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The First Born Triple Differential Cross-Section for Ionization of H(3P) by Electron Impact in the Asymmetric Coplanar Geometry

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Abstract

First Born triple differential cross sections (TDCS) for ionization of metastable 3P-state hydrogen atoms by electrons are calculated for various kinematic conditions in the asymmetric coplanar geometry. A multiple scattering theory is used in this study. The present results are compared with other existing related theoretical results for ionizations of hydrogen atoms from metastable 2S-state and 2P-state, showing a good qualitative agreement. There is no available theoretical study for ionization of metastable 3P-state hydrogen atoms by electrons. We are expecting that the present results provide a wide scope for further study of such ionization problems.

Keywords

Electron, Ionization, Cross-Section, Scattering

1. Introduction

Hydrogen atom is one of the most abundant elements in the universe and is one of the simplest elements. Under some conditions, hydrogen atom occurs as ion, where its unusual properties make it of particular interest to chemists, physicists and astronomers as well as applied mathematicians.

Atoms in metastable states possess certain characteristic properties, such as long lifetimes, capability of transferring large amounts of energy [1], low excitation and ionization potentials, leading to extremely large

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scattering cross-sections. From this point of view, electron impact ionization of metastable atoms is finding potential importance for understanding of mechanisms occurring in many research areas, e.g., astrophysics, plasma physics and also in life sciences.

Total differential cross section for the ionization of atoms and molecules by electron impact is one of the essential sets of data needed in a wide range of various applications. Electron impact ionization of hydrogen atoms by electrons was investigated first by Bethe [2] and the ionization of metastable 2S-state hydrogen atoms by electron impact was discussed first using Ehrhardt coplanar geometry [3]-[6]. After that a huge amounts of theoretical and experimental investigation make this field more interesting.

Ionization of hydrogen atoms by electrons have been successfully used during the last five decades to investigate the details of the ionization process both in the ground state [7]-[13] and metastable states [14]-[21] of atomic hydrogen. The TDCS for the (e, 2e) processes were widely studied for the ground state hydrogen atom both experimentally [22]-[24] and theoretically [25]-[29].

Presently we have quantum mechanically discussed the TDCS of the metastable 3P-state hydrogen atom by electrons considering at intermediate and high energies due to the multiple scattering theory of Das [9] and Das and Seal [10] which also has important effects on other metastable atomic hydrogen. Though there is the scarcity of any theoretical and experimental results on TDCS for ionization of hydrogen atoms by electrons from metastable 3P-state, the present First Born results for ionization from the 3P-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.

2. Theory

Ionization cross sections are obtained by taking the ratio of the number of ionization events per unit time and per unit target to the incident electron flux. The most detailed information presently available is about the single ionization processes of the following type:

$$\mathrm{e}^- + \mathrm{H}(3\mathrm{P}) \to \mathrm{H}^+ + 2\mathrm{e}^- \tag{1}$$

where the symbol 3P denotes the hydrogenic metastable state and has been obtained in the coplanar geometry by analyzing 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 $\bar{p}_1$ and $\bar{p}_2$ emitted respectively into the solid angles $\mathrm{d}\Omega_1$ and $\mathrm{d}\Omega_2$ centred about the directions (θ_1,ϕ_1) and (θ_2,ϕ_2). The TDCS is usually denoted by the symbol $\dfrac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_1}$.

For unpolarized incident electrons and targets, it is a function of the quantities E_i, E_1 or E_2, θ_1, θ_2 and $\phi=\phi_1-\phi_2$. By integrating the TDCS over $\mathrm{d}\Omega_1$, $\mathrm{d}\Omega_2$ or $\mathrm{d}E_1$, one can form various double and single differential cross sections. Finally, the total ionization cross section is obtained by integrating over all outgoing scattering angles and energies, and depends only E_1 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 multiple scattering theory of ionization of hydrogen atoms by electrons is described in detail [10] [16] [17] [20] and [30]. Here we will describe the method very briefly, for the particular case of hydrogenic 3P-state at intermediate and high energies.

The direct T-matrix element for ionization of hydrogen atoms by electrons [10], may be written as,

$$T_{fi} = \left\langle \Psi_f^{(-)}(\bar{r}_1,\bar{r}_2) \middle| V_i(\bar{r}_1,\bar{r}_2) \middle| \Phi_i(\bar{r}_1,\bar{r}_2) \right\rangle. \tag{2}$$

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

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

and

$$\Phi_i(\bar{r}_1,\bar{r}_2)=\frac{\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}}{(2\pi)^{3/2}}\phi_{3P}(\bar{r}_1).$$

where

$$\phi_{3P}(\bar{r}_1)=\frac{\sqrt{2}}{81\sqrt{\pi}}\left(6r_1-r_1^2\right)\cos\theta\mathrm{e}^{-r_1/3}=\sqrt{\frac{2}{6561\pi}}\left(6r_1-r_1^2\right)\cos\theta\mathrm{e}^{-\lambda_1 r_1}. \tag{3}$$

Here $\lambda_1=\frac{1}{3}$, $\phi_{3P}(\bar{r}_1)$ is the hydrogenic 3P state wave function and $\Psi_f^{(-)}(\bar{r}_1,\bar{r}_2)$ is the final three-particle scattering state wave function [10] and co-ordinates of the two electrons are $\bar{r}_1$ and $\bar{r}_2$ respectively.

Here the approximate wave function $\Psi_f^{(-)}$ is given by

$$\Psi_f^{(-)}(\bar{r}_1,\bar{r}_2)=N(\bar{p}_1,\bar{p}_2)\left[\phi_{\bar{p}_1}^{(-)}(\bar{r}_1)\mathrm{e}^{i\bar{p}_2\cdot\bar{r}_2}+\phi_{\bar{p}_2}^{(-)}(\bar{r}_2)\mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1}+\phi_{\bar{p}}^{(-)}(\bar{r})\mathrm{e}^{i\bar{P}\cdot\bar{R}}-2\mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1+i\bar{p}_2\cdot\bar{r}_2}\right]\Big/(2\pi)^3 \tag{4}$$

Here

$N(\bar{p}_1,\bar{p}_2)$ is normalization constant, $\bar{r}=\frac{\bar{r}_2-\bar{r}_1}{2}$, $\bar{R}=\frac{\bar{r}_1+\bar{r}_2}{2}$,

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

and $\phi_q^{(-)}(\bar{r})$ is Coulomb wave function.

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

$$T_{fi}=T_B+T_{B'}+T_i-2T_{PB} \tag{5}$$

where

$$T_{\mathbf{B}}=\left\langle\phi_{p_1}^{(-)}(\bar{r}_1)\mathrm{e}^{i\bar{p}_2\cdot\bar{r}_2}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{6}$$

$$T_{B'}=\left\langle\phi_{p_2}^{(-)}(\bar{r}_2)\mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{7}$$

$$T_i=\left\langle\phi_p^{(-)}(\bar{r})\mathrm{e}^{i\bar{P}\cdot\bar{R}}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{8}$$

$$T_{PB}=\left\langle\mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1+i\bar{p}_2\cdot\bar{r}_2}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle. \tag{9}$$

For first Born approximation Equation (6) may be written as

$$T_{\mathbf{B}}=\frac{1}{162\pi^2}\left\langle\phi_{p_1}^{(-)}(\bar{r}_1)\mathrm{e}^{i\bar{p}_2\cdot\bar{r}_2}\left|\frac{1}{r_{12}}-\frac{1}{r_2}\right|\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}\left(6r_1-r_1^2\right)\cos\theta\mathrm{e}^{-r_1\lambda_1}\right\rangle$$

$$\begin{aligned}
T_B&=\frac{1}{162\pi^2}\int\phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\left(\frac{1}{r_{12}}-\frac{1}{r_2}\right)\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}\left(6r_1-r_1^2\right)\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2\\
&=\frac{1}{162\pi^2}\int\phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_{12}}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}6r_1\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2\\
&\quad-\frac{1}{162\pi^2}\int\phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_2}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}6r_1\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2\\
&\quad-\frac{1}{162\pi^2}\int\phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_{12}}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}r_1^2\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2\\
&\quad+\frac{1}{162\pi^2}\int\phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_2}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}r_1^2\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2
\end{aligned}$$

$$T_{\mathbf{B}}=\mathrm{tb1}+\mathrm{tb2}+\mathrm{tb3}+\mathrm{tb4} \tag{10}$$

where

$$\text{tb1} = \frac{1}{162\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_{12}}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}6r_1\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2$$

$$\text{tb2} = -\frac{1}{162\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_2}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}6r_1\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2$$

$$\text{tb3} = -\frac{1}{162\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_{12}}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}r_1^2\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2$$

$$\text{tb4} = \frac{1}{162\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)\mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_2}\mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2}r_1^2\cos\theta\mathrm{e}^{-\lambda_1 r_1}\mathrm{d}^3r_1\mathrm{d}^3r_2.$$

For First Born approximation, we have calculated the terms of Equation (10).

After analytical calculation by using the Lewis integral [31], we evaluated the above expressions numerically using the computer language. Finally the triple differential cross-sections for T-Matrix element is given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_1} = \frac{p_1 p_2}{p_i}\left|T_{fi}\right|^2. \tag{11}$$

3. Results and Discussions

The first Born TDCS are presented here for some varied kinematic conditions. In this study, the incident energy E_i is taken fixed as 250 eV and the ejected energy E_1 is fixed as 5 eV. The present First Born TDCS results are represented in **Figure 1** to **Figure 6**, where we have plotted the electron impact by varying the angle of ejection (θ_1) of the ejected electron. In all figures, the reason 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 have considered here $\theta = 0^\circ$ to $\theta = 360^\circ$.

In all figures, the present First Born results in the metastable 3P-state hydrogen atoms exhibit two sharp peak structures in recoil region and loaded peaks in binary region.

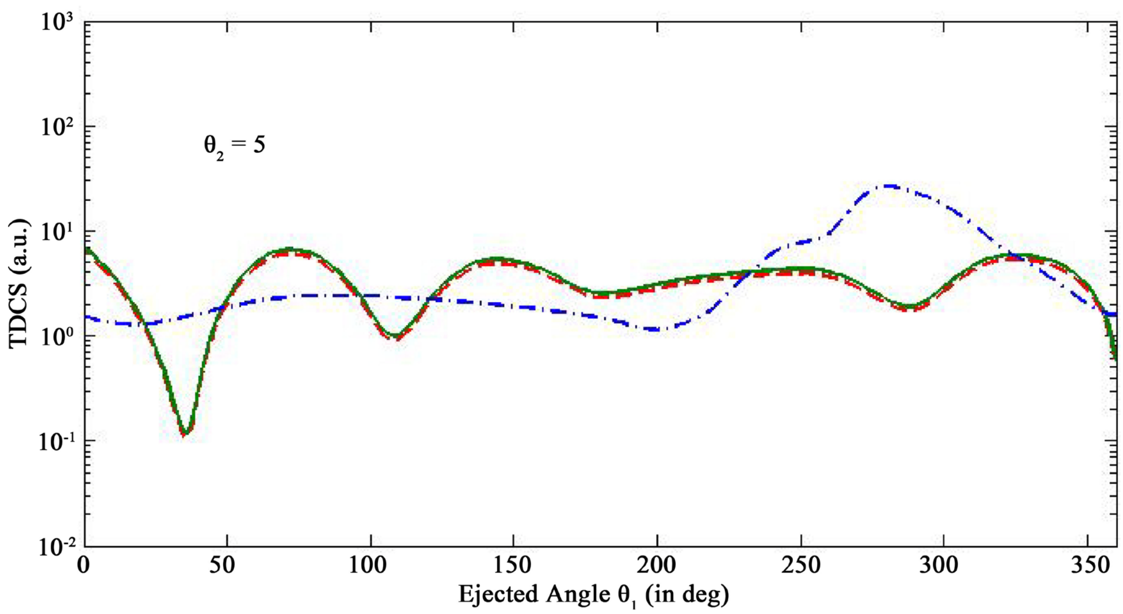

Figure 1. The TDCS for ionization of atomic hydrogen by 250 eV electron impact for scattering angle $\theta_2 = 5^\circ$ varies against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5\ \text{eV}$. Theory: Full curve (Green): Present first born result, dash curve (Red): 2P-state first born result [20] and dash dotted curve (Blue): 2S-state first born result [17].

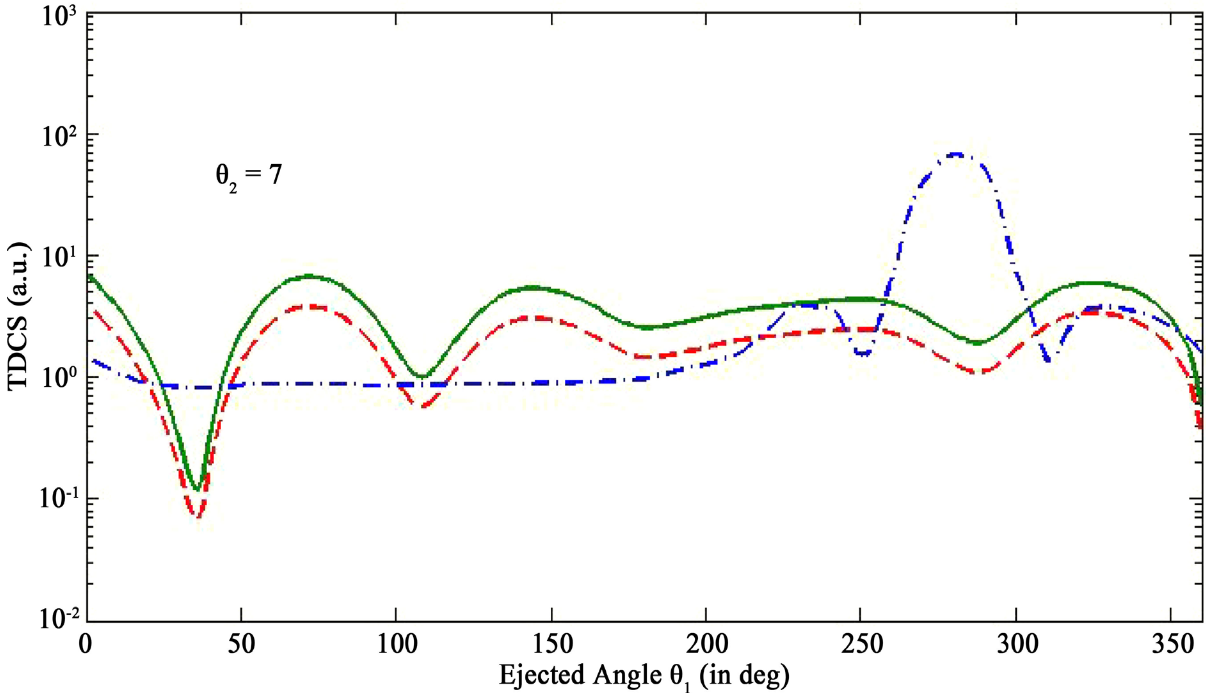

Figure 2. The TDCS for ionization of atomic hydrogen by 250 eV electron impact for scattering angle $\theta_2 = 7^\circ$ varies against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5\ \text{eV}$. Theory: Full curve (Green): Present first born result, dash curve (Red): 2P-state first born result [20] and dash dotted curve (Blue): 2S-state first born result [17].

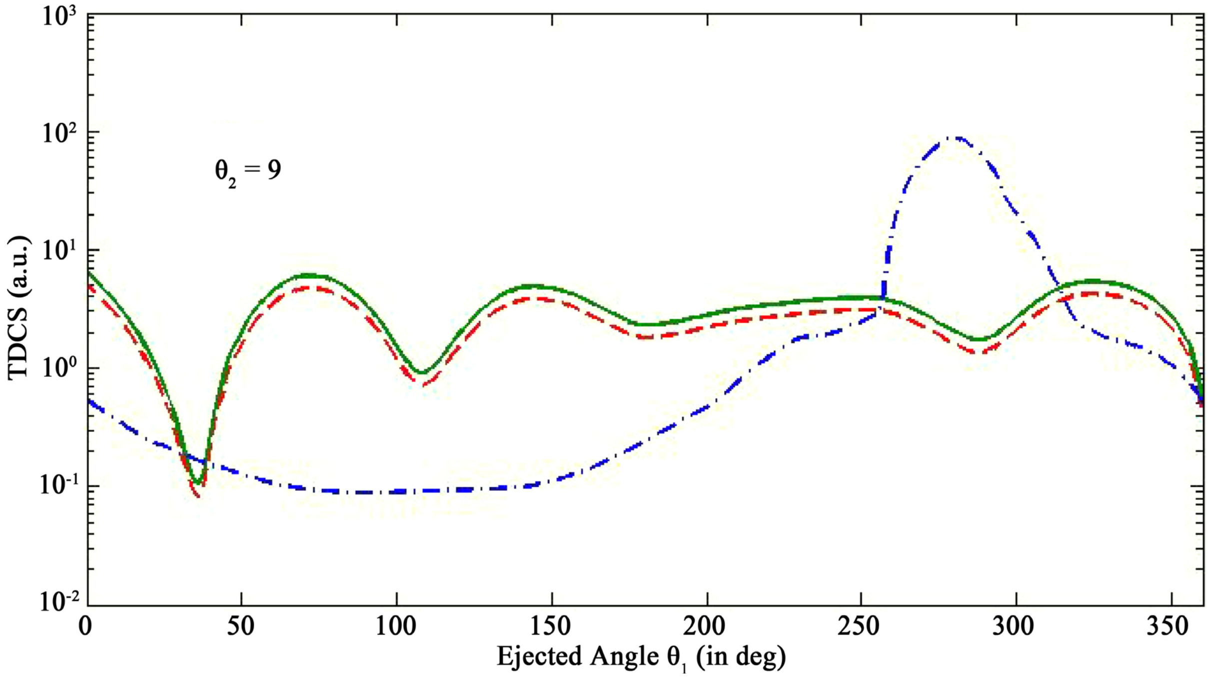

Figure 3. The TDCS for ionization of atomic hydrogen by 250 eV electron impact for scattering angle $\theta_2 = 9^\circ$ varies against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5\ \text{eV}$. Theory: full curve (Green): Present first born result, dash curve (Red): 2P-state first born result [20] and dash dotted curve (Blue): 2S-state first born result [17].

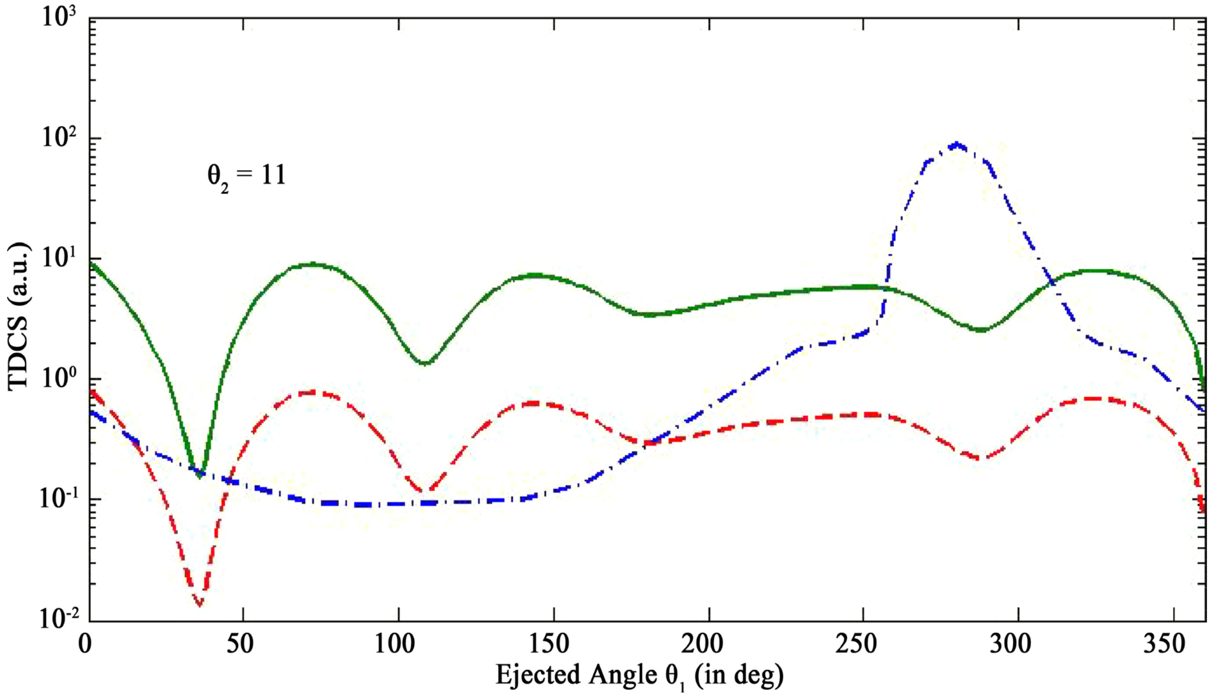

Figure 4. The TDCS for ionization of atomic hydrogen by 250 eV electron impact for scattering angle $\theta_2 = 11^\circ$ varies against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5\ \text{eV}$. Theory: full curve (Green): Present first born result, dash curve (Red): 2P-state first born result [20] and dash dotted curve (Blue): 2S-state first born result [17].

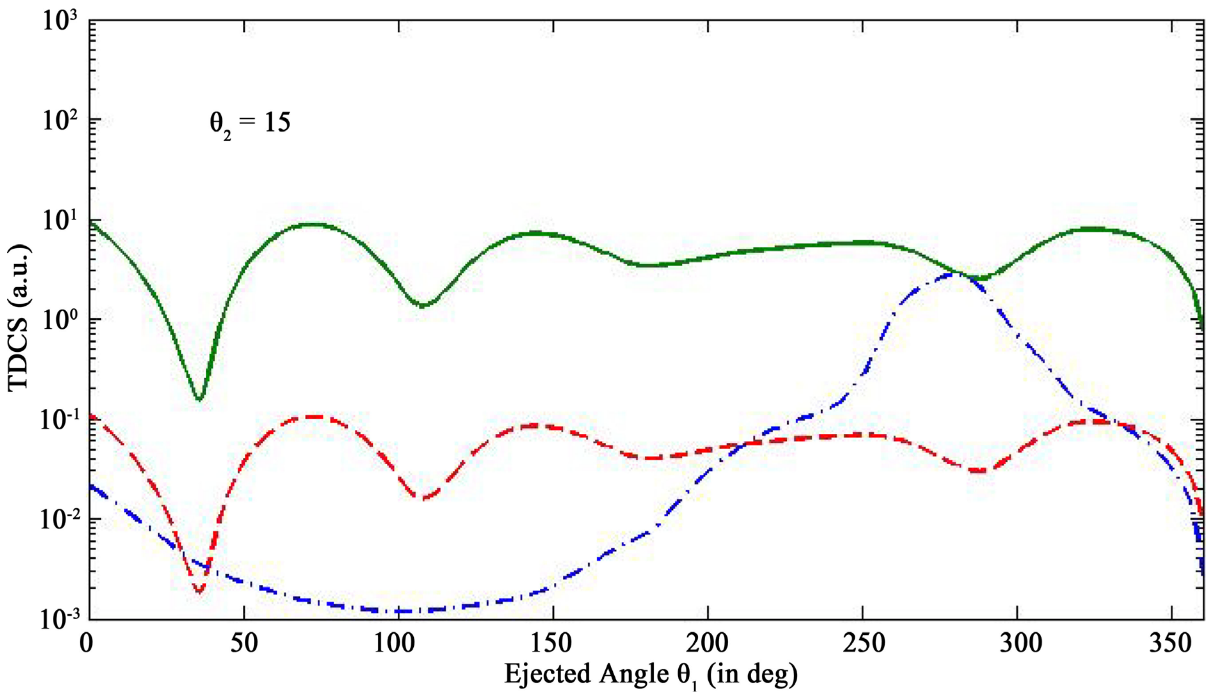

Figure 5. The TDCS for ionization of atomic hydrogen by 250 eV electron impact for scattering angle $\theta_2 = 15^\circ$ varies against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5\ \text{eV}$. Theory: full curve (Green): Present first born result, dash curve (Red): 2P-state first born result [20] and dash dotted curve (Blue): 2S-state first born result [17].

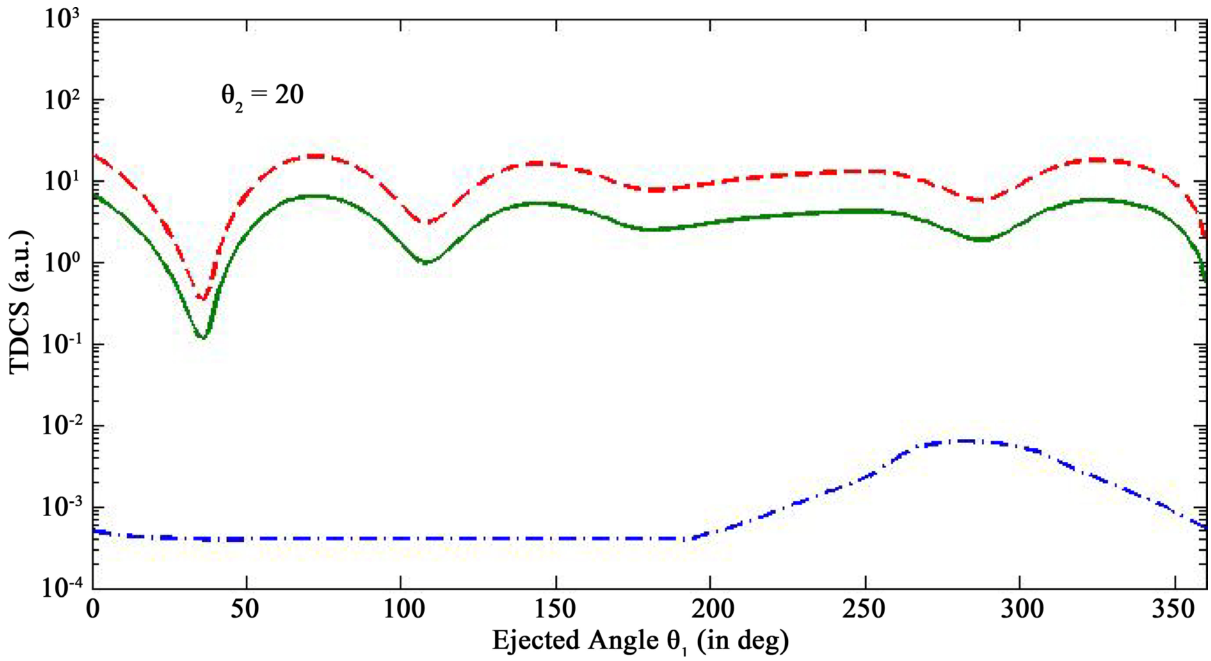

Figure 6. The TDCS for ionization of atomic hydrogen by 250 eV electron impact for scattering angle $\theta_2 = 20^\circ$ varies against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5\text{ eV}$. Theory: full curve (Green): Present first born result, dash curve (Red): 2P-state first born result [20] and dash dotted curve (Blue): 2S-state first born result [17].

Figure 1 revealed with coincidence of metastable 2P [20] and the present 3P-states hydrogen atoms by electron impact whereas, metastable 2S -state results [17] show dissimilar peak-pattern in recoil region but completely opposite peak pattern in binary region.

In **Figure 2** and **Figure 3** the present First Born results are almost closer to the results of Dhar and Nahar [20] for all ejected angles. But in the binary region the peak values of 2S-state [17] are very sharp than the present results.

In **Figure 4** and **Figure 5**, the present results are exposed with larger magnitude in both recoil and binary regions than the corresponding compared results of 2S and 2P metastable states [17] [20].

In **Figure 6**, both present results of metastable 3P and metastable 2P-states [20] results display higher magnitude peak positions than the metastable 2S-state [17] results. But interestingly, with the increase of scattering angle, the present First Born results represent lower magnitude than the metastable 2P-state results [20].

Finally, we notice that in our present results and the 2P-metastable state results [20] in both recoil and binary regions, peaks are nearly similar pattern same with different magnitude almost for all scattering angles. But in the binary region the opposite peak values of 2S-metastable state [17] are very sharp than the corresponding 2P-state [20] and 3P-state results.

A table (please see **Table 1**) of comparison results for ionization of hydrogenic 2S-state, 2P-state and 3P-state atoms by electron is given here.

4. Conclusion

In the present calculation, we have computed the TDCS for ionization of metastable 3P-state hydrogen atoms by incident electron energy 250 eV electron impact using the multiple scattering theory of Das & Seal [10]. On the basis of the present calculation, we can first conclude that the present results represent good qualitative agreement with the available hydrogenic ground state as well as metastable 2P-state and 2S-state results. The present results provide a significant contribution in the field of metastable 3P-state ionization problem. The metastable 3P-state TDCS results are much higher than the corresponding 2S-state cross sections. We are expecting that the present study makes more significant contribution to the study of atomic scattering problems using the multiple

Table 1. Triple differential cross sections (TDCS) for ionization of atomic hydrogen atoms by electron impact at metastable 3P-state are obtained by using Equation (11). The incident energy is 250 eV, the scattering angle is $\theta_2 = 9^\circ$ and the ejected electron energy is $E_1 = 5\ \text{eV}$. In the given table we present 3P-state First Born results and compared 2P-state&2S-state first Born results.

Ejected angle(θ_1)	2S	2P	3P
0	1.1501	5.1354	7.2001
36	0.4791	0.0841	0.1179
72	0.3101	4.8045	6.7357
108	0.3275	0.7241	1.0154
144	0.3665	3.8972	5.4639
180	0.5391	1.8393	2.5787
216	2.1587	2.6473	3.7109
252	2.3911	3.1421	4.4046
288	110.00	1.3769	1.9305
324	2.9969	4.2969	6.0240
360	1.2911	0.4133	0.5794

scattering theories. In the future calculations, other kinematic conditions or other atomic species will also be interesting and significant.

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