Triple differential cross section for electron impact ionization of hydrogen atom

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Abstract.
The electron impact ionization of atomic hydrogen is calculated for incident electron energy 76.46 eV. The Hartree-Fock approximation is used to calculate the initial state which includes both bound and continuum wave functions. The final state continuum electron wave functions are obtained in the potential of hydrogen ion. The interaction between the two final state continuum electrons is approximated with the screening potential determined variationally.
1. Introduction

It is of fundamental importance to study triple differential cross sections for the ionization of atoms both theoretically and experimentally, as TDCS provide valuable information about the structure of atoms between the three bodies. Several studies have been performed earlier on several targets using different approximations. Hydrogen has been chosen for detailed investigation because of their simple structure. Among the various theoretical approaches, the convergent close coupling method (CCC), the time dependent close coupling (TDCC) method and the exterior complex scaling (ECS) approach are considered to produce accurate results. The multichannel R-matrix theory, the distorted wave method and the distorted partial wave approach also produce reliable results. The TDCS at low and intermediate energies are studied by Braunner et al. using the final state wave functions which is correct asymptotically.

Previously we investigated TDCS of H atom by electron impact at several incident energies for the simplified case when the two final state continuum electrons leave in the opposite direction using our extended MCHF method. The initial state is calculated in the HF approximation and the final state wave function are obtained in the HF and the variationally determined screening approximation for both equal and unequal sharing of excess energy by the two final state continuum electrons. Both HF and the SP results are found to be very close to each other indicating that when the two final state continuum electrons leave in the opposite direction. The results are found to be very good with relative experimental measurement and the other accurate calculations.

Non-perturbative methods e.g ECS, CCC, and TDCC approaches are known to provide more accurate results only for ionization of simple targets such as H and He than those provided by the SP approximation. Although nonpertubative methods can explain the experimental measurement very accurately but they have limitations for multi-electron targets or complex atoms. The application of the present, one of the perturbative approaches, on the otherhand, can be applied to multi- electron targets, when non-perturbative methods have difficulty.

The application of the present approach, one of the perturbative approaches for electron atom ionization provide a first step in testing ionization from complex targets for which non-perturbative methods have not been applied. So far, our calculations with the SP approximation are performed for a simple geometry when the two final state continuum electrons are leaving in the opposite direction. All calculations found that results obtained in the SP approximation provide very good results with the experiment and the other accurate calculation. As already mentioned, investigation on TDCS for electron impact ionization of H and He atoms using the HF and the SP approximation for $\theta_{12} = \pi$ symmetry have been reported. It has been found that the results are very encouraging. It was also found that in the case of H and He the electron correlation between the two final state continuum elecons are small when the two continuum electrons leave in the opposite direction. In this paper we investigated the application of the SP approximation to study the TDCS of H for incident electron energy 76.46 eV with two
The study of electron impact ionization of atoms has been the subject of fundamental interest and importance both theoretically and experimentally as they provide valuable information about the structure of atoms and electron dynamics between the three bodies. Several studies have already been made earlier on several targets using different approximations. Among many targets hydrogen and helium have been investigated in detail because of their simple nature. Theoretical few approximations which produce accurate results are the convergent close coupling (CCC) method [1], the time-dependent close coupling method [2] and the exterior complex scaling [3] approach. Few other theoretical methods which provide reliable results are the multichannel R-matrix theory [4], distorted wave method [5] and the distorted partial wave approach [6]. In addition, Braunner et al. [7, 8] used the exact asymptotically correct final state wave function to study triple differential cross section (TDCS) for electron impact ionization of H and He at low and intermediate energies. Temkin [9] studied theoretically the behavior of electron impact ionization of atoms by developing the Coulomb dipole theory. All these theoretical models paid their attention to improve the final state wave function more accurately. We reported [10, 11] earlier the results of our study for the TDCS of H by electron impact at several incident energies for the case when the two final state continuum electrons leave in the opposite direction using the Hartree-Fock (HF) and the Screening potential (SP) approximations. Recently we performed calculations on low energy electron impact ionization of helium atom using MCHF method [12]. In another recent paper [13], we considered target correlation and polarization effects on electron impact ionization of helium atoms. We found that polarization of the target by the incoming electron has considerable effects on the electron impact ionization of He atom. Experimentally, Ren et al. [14] has made both experimental and theoretical study on electron impact ionization of He by the 70.6 eV incident electron, which covers entire solid angle for the emitted electron and the collision kinematics. They compared the absolutely normalized triple differential experimental cross section with the theoretical calculation obtained by CCC and TDCC methods and found excellent agreement.

In this paper we are interested in the calculation of the TDCS of H at 76.46 eV incident energy for equal sharing of 62.86 eV excess energy. It is very important to calculate the initial and the final state wave functions accurately to obtain accurate TDCS. As mentioned earlier, most of the methods were designed mainly to treat the final state correlation accurately. In this work we have carried out calculation of the TDCS of H-target at 76.46 eV incident electron energy for the case when the two final state outgoing electrons share the 62.46 eV excess energy equally. The main purpose of this investigation is to test the screening potential approximation on TDCS at the incident energy and to compare our results with the available experimental and the other theoretical data. The final state interaction potential between the two final state continuum electrons is included using the variationally determined screening potential
2. Theory

A. Triple Differential Cross Sections

The description of the MCHF theory of electron impact ionization of atoms is provided in earlier papers [10, 11]. Briefly, the triple differential cross section for electron impact ionization of atoms is given by [6]

\[
\frac{d^3\sigma}{dE_2d\Omega_1d\Omega_2} = \frac{(2\pi)^4}{k^2} k_1 k_2 | < \Psi_f^- | V | \Phi_i^+ > |^2
\]

where \( \vec{k} \) is the momentum of the incident electron and \( \vec{k}_1 \) and \( \vec{k}_2 \) are the momenta of the two continuum electrons in the final state. \( \Phi_i^+ \) and \( \Psi_f^+ \) represent the initial and final state wave functions of the system respectively. \( E_i = \frac{k_i^2}{2} \) is the kinetic energy of the \( i^{th} \) final state continuum electron. The solid angles \( d\Omega_1 \) and \( d\Omega_2 \) are associated with the two final state continuum electrons. The perturbation \( V \) is the difference between the exact Hamiltonian and the approximate Hamiltonian used to construct and describe approximately the initial state \( \Phi_i^+ \) and is approximately defined as [6]

\[
V = \sum_{i=1}^{N} \frac{1}{|r_{N+1} - r_i|} - V_{HF}^{N+1}(r_{N+1})
\]

where the first term on the right hand side of this equation is the coulomb interaction between the incident electron and the N-target electrons and the second term is a multi-configuration Hartree-Fock approximation to this interaction which is used to construct the initial state \( \Phi_i^+ \). The initial state \( \Phi_i^+ \) is described by the orbital and spin angular momentum \( L_0 \) and \( S_0 \) of the target and by the momenta \( \vec{k} \) and orbital angular momentum \( l \) of the incident electron. The final state wave function \( \Psi_f^- \) is characterized by the orbital and spin angular momenta \( L_c \) and \( S_c \) of the (N-1) electron of the core ion and by the momenta \( \vec{k}_1 \) and \( \vec{k}_2 \) and by orbital angular momenta \( l_1, l_2 \) of the two continuum electrons.

Using the partial wave expansion of the incident electron and each of the two final state continuum electron wave functions we expand the initial state \( \Phi_i^+ \) and the final state \( \Psi_f^- \) wave function for the (N+1) electron system. The triple differential cross section then reduces to

\[
\sigma_{He}^{(3)} = \frac{4\pi}{k^2 |L_0||S_0|} \sum_S \sum_L |(2L + 1)A(LS\vec{k}_1\vec{k}_2)|^2
\]
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where

\[
A(LS\hat{k}_1\hat{k}_2) = \sum_{l_1l_2 m_1m_2} \sum_{l_1+l_2} e^{i(\delta_1+\sigma_1+\delta_2+\sigma_2)} 
\]

\[
\times \begin{pmatrix} l_1 & l_2 & L \\ m_1 & m_2 & 0 \end{pmatrix} Y_{l_1m_1}(\theta_1, \phi_1)Y_{l_2m_2}(\theta_2, \phi_2) < \psi_f | V | \psi_i > \tag{4}
\]

with \([x] = (2x+1)\)

\[
\psi_i \equiv \Psi_i((L_0l)LT(M_0\frac{1}{2}))ST(Ms)T,
\]

\[
\psi_f \equiv \Psi_f([L_{c}(l_1l_2)L]LT(M_0\frac{1}{2})S | ST(Ms)T)
\]

Here \(L\) and \(S\) are the orbital and spin angular momenta of the final-state continuum pair and \(L_T M_T\) and \(S_T M_{St}\) are the total orbital and spin angular momenta of the system.

B. Wave functions for the Continuum electrons

The multi-channel multi-configuration Hartree-Fock (MCHF) method is described earlier [15]. The total wave function in the HF approximation [11] at energy \(E = E_i + k^2/2\) and term value \(LS\) can be expressed as [15]

\[
\Psi_E = \Phi(\gamma_i L_i S_i; N)F_{k_1l_1} \tag{5}
\]

where \(\Phi(\gamma_i L_i S_i; N)\) represents \(N\)-electron target wave function having energy \(E_i\), configuration \(\gamma_i\) and the term \(L_i\) and \(S_i\) coupled with a single electron wave function \(F_{k_1l_1}\) having energy \(\frac{1}{2}k_1^2\) (in atomic units) and orbital angular momentum \(l_i\) to form an antisymmetric configuration for the \((N+1)\) electron system with a designated term value. The above wave function is defined in terms of a set of radial functions \(P_i(r), i = 1, \ldots, m\). As for example, \(F_{k_1l_1} = \frac{P_{r}(r)}{r}Y_{l_1m_1}(\theta_1, \phi_1)\chi_{ms}\) where \(Y_{l_1m_1}(\theta_1, \phi_1)\) is the spherical harmonic and \(\chi_{ms}\) is the spin function. The set of radial functions \(P_i(r), i = 1, \ldots, m_t\) describing the targets are obtained from the HF bound state calculations for the targets and are kept fixed. The set of radial functions describing the continuum orbitals are determined variationally. These radial functions are the solutions of the integro-differential equations of the form [15],

\[
\frac{d^2}{dr^2} + \frac{2Z}{r} - \frac{l_i(l_i+1)}{r^2} P_i(r) = \frac{2}{r}[Y_i(r)P_i(r) + X_i(r) + I_i(r)] + \sum_{\nu} \epsilon_{i\nu} P_{\nu}(r) \tag{6}
\]

which has the same form as the Hartree-Fock equation for a singly occupied orbital of a bound state system, the only difference being the specified binding energy, \(\epsilon_{ii} = \frac{k_i^2}{2}\) and the boundary condition at infinity.

In this equation \(\frac{2}{r}Y_i(r)\) is a part of direct potential, \(\frac{2}{r}X_i(r)\) is the exchange function and \(\frac{2}{r}I_i(r)\) represents terms arising from interactions between the configurations. The
off-diagonal energy parameter $\epsilon_{ii'}$ are related to Lagrange multipliers that ensure orthogonality between the continuum and the bound electrons of the target having the same symmetry. These operators have their usual meanings as for bound state problems.

In the single channel case, the radial function $P_i(r)$ satisfies the boundary conditions,

\[
P_i(r) \rightarrow r^{l_i + 1}, \quad P_i(r) \rightarrow \frac{2}{\pi k_i} \sin(k_i r - \frac{l_i \pi}{2} + \delta_i)
\]

if the target is an atom and

\[
P_i(r) \rightarrow r^{l_i + 1} \sqrt{\frac{2}{\pi k_i}} \sin(k_i r - \frac{l_i \pi}{2} + \frac{q}{k_i} \ln 2k_i r + \sigma_i + \delta_i)
\]

if the target is an ion. Here $\sigma_i = \arg[\Gamma(l_i + 1 - \frac{q}{k_i})]$ is the coulomb phase shift. $q = Z-N$ is the net charge of the ion.

The integro-differential equation (6) is solved numerically by the iterative method similar to the bound state problem. The self-consistent field procedure is applied to compute the continuum wave functions. The continuum radial function is normalized by fitting the computational values at two adjacent points to the regular and irregular Bessel or Coulomb functions depending on the target as soon as the region is reached where the direct and exchange potentials are vanishingly small. This may be at a considerably smaller value of $r$ than the asymptotic form represented by the boundary conditions specified in equations (7) and (8.).

3. Approximations used to calculate initial and the final state wave functions.

In this paper, we have considered the HF approximation to calculate the incident electron wave function. For the final state continuum electron wave functions the HF and the screening potential (SP) approximations are used.

Initial State: In the present case, the target considered is the hydrogen atom. We first calculated the initial state hydrogen atom wave function in the Hartree-Fock (HF) approximation. As already mentioned, the initial state wave function $\Phi_i^+$ is expanded in terms of antisymmetrized LS coupled wave function of the N electron target and the single electron wave function of the incident electron. The continuum radial wave functions are calculated by solving the integro-differential eqn(6) with the HF potential of the target hydrogen atom under the specified boundary conditions, where the target electron wave function is kept frozen at incident electron energy 76.46 eV for angular momentum from $l = 0$ to $l = 6$. 
Final State: To examine the effect of electron correlation in the final state, the final state continuum electron wave function is calculated in two approximations. (i) the HF approximation and (ii) the screening potential (SP) approximation. It should be mentioned that the screening potential approximation is an approximation to the actual Coulomb interaction potential between the two continuum electrons. It accounts for partial electron correlation. In the screening potential approximation the exact Coulomb interaction between the two continuum electrons in the final state is replaced by a variationally determined angle dependent screening potential due to mutual screening \[ \text{[16, 17]} \] of the nucleus by the ejected electrons using effective charges which satisfy proper asymptotic boundary conditions. On the other hand, in the HF approximation we ignored this interaction between the two final state continuum electrons. The difference between the wave functions calculated with these two approximations will determine the effect of distortion in the final state wave functions. The screening potential for the two continuum electrons are determined by the effective screening charges $\Delta_1$ and $\Delta_2$ which are obtained by the condition \[ \text{[6, 16, 17]} \]

$$\frac{Z_T - \Delta_1}{k_1} + \frac{Z_T - \Delta_2}{k_2} = \frac{Z_T}{k_1} + \frac{Z_T}{k_2} - \frac{1}{k_1 - k_2} \quad (9)$$

where $Z_T$ is the net asymptotic charge of the ionized target. The effective screening charges which satisfy the above relation are obtained as \[ \text{[6, 16, 17]}, \]

$$\Delta_i = \frac{(\vec{k}_i, \vec{k}_{ij})k_i}{k_{ij}^3} \quad (i = 1, 2). \quad (10)$$

where $\vec{k}_{ij} = \vec{k}_i - \vec{k}_j, j \neq i, \text{esium atom}$ with $k_{ij} = |\vec{k}_{ij}|$

The wave function for each of the final state continuum electrons in the SP approximation are calculated using the same numerical procedure as adopted in the multi-configuration Hartree-Fock method \[ \text{[13, 12]} \] for bound and continuum electrons at each relative angle between the two continuum electrons ejected at equal energy for the angular momentum $l = 0$ to $l = 6$ for the partial wave $L = 1 - 6$ and $S = 0 - 1$.

3. Results

In this case, we discuss the triple differential cross section for electron impact ionization of hydrogen atom with the initial state calculated in the HF approximation at 76.46 eV incident electron energy and the final state in the HF and the screening potential (SP) approximation with the excess energy 62.86 eV shared equally by the two final state continuum electrons at a scattered electron angle $\theta_1 = 30^0$ in both inplane and out of plane.

Equal energy: $E_1 = E_2 = 31.43eV$
Figure 1. Comparison of present triple differential cross sections of He in the scattering plane for equal energy sharing $E_1 = E_2 = 31.43\,eV$, as a function of ejected electron angle ($\theta_1$) for the scattered electron angle $\theta_1$ fixed at $\theta_1 = 30^0$.

Figure represents the TDCS calculated in the HF and the SP approximations for the 62.86 eV excess energy sharing equally between the two final state electrons in the scattering plane at fixed scattered electron angle $\theta_1 = 30^0$.

4. Conclusion

We studied the ionization of hydrogen atom by 76.46 eV electron in the HF and the SP approximation. We calculated the triple differential cross sections with the final state continuum electrons sharing 62.86 eV excess energy equally for a fixed scattered electron angle. We use HF approximation for the initial state and both HF and SP approximations for the final state. The interaction potential between the two final state continuum electrons is approximated by variationally determined screening potential. It only accounts for partial potential and can not be considered as a correct electron correlation between two final state continuum electrons. We could not compare the present results with experiment as the available experimental results are not reliable.

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References

[1] I. Bray, J. Phys. B 33, 581 (2000).
[2] J. Colgan, M.S. Pindzola, F.J. Robicheaux, D.C. Griffin, and M. Baertschy, Phys. Rev. A 65, 042721 (2002).
[3] T.N. Resigno, M. Baertschy, W.A. Isaacs and C.W. McCurdy, Science 280, 2474 (1999).
[4] K. Bartschat and P.G. Burke, J.Phys. B 20, 3191 (1987).
[5] D.H. Madison, R.V. Calhoun and W.N. Shelton, Phys. Rev. A 16, 552 (1977).
[6] Cheng Pan and A.F. Starace, Phys. Rev. Lett. 67, 185 (1991); Phys. Rev. A 45, 4588 (1992).
[7] M. Brauner, J.S. Briggs and H. Klar, J.Phys. B 22, 2265 (1989).
[8] M. Brauner, J.S. Briggs, H. Klar, J.T. Broad, T. Rosel, K. Jung and H. Ehrhardt, J.Phys. B 24, 657 (1991).
[9] A. Temkin, Phys. Rev. Lett. 49, 365 (1982).
[10] H.P. Saha, J.Phys.B 41, 055201 (2008).
[11] H.P. Saha, Phys. Rev. A 77, 062705 (2008).
[12] H.P. Saha, Phys. Rev. A 82, 042703(2010).
[13] Hari P. Saha, J. Phys. B 44, 065202 (2011).
[14] Ren et. al., Phys. Rev. A 83, 052711 (2011).
[15] H.P. Saha and D.J. Murray, J. Phys. B 38, 3015 (2005).
[16] M.R.H. Rudge and Seaton, Proc. Roy. Soc. London, A 283, 262(1965).
[17] S. Jetzke, J. Zaremba, and F.H.M. Faisal, Z.Phys. D 11, 63 (1989); F.H.M. Faisal, Atoms in Strong Fields, edited by C.A. Nicolaides, C.W. Clark and M.H. Nayfeh (Plenum, New York, 1990), pp 407-424.