

# Ionization of Metastable 2P-State Hydrogen Atoms by Electron Impact for Coplanar Asymmetric Geometry

S. Dhar\*, N. Nahar

Department of Mathematics, Chittagong University of Engineering and Technology, Chittagong, Bangladesh

Email: \*[sdhar@cuet.ac.bd](mailto:sdhar@cuet.ac.bd), \*[sdhar03@yahoo.com](mailto:sdhar03@yahoo.com)

Received 15 September 2014; revised 9 October 2014; accepted 9 November 2014

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## Abstract

The triple differential cross-sections of First Born approximation have been calculated for ionization of metastable 2P-state hydrogen atoms by electron impact in the asymmetric coplanar geometry. In this study a multiple scattering theory of ionization of hydrogen atoms is used. The latest results of the present method are compared with other calculations. It will be added for new experimental study of ionization of hydrogen atoms in their metastable states.

## Keywords

Ionization, Scattering, Cross-Section, Electron

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## 1. Introduction

Atomic ionization of atoms by charged particles like electron or positron forms an important class of Atomic Physics. Accurate determination of cross-section results of various types such as single, double and triple differential with varied kinematics conditions [1]-[12] offers very interesting and challenging problems to Applied Mathematics. With the availability of new experimental results over the last four decades a new dimension has been added in this field of research such as Astrophysics, Plasma Physics and Fusion research technology. It now appears that the investigation of ionization from metastable 2S-state [13]-[15] hydrogen atoms and ionization of medium heavy atoms [16]-[19] as well as linear superposition of 2S- and 2P-state [20]-[22] of hydrogen atoms by charged particles is equally interesting and the time is not far off when experimental results will be available in this field. Lewis integral [23] is used in the present calculation. At present, beyond the First Born

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\*Corresponding author.

results there exists the second Born calculations [12] [21] for small momentum transfer asymmetric scattering at the intermediate incident energies 150 eV, 250 eV and 400 eV. Here we presented a few new sets of theoretical results following the multiple scattering theory [1] [9]. It may be noted that using this multiple scattering theory [1] [9] gives good cross-section results for the electron-atom ionization both in the ground state [9]-[12] and in the metastable 2S state [13]-[15] and many other calculations, the references of which are not given here. The energy spectrum of scattered electrons in the K-shell ionization of medium-heavy atoms by fast electrons is nicely represented [16]-[19] by the use of scattering state wave function of Das and Seal [1] [9] multiplied by a suitable spinor. So the present First Born results for ionization from the 2P state may also be expected to be good, interesting and significant. The present calculation reveals new features in the cross-section curves which may be confirmed by experiments. The physical origin of the findings of the different features is presented here.

## 2. Theory

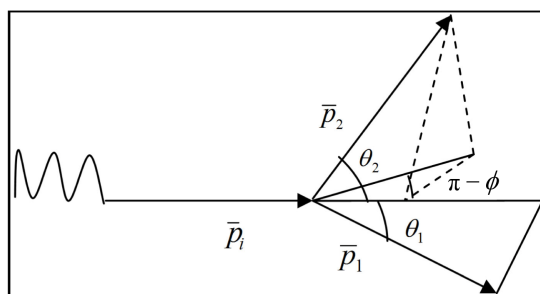
The most detailed information presently available about single ionization processes of the following type,



where, the symbol  $i$  denotes the initial state of the target, has been obtained in the coplanar geometry by analyzing triple differential cross sections (TDCS) measured in  $(e, 2e)$  coincidence experiments. The TDCS is a measure of the probability that in an  $(e, 2e)$  reaction an incident electron of momentum  $\bar{p}_i$  and energy  $E_i$  will produce on collision with the target two electrons having energies  $E_1$  and  $E_2$  and momenta  $\bar{p}_1$ ,  $\bar{p}_2$ , emitted respectively into the solid angles  $d\Omega_1$  and  $d\Omega_2$  centered about the directions  $(\theta_1, \phi_1)$  and  $(\theta_2, \phi_2)$ .

The TDCS is usually denoted by the symbol  $d^3\sigma/d\Omega_1 d\Omega_2 dE_2$ . For unpolarized incident electrons and targets, it is a function of the quantities  $E_i$ ,  $E_1$  or  $E_2$ ,  $\theta_1$ ,  $\theta_2$  and  $\phi = \phi_1 - \phi_2$ . By integrating the TDCS over  $d\Omega_1$ ,  $d\Omega_2$  or  $dE_2$  one can form various double and single differential cross sections. We will calculate the same. Finally, the total ionization cross section is obtained by integrating over all outgoing scattering angles and energies, and depends only on  $E_i$ , the incident electron energy.

It is useful when studying  $(e, 2e)$  coincidence experiments to distinguish between several kinematical arrangements, since these have important implications for the theoretical analysis of the collision as we shall see later. A first distinction can be made between coplanar geometries-such that the momenta  $\bar{p}_i$ ,  $\bar{p}_1$  and  $\bar{p}_2$  are in the same plane-and non-coplanar geometries such that the momentum  $\bar{p}_2$  is out of the  $(\bar{p}_i, \bar{p}_1)$  reference plane.



The kinematics of an  $(e, 2e)$  reaction. The incident electron momentum is  $\bar{p}_i$  and the momenta of the outgoing electrons are  $\bar{p}_1$ ,  $\bar{p}_2$  respectively. Also shown are the angles  $\theta_1$  and  $\theta_2$  with respect to the incident direction and the angle  $\pi - \phi$  measuring the direction in coplanar situation.

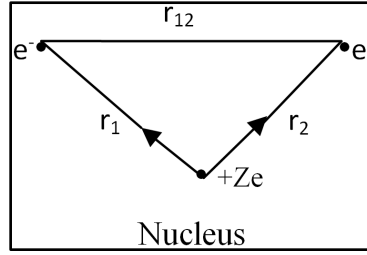
The multiple scattering theory of ionization of hydrogen atoms by electrons is described in detail [1] [11] [12] [14]. Here we will describe the method very briefly, for the particular case of hydrogenic 2P states at intermediate and high energies. The direct T-matrix element for ionization of hydrogen atoms by electrons, may be written as,

$$T_{fi} = \langle \Psi_f^{(-)}(\bar{r}_1, \bar{r}_2) | V_i(\bar{r}_1, \bar{r}_2) | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \quad (2)$$

where, the perturbation potential  $V_i(\bar{r}_1, \bar{r}_2)$  is given by,

$$V_i(\bar{r}_1, \bar{r}_2) = \frac{1}{r_{12}} - \frac{Z}{r_2}$$

for hydrogen atom nuclear charge ( $Z=1$ ),  $r_1$  and  $r_2$  are the distances of the two electrons from the nucleus and  $r_{12}$  is the distance between the two electrons.



Interaction between two electrons and nucleus.

The initial channel unperturbed wave function is,

$$\Phi_i(\bar{r}_1, \bar{r}_2) = \frac{e^{i\bar{p}_i \cdot \bar{r}_2}}{(2\pi)^{3/2}} \varphi_{2p}(\bar{r}_1) = \frac{e^{i\bar{p}_i \cdot \bar{r}_2}}{8\sqrt{2}\pi^2} r_1 \cos \theta e^{-\bar{r}_1 \lambda_i} \quad (3)$$

where,  $\varphi_{2p}(\bar{r}_1) = \sqrt{\frac{1}{32\pi}} \bar{r}_1 \cos \theta e^{-\bar{r}_1/2} = \sqrt{\frac{1}{32\pi}} \bar{r}_1 \cos \theta e^{-\lambda_i \bar{r}_1}$  is the hydrogenic  $2p$  wave function,  $\bar{p}_i$  is the incident electron momentum, and  $\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$  is the final three-particle scattering state with the electrons being in the continuum with momenta  $\bar{p}_1$ ,  $\bar{p}_2$ . Co-ordinates of the two electrons are taken to be  $\bar{r}_1$  and  $\bar{r}_2$ . Here  $\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$  is approximated by a wave function  $\psi_f^{0(-)}$  is given by [1],

$$\psi_f^{0(-)}(\bar{r}_1, \bar{r}_2) = N(\bar{p}_1, \bar{p}_2) \left[ \varphi_{\bar{p}_1}^{(-)}(\bar{r}_1) e^{i\bar{p}_2 \cdot \bar{r}_2} + \varphi_{\bar{p}_2}^{(-)}(\bar{r}_2) e^{i\bar{p}_1 \cdot \bar{r}_1} + \varphi_{\bar{p}}^{(-)}(\bar{r}) e^{i\bar{p} \cdot \bar{R}} - 2e^{i\bar{p}_1 \cdot \bar{r}_1 + i\bar{p}_2 \cdot \bar{r}_2} \right] / (2\pi)^3 \quad (4)$$

where,

$$\bar{r} = \frac{\bar{r}_1 - \bar{r}_2}{2}, \quad \bar{R} = \bar{r}_1 + \bar{r}_2, \quad \bar{p} = (\bar{p}_2 - \bar{p}_1), \quad \bar{P} = \bar{p}_2 + \bar{p}_1$$

The normalization constant  $N(\bar{p}_1, \bar{p}_2)$  is given by,

$$|N(\bar{p}_1, \bar{p}_2)|^{-2} = \left| 7 - 2[\lambda_1 + \lambda_2 + \lambda_3] - \left[ \frac{2}{\lambda_1} + \frac{2}{\lambda_2} + \frac{2}{\lambda_3} \right] + \left[ \frac{\lambda_1}{\lambda_2} + \frac{\lambda_1}{\lambda_3} + \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{\lambda_3} + \frac{\lambda_3}{\lambda_1} + \frac{\lambda_3}{\lambda_2} \right] \right| \quad (5)$$

where,

$$\begin{aligned} \lambda_1 &= e^{\pi\alpha_1/2} \Gamma(1 - i\alpha_1), & \alpha_1 &= 1/p_1, \\ \lambda_2 &= e^{\pi\alpha_2/2} \Gamma(1 - i\alpha_2), & \alpha_2 &= 1/p_2, \\ \lambda_3 &= e^{\pi\alpha/2} \Gamma(1 - i\alpha), & \alpha &= -1/p. \end{aligned}$$

Here  $\phi_q^{(-)}(\bar{r})$  is the Coulomb wave function given by,

$$\phi_q^{(-)}(\bar{r}) = e^{\pi\alpha/2} \Gamma(1 + i\alpha) e^{iq \cdot \bar{r}} F_1(-i\alpha, 1, -i[qr + \bar{q} \cdot \bar{r}])$$

where,

$$\alpha_1 = \frac{1}{p_1} \text{ for } \bar{q} = \bar{p}_1, \quad \alpha_2 = \frac{1}{p_2} \text{ for } \bar{q} = \bar{p}_2 \text{ and } \alpha = -\frac{1}{p} \text{ for } \bar{q} = \bar{p}.$$

Now applying Equations (3) and (4) in Equation (2), we get

$$T_{fi} = T_B + T'_B + T_i - 2T_{PB} \quad (6)$$

where,

$$T_B = \left\langle \phi_{p_1}^{(-)}(\bar{r}_1) e^{i\bar{p}_2 \cdot \bar{r}_2} |V_i| \Phi_i(\bar{r}_1, \bar{r}_2) \right\rangle \quad (7)$$

$$T'_B = \left\langle \phi_{p_2}^{(-)}(\bar{r}_2) e^{i\bar{p}_1 \cdot \bar{r}_1} |V_i| \Phi_i(\bar{r}_1, \bar{r}_2) \right\rangle \quad (8)$$

$$T_i = \left\langle \phi_p^{(-)}(\bar{r}) e^{i\bar{p} \cdot \bar{R}} |V_i| \Phi_i(\bar{r}_1, \bar{r}_2) \right\rangle \quad (9)$$

$$T_{PB} = \left\langle e^{i\bar{p}_1 \cdot \bar{r}_1 + i\bar{p}_2 \cdot \bar{r}_2} |V_i| \Phi_i(\bar{r}_1, \bar{r}_2) \right\rangle \quad (10)$$

For First Born approximation, we will calculate  $T_v$  matrix amplitude of Equation (7) using [8],

$$\begin{aligned} T_B &= \frac{1}{8\sqrt{2}\pi^2} \left\langle \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2 \cdot \bar{r}_2} \left| \frac{1}{r_{12}} - \frac{1}{r_2} \right| e^{i\bar{p}_i \cdot \bar{r}_2} r_1 \cos \theta e^{-\lambda_1 r_1} \right\rangle \\ &= \frac{1}{8\sqrt{2}\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2 \cdot \bar{r}_2} \left( \frac{1}{r_{12}} - \frac{1}{r_2} \right) e^{i\bar{p}_i \cdot \bar{r}_2} r_1 \cos \theta e^{-\lambda_1 r_1} d^3 r_1 d^3 r_2 \\ &= \frac{1}{8\sqrt{2}\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2 \cdot \bar{r}_2} \frac{1}{r_{12}} e^{i\bar{p}_i \cdot \bar{r}_2} r_1 \cos \theta e^{-\lambda_1 r_1} d^3 r_1 d^3 r_2 \\ &\quad - \frac{1}{8\sqrt{2}\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2 \cdot \bar{r}_2} \frac{r_1}{r_2} e^{i\bar{p}_i \cdot \bar{r}_2} \cos \theta e^{-\lambda_1 r_1} d^3 r_1 d^3 r_2. \end{aligned}$$

After analytical calculation by using the Lewis integral [23], we evaluated these expressions numerically using Gaussian quadrature formula. The triple differential cross-section (TDCS) is finally given by

$$\frac{d\sigma}{d\Omega_1 d\Omega_2 dE_2} = \frac{P_1 P_2}{P_i} |T_{fi}|^2 \quad (11)$$

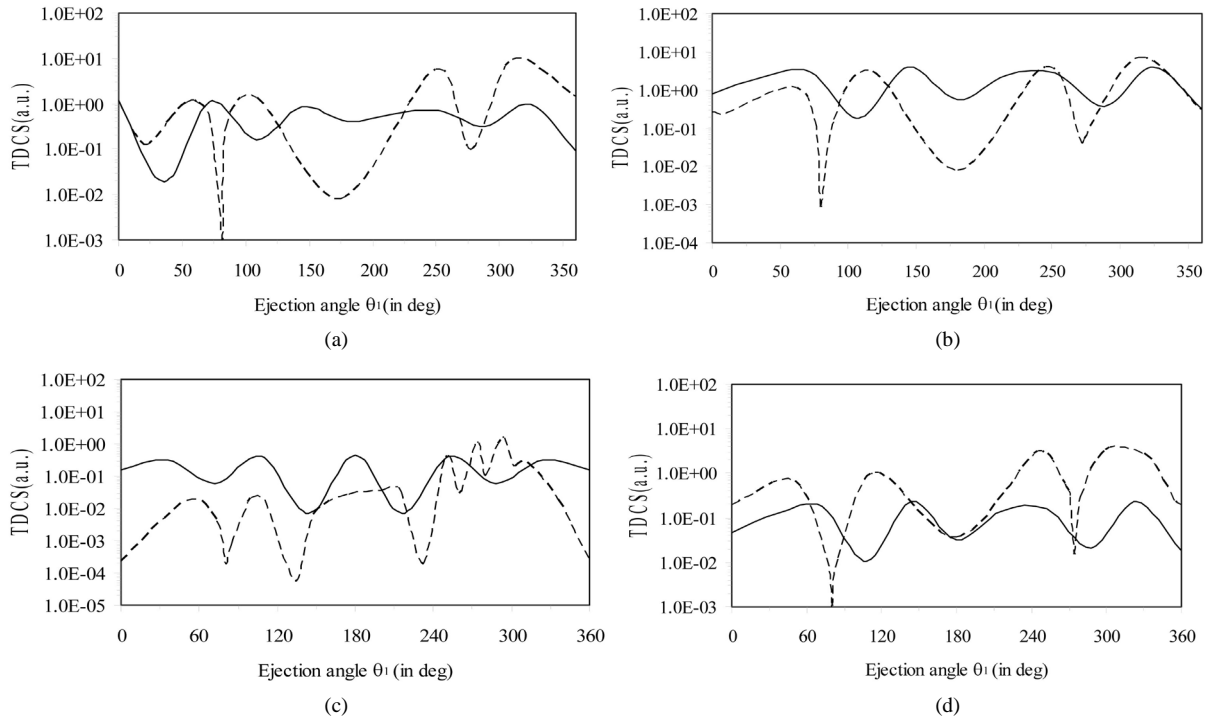
where  $E_2$  is the energy of the incident electron. Therefore, in our present calculation we have computed the TDCS, given by Equation (11).

### 3. Results and Discussion

We have presented here First Born approximation Triple differential cross-section (TDCS) for the process (1) at intermediate incident energies  $E_i = 150$  eV and  $E_i = 250$  eV for some varied ejected angles and fixed scattering angles. The present results have been displayed in nine figures where we have plotted the electron impact TDCS by varying the angle of ejection ( $\theta_1$ ) of the ejected electron. In all figures, the region for  $\theta_1 (0^\circ - 150^\circ)$  and  $\phi = 0^\circ$ , refers to the recoil region, while  $\theta_1 (150^\circ - 360^\circ)$  and  $\phi = 180^\circ$  refers to the binary region. We considered here  $\theta = 0^\circ$  to  $\theta = 360^\circ$ .

The present First Born approximation TDCS results in the metastable 2P-state hydrogen atoms are presented in the **Figures 1(a)-(d)**, and **Figures 2(a)-(e)** for scattering in a plane. Here the incident electron energy is  $E_i = 250$  eV and scattering angles are  $\theta_2 = 3^\circ (1a), 5^\circ (2a), 7^\circ (2b), 9^\circ (2c), 11^\circ (2d), 15^\circ (2e), 10^\circ (1c)$  and ejection angle  $\theta_1$  varies from  $0^\circ$  to  $360^\circ$  (measured oppositely from the forward direction compared to that for scattering angle  $\theta_2$ ). We also computed TDCS for the same state for the incident energies  $E_i = 150$  eV and  $E_i = 400$  eV and scattering angles are  $\theta_2 = 3^\circ$  and  $\theta_2 = 4^\circ$ , presented in **Figure 1(b)** and **Figure 1(d)** respectively.

When we compared the present First Born results to the linear superposition of the 2S-state and 2P-state ionization [21], it is noted that the TDCS exhibits a distinct four loaded structure where both the binary and recoil regions consist of two distinct peaks of comparable magnitudes as shown in **Figures 1(a)-(d)**. In the present First Born TDCS (see **Figures 1(a)-(d)** and **Figures 2(a)-(e)**), for the metastable 2P-state ionization, exhibit two distinct peaks both in the recoil and the binary, at all incident energies ( $E_i = 150$  eV, 250 eV and 400 eV). The



**Figure 1.** (a) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 3^\circ$ . Solid curve: present First Born result, Dashed curve: result of Deb *et al.* [21]; (b) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 150$  eV,  $E_1 = 5$  eV,  $\theta_2 = 3^\circ$ . Solid curve: present First Born result, Dashed curve: result of Deb *et al.* [21]; (c) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 10^\circ$ . Solid curve: present First Born result, Dashed curve: result of Deb *et al.* [21]; (d) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 400$  eV,  $E_1 = 5$  eV,  $\theta_2 = 4^\circ$ . Solid curve: present First Born result, Dashed curve: result of Deb *et al.* [21].

binary peak arises due to the electron-electron interaction while the recoil peak is due to the projectile nucleus interaction.

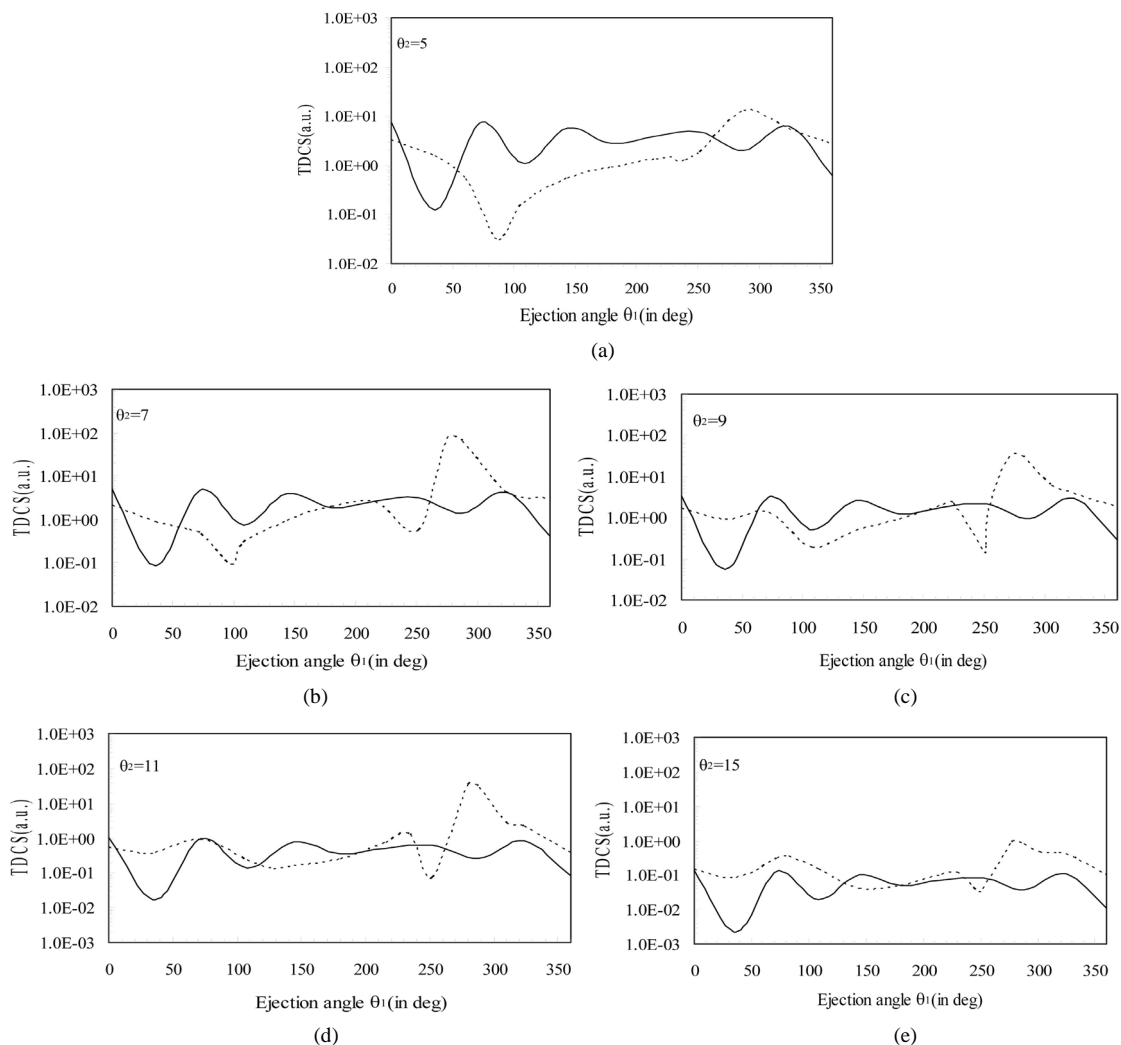
The present First Born TDCS in the metastable 2P-state ionization for the incident energy  $E_i = 250$  eV and higher scattering angles shows dissimilar magnitude peaks in the recoil region (see **Figures 2(a)-(e)**). Hence these **Figures 2(a)-(e)** reveal that at the incident energy  $E_i = 250$  eV and the higher scattering angles the collision becomes almost recoil peaks less prominent in the metastable 2S-state [13] than the present metastable 2P-state calculation results. It may be expected. But here, in the binary region, the present peak values are slightly smaller than the corresponding compared 2S-state results of Dhar [13].

The present binary peaks are shifted to the higher ejected scattering angles in the recoil region (see **Figures 1(a)-(d)**). But in the binary regions peaks are nearly similar pattern same with different magnitudes.

It is clear that the present First Born TDCS results almost agree with the linear combination of the 2S- and 2P-state results of Deb *et al.* [21] and the previous that of the metastable 2S-state results of Dhar [13]. But in some cases our results disagree in the recoil regions.

Amplitude corresponds to other three terms in the Equation (6) are also calculated and will be reported in near future.

The physical origins of finding cross-section results for 150 eV, 250 eV and 400 eV energies are presented. Here the amplitude (the First Born amplitude) corresponds to the first term on the right hand side of Equation (6) in which the scattered electrons of momentum  $\bar{p}_2$  are described by a plane wave while the ejected electrons of momentum  $\bar{p}_1$  are described by a coulomb wave. Also the physical origin of the peaks in the cross-section curves has been investigated, scattering first by atomic nucleus or atomic electron and then by atomic electron for the second time.



**Figure 2.** (a) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 5^\circ$ . Solid curve: present First Born result, Dashed curve: 2S-state result [13]; (b) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 7^\circ$ . Solid curve: present First Born result, Dashed curve: 2S-state result [13]; (c) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 9^\circ$ . Solid curve: present First Born result, Dashed curve: 2S-state result [13]; (d) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 11^\circ$ . Solid curve: present First Born result, Dashed curve: 2S-state result [13]; (e) The TDCS impact as a function of the ejected electron angle ( $\theta_1$ ) at  $E_i = 250$  eV,  $E_1 = 5$  eV,  $\theta_2 = 15^\circ$ . Solid curve: present First Born result, Dashed curve: 2S-state result [13].

## 4. Conclusion

In the present study we have calculated triple differential cross sections (TDCS) for ionization of metastable 2P-state hydrogen atoms by 150 eV, 250 eV and 400 eV electron impact. It reveals additional possible features of the cross-section curves for small momentum transfer. Hence the present calculation provides significant contribution in the field of metastable 2P-state ionization problem. Thus, new experimental results will be more interesting and significant for metastable 2P-state hydrogen atoms by electrons scattering problems.

## Acknowledgements

The computational works have been performed in the Simulation Lab of the Department of Mathematics, Chit-

tagong University of Engineering and Technology.

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