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Coplanar (e, $3e$) differential cross-section of He atom

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Abstract. We present in this paper the results of our calculation of five-fold differential cross-section (FDCS) for $(e, 3e)$ process on He atom in low momentum transfer and high electron impact energy in shake-off mechanism. The formalism has been developed in Born approximation using plane waves, Byron and Joachain as well as Le Sech and correlated BBK-type wave functions respectively for incident and scattered, bound and ejected electrons. The angular distribution of FDCS of our calculation is presented in various modes of coplanar geometry and comparison is made with the available experimental data. We observe that the present calculation is able to reproduce the trend of the experimental data. However, it differs in magnitude from the experiment. The present theory does not predict four-peak structure in *summed mutual angle mode* for lower excess ejected electron energies. We also discuss the importance of momentum transfer, post-collision interaction (PCI) and ion participation in the $(e, 3e)$ process in constant θ_{12} mode.

Keywords. ($e, 3e$) Process; coplanar geometry; five-fold differential cross-section; shake-off mechanism.

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1. Introduction

The main objective of electron impact double ionization study of atoms, hereafter referred to as $(e, 3e)$ process, is to investigate the reaction mechanisms which are responsible for double ionization, structure of the target and electron–electron correlation in the bound as well as in the continuum states. The archetypal system for such a type of study is the He atom, which has the simplest two-electron configuration. The ($e, 3e$) study on He atom is an interesting problem as it involves three electrons and He^{2+} ion (which does not have any relevant internal structure) in the final channel which constitutes a pure four-body problem. The long range potential, which plays an important role in the interactions among these particles, makes the correct treatment of this many-body problem extremely difficult. Measurements of the coincidence angular distributions provide an essential insight in this problem. The measured quantity in ($e, 3e$) process is the five-fold differential cross-section (FDCS), whereas in the ($e, 2e$) process it is the triple differential cross-section (TDCS).

Three mechanisms are involved in the direct ejection of two target electrons: the shake-off (SO), the two-step 1 (TS1) and the two-step 2 (TS2) mechanisms. In the shake-off mechanism the incident electron interacts with one of the bound electrons and ejects it, the second electron is no longer an eigenstate of the target as there is a sudden change in the potential. This will induce the second electron to get ejected after a relaxation process [1,2]. The other two mechanisms (TS1 and TS2) in $(e, 3e)$ process involve interaction in two steps. The first step is common for the two mechanisms, in which the incident electron ejects one of the target electrons. The difference between the two mechanisms is in the second step. In the TS1 mechanism it is the ejected electron which ejects the other target electron whereas in the TS2 mechanism it is the scattered electron which ejects the other target electron [3].

Numerous theoretical studies of $(e, 3e)$ processes have been carried out on He atom [4–14], since the first measurement on Ar atom by Lahmam-Bennani *et al* [15]. Dal Cappello and Le Rouzo [4] have pointed out the importance of correlation in the final state in the $(e, 3e)$ process on He atom using orthogonalized plane and Coulomb wave functions for the ejected electrons. Berakdar and Klar [5] have investigated the dynamical and kinematical origins of the maxima and minima in the angular distribution of the FDCS using the wave function of Garibotti and Miragila [16] for the ejected electrons. Srivastava *et al* [6] have studied the FDCS for $(e, 3e)$ process on He atom in Bethe-ridge kinematics to show that it is very sensitive to the correlation of bound electrons. Popov *et al* [7] have investigated the $(e, 3e)$ process in the electron momentum spectroscopy (EMS) kinematics to understand the electron–electron correlation in the target. Defrance *et al* [8] have developed the theoretical formalism to compute the FDCS in the first Born approximation using Hylleraas-type wave function for the target atom and also obtained the expression for the total double ionization cross-section by analytic integration of the FDCS over solid angles of the outgoing electrons and energies of the ejected electrons.

The calculations performed by the workers [4–8] have been done for the kinematical arrangements of theoretical interest and have not been compared with the coincidence $(e, 3e)$ experiments. A number of workers [9–14] have developed theoretical formalism after the first measurement on He atom by Taouil *et al* [17] and also compared with the coincidence $(e, 3e)$ experiments. Lahmam-Bennani *et al* [9] have developed the formalism using correlated four-body final state wave function (C4FS) to interpret the experimental trend and origin of dips and peaks in the experimental data. Kheifets *et al* [10] have investigated the angular profile of FDCS for the $(e, 3e)$ process on He atom in convergent close-coupling (CCC) formalism and also discussed the similarities and differences between $(e, 3e)$ process and photo-double ionization (PDI). They also observed that the experimental four-peak structure in summed mutual angle mode is not reproduced by the CCC theory for $(4 + 4$ eV) excess ejected electron energies. Grin *et al* [11] have investigated $(e, 3e)$ process in the second Born approximation and showed the asymmetry in the angular profile of FDCS about the direction of momentum transfer. Lahmam-Bennani *et al* [12] measured the coplanar $(e, 3e)$ cross-section of He atom at 1 KeV and compared it with CCC and 3-Coulomb wave function (3C) theories. Khiefets *et al* [13] have compared the CCC theory and the 3C theory and pointed out that the difference between the 3C and CCC calculations is sensitive to the amount of momentum transfer to the target. The existence of the contribution from the higher order processes in the $(e, 3e)$ reaction has been suggested by Lahmam-Bennani *et al* [14] using double coincidence $(e, 3\text{-}1e)$ experiment on He atom at 640 KeV electron impact energy. Recently Muktavat and Srivastava [18]

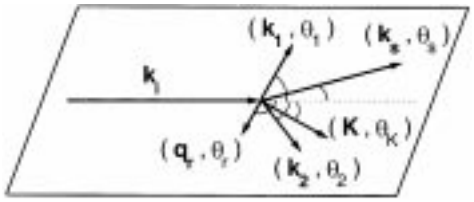

Figure 1. Schematic diagram of $(e,3e)$ process on He atom showing the momenta of the incident, scattered and ejected electrons 1, 2 and He^{2+} ion by $\mathbf{k_i}, \mathbf{k_s}, \mathbf{k_1}, \mathbf{k_2}$ and $\mathbf{q_r}$ respectively and θ_s, θ_1 and θ_2, θ_r and θ_K are the angles of the scattered, ejected electrons 1 and 2, He^{2+} ion and momentum transfer $\mathbf{K}$ with respect to the incident direction.

have studied FDCS on metastable para-helium He (2^1S) and ortho-helium He (2^3S) in various kinematical modes of coplanar geometry. The extensive study of $(e,3e)$ reaction on He atom [9–14,18] led Dorn *et al* [19,20] to perform new $(e,3e)$ experiments using electron-recoil–ion coincidence technique. Dorn *et al* [19] have not observed four-peak structure in the summed mutual angle mode in the kinematics close to the optical limit within the accessible range of the experiment.

In this paper, we present an outline of the theory to calculate five-fold differential cross-section (FDCS) in the shake-off mechanism for He target in §2. The formalism has been developed in Born approximation using plane waves, Byron and Joachain as well as Le Sech and correlated BBK-type wave functions respectively for incident and scattered, bound and ejected electrons. The results of the present calculation in *θ-variable, summed mutual angle, symmetric geometry*, and *constant* θ_{12} *modes* is presented in §3 and is also compared with the available experimental data. Finally, we summarise and discuss the results of our calculations in §4.

We depict in figure 1 the coplanar $(e,3e)$ process in an atom to explain the various symbols used in this communication and the momentum and energy conservation laws are expressed as

$$\mathbf{k_i} = \mathbf{k_s} + \mathbf{k_1} + \mathbf{k_2} + \mathbf{q_r} \tag{1}$$

and

$$E_i = E_s + E_1 + E_2 + \varepsilon_0^{++}(\mathrm{He}) \tag{2}$$

where E_i, E_s, E_1 and E_2 are the energies of the incident, scattered and ejected electrons 1 and 2, respectively and ε_0^{++} is the binding energy of two electrons of He (79 eV), while $\mathbf{k_i}, \mathbf{k_s}, \mathbf{k_1}$ and $\mathbf{k_2}$ are the momenta of the corresponding electrons and $\mathbf{q_r}$ is the recoil momentum of the target nucleus. Other kinematical parameters of interest are the total shared energy $E = E_s + E_1 + E_2$, shared momentum by the pair of the ejected electrons $\mathbf{K_R} = \mathbf{k_1} + \mathbf{k_2}$ and the momentum transfer $\mathbf{K} = \mathbf{k_i} - \mathbf{k_s}$.

2. Theory

We present in this section, the theoretical formalism to calculate the FDCS of $(e,3e)$ process in He atom under the conditions of high electron impact energy and small momentum transfer. The present formalism has been developed with the following assumptions:

1. The incident and scattered electrons are described by plane waves.
2. The bound electrons are described by the Byron and Joachain [21] as well as by Le Sech wave functions [22].
3. The ejected electrons are described by the correlated approximate BBK [23] type wave function with effective charges as given by Lahmam–Bennani *et al* [9].

The five-fold differential cross-section (FDCS) for the shake-off mechanism in first Born approximation is given as

$$\frac{\mathrm{d}^5\sigma}{\mathrm{d}\Omega_\mathrm{s}\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_1\mathrm{d}E_2} = (2\pi)^4\frac{k_\mathrm{s}k_1k_2}{k_\mathrm{i}}|T_\mathrm{fi}|^2, \tag{3}$$

where $\mathrm{d}\Omega_\mathrm{s}, \mathrm{d}\Omega_1$ and $\mathrm{d}\Omega_2$ are solid angle elements of scattered, first and second ejected electrons respectively and

$$T_\mathrm{fi} = \frac{-1}{2\pi^2}\cdot\frac{1}{K^2}\cdot M_\mathrm{fi}. \tag{4}$$

We can express M_fi as,

$$M_\mathrm{fi} = \langle\psi_\mathrm{f}^{\perp}(\mathbf{r_1},\mathbf{r_2})|\exp(i\mathbf{K}\cdot\mathbf{r_1}) + \exp(i\mathbf{K}\cdot\mathbf{r_2})|\psi_i(\mathbf{r_1},\mathbf{r_2})\rangle, \tag{5}$$

where $\mathbf{r_1}$ and $\mathbf{r_2}$ are the position vectors of the two ejected electrons with respect to the nucleus which is assumed to be located at the origin. We have used the target wave function $\psi_\mathrm{i}(\mathbf{r_1},\mathbf{r_2})$, given by Byron and Joachain (BJ) [21] and Le Sech wave function [22]. The analytic form of the BJ wave function is simple and is obtained by fitting it to the Hartree–Fock ground-state wave function:

$$\psi_\mathrm{i}(\mathbf{r_1},\mathbf{r_2}) = \phi_1(r_1)\cdot\phi_2(r_2), \tag{6}$$

where $\phi_\mathrm{i}(r_\mathrm{i}) = (4\pi)^{-1/2}(A\mathrm{e}^{\alpha r_\mathrm{i}} + B\mathrm{e}^{-\beta r_\mathrm{i}})$ and $A = 2.60505$, $B = 2.08144$, $\alpha = 1.41$ and $\beta = 2.61$.

The Le Sech wave function of He atom has two variational parameters and includes radial as well as angular correlation between the target electrons. The wave function has the following form:

$$\psi_\mathrm{i}(\mathbf{r_1},\mathbf{r_2}) = N\mathrm{e}^{-Zr_1}\mathrm{e}^{-Zr_2}[\cosh(\lambda r_1) + \cosh(\lambda r_2)][1 + 0.5\mathbf{r_{12}}\mathrm{e}^{-\mathbf{ar_{12}}}], \tag{7}$$

where $\lambda = 0.7$ and $a = 0.17$ and N is the normalization constant. We have dropped the angular correlation factor $\mathbf{r_{12}}$ in computing the matrix element (5), needed for evaluation of FDCS using analytically evaluated radial integrals. The ejected electrons are described by the correlated approximate BBK [23] type wave function which is orthogonalized to the initial state wave function and is given as

$$|\psi_\mathrm{f}^{\perp}(\mathbf{r_1},\mathbf{r_2})\rangle = |\psi_\mathrm{f}(\mathbf{r_1},\mathbf{r_2})\rangle - \langle\psi_\mathrm{i}(\mathbf{r_1},\mathbf{r_2})|\psi_\mathrm{i}(\mathbf{r_1},\mathbf{r_2})\rangle, \tag{8}$$

where

$$\psi_\mathrm{f}(\mathbf{r_1},\mathbf{r_2}) = \frac{C}{\sqrt{2}}[\psi_{\mathbf{k_1}}(z_1,\mathbf{r_1})\psi_{\mathbf{k_2}}(z_2,\mathbf{r_2}) + \psi_{\mathbf{k_2}}(z_2,\mathbf{r_1})\psi_{\mathbf{k_1}}(z_1,\mathbf{r_2})], \tag{8a}$$

$$C = \exp(-\pi\eta/2)\Gamma(1-i\eta) \tag{8b}$$

and $\eta = 1/|\mathbf{k_1} - \mathbf{k_2}|$, which takes into account the correlation between the ejected electrons.

The Coulomb wave function $\psi_{\mathbf{k}_j}(z_j, \mathbf{r})$, of the outgoing electron is given by

$$\psi_{\mathbf{k}_j}(z_j, \mathbf{r}) = C_1 \exp(i\mathbf{k}_j \cdot \mathbf{r}_j)\, {}_1F_1(i\alpha_j, 1, -i(k_j r + \mathbf{k}_j \cdot \mathbf{r})), \tag{9}$$

where $C_1 = (2\pi)^{-3/2}\Gamma(1 - i\alpha_j)\exp(-\pi\alpha_j/2)$ and ${}_1F_1(i\alpha_j, 1, -i(k_j r + \mathbf{k}_j \cdot \mathbf{r}))$ are the hypergeometric functions while $\Gamma(1 - i\alpha_j)$ is a gamma function and $\alpha_j = -Z_j/k_j$. The effective charges used [9] are given by the expressions

$$Z_1 = Z + \frac{Z}{2} \cdot \frac{k_1}{k_s} - \frac{k_1}{|\mathbf{k_s} - \mathbf{k_1}|}, \tag{10a}$$

$$Z_2 = Z + \frac{Z}{2} \cdot \frac{k_2}{k_s} - \frac{k_2}{|\mathbf{k_s} - \mathbf{k_2}|}. \tag{10b}$$

The matrix element M_{fi} (5) can be expressed in terms of the integrals of the following two types,

$$I_1 = \int \mathrm{e}^{i\mathbf{K}\cdot\mathbf{r}} \mathrm{e}^{-i\mathbf{k}_j\cdot\mathbf{r} - Cr}\, {}_1F_1(-i\alpha_j, 1, i(k_j r + \mathbf{k}_j \cdot \mathbf{r}))\mathrm{d}^3\mathbf{r}, \tag{11a}$$

and

$$I_2 = \int \mathrm{e}^{-i\mathbf{k}_j\cdot\mathbf{r} - Cr}\, {}_1F_1(-i\alpha_j, 1, i(k_j r + \mathbf{k}_j \cdot \mathbf{r}))\mathrm{d}^3\mathbf{r}. \tag{11b}$$

We calculate the matrix element (5) numerically using analytically evaluated integrals of the type (11a) and (11b) and for brevity, explicit expressions are not given here. The present theoretical model is similar to the one used by Defrance *et al* [8] except in the use of BJ and Le Sech wave functions and the effective charges as given by eqs (10a) and (10b). Further, Defrance *et al* [8] have used the model for calculating the total ionization cross-section of He-like ions while we use it in the calculation of FDCS in (*e*, 3*e*) reaction on He atom.

3. Results and discussion

In this section we present the results of our calculation of FDCS of (*e*, 3*e*) process on He atom in various modes in coplanar geometry. We display the angular profile computed using BJ and Le Sech wave functions by dashed and solid curves respectively in figures 2 – 7 (except in figures 4 and 5 where we use only Le Sech wave function). We also compare the results of the present calculations with the available experimental data [9,10,19], which is depicted by the symbol (•) in the figures.

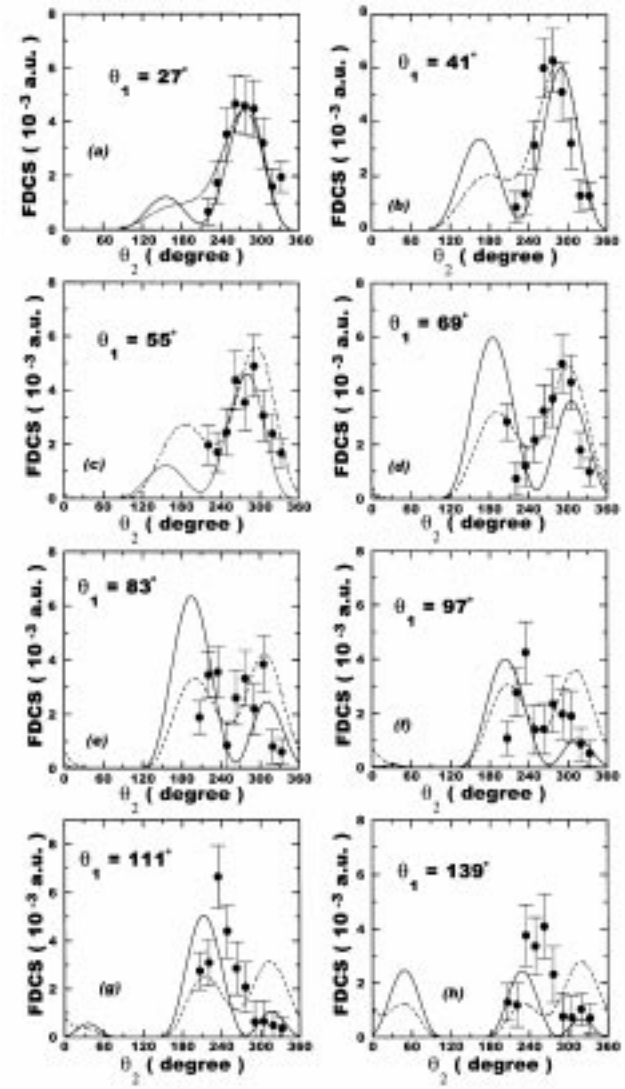

Figure 2. Five-fold differential cross-section (FDCS) is plotted as a function of θ_2 in θ_1-mode for He atom in coplanar geometry. The kinematics used in the depicted calculation is: $E_i = 5599$ eV, $E_s = 5500$ eV, $E_1 = E_2 = 10$ eV, $\theta_s = 0.45^\circ$ and θ_1 is given in each frame. The solid and dashed curves represent the results of our calculation using Le Sech and BJ wave functions, respectively and experimental data [9,10] by the symbol (•).

3.1 *θ-variable mode*

The experimental data [9,10] is available in θ-variable mode in which the angular profile of FDCS has been measured in two ways: in θ_1- as well as θ_2-modes. In the θ_1-mode, one

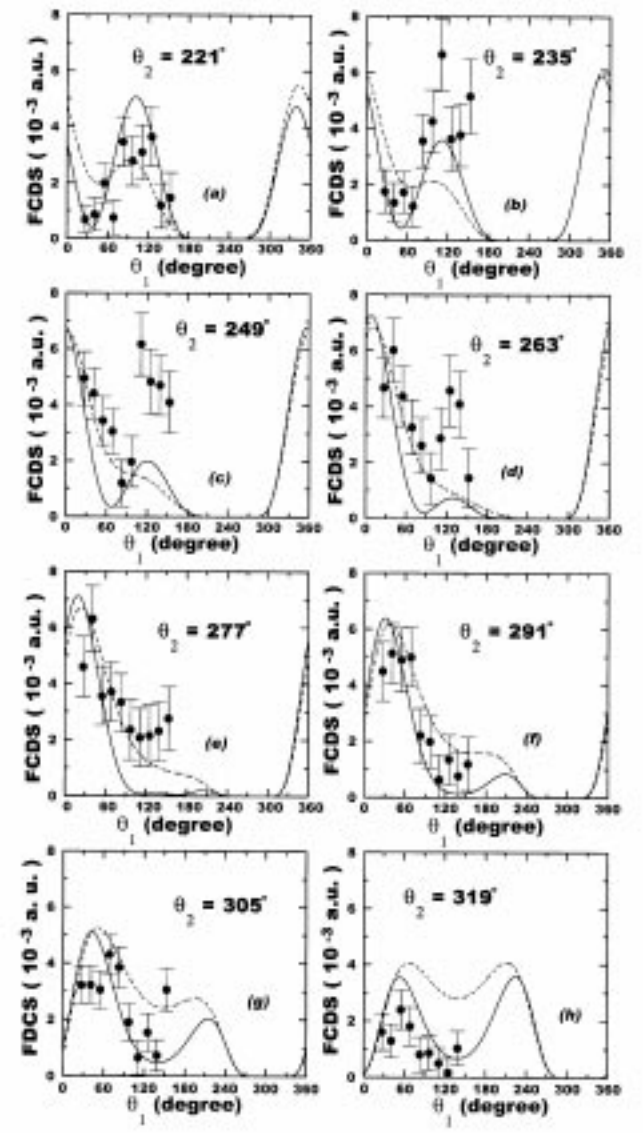

Figure 3. Same as in figure 2, but in θ_2-mode and keeping one of the ejected electrons fixed in the lower two quadrants.

of the two ejected electrons is kept fixed in the upper two quadrants ($27^\circ \leq \theta_1 \leq 139^\circ$) and the measured angular profile of FDCS is in the lower two quadrants ($200^\circ \leq \theta_2 \leq 360^\circ$) whereas in the θ_2-mode one of the ejected electrons is kept fixed in the lower two quadrants ($200^\circ \leq \theta_2 \leq 360^\circ$) and the measured angular profile of FDCS is in the upper two quadrants ($27^\circ \leq \theta_1 \leq 139^\circ$). We show the available experimental FDCS data for θ_1-mode

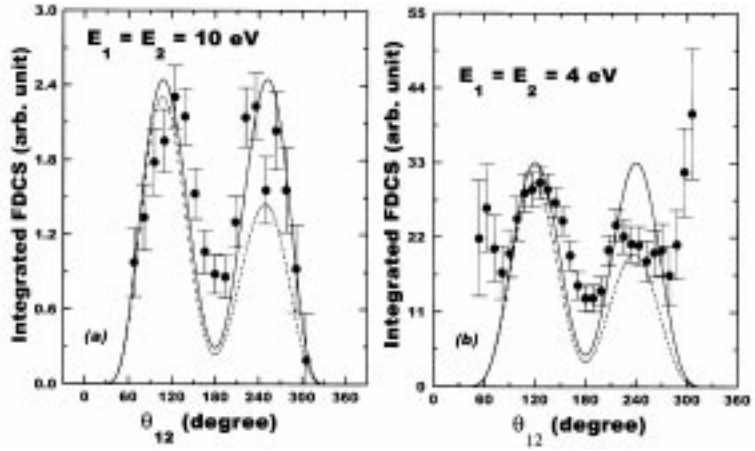

Figure 4. The angular behaviour of the integrated FDCS with mutual angle θ_{12} between the ejected electrons in summed mutual angle mode for (a) $E_i = 5599$ eV, $E_1 = E_2 = 10$ eV and (b) $E_i = 5587$ eV, $E_1 = E_2 = 4$ eV. Solid and dashed curves represent the results of the present calculation using Le Sech wave function in full and accessible angular range of the experiment [10]. The other kinematical parameters are: $E_s = 5500$ eV and $\theta_s = 0.45°$.

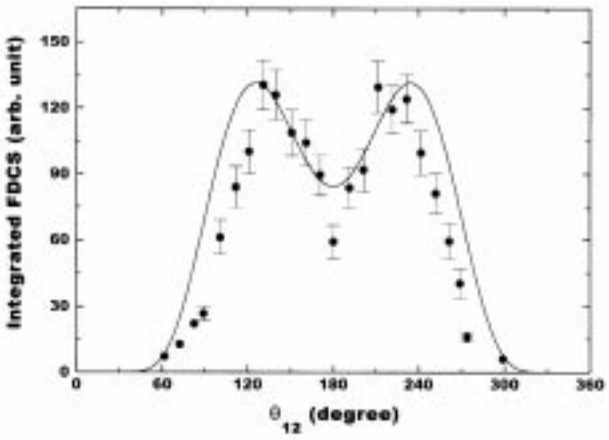

Figure 5. Same as in figure 4 except for the parameters $E_i = 2000$ eV, $E_s = 1911$ eV, $E_1 = E_2 = 5$ eV and momentum transfer $K = 0.6$ a.u. The experimental data from Dorn *et al* [19] has been depicted by the symbol (•).

in figure 2 and for θ_2-mode in figure 3 along with our calculation using two types of target wave functions (BJ and Le Sech wave functions). The trend of the angular distribution is well-described by the present theory (see figures 2 and 3). However, discrepancy exists in the magnitude of the cross-section and it is found to be very sensitive to the initial state description of the target. These observations are consistent with the previous findings of

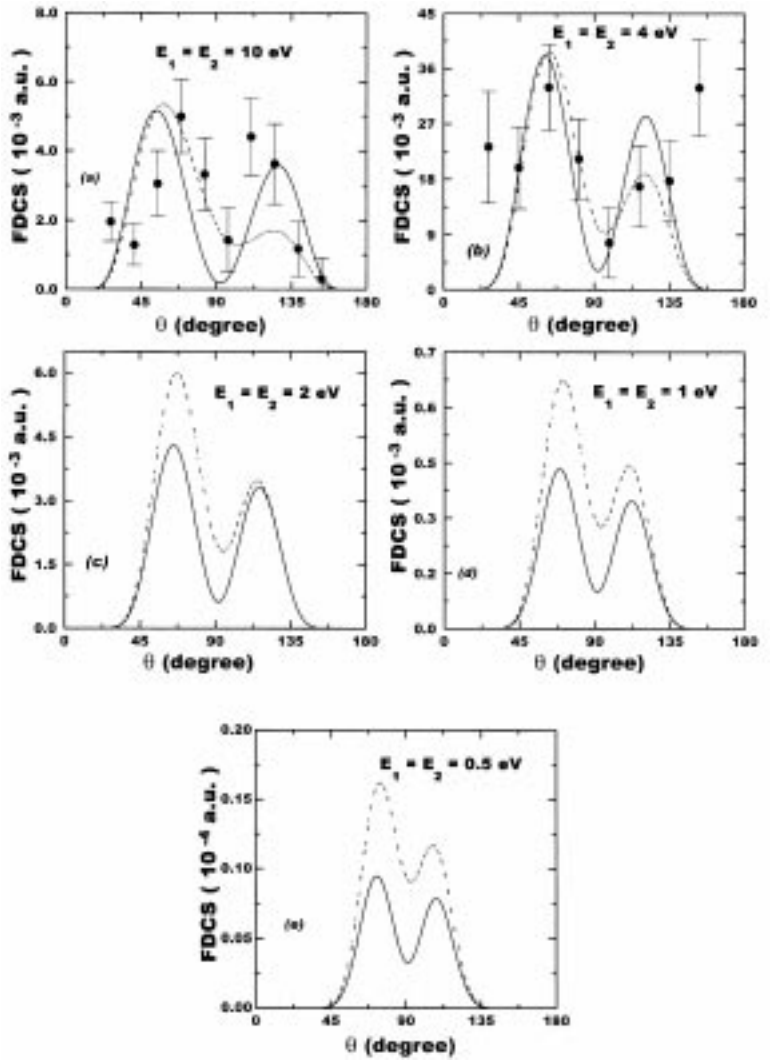

Figure 6. The angular behaviour of FDCS as a function of $\theta_1 = -\theta_2 = \theta$ in symmetric geometric mode with the symmetrically ejected electron energies shown in each frame. The kinematical parameters are: $E_s = 5500$ eV and $\theta_s = 0.45°$. The solid and dashed curves represent the results of our calculation using Le Sech and BJ wave functions, respectively and the experimental data [27] by the symbol (•).

Lahmam-Bennani *et al* [9] who have used Slater and Hylleraas wave functions in their studies. The depicted cross-sections in figures 2 and 3 have been scaled by $\frac{1}{2}$ and 3 respectively for calculations done using BJ- and Le Sech-type target wave functions. As in the present kinematics the momentum transfer is very small (0.24 a.u.), so it is natural to compare the present calculation with the photo-double ionization (PDI) process. In the PDI process on

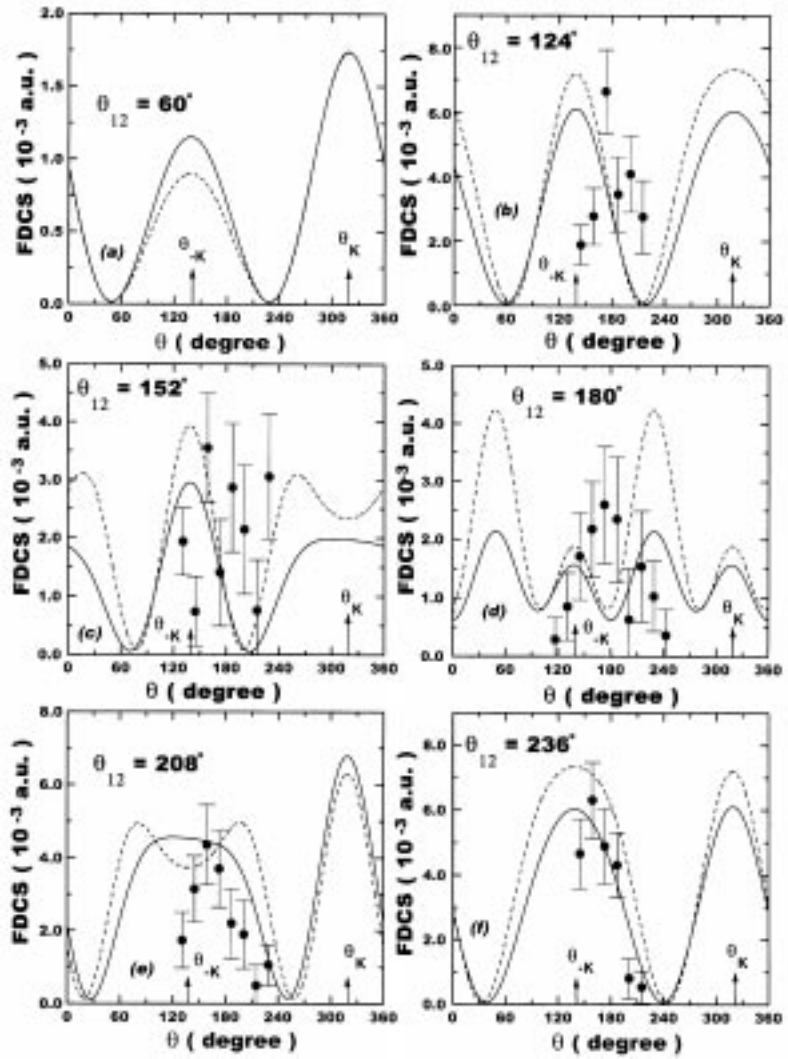

Figure 7. The angular behaviour of FDCS with the bisector angle θ in constant θ_{12} mode and θ_{12} is shown in each frame. The kinematical parameters are: $E_i = 5599$ eV, $E_s = 5500$ eV, $E_1 = E_2 = 10$ eV, $\theta_s = 0.45°$. The solid and dashed curves represent the results of our calculation using Le Sech and BJ wave functions, respectively and the experimental data [27] by the symbol (•).

He atom, the symmetrically energetic ejected electron pair in the same direction as well as in the opposite direction is prohibited. The explanation for non-emission of the electron pair in the same direction is trivial and is a direct consequence of the Coulomb repulsion between the electrons, which prohibits two electrons to get ejected in the same direction with the same energy whereas the dipole selection rule prohibits back-to-back emission of

the ejected electrons [24]. These rules restrict the angular profile of PDI to a two-peak structure. As expected, this two-peak structure is well-described in the present calculation of angular profile of FDCS of the (*e*, 3*e*) process (see figures 2 and 3) on He atom. However, the dipole selection rule is only approximated here and the node at $\theta_{12} = 180^\circ$ is filled by the non-dipolar contribution. We also observe that this contribution is different for different ejected electron angles. This has already been reported by Lahmam-Bennani *et al* [9] and Kheifets *et al* [10] in θ-variable mode and later we show the dependence of non-dipolar contribution with the angles of the ejected electrons in constant θ_{12} mode (figure 7d). It is found that for $\theta_1 = 139^\circ$ (i.e. opposite to the direction of the momentum transfer), this non-dipolar contribution create a small peak at the node point (figure 2h). We further observe that the height of the contribution of the node is sensitive to the choice of the initial state wave function and it is more in the case where the BJ wave function has been used instead of the Le Sech wave function. We also observe some discrepancy between the present theory and the experiments (see figures 2f, 3c, 3d and 3e) which suggests the incorporation of non-first Born processes in the theory. The importance of these processes have already been pointed out in the $(e, 3e)$ process on heavier noble gases [25,26] and recently on He atom [14].

3.2 *Summed mutual angle mode*

We present in this subsection the results of our calculation in summed mutual angle mode and the variation of the integrated FDCS as a function of mutual angle θ_{12}. The angular profile of the integrated FDCS with the mutual angle θ_{12} is depicted in figure 4 for excess ejected electron energies of $(10 + 10$ eV) as well as for $(4 + 4$ eV). The results of the present calculation is reminiscent of the two-peak structure in PDI process on He and also for a node at $\theta_{12} = 180^\circ$. The results of the present calculation for $(10 + 10$ eV) is found to be in good agreement with the experimental data of Kheifets *et al* [10]. However for lower excess ejected electron energies $(4 + 4$ eV), the present calculation is unable to reproduce two additional possible peaks around $\theta_{12} = 60^\circ$ and 320° as predicted by the experiment [10]. This disagreement remains even on performing the integrated FDCS calculation in the useful range of the experiment. The disagreement has also been reported by Kheifets *et al* [10] who have performed CCC calculation using first Born approximation (FBA). The present as well as CCC-type calculations are in the first Born approximation (although present calculation goes beyond FBA due to the use of effective charges, but its effect is very less on the profile [10]) and thus this disagreement may be attributed to the existence of higher-order processes in the double ionization mechanism. This disagreement led Dorn *et al* [19] to perform an experiment in this mode using the electron-recoil-ion coincidence technique. They have not observed any four-peak structure within the accessible angular range. We have also performed the calculation for the same kinematics as used by Dorn *et al* [19] and have not found four-peak structure in the integrated FDCS versus θ_{12} curve (see figure 5). The same type of behaviour is also observed in the CCC calculation done for full as well as in the accessible range of the experiment [19]. So the controversy remains and we suggest more theoretical studies beyond the first Born approximation to settle the disagreement.

3.3 *Symmetric geometry mode*

We have also investigated the angular behavior of FDCS in symmetric geometry mode in which the ejected electron angles $(\theta_1 = -\theta_2 = \theta)$ are varied symmetrically and our results are shown in figure 6. We have also compared the results of the present calculation with the unpublished experimental data of Lahmam-Bennani [27] for excess ejected electron energies of $(10 + 10$ eV) and $(4 + 4$ eV) and are shown in figures 6a and 6b. We observe that the present theory well describes the experimental trend and the scaled computed FDCS are within the error limits, especially the relative height of the two peaks. However, for lower excess ejected electron energies of $(4 + 4$ eV), the angular profile obtained by the present theory is unable to reproduce the experimental trend around $\theta = 25^\circ$ and 150°. This may be due to the existence of higher-order processes involved in the reaction dynamics, which has been reported [10] to play an important role for lower excess ejected electron energies. We have also performed the calculation for the lower excess ejected electron energies (i.e. from (2+2 eV) to (0.5+0.5 eV) and observed the following trend:

- We observe a two-peak structure and a node around $\theta = 90^\circ$. Thus we can conclude that both the ejected electrons are ejected either in the forward direction with respect to the incident direction (i.e. forward peak) or in the backward direction (i.e. backward peak). The node around $\theta = 90^\circ$ is similar to the one observed in PDI process wherein dipole selection rule prohibits electrons to get ejected in the back-to-back direction. However due to finite momentum transfer in (e, $3e$) process, the zero point at $\theta = 90^\circ$ gets filled by the non-dipolar contribution.
- We have also observed that the magnitude of the cross-section increases with the decrement of symmetrically ejected excess electron energies from 10 eV to 4 eV, while it decreases from 4 eV to 0.5 eV. This type of behaviour of FDCS with the energy demands further theoretical as well as experimental investigations as a function of excess ejected electron energies.

3.4 *Constant θ_{12} mode*

In the constant θ_{12} mode, the mutual angle between the ejected electrons is kept constant ($\theta_{12} = \theta_1 - \theta_2$ is constant) and the variation of the FDCS is investigated as a function of θ $(\theta = (\theta_1 + \theta_2)/2)$ from 0° to 360°. The results of the present calculation have been depicted in figure 7 for various constant θ_{12} angles and compared with the unpublished data of Lahmam-Bennani [27]. The kinematics used in the present studies is such that the escape angles are $\theta_{1,2} = \theta \pm (\theta_{12}/2)$ and for fixed scattering angle (θ_s) (which fixes the momentum transfer direction (θ_k)). The angular profile has been found to contain two peaks in most cases of constant θ_{12} angles, one in the direction of momentum transfer and the other in the direction opposite to momentum transfer. This means that the pair of ejected electrons has the tendency to get ejected either in the direction of momentum transfer (the so-called 'binary peak') or opposite to it (the so-called 'recoil peak'). Ejection of the pair of ejected electrons in the direction of momentum transfer or opposite to it is analogous to an (e, $2e$) process in which single electron tends to get ejected either in the direction of momentum transfer direction (binary peak) or in its opposite direction (recoil peak) with the scattered electron being in a fixed direction. The origin of 'binary'

and 'recoil' peaks can be understood if we concentrate ourselves to the shared momenta $\mathbf{K_R} = \mathbf{k_1} + \mathbf{k_2}$ carried by the pair of ejected electrons which is in the direction of θ for the case $|\mathbf{k_1}| = |\mathbf{k_2}|$. So the variation of FDCS with θ is equivalent to the variation of FDCS with the direction of shared momenta $\mathbf{K_R}$.

(i) When $\mathbf{K_R}$ is in the direction of $\mathbf{K}$ ($\mathbf{K} = \mathbf{k_1} + \mathbf{k_2} + \mathbf{q_r} = \mathbf{K_R} + \mathbf{q_r}$), the recoil momentum $q_r = K - K_R$ is minimum and the momentum carried out by the pair of ejected electrons is maximum. This results in the formation of 'binary peak' in the FDCS of the (e, 3e) process on He atom in the direction of momentum transfer.

(ii) When $\mathbf{K_R}$ is in the direction opposite to the direction of momentum transfer, the recoil momentum $q_r = K + K_R$ is maximum and hence the ion has an active role in the (e, 3e) process. This results in the recoil of the ejected electron pair by the massive ion and is directed opposite to the direction of momentum transfer (θ_{-K}). This will result in the formation of 'recoil peak' in the direction opposite to the direction of momentum transfer.

With the increment of θ_{12} from 0° to 180° (i.e. with the variation of post-collision interaction (PCI)), the magnitude of $\mathbf{K_R}$ decreases, i.e. the momentum carried by the pair of the ejected electrons decreases. This will result in the lesser dominance of the 'binary peak' over the 'recoil peak' with the increment of θ_{12}. Further the 'recoil peak' becomes almost equal to the 'binary peak' at $\theta_{12} = 124°$ and dominates for higher θ_{12} angles up to 180°. We have also observed that the FDCS is large for $\theta_{12} = 124°$, 152° and 236° (see figures 7b, 7c and 7f) in which the recoil peak plays an important role. This also strengthens the earlier comments made by Lahmam-Bennani *et al* [9] about the importance of the ion participation in the (e, 3e) process and less probability of free binary collision between the incident electron and the pair of ejected electrons in the optical limit.

The case $\theta_{12} = 180°$ is very interesting (see figure 7d) as it gives direct visualization of non-dipolar contribution with the escaping angles. We observe that the non-dipolar contribution to the FDCS exists for all escaping angles and it does not become zero for any value of θ. We further observe that the 'binary' and 'recoil' peaks get split and two additional peaks are formed and these two additional peaks are more pronounced as compared to the 'binary' and 'recoil' peaks. These additional peaks are located at $\theta = 49°$ and 229°, which corresponds to $\theta_1 = 139° = \theta_{-\mathbf{K}}$ and $\theta_2 = 319° = \theta_{\mathbf{K}}$ for $\theta = 49°$ and for $\theta = 229°$, $\theta_1 = 319° = \theta_{\mathbf{K}}$ and $\theta_2 = 139° = \theta_{-\mathbf{K}}$. So we conclude that the non-dipolar contribution is maximum when one electron is ejected in the direction of momentum transfer and simultaneously the other electron is ejected opposite to the momentum transfer direction.

If we closely observe the angular profile in this mode, we observe that there exists a symmetry about the direction of momentum transfer. This symmetry exists for any first Born approximation calculation. So breaking of symmetry about the direction of momentum transfer will indicate the role of higher-order projectile–target interactions (TS2 mechanism) in the (e, 3e) reaction. In the TS2 mechanism, the incident electron interacts with the bound electrons successively thus resulting in the transfer of momentum twice so that the symmetry about the direction of momentum transfer is destroyed. We have compared the results of the present calculation with the unpublished experimental data of Lahmam-Bennani [27] and found that for all the cases, the position of the 'recoil peak' in the experimental data is shifted towards higher angles. Recently, a similar type of shifting in the position of the recoil peak has been observed experimentally by Dorn *et al* [19]. Hence the present finding also supports the earlier observation made by them that the shift-

ing in the recoil peak indicates the possibility of the existence of higher-order processes in the (e, 3e) reaction on the heluim atom.

In summary, further experimental as well as theoretical efforts in this geometrical mode will elucidate the importance of the higher-order processes, active participation of the ion in the optical limit and the effect of post-collision interaction between the ejected electrons on the 'binary' and 'recoil' peaks.

4. Conclusions

We have performed theoretical calculation in first Born approximation to compute FDCS in (e, 3e) process on He atom under the conditions of high electron impact energy and low momentum transfer using approximated 3-Coulomb wave function approach. We conclude from the present studies of the (e, 3e) process on helium atom in the θ-variable mode that the present calculation can explain the trend of the angular profile of the experimental data. However, discrepancy exists in the magnitude of FDCS and also depends on the choice of the target wave function description. Our study also confirms the results of the earlier theoretical and experimental investigations that the non-dipolar contribution depends not only on the incident electron impact energy and momentum transfer direction but also on the direction of the ejected electrons.

Our theory, like CCC calculation, in FBA does not predict four-peak structure in summed mutual angle mode and is not in agreement with the experimental observations [10]. It may be mentioned that the four-peak structure has not been observed in the experiment of Dorn *et al* [19] within the accessible range of the experiment. So the resolution of this controversy demands new experiments as well as theoretical efforts beyond the first Born approximation. We observe the forward and backward peaks in the angular profile of FDCS in the symmetric geometry mode and we also observe that the backward peak plays an important role for lower excess ejected electron energies.

'Binary' and 'recoil' peaks like distribution has been observed in the angular profile of FDCS with the variation of the bisector angle of the constant mutual angle in constant θ_{12} mode. The origin of 'binary' and 'recoil' peaks is given in terms of the momenta shared by the pair of ejected electrons and we observe that the relative contribution from 'binary' and 'recoil' peaks depend on the variation of θ_{12} (i.e on the post-collision effect). We also confirm that the recoil peak plays an important role in the (e, 3e) process on He in the low momentum transfer condition with less possibilities for the free binary-like collision between the incident electron and the pair of ejected electrons. Comparison of the present results with the unpublished experimental data of Lahmam-Bennani [27] in the constant θ_{12} mode indicates the importance of higher-order projectile–target interactions for the present kinematics. Some discrepancies between theory and experiment demands the incorporation of higher-order processes in the present FBA calculation on the helium atom.

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