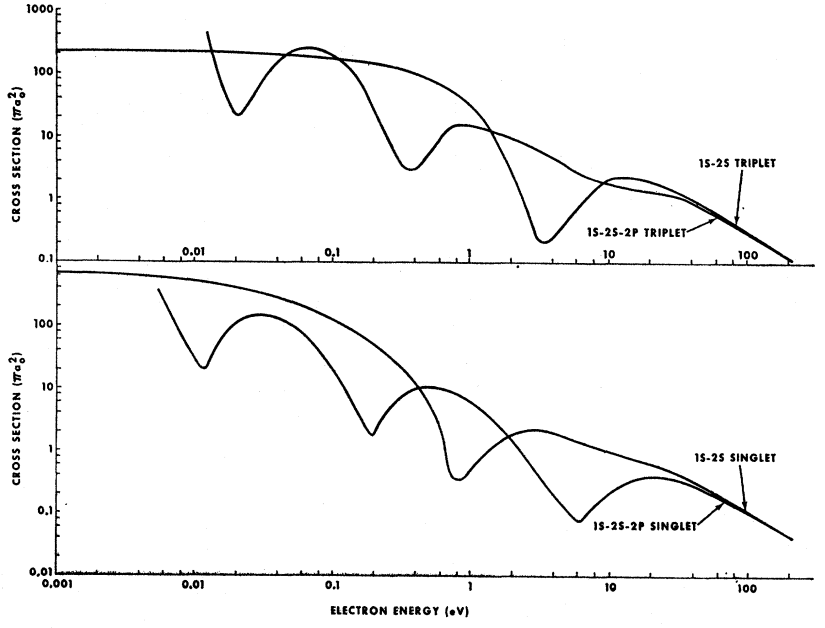

FIG. 4. $L=0$, $2s \rightarrow 2s$ elastic cross section. Curves are designated as in Fig. 2.

[21] M. Gailitis and R. Damburg, Proc. Phys. Soc. (London) 82, 192 (1963). [*Note added in proof:* When the energy difference between the $2s$ and the $2p$ states are neglected in the $1s-2s-2p$ couplings, Gailitis and Damburg have shown that at the threshold the $1s \rightarrow 2s$ excitation cross section does not go to zero (cf. Fig. 2).]

TABLE II. The singlet $L=0$, $1s \rightarrow 2s$ excitation cross section near threshold. k_2 is the wave number of the inelastically scattered wave, and E is the corresponding energy in meV. Q_1 and Q_2 are the cross sections according to the $1s-2s$ and the $1s-2s-2p$ couplings, respectively.

k_2	0	0.01	0.02	0.025	0.030	0.035	0.04
E (meV)	0	1.36	5.44	8.50	12.2	16.7	21.8
Q_1	0	0.0168	0.0298		0.0377		0.0423
Q_2	0		0.0149	0.0259	0.0349	0.0405	0.0353
k_2	0.045	0.050	0.060	0.070	0.080	0.090	0.100
E (meV)	27.5	34.0	49.0	66.6	87.0	110	136
Q_1		0.0446	0.0441	0.0435	0.0423	0.0412	0.0405
Q_2	0.0346	0.0405	0.0391	0.0361	0.0395	0.0392	0.0385

TABLE III. $2p-2p$ 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 couplings 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 couplings 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
	D. $L-l_1-l_2$ even, Born approximation									
	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$L=7$	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

TABLE III—(*continued*)

E. $L-l_1-l_2$ even, exchange neglected $1s-2s-2p$ eigenstates couplings approximation

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$L=7$	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	0.8438	0.6912		11.37	19.56
1.80	0.5612	1.385	1.238	0.8299	0.5109	0.3005	0.2022		5.028	9.382

F. $L-l_1-l_2$ even, $1s-2p$ eigenstates couplings approximation

Singlet

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$L=7$	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

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$L=7$	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. $L-l_1-l_2$ even, $1s-2s-2p$ eigenstates couplings approximation

Singlet

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$L=7$	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	0.7903		13.047	
0.83	0.7424	1.316	1.579	1.518	1.079	0.7580	0.5313		7.524	
1.23	0.2813	0.6752	0.6254	0.3663	0.2726	0.2289	0.1916		2.641	
1.80	0.1357	0.3339	0.2862	0.1816	0.1065	0.0659	0.0471	0.0383	1.1952	
2.87	0.0513	0.1053	0.0930	0.0739	0.0553	0.0391	0.0268	0.0181	0.4628	
3.91	0.0267	0.0451	0.0422	0.0373	0.0318	0.0261	0.0212	0.0166	0.2470	

Triplet

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	$L=7$	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	0.9741	2.290	2.465	1.599	0.9568	0.6421	0.4924		9.419	20.11
1.80	0.4291	1.055	0.9303	0.6614	0.4150	0.2540	0.1639	0.1180	4.027	9.531
2.87	0.1564	0.3217	0.2907	0.2330	0.1780	0.1291	0.0907	0.0623	1.4619	3.945
3.91	0.0805	0.1366	0.1285	0.1143	0.0982	0.0810	0.0655	0.0524	0.7570	

section. The $1s-2s$ coupling approximation gives a value of $944\pi a_0^2$ at zero-incident energy, while the corresponding value in the Born approximation is $786\pi a_0^2$. The high value of this cross section at zero energy is in sharp contrast with its geometrical cross section. The zero energy $2s \rightarrow 2s$ cross section in the $1s-2s-2p$ coupling approximation, because of the r^{-2} potential, is difficult to find. The $2s \rightarrow 2s$ cross section has certain maxima and minima at low energy which is not found in the $1s \rightarrow 1s$ cross section. Figure 4 shows the $L=0$, singlet and triplet $2s \rightarrow 2s$ cross section in the two approximations. While there is one minimum in the $1s-2s$ coupling approximation there are three minima in the $1s-2s-2p$ coupling approximation. It is thought that the existence of these minima is due to a wider

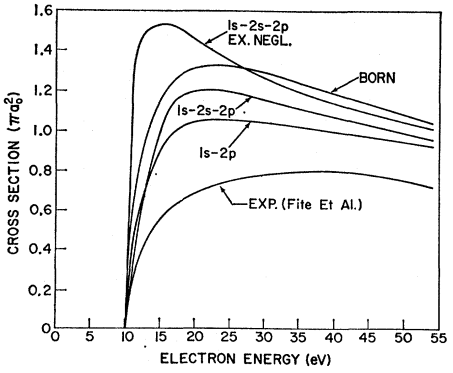

FIG. 5. $1s \rightarrow 2p$ total excitation cross section. $1s-2p$ refers to $1s-2p$ eigenstates coupling approximation. $1s-2s-2p$ has similar meaning. EX. NEGL. refers to exchange neglected case. BORN is the Born approximation. EXP. refers to experiment.

TABLE IV. $2s-2p$ excitation cross sections.

k_2	A. Born approximation								
	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	Σ	Q_T[a]
0.245	210.45	465.14	449.77	343.68	148.60	209.74	158.31	1985.69	13560
0.500	6.2469	30.729	57.561	64.948	54.469	49.590	40.391	303.935	3465.0
0.678	0.92003	6.6619	16.736	24.356	25.702	24.598	21.122	120.096	1930.9
0.831	0.24580	2.1480	6.4066	11.011	13.641	14.135	12.973	60.560	1308.4
1.225	0.02039	0.20887	0.78437	1.7481	2.7859	3.6015	3.9501	13.099	620.51
1.803	0.00187	0.01900	0.07823	0.20201	0.38645	0.59807	0.78354	2.0692	294.95
2.872	0.00011	0.00107	0.00444	0.01211	0.02545	0.04450	0.06688	0.15456	120.26
3.905	0.00002	0.00017	0.00067	0.00182	0.00389	0.00699	0.01096	0.02452	66.509

B. Exchange neglected $1s-2s-2p$ eigenstates couplings approximation

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	Σ	Q_T
0.245	5.311	12.59	23.21					41.11	12476
0.500	0.8651	10.55	1.143	18.92	26.25			57.73	3308.8
0.678	1.150	5.907	0.5760	7.168	12.28	14.46	15.08	56.62	1867.4
0.831	1.249	2.859	0.3831	3.158	6.664	8.591	9.391	32.295	1280.1
1.225	0.3847	0.4266	0.0881	0.4560	1.403	2.328	3.022	8.108	615.52
1.803	0.0654	0.0516	0.0142	0.0553	0.1846	0.3930	0.6183	1.3824	294.26

C. $1s-2s-2p$ eigenstates couplings approximation

Singlet

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	Σ_S
0.245	2.243	4.424	3.276					9.943
0.500	0.1241	1.605	1.348	6.360	7.159			16.596
0.678	0.0362	1.446	0.5518	3.056	3.693	3.911		12.694
0.831	0.1866	0.9881	0.2615	1.488	2.144	2.433	2.505	10.006
1.225	0.1048	0.1516	0.0384	0.1639	0.4584	0.7031	0.8529	2.473
1.803	0.0175	0.0157	0.0046	0.0148	0.0530	0.1108	0.1726	0.3890
2.872	0.0014	0.0010	0.0004	0.0010	0.0032	0.0075	0.0133	0.0278
3.905	0.0002	0.0002	0.0001	0.0002	0.0005	0.0012	0.0019	0.0043

Triplet

	$L=0$	$L=1$	$L=2$	$L=3$	$L=4$	$L=5$	$L=6$	Σ_T	$\Sigma_S+\Sigma_T$	Q_T
0.245	0.0000	10.40	56.74					67.14	77.083	12512
0.500	2.322	7.125	2.357	3.838	17.01			32.652	49.248	3300.3
0.678	1.590	2.363	0.3333	1.442	6.810	9.868		22.406	35.100	1867.0
0.831	0.9885	1.125	0.1226	0.8444	3.411	5.518	6.556	18.566	28.572	1276.4
1.225	0.2648	0.2173	0.0402	0.2297	0.7623	1.423	1.987	4.924	7.397	614.8
1.803	0.0455	0.0310	0.0094	0.0383	0.1223	0.2544	0.4070	0.9079	1.297	294.18
2.872	0.0040	0.0024	0.0009	0.0031	0.0095	0.0208	0.0359	0.0766	0.1044	120.21
3.905	0.0007	0.0004	0.0002	0.0005	0.0015	0.0035	0.0063	0.0131	0.0174	66.520

[a] $Q_T=\frac{72}{k_2^2}[14.8451-\mu+\ln k_2^2]$, $\mu=\frac{2}{7}\left(1-\frac{1}{\eta^7}\right)+\frac{1}{2}\sum_{n=1}^{5}\frac{1-\eta^{-n}}{n}+\frac{1}{2}\ln\eta$, $\eta=1+4k_2^2$ (Ref. 24).

potential range in the $2s\rightarrow 2s$ scattering, a case which does not exist in the $1s\rightarrow 1s$ scattering.[21a]

In Fig. 5 the four calculated curves for the $1s\rightarrow 2p$ excitation cross section are compared with the measurement of Fite, Stebbings, and Brackmann.[22,23] The $1s-2s-2p$ and the Born curves are the same as in Refs. 4(a), 4(b), but the $1s-2s-2p$ exchange neglected, and the $1s-2p$ curves are not calculated in these references. As concluded before, the calculated curves are higher than the experimental. Moreover, we notice that, similar to the $1s\rightarrow 2s$ excitation cross section, the inclusion of the exchange lowers the value of the cross section at threshold.

The calculation of the $2p\rightarrow 2p$ elastic cross section is more complicated than the cases so far considered. For a given total angular momentum L, the angular momentum of the partial wave which is scattered from the $2p$ state may be $L-1$, L, and $L+1$. The first and the third values correspond to a wave function which has the same parity as the wave functions in the $1s$ and the $2s$ channels. In this case $L-l_1-l_2$ is even. The second value corresponds to a wave function with a different parity, and the only process that occurs with this parity is the $2p$ elastic scattering. In this case $L-l_1-l_2$ is odd. We have calculated the $2p\rightarrow 2p$ cross sections for the two cases, and they are listed in Table III. The total cross section is shown in Fig. 6. Because of the r^{-2}

[21a] *Note added in proof.* Figures 2 and 4 show that in the $1s-2s-2p$ couplings if E_{n-1} and E_n represent the energy with respect to the threshold of the two neighboring maxima or minima then $E_n/E_{n-1}\cong$const. This may be attributed to the r^{-2} potential which is due to the coupling between the $2s$ and the $2p$ states. For further details see Ref. 21.

[22] W. L. Fite and R. T. Brackmann, Phys. Rev. **112**, 1151 (1958).

[23] W. L. Fite, R. F. Stebbings, and R. T. Brackmann, Phys. Rev. **116**, 356 (1959).

potential it is difficult to find the zero energy value of this cross section.

The $2s \rightarrow 2p$ transition cross section has application in some plasma, and stellar atmosphere, calculations. The total cross section using the Born approximation is given by Seaton.[24] In Table IV we list the partial cross section using the close couplings approximation. This table may be found useful in problems in which plasma shielding occurs; where only electrons with an impact parameter within a given range can induce the $2s \rightarrow 2p$ transition.

It may be noted that the cross sections for the inverse processes $2s \rightarrow 1s$, $2p \rightarrow 1s$, and $2p \rightarrow 2s$ may be calculated by Eq. (3.20) and the symmetry of the T matrix.

Tables for the processes $1s \rightarrow 1s$, $1s \rightarrow 2s$, $1s \rightarrow 2p$, and $2s \rightarrow 2s$ will not be given here as the most important cases have been reported by Burke, Schey, and Smith.[4(a)(b)] These tables in various approximations are given in Ref. 6.

In all tables listed here k_1 is the wave number in the $1s$, and k_2 is the wave number in the $2s$ or the $2p$ channels. The energy, in electron volts, of the incident electron in each channel is given by $E=13.6k^2$, where k could be k_1 or k_2. All cross sections are in units of πa_0^2. In Tables III and IV, $\sum$ is the sum of the partial cross sections calculated. The total cross section Q_T is obtained by adding the contribution of higher partial waves than those calculated using the regular Born approximation. This could easily be done with the help of the table of the Born approximation.

V. CONCLUSION

The noniterative technique employed here can be applied to a large class of problems containing exchange integrals. The method is particularly useful when exchange potential is comparable to direct potential, in which case the convergence of iteration is slow.

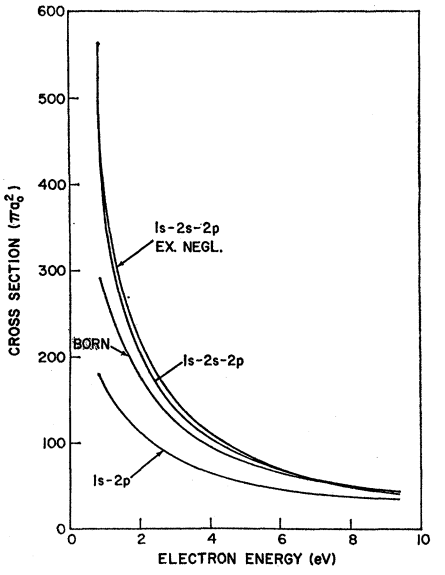

FIG. 6. $2p \rightarrow 2p$ total elastic cross sections. Curves are designated as in Fig. 5. The cross section at zero energy is finite but is not found here.

ACKNOWLEDGMENTS

The programming of the numerical integration of the radial differential equations on IBM-7090 computer has been performed by Edward Sullivan; through his meticulous and systematic programming the solution of the present problem has become available.

I am indebted to Dr. A. Temkin for many fruitful and illuminating discussions. I also wish to thank Professor Myers of the University of Maryland for a clarifying discussion.

APPENDIX I: ELEMENTS OF THE POTENTIAL MATRIX

(i) $L-l_1-l_2$ Even

Elements of D_{ij}

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

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

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

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

[24] M. J. Seaton, Proc. Phys. Soc. (London) A68, 457 (1955).

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

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

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

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

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

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

Elements of F_{ij}

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

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

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

$$F_{44}=\frac{3\beta}{2L+3}\left[\frac{1}{(2L+1)^2}\left(\frac{R_{21}}{r^L}\int_0^r R_{21}r'^{L+1}dr'-R_{21}r^{L+1}\int_0^r\frac{R_{21}}{r'^L}dr'\right)+\frac{L+2}{2L+5}\left(\frac{R_{21}}{r^{L+2}}\int_0^r R_{21}r'^{L+3}dr'-R_{21}r^{L+3}\int_0^r\frac{R_{21}}{r'^{L+2}}dr'\right)\right],$$

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

$$F_{21}=F_{12}[R_{10}\rightleftharpoons R_{20}],$$

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

$$F_{31}=F_{13}[R_{10}\rightleftharpoons R_{21}],$$

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

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

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

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

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

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

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

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

Elements of g_{ij} and h_{ij}

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

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

$$g_{33}{}^1=\frac{3\beta R_{21}r^{L+1}}{(2L-1)(2L+1)^2},\qquad h_{33}{}^1=\frac{R_{21}}{r^L},$$

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

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

$$g_{44}{}^2=\frac{3\beta(L+2)R_{21}r^{L+3}}{(2L+3)(2L+5)},\qquad h_{44}{}^2=\frac{R_{21}}{r^{L+2}},$$

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

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

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

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

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

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

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

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

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

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

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

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

(ii) $L-l_1-l_2$ Odd

$$D_{55}=-\left[\frac{1}{r}+\frac{3}{4}+\frac{r}{4}+\frac{r^2}{24}\right]e^{-r}-6\left[\frac{1}{r^3}-\left(\frac{1}{r^3}+\frac{1}{r^2}+\frac{1}{2r}+\frac{1}{6}+\frac{r}{24}+\frac{r^2}{144}\right)e^{-r}\right],$$

$$F_{55}=-\frac{3\beta}{2L+1}\left[\frac{1}{2L-1}\left(\frac{R_{21}}{r^{L-1}}\int_0^r R_{21}r'^L dr'-R_{21}r^L\int_0^r\frac{R_{21}}{r'^{L-1}}dr'\right)-\frac{1}{2L+3}\left(\frac{R_{21}}{r^{L+1}}\int_0^r R_{21}r'^{L+2}dr'-R_{21}r^{L+2}\int_0^r\frac{R_{21}}{r'^{L+1}}dr'\right)\right],$$

$$g_{55}{}^1=-\frac{3\beta R_{21}r^L}{(2L+1)(2L-1)},\qquad h_{55}{}^1=R_{21}\left[\frac{1}{r^{L-1}}-\frac{\frac{1}{4}+k_2{}^2}{2}\delta(L,1)r\right],$$

$$g_{55}{}^2=\frac{3\beta R_{21}r^{L+2}}{(2L+1)(2L+3)},\qquad h_{55}{}^2=\frac{R_{21}}{r^{L+1}}.$$

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

APPENDIX II: SINGULARITY OF THE DETERMINANT OF EQ. (2.17) FOR $L=0$ AND 1

(i) $L=0$ Case

By making use of the definition of D_{ij} and F_{ij} and Eq. (2.18), the following relation can be derived from Eq. (2.14):

$$\int_0^\infty\left[rR_{20}\left(\frac{d^2}{dr^2}+k_1{}^2\right)v_1-\beta rR_{10}\left(\frac{d^2}{dr^2}+k_2{}^2\right)v_2\right]dr=-\frac{2}{\sqrt{3}}[a_{13}B_{24}-\beta a_{23}B_{14}],\tag{II.1}$$

where the superscript μ is suppressed when there is only one value for μ and

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

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

Integrating the left-hand side of Eq. (II.1) by parts, and making use of Eqs. (2.11) and (2.18), we obtain

$$\int_0^\infty\left[rR_{20}\left(\frac{d^2}{dr^2}+k_1{}^2\right)v_1-\beta rR_{10}\left(\frac{d^2}{dr^2}+k_2{}^2\right)v_2\right]dr=-2[B_{21}-\beta B_{12}].\tag{II.4}$$

We conclude that

$$B_{21}-\beta B_{12}=\frac{1}{\sqrt{3}}[a_{13}B_{24}-\beta a_{23}B_{14}].\tag{II.5}$$

Equation (II.5) connects the right-hand sides of four equations of Eqs. (2.17) specified by $ij=21$, 12, 24, 14. A similar relation should hold among the left-hand sides of these equations. This in fact is the case and by making use of the first of Eqs. (2.18) it can be shown directly that equations similar to Eq. (II.5) hold among the elements of each column klv of the left-hand sides of Eqs. (2.17) specified by $ij=21$, 12, 24, 14. We conclude that one of the Eqs. (2.17) is linearly dependent on others and the determinant of Eqs. (2.17) is singular.

(ii) $L=1$ Case

Similar to the previous case, the following relation can be derived from Eqs. (2.14):

$$\int_0^\infty\left[rR_{21}\left(\frac{d^2}{dr^2}+k_1{}^2-\frac{2}{r^2}\right)v_1-\beta rR_{10}\left(\frac{d^2}{dr^2}+k_2{}^2\right)v_3\right]dr=-\tfrac{2}{3}[\beta a_{13}B_{11}+\beta a_{23}B_{12}-a_{13}B_{33}{}^1+\sqrt{2}(a_{13}B_{34}-\tfrac{3}{5}\beta a_{33}B_{14})],\tag{II.6}$$

where

$$a_{33}=\int_0^\infty R_{21}{}^2 r^4 dr=30. \tag{II.7}$$

Integrating the left-hand side of Eq. (II.6) by parts, and making use of Eqs. (2.11) and (2.18), we obtain

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2}+k_1{}^2-\frac{2}{r^2}\right)v_1-\beta r R_{10}\left(\frac{d^2}{dr^2}+k_2{}^2\right)v_3\right]dr=-2[B_{31}-\beta B_{13}]. \tag{II.8}$$

Combining Eqs. (II.6) and (II.8), we get

$$B_{31}-\beta B_{13}=\tfrac{1}{3}[\beta a_{13}B_{11}+\beta a_{23}B_{12}-a_{13}B_{33}{}^1+\sqrt{2}(a_{13}B_{34}-\tfrac{3}{5}\beta a_{33}B_{14})]. \tag{II.9}$$

Finally, Eqs. (2.14) give the following relation:

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2}+k_2{}^2-\frac{2}{r^2}\right)v_2-\beta r R_{20}\left(\frac{d^2}{dr^2}+k_2{}^2\right)v_3\right]dr=-\tfrac{2}{3}[\beta a_{23}B_{22}+\beta a_{13}B_{21}-a_{23}B_{33}{}^1+\sqrt{2}(a_{23}B_{34}-\tfrac{3}{5}\beta a_{33}B_{24})]. \tag{II.10}$$

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

$$\int_0^\infty \left[rR_{21}\left(\frac{d^2}{dr^2}+k_2{}^2-\frac{2}{r^2}\right)v_2-\beta r R_{20}\left(\frac{d^2}{dr^2}+k_2{}^2\right)v_3\right]dr=-2[B_{32}-\beta B_{23}], \tag{II.11}$$

whereupon we get

$$B_{32}-\beta B_{23}=\tfrac{1}{3}[\beta a_{23}B_{22}+\beta a_{13}B_{21}-a_{23}B_{33}{}^1+\sqrt{2}(a_{23}B_{34}-\tfrac{3}{5}\beta a_{33}B_{24})]. \tag{II.12}$$

Similar to the case $L=0$, Eqs. (II.9, 12) indicate that two of the Eqs. (2.17) are linearly dependent on others and the determinant of Eqs. (2.17) is singular.

To remove the singularity in $L=0$ case, one of the $C_{kl'}$ is chosen arbitrarily, and a degenerate equation is removed from Eqs. (2.17). Similarly, in the $L=1$ case two of the $C_{kl'}$ are chosen arbitrarily and two degenerate equations are removed from Eqs. (2.17).

APPENDIX III: ELEMENTS OF THE MATRIX OF THE SUM OF THE ASYMPTOTIC COULOMB AND CENTRIFUGAL POTENTIALS

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

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

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

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

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