(e, 2e) processes on Ne, Ar and Xe targets

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Abstract. Recently, there have been several attempts to explain the features of triple differential cross section (TDCS) for the (e, 2e) processes on inert targets Ne, Ar and Xe but there are still certain discrepancies in theoretical results and measurements, which require more theoretical efforts to understand the collision dynamics of these targets. We present in this paper the results of our modified distorted wave Born approximation (DWBA) calculation of TDCS for the ionization of Ne (2p), Ar (3p) and Xe (5p) targets. We modify the standard DWBA formalism by including the correlation-polarization potential (which is function of electron density) and compare our computed results with the available experimental and theoretical data. We observe that the polarization potential is able to improve the agreement with experimental results.

1. Introduction
Kinematically complete studies of electron-impact single ionization (i.e. (e, 2e) processes) of atoms and ions provide important information about target structure, target wavefunction and collision dynamics. Since the experiment of Ehrhardt et al. [1] extensive studies have been performed for the electron impact single ionization of hydrogen [2] and helium [3] atoms in different geometrical arrangements. Apart from hydrogen and helium atoms, (e, 2e) studies have been performed on a number of targets using different theoretical approaches (see review articles [4-7]). The study of (e, 2e) processes on heavier atoms, particularly noble gas atoms, has been a subject of recent interest as it introduces physical effects like exchange between active and passive electrons, target polarization etc. which are not evident from the ionization of lighter atoms. There have been numerous theoretical and experimental efforts to explain the trends of triple differential cross section (TDCS) of (e, 2e) processes on Ne, Ar and Xe targets (Waterhouse et al. (1998) [8], Haynes and Lohmann (2000, 2001a, 2001b) [9-11], Biava et al. 2002 [12], Haynes et al. (2003) [13], Stevenson et al. (2005, 2009) [14-15] and Stevenson and Lohmann (2006, 2008) [16,17]. Various theoretical studies have been done to describe the features of the measurement of TDCS in the above mentioned studies. Purohit et al. [18] reported the results of modified distorted wave Born approximation (DWBA) for the ionization from 3s shell of argon atom. Prideaux and Madison [19] have considered the treatment of exchange and post collision interaction (PCI) in the DWBA approach. The hybrid DWBA-R matrix (hereafter referred as DWB2-RM) has been applied to 3p and 3s shell ionization of argon [20], 2p shell ionization of neon [15] and 5p shell ionization of xenon target [15]. DWBA approach which included PCI by a simple Gamow factor (DWBA-G) has also been reported [15, 21]. The distorted wave and 3DW (three distorted wave) approaches [22] reported the results of (e, 2e) processes on Ar(3p). Recently Otranto (2009) [23] reported the results of TDCS for the ionization from the 3p shell of argon atom. All the
above mentioned theoretical studies have mixed degree of success in explaining the experimental trends of TDCS for Ne, Ar and Xe targets.

We report the results of our modified distorted wave Born approximation calculations (DWBACPE) for Ne (2p), Ar (3p) and Xe (5p) targets. We modify the standard DWBA formalism by inclusion of correlation-polarization potential as a function of electron density. We present the results of our DWBACPE calculations at incident electron energy 150 eV for Ne (2p) and Xe (5p) atoms and at incident electron energy 113.5 eV for Ar (3p) target. We compare the results of TDCS with the recent available measurements of Stevenson et al (2009) [15] for Ne (2p), Xe (5p) and Stevenson and Lohmann (2008) for Ar (3p) [17]. We also compare the results of our DWBACPE calculations with the recently available theoretical studies [15, 17].

2. Theory
The triple differential cross section for (e, 2e) process on a target may be written as

\[
\frac{d^3\sigma}{d\Omega_1 \, d\Omega_2 \, dE_i} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{\alpha \nu} |T(k_1, k_2, k_0)|^2
\]

with

\[
T(k_1, k_2, k_0) = \langle k_1 k_2 | T | \psi_{\alpha l} k_0 \rangle.
\]

The expression in Eq. (1) includes a sum over final and average over initial magnetic and spin state degeneracy. The T matrix in Eq.(1) is the reaction amplitude, it couples the initial states \(\psi_i\) and the final states. T includes interaction between the incident and target electrons and the nucleus. It is the part of the TDCS that is the subject of approximation. The T-matrix element which represent the ionization amplitude is conveniently written in terms of distorted waves as

\[
\langle k_1 k_2 | T | \psi_{\alpha l} k_0 \rangle = \langle X_1^{(-)}(k_1) X_2^{(-)}(k_2) | v_1 + v_3 - U | \psi_i X_0^{(+)}(k_0) \rangle
\]

The electron-electron potential \(v_3\) is responsible for ionization and U is the distorting potential. Use of orthogonality between orbital \(\psi_i\) and distorted wave for ejected electron eliminates \(v_1\) and \(U\) from the expression of T matrix element. As mentioned earlier the initial state \(\psi_i\) contains an electron bound to the atom core with separation energy \(E_b\). The distorted waves for the incident and scattered electrons, \(X_0^{(+)}(k_0)\) and \(X_1^{(+)}(k_1)\), respectively, are calculated in a potential \(U = \langle \psi_i | v_1 + v_3 | \psi_i \rangle\).

Equation (1) in terms of direct and exchange amplitudes may be written as

\[
\frac{d^3\sigma}{d\Omega_1 \, d\Omega_2 \, dE_i} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{\alpha \nu} \left( |f|^2 + |g|^2 - \text{Re}(f^* g) \right)
\]

where

\[
f = \langle X_1^{(-)}(k_1, r_1) X_2^{(-)}(k_2, r_2) | v_3 | X_0^{(+)}(k_0, r_1) \psi_{\alpha l}(r_2) \rangle,
\]

\[
g = \langle X_1^{(-)}(k_1, r_2) X_2^{(-)}(k_2, r_1) | v_3 | X_0^{(+)}(k_0, r_1) \psi_{\alpha l}(r_2) \rangle
\]

here \(v_3 = \frac{1}{|r_1 - r_2|}\) is the interaction potential between the incident and target electrons responsible for the ionization, \(X_0^{(+)}\) is the distorted wavefunction for the incident electron, \(X_1^{(-)}\) and \(X_2^{(-)}\) represent the distorted wavefunctions for the two outgoing electrons and each is orthogonalized with respect to
Equations (4) and (5) are direct and exchange amplitudes for ionization from the \( (n,l) \) shell of the target atom where \( \psi_{nl} \) is the corresponding target orbital from which ionization is taking place and \( n \) and \( l \) are the principal and orbital quantum number respectively. We have used Hartree-Fock orbitals of Clementi and Roetti [24] for \( \psi_{nl} \). The distorted wavefunction for the incident electron is generated in the equivalent local ground state potential of the atom whereas the distorted wavefunctions for the outgoing electrons are generated in the equivalent local ground state potential of the ion. For the work reported here we have made a careful check to ensure that the cross sections converge satisfactorily. The spin-averaged static-exchange potential [25] with the exchange potential taken in the equivalent local approximation is given as

\[
V_x(r) = 0.5[E_0 + V_D(r)] - \{[E_0 + V_D(r)]^2 - 2\pi \rho(r)^2\}^{1/2}
\]  

(6)

where \( \rho(r) \) is the electron density. The direct distorting potential \( V_D(r) \) for the incident electron is obtained from the target radial orbital \( u_{nl}(r) \) [26] as

\[
V_D(r) = -\frac{Z}{r} + \sum_{n,l} N_{nl} \int dr [u_{nl}(r')]^2 / r_+, \tag{7}
\]

where \( r_+ \) is the greater of \( r \) and \( r' \). The details about the integration of the radial matrix element are described by McCarthy [26] and we have not given here for brevity. The equivalent local ground state potential \( V_{00} \), which is the distorting potential, is the sum of exchange and direct potentials and is expressed as follows;

\[
U = V_0(r) + V_D(r), \tag{8}
\]

\[
U = V_D(r) + 0.5[E_0 + V_D(r)] - \{[E_0 + V_D(r)]^2 - 2\pi \rho(r)^2\}^{1/2}. \tag{9}
\]

We have modified the distorting potential (eq. (9)) used to calculate distorted waves \( X^{(+)} \) and \( X^{(-)} \) by addition of correlation-polarization potential \( V_{CP} \) to see the effect of electron correlation and target polarization on the trend of TDCS (DWBACPE calculations). The fundamental form of the short range correlation plus long range polarization potential may be approximated by means of local density functional theory (Padial and Norcross [27], Perdew and Zunger [28] and Yuan and Zhang [29]) as follows

\[
V_{CP}(r) = V_{SR}(r), \quad r \leq r_0
\]

\[
= -\frac{\alpha_d}{2r^2}, \quad r > r_0 \tag{10}
\]

where \( \alpha_d \) is dipole polarizability of the target and we have used short range correlation potential similar to [27].

3. Results and discussion

We present the results of triple differential cross section (TDCS) for electron impact ionization of Ne (2p) target in coplanar asymmetric geometry at incident electron energy 150 eV in Figure 1. We present the results of our standard DWBA and DWBACPE calculations by dash-dot-dotted and solid curves respectively. The other results plotted are DW2-RM (dashed curve) and DWBA-G (dotted curve) calculations [15]. The experimental results [15] (full circles) are shown for comparison. For a better comparison the DWBA-G results have been multiplied by a factor of 0.78 while plotting for Ne (2p) results. The experimental results have been normalized to the second binary lobe of our DWBACPE calculations for better comparison of TDCS shape since the absolute experimental results are not available. At scattering angle \( \theta_s = -15^0 \) a deep minimum in the binary peak region is observed (Fig. 1a) in the experimental data and all the theoretical calculations including present
DWBA calculations. This corresponds to signature of the p orbital momentum distribution in the Bethe ridge kinematics.

Figure 1: TDCS of Ne (2p) atom at incident electron energy $E_0 = 150$ eV and ejected electron energy $E_1 = 10$ eV at various scattering angles $\theta_1$. Solid curve is our DWBACPE calculation, dash dot dotted curve is the standard DWBA calculation, dashed curve is DW2-RM and dotted curve is DWBA-G calculations [15]. The experimental results [15] are shown by full circles.
The depth of minimum decreases as scattering angle is decreased from $\theta_1 = -15^0$ to $-10^0$ and further to $-5^0$. Our DWBA and DWBACPE calculations are able to produce good agreement with the direction of primary and secondary binary peaks but there is a shift in the direction of recoil peak. The DWBACPE calculations which include correlation-polarization potential are able to improve the agreement with the experimental data. The DW2-RM [15] calculations are able to produce better binary to recoil peak ratio but the direction of binary peaks are not as observed in the experimental data. The DWBA-G [15] calculations overestimate the recoil peak whereas underestimate the binary peak at the scattering angles $\theta_1 = -15^0$ and $-10^0$. Our DWBACPE results provide a good agreement in terms of direction of binary peak but there are still certain discrepancies in terms of direction of recoil peak and the binary to recoil peak ratio for the ionization of Ne (2p) target.

![TDCS of Ar (3p) atom](image)

Figure 2: TDCS of Ar (3p) atom at incident electron energy $E_0 = 113.5$ eV and ejected electron energy $E_1 = (a) 2$ eV and (b) 5 eV at various scattering angles $\theta_1$. Solid curve is our DWBACPE calculation, dash dot dotted curve is standard DWBA calculation, dashed curve is DW2-2st.-MC and dotted curve is 3DW calculations taken from [17]. The solid circles are experimental results of [10] and the open shapes are the results of [17].
The results of TDCS in the coplanar asymmetric (e, 2e) processes on Ar (3p) atoms are presented in Figure 2. The DWBACPE and standard DWBA calculations are depicted by the solid and dash-dot-dotted curves respectively. The other calculations plotted are DW2-2state-MC (dashed curve) and 3DW (dotted curve) taken from [17]. The solid circles are experimental results of [10] and the open shapes are experimental results of [17]. The experimental data have been normalized to our DWBACPE calculations at the secondary binary peak. We observe that at ejected electron energy 2 eV (Fig. 2a) the DWBACPE, standard DWBA and 3DW calculations are able to provide good agreement with both the binary peaks, however all of these calculations underestimate the dip near the momentum transfer direction. As it has been mentioned in the discussion of Ne (2p) ionization, the dip near the momentum direction is signature of ionization from p-orbital. It is interesting to observe that the inclusion of correlation-polarization potential improves the agreement with the measurements in the binary peak region. The agreement in the recoil peak direction is not so good in the present DWBACPE and standard DWBA calculations. We believe that that inclusion of PCI in the DWBA calculations may improve the agreement with the experimental results. The DW2-2state-MC calculation gives good agreement with the experimental results in the second binary peak region however it overestimates the first binary peak and the direction is also not correct. The DW2-2state-MC calculation gives better agreement in the recoil peak region in comparison to the other calculations at ejected electron energy 2 eV.

In case of ionization from the 3p shell of argon at ejected electron energy 5 eV (Fig. 2b) the present DWBACPE, standard DWBA and 3DW calculations are able to give nearly correct trend of TDCS in the binary peak region, however there are significant discrepancies in terms of magnitude and direction in the recoil peak region. The DW2-2state-MC calculation is able to produce most of the trends of TDCS at ejected electron energy 5 eV.

The results of triple differential cross sections (TDCS) for the electron impact ionization of Xe (5p) are presented in Figure 3. The results of our standard DWBA and DWBACPE calculations are depicted by dash-dot-dotted and solid curve respectively. The other results shown are DW2-RM (dashed curve) and DWBA-G (dotted curve) calculations [15]. The experimental results [15] (full circles) are also shown for comparison. The DWBA-G results have been multiplied by a factor of 1.35 for a better comparison. The experimental results have been normalized to the binary peak of our DWBACPE calculations for better comparison of TDCS shape. As in the case of ionization of Ne (2p) target, the ionization of Xe (5p) at $\theta_i = -15^\circ$ corresponds to the Bethe ridge condition. The trace of p-orbital momentum distribution is very weak for the Xe target at $\theta_i = -15^\circ$ and it disappears as scattering angle is reduced (Figs. 3b, 3c). Our DWBACPE calculations which include correlation-polarization potential give an improved agreement with the experimental data in the binary peak direction in comparison to standard DWBA and other available theoretical calculations. However, our calculations and all other available theoretical calculations underestimate the TDCS in the recoil peak region.

We have presented the results of TDCS of the (e, 2e) processes on Ne (2p), Ar (3p) and Xe (5p) targets in the modified distorted wave Born approximation formalism by including the correlation-polarization potential (as a function of electron density) in the standard DWBA formalism. We have also compared the results of our present calculations with the recent available theoretical and experimental results. We observe that there is mixed degree of agreement between various theoretical and experimental results. Particularly, our DWBACPE calculation is able to produce good agreement in the binary peak region for the ionization from Ar (3p) and Xe (5p) targets, however the agreement in case of ionization from Ne (2p) target is not so good. This may be due to increase in the polarizabilities from Ne to Ar and Xe targets so the effect of polarization potential on the trend of TDCS is more significant for Ar and Xe targets. We conclude that polarization of target is an important effect at the incident electron energies considered in the present investigation. Still there are certain discrepancies in the trend of TDCS of noble gas targets Ne, Ar and Xe which require further investigation of (e, 2e) processes on these targets. We strongly believe that the inclusion of PCI,
second order processes and better treatment of polarization phenomenon may improve the trends of TDCS.

Figure 3: TDCS of Xe (5p) atom at incident electron energy $E_0=150$ eV and ejected electron energy $E_1=10$ eV at various scattering angles $\theta_1$. Solid curve is our DWBACPE calculation, dash dot dotted
curve is the standard DWBA calculation, dashed curve is DW2-RM and dotted curve is DWBA-G calculations [15]. The experimental results [15] are shown by full circles.

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