Coplanar Doubly Symmetric (e, 2e) Process on Alkali Atoms

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Abstract
We have performed theoretical calculations for triple differential cross sections (TDCS) for the (e, 2e) process in doubly symmetric geometry at excess energies of 6, 10, 15, 20, 30, 40, 50 and 60 eV for lithium, and at selected excess energies 15, 20, 50 and 60 eV for sodium and potassium targets. The process has been described using distorted-wave Born approximation theory. Post-collision interaction is included through an angle-dependent effective charge model using two different approximations. Our theoretical results are found to qualitatively reproduce the reported experimental data.

1. Introduction
The TDCS for electron impact ionization of hydrogen and helium have been measured and studied now for more than three decades. Various methods, such as the convergent close-coupling method [1-5], exterior complex scaling method [6-8], hyperspherical R-matrix approach [9,10], time-dependent approach [11,12] and the distorted-wave Born approximation (DWBA) have been applied and tested [13]. The DWBA has been very successful and most widely used method [13-24]. The studies on electron impact ionization of heavier atoms are rather more involved and complex because of the presence of passive electrons. Due to this reason very few theoretical and experimental results for heavier atoms have been reported in the literature.

The most recent measurements of Murray [25] on the angular distribution of TDCS for (e,2e) on sodium and potassium for doubly symmetric kinematics in the excess electron energy range 6 - 60 eV have evoked fresh interest. These are first (e, 2e) results on alkali atoms. In the light of Murray's experiment [25] we have taken up this problem here in this paper and theoretically analyzed the (e, 2e) process in alkali atoms viz. Li, Na and K using DWBA theory. In the next section we briefly describe our DWBA calculation along with the procedure of including exchange distortion and post-collision interaction (PCI) in our study. The results are presented in Section (3).

2. Theory
The lithium, sodium and potassium atoms are monovalent and have been treated as single active-electron targets. In DWBA, the TDCS for the ionization of alkali atoms by electrons with energy $E_i$ (momentum $k_i$) can be defined in terms of direct ($f$) and exchange ($g$) amplitudes as follows.

$$\frac{d^3\sigma}{dE_i d\Omega_s d\Omega_b} = (2\pi)^4 \frac{k_x k_y k_z}{k_i} \left( \frac{1}{4} |f + g|^2 + \frac{3}{4} |f - g|^2 \right).$$

where
Here $\chi_a^{(-)}(r_0)\chi_b^{(-)}(r_0)$ are normalized final state distorted waves of the two outgoing electrons having momenta $k_a$ and $k_b$ respectively. These are eigenfunctions of the distorting potentials $U_a$ and $U_b$. The distorted wave for the incident electron, $\chi_i^{(+)}$ is normalized eigenfunction of the initial state distorting potential $U_i$, $\psi_i(r_i)$ is Hartree-Fock wave function of the valence electron of the target. Here $r_i$ and $r_0$ are respectively the position vectors of the projectile electron and the valence electron of the target with respect to the target nucleus. The energies are related by the conservation relation

$$E_i = I + E_a + E_b,$$  \hspace{1cm} (4)

where $I$ is ionization potential of the targets. The initial state distorting potential $U_i$ is the sum of the static potential $U_{\text{atom}}$ of alkali atoms as felt by the incident electron and local exchange potential $U_{\text{exch}}$ [26] given by

$$U_{\text{exch}} = \frac{1}{2}\left\{(E - V) - \left[(E - V)^2 + 8\pi \rho_0\right]\frac{\rho}{r}\right\},$$  \hspace{1cm} (5)

where $E = E_i$, $V(r) = U_{\text{atom}}(r)$ and $\rho_0 = \frac{1}{2}\sum_j |\phi_j|^2$. The summation is over all atomic electrons.

The PCI has been included through angle-dependent effective charges and we have used here two models to fix the effective charges. These are described below:

1. The first model which we have considered was suggested by Jones et al [16] (referred hereafter as JMS model). They have made the physical argument that each of the effective charges contains the interaction with the other electron and have obtained

$$Z_a = Z_b = 1 - \frac{1}{2\sin\left(\frac{\theta_{ab}}{2}\right)},$$  \hspace{1cm} (6)

for equal energy final state electrons ‘a’ and ‘b’. The angle $\theta_{ab}$ is the angular separation between these two electrons. We have also used this JMS model in our calculation on calcium [27].

2. Our second model referred to as the $R$ model has been proposed by Rudge [28] in his study for e-H scattering. It satisfies the Rudge-Seaton-Peterkop formula [29]. The effective charges in this model are given by

$$Z_j = 1 - \frac{|k_j|^3}{(k_a^2 + k_b^2)|k_a - k_b|}, \hspace{1cm} j = a, b,$$  \hspace{1cm} (7)
For the doubly symmetric kinematics as in the present case, this reduces to
\[ Z_a = Z_b = 1 - \frac{1}{4 \sin \left( \frac{\theta_{ab}}{2} \right)} \]  

(8)

Both the above models ensure a vanishingly small cross section as the angular separation \( \theta_{ab} \) goes to zero. It should however be noted that any model using effective charges shall lead to nonphysical result i.e. the effective charge vanishes whenever the contribution representing electron-nucleus interaction cancels the contribution coming from electron-electron interaction. This is because these effective charges lead to a radial force on the electrons whereas in the final state comprising of three charged particles, the force on the electrons is not radial.

The distorting potentials \( U_a \) and \( U_b \) are made to satisfy the following limiting physical conditions as in [16]
\[
U_a (r) = U_b (r) \rightarrow \begin{cases} - \frac{Z_a}{r} & \text{as } r \to \infty \\ - \frac{Z}{r} & \text{as } r \to 0 \end{cases}
\]

(9)

by using the combination
\[
U_a (r) = Z_a U_{ion} (r) + (1 - Z_a) U_{atom} (r).
\]

(10)

\( Z \) in Eq.(9) is target nuclear charge and \( U_{ion} \) in Eq.(10) is the static potential of residual ions. The distorting potentials \( U_a \) and \( U_b \) in the final channel have been constructed differently than the distortion potential in the initial channel as they need to satisfy the conditions at close encounter as well as mimic PCI. The exchange potential
\[
U_{exchf} = \frac{1}{2} \left\{ (E - V) - \left[ (E - V)^2 + 8 \pi \rho_c \right]^{0.5} \right\} + \frac{1}{2} \left\{ (E - V) - \left[ (E - V)^2 + (-1)^S \cdot 8 \pi \rho_v \right]^{0.5} \right\}
\]

(11)

is then added following Biava et al [30] to \( U_a \) (and \( U_b \)) with \( V= U_a \) or \( U_b \), \( E = E_a \) or \( E_b \), \( \rho_c = \frac{1}{2} \sum_j |\phi_j|^2 \) (the summation \( j \) refers here to core electrons only), \( \rho_v = |\phi_v|^2 \) and \( S=0(1) \) for singlet (triplet) scattering amplitude.

Finally the scattering amplitudes \( f \) and \( g \) are calculated by using the usual partial wave expansion for distorted waves and angular momentum algebra [21] in Eqs. (2) and (3) and the TDCS are obtained.

3. Results and Discussions

Figure 1 shows our results for potassium at selected excess energies 15, 20, 50 and 60eV using JMS and \( R \) models along with the experimental data of Murray [25]. The relative experimental data of Murray [25] have been normalized to our results at \( \theta_a = \theta_b = 90^0 \) where the two outgoing electrons and the residual ion are collinear. Further, in order to have a meaningful comparison and the same normalization of the experimental data with our theoretical results from both the models, we have multiplied our results of the JMS model by appropriate factors as given in the figure caption. Our results in both the models
broadly reproduce the general features such as a forward peak at $\theta \sim 45^\circ$ due to direct binary collision between the projectile and target electrons, a back-scatter peak at $\theta \sim 135^\circ$ which becomes weaker as the incident energy increases and an enhancement at $\theta \sim 90^\circ$ due to PCI which decreases as the energy of the outgoing electrons increase indicating decreasing importance of PCI effects. The results of the $R$ model show a better overall agreement with the experimental data. This suggests the importance of PCI effects and perhaps also the usefulness of the Rudge-Seaton-Peterkop condition [29].

Figure 1. Triple differential cross sections (in a.u.) for the ionization of potassium in the doubly symmetric kinematics at excess energies $E_{ex} = 15\text{eV}$ (a), $20\text{eV}$ (b), $50\text{eV}$ (c) and $60\text{eV}$ (d). Present results ($R$ model), present results ($JMS$ model) and experimental data of Murray [25] normalized to our $R$ model results at the scattering angle $\theta_a = \theta_b = 90^\circ$. The $JMS$ model results have been multiplied by factors given here for figures (a) 4.69, (b) 1.75, (c) 93.0 and (d) 108 such that the $JMS$ model results at $\theta_a = \theta_b = 90^\circ$ become equal to the corresponding $R$ model results. At $E_{ex} = 50\text{eV}$, the experimental data have been normalized to our theoretical model results at $\theta_a = \theta_b = 85^\circ$ for a better comparison.
Figure 2 presents a similar comparison of our results in the JMS and R models with the experimental data of Murray [25] for sodium. Again their relative measurements are normalized to our R model results at $\theta_a = \theta_b = 90^0$. The general features of the results are similar to those of potassium. The results in both the models qualitatively reproduce the general features of the angular distribution equally well. The binary peak here at $\theta = 45^0$ is broader as compared to that for potassium.

![Figure 2](image-url)

**Figure 2.** Same as in Fig. 1 but for sodium. The experimental data have been normalized to our $R$ model results at the scattering angle $\theta_a = \theta_b = 90^0$. The JMS model results have been multiplied by factors given here for figures (a) 0.654, (b) 0.642, (c) 0.781 and (d) 0.771 such that the JMS model results at $\theta_a = \theta_b = 90^0$ become equal to the corresponding $R$ model results.

Since there are no experimental results reported for the (e, 2e) process in lithium we have presented in figure 3, a comparison of our results in the JMS and R models only. We have shown our results in the range of excess energies 6-60 eV. From the figure we find that for lithium the two models do not give very different results as was seen for sodium and potassium, although the overall behavior of TDCS is similar as shown in figures 1 and 2. We hope that future experiments will be able to confirm our theoretical results for lithium.
4. Conclusion

Finally we conclude that our DWBA results are able to reproduce general features of the experimental data. Our results also show the importance of proper accounting of PCI effects. From our present calculation it seems that the $R$ model which shows better over all agreement with the experimental data describes the PCI effects better than the $JMS$ model.

Figure 3. Same as in Fig. 1 but for lithium at $E_{ex} = 6eV$ (a), 10eV (b), 15eV (c), 20eV (d), 30eV (e), 40eV (f), 50eV (g) and 60eV (h) (The results of the $JMS$ model are not multiplied by any factor).
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References
[1] Bray I and Stelbovics A T 1992 Phys. Rev. A 46 6995
[2] Bray I and Fursa D V 1996 Phys. Rev. A 54 2991
[3] Bray I 1997 Phys. Rev. Lett. 78 4721
[4] Bray I 1999 J. Phys. B 32 L119
[5] Bray I 2000 J. Phys. B: At. Mol. Opt. Phys. 33 581
[6] McCurdy C W, Rescigno T N and Byrum D 1997 Phys. Rev. A 56 1958
[7] Rescigno T N, Baertschy M, Isaacs W A and McCurdy C W 1999 Science 286 2474
[8] Baertschy M, Rescigno T N, Isaacs W A, Li X and McCurdy C W 2001 Phys. Rev. A 63 022712
[9] Malegat L, Selles P and Kazansky A K 1999 Phys. Rev. A 60 3667
[10] Malegat L, Selles P and Kazansky A K 2000 Phys. Rev. Lett. 85 4450
[11] Pindzola M S and Robicheaux F 1998 Phys. Rev. A 57 318
[12] Pindzola M S and Robicheaux F 2000 J. Phys. B: At. Mol. Opt. Phys. 33 L427
[13] Jones S and Madison D H 2000 Phys. Rev. A 62 042701
[14] Pan C and Starace A F 1991 Phys. Rev. Lett. 67 185
[15] Pan C and Starace A F 1992 Phys. Rev. A 45 4588
[16] Jones S, Madison D H and Srivastava M K 1992 J. Phys. B: At. Mol. Opt. Phys. 25 1899
[17] Rosel T, Roder J, Frost L, Jung K, Ehrhardt H, Jones S and Madison D H 1992 Phys. Rev. A 46 2539
[18] Pan C and Starace A F 1993 Phys. Rev. A 47 2389
[19] Whelan C T, Allan R J and Walters H R J 1993 J Physique 3 39
[20] Whelan C T, Allan R J, Rasch J, Walters H R J, Zhang X, Roder J, Jung K and Ehrhardt H 1994 Phys. Rev. A 50 4394
[21] Gupta S and Srivastava M K 1995 J. Phys. B: At. Mol. Opt. Phys. 29 323
[22] Rouet F, Tweed R J and Langlois J 1996 J. Phys. B: At. Mol. Opt. Phys. 29, 1767
[23] Haynes M A, Lohmann B, Prideaux A and Madison D H 2003 J. Phys. B: At. Mol. Opt. Phys. 36, 811
[24] Prideaux A and Madison D H 2003 Phys. Rev. A 67 052710
[25] Murray A J 2005 Phys. Rev. A 72 062711
[26] Furness J B and McCarthy J E 1973 J. Phys. B: At. Mol. Opt. Phys. 6 2280
[27] Chauhan R K, Srivasatava M K and Srivastava R 2005 Phys. Rev. A 71 032708
[28] Rudge M R H 2000 J. Phys. B: At. Mol. Opt. Phys. 33 1223
[29] Rudge M R H 1968 Rev. Mod. Phys. 40 564
[30] Biava D A, Saha H P, Engel E, Dreizler R M, McEachran R P, Haynes M A, Lohmann B, Whelan C T and Madison D H 2000 J. Phys. B: At. Mol. Opt. Phys. 35 293