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Triple Differential Cross-Sections for Ionization of H(3d) by Incident Electron

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Abstract

Triple differential cross sections (TDCS) are estimated for the ionization of metastable 3d-state hydrogen atoms by electron at 250 eV for various kinematic conditions pursuing a multiple scattering theory. The present new results are compared with the theoretical results of hydrogenic different metastable states as well as the hydrogenic ground state experimental data. Obtained new finding results are in good qualitative agreement with those of compared theories. The present results give an immense opportunity for experimental trial in the field of ionization problems.

Keywords

Electron, Ionization, Cross-Sections, Scattering

1. Introduction

The theoretical non-relativistic studies for the atomic ionization by fast particle were first treated by Bethe [1]. Electron impact ionization by electrons processes is used in a diverse range of fields, such as radiation physics, plasma physics as well as astrophysics. Over the last four decades, the theoretical and experimental study in electron atom ionization collision on different cross sections has become progressively interesting for non-relativistic [2]-[29] as well as relativistic [30] [31] [32] [33] [34] energies. The atomic hydrogen ionization by fast particle is a good form for perturbation theory due to the availability of experimental results. In this context, the electron-electron coincidence experiments called (e, 2e) experiments, provide a clear concept of the kinematics of the collisions by giving information about the direction of the scattered and ejected electrons. During the last five decades, ionization of hydrogen atom by electron has been considered to explore the details of the ionization process both in the ground state [2]-[15] and metastable states [16]-[29] of atomic hydrogen.

In the field of electron, impact ionization is to develop a general theoretical framework, which will provide the accurate ionization cross sections for many atoms over a practically relevant impact energy range. Due to its perplexity, the fully quantum mechanical treatment of atomic ionization by electron is possible for the artless cases of hydrogen atom. In this work, atomic hydrogen is used as target in order to perceive the ionization mechanism of atomic system by electron impact energy.

Hydrogenic metastable 3d state is an excited state which has a relatively long lifetime than the other excited states. A metastable sate has a higher energy than the ground state. The lifetime of excited state is given by [35]

$$T_i = \left(\sum A_{ij}\right)^{-1}$$

where A_{ij} is Einstein A coefficient. The lifetime of metastable 3d state of hydrogen atom is 2.3×10^{-7} s.

A multiple scattering theory [5] [15] has been applied in the present calculation of the triple differential cross sections (TDCS) in the metastable 3d-state hydrogen atom ionization by 250 eV electron energy. Lewis integral [36] has been used in the present study for analytical calculation.

The existent new study results will present a new dimension on ionization of hydrogenic metastable states. Current results are compared with previous related theories [18] [27] and [29].

2. Theory

Electron-impact ionization cross section is estimated by taking the ratio of the number of ionization elements per unit time and per unit target to the incident electron flux.

Ionization of atomic hydrogen by electron in most elaborate form is presently available of following type

$$e^- + H(3d) \rightarrow H^+ + 2e^- \tag{1}$$

Here 3d denotes the hydrogenic metastable state and has been attained in the coplanar geometry by examining TDCS measured in (e, 2e) coincidence experiments.

The triple differential cross section is denoted by the symbol $\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1}$.

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.

The direct T-matrix element for ionization of hydrogen atoms by electrons, following Das and Seal [15] may be written as

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

here, $\bar{r}_1$ and $\bar{r}_2$ represent the coordinates of the atomic active electron and the incident electron, $(\bar{p}_1,\bar{p}_2)$ and (E_1,E_2) represent the momenta and energies of the two electrons in the final state and $(\bar{p}_i,E_i)$ are the momentum and the energy of the incident electron.

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

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

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

We have the initial channel unperturbed wave function is

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

where

$$\phi_{3d}(\bar{r}_1)=\frac{1}{81\sqrt{6\pi}}(r_1^2)(3\cos^2\theta-1)\mathrm{e}^{-r_1/3}=\frac{1}{324\sqrt{3\pi^2}}(r_1^2)(3\cos^2\theta-1)\mathrm{e}^{-\lambda_1 r_1}.$$

$$\Phi_i(\bar{r}_1,\bar{r}_2)=\frac{1}{324\sqrt{3\pi^2}}(r_1^2)(3\cos^2\theta-1)\mathrm{e}^{-\lambda_1 r_1} \tag{3}$$

here $\lambda_1=\frac{1}{3}$, $\phi_{3d}(\bar{r}_1)$ is the hydrogenic 3d-state wave function and $\Psi_f^{(-)}(\bar{r}_1,\bar{r}_2)$ is approximate wave function is given by [15]

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

where

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

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

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

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

where

$$\lambda_1=\mathrm{e}^{\pi\alpha_1/2}\Gamma(1-i\alpha_1),\quad \alpha_1=\frac{1}{p_1}$$

$$\lambda_2=\mathrm{e}^{\pi\alpha_2/2}\Gamma(1-i\alpha_2),\quad \alpha_2=\frac{1}{p_2}$$

$$\lambda_3=\mathrm{e}^{\pi\alpha/2}\Gamma(1-i\alpha),\quad \alpha=-\frac{1}{p}$$

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

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

with

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

and

$$\alpha = -\frac{1}{p} \text{ for } \bar{q} = \bar{p}$$

Now Equation (2) becomes

$$T_{fi} = T_B + T_{B'} + T_i - 2T_{PB} \tag{6}$$

where

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

$$T_{B'} = \left\langle \phi_{p_2}^{(-)}(\bar{r}_2)e^{i\bar{p}_1\cdot\bar{r}_1}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{8}$$

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

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

here Equation (6) is called First Born term and it may be written as

$$T_B = \frac{1}{324\sqrt{3}\pi^2}\left\langle \phi_{p_1}^{(-)}(\bar{r}_1)e^{i\bar{p}_2\cdot\bar{r}_2}\left|\frac{1}{r_{12}}-\frac{1}{r_2}\right|e^{i\bar{p}_i\cdot\bar{r}_2}(r_1^2)(3\cos^2\theta-1)e^{-r_1\lambda_1}\right\rangle$$

$$= \frac{1}{324\sqrt{3}\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)e^{-i\bar{p}_2\cdot\bar{r}_2}\left(\frac{1}{r_{12}}-\frac{1}{r_2}\right)e^{i\bar{p}_i\cdot\bar{r}_2}(r_1^2)(3\cos^2\theta-1)e^{-\lambda_1 r_1}d^3r_1d^3r_2$$

$$T_B = \frac{1}{324\sqrt{3}\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)e^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_{12}}e^{i\bar{p}_i\cdot\bar{r}_2}r_1^2(3\cos^2\theta-1)e^{-\lambda_1 r_1}d^3r_1d^3r_2$$

$$-\frac{1}{324\sqrt{3}\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)e^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_2}e^{i\bar{p}_i\cdot\bar{r}_2}r_1^2(3\cos^2\theta-1)e^{-\lambda_1 r_1}d^3r_1d^3r_2$$

$$T_B = \mathrm{tb1} + \mathrm{tb2} \tag{11}$$

where

$$\mathrm{tb1} = \frac{1}{324\sqrt{3}\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)e^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_{12}}e^{i\bar{p}_i\cdot\bar{r}_2}r_1^2(3\cos^2\theta-1)e^{-\lambda_1 r_1}d^3r_1d^3r_2$$

$$\mathrm{tb2} = -\frac{1}{324\sqrt{3}\pi^2}\int \phi_{p_1}^{(-)*}(\bar{r}_1)e^{-i\bar{p}_2\cdot\bar{r}_2}\frac{1}{r_2}e^{i\bar{p}_i\cdot\bar{r}_2}r_1^2(3\cos^2\theta-1)e^{-\lambda_1 r_1}d^3r_1d^3r_2$$

Using the Lewis integral [36], we have evaluated First Born term T_B of Equation (7).

Similarly, we have calculated analytically the above Equations (8), (9) and (10) for second Born results using the Lewis integral [36]. After that we have computed the above equations using Gaussian quadrature formula. Finally the triple differential cross-sections for T-Matrix element is given by

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{p_1 p_2}{p_i}\left|T_{fi}\right|^2 \tag{12}$$

3. Results and Discussions

In this section, We have calculated in this work the triple differential cross-sections (TDCS) at high incident energy $E_i = 250\ \text{eV}$ for various ejected angles θ_1 and fixed scattering angles θ_2. Triple differential cross sections for ionization of metastable 3d-state hydrogen atoms by incident electron are presented at different energies. The existent results are compared with the ionization of hydrogen atoms by electrons from ground state theoretical results of Dal *et al.* [16], the BBK model of Brauner *et al.* [11] and the experiment results of Ehrhardt *et al.* [2]. Also the earlier works on hydrogenic 2S-state [18], 3S-state [27] and recent works on hydrogenic 3P-state [29] ionization results are exhibited here for comparison. The present results of triple differential cross section are presented in the following nine figures where we have designed the electron impact TDCS varying against the angle of ejection (θ_1) of the ejected electron.

In this study, the ejected angle θ_1 varies from 0˚ to 360˚ considered as horizontal axis where scattering angles θ_2 is fixed and referred as vertical axis. The present results of hydrogenic metastable 3d state by electron are designed corresponding to the different scattering angles $\theta_2 = 30^\circ$ **Figure 1(a)** for ejected electron energies $E_1 = 5$, 15˚ **Figure 1(b)**, 25˚ **Figure 1(c)** for ejected electron energies $E_1 = 50\ \text{eV}$ considering the ejected angle θ_1 from 30˚ to 100˚ and the scattering angle $\theta_2 = 5^\circ$ **Figure 2(a)**, 7˚ **Figure 2(b)**, 9˚ **Figure 2(c)**, 11˚ **Figure 3(a)**, 15˚ **Figure 3(b)** and 20˚ **Figure 3(c)** for ejected electron energies $E_1 = 5\ \text{eV}$.

The incident electron energy of $E_i = 250$ is taken here. In all figures, $\theta_1\left(0^\circ - 150^\circ\right)$ and $\phi = 0^\circ$ is considered as recoil region while $\theta_1\left(150^\circ - 360^\circ\right)$ and $\phi = 180^\circ$ is referred as binary region.

In **Figure 1(a)**, the present results shows a qualitative comparison with the present first Born result (black), the hydrogenic ground state result of BBK model [11], the second Born approximation [16], the hydrogenic ground state experimental data [2], 3S-state results [27] and recent works on hydrogenic 3P-state [29] ionization results. The peak values of present results and first Born results show good qualitative agreement with those of the compared results in the recoil region but show somewhere dissimilar in the binary region. This may be happened due to the change of the hydrogenic metastable states by electrons. Here in the recoil region the peak values of present and first Born and 3P-state results [29] are about double results of the other compared results. The binary peak values of the present results slightly shifted right from other compared results.

In **Figure 1(b)**, the peak value of present and first Born results are lower than the hydrogenic ground state experimental results [2], hydrogenic metastable 3P-state results [29] and hydrogenic metastable 3S-state results [27]. Also the peak values shifted slightly to the higher ejected angle near about $\theta_1 = 72^\circ$. The peak pattern of the present result shows exactly similar conduct with the hydrogenic ground state BBK results [11] with slight shift.

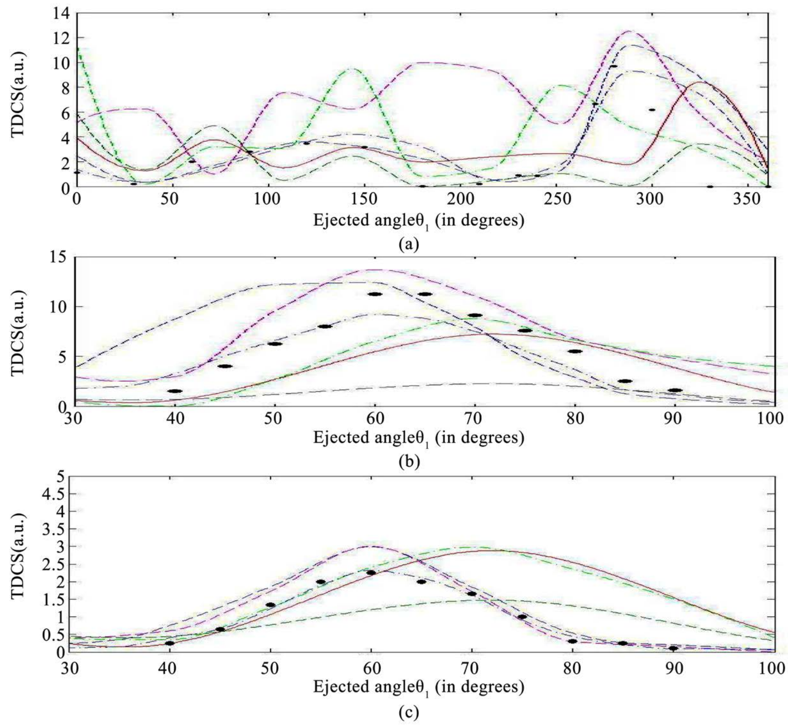

Figure 1. Triple-differential cross sections (TDCS) with versus ejected electron angle θ_1 for atomic hydrogen by electron energy 250 eV with (a) $E_1 = 5\text{ eV}$ and $\theta_2 = 3^\circ$, (b) $E_1 = 50\text{ eV}$ and $\theta_2 = 15^\circ$, (c) $E_1 = 50\text{ eV}$ and $\theta_2 = 25^\circ$. Theory: Continuous curve (Red) illustrate Present result, Dash curve (Black) exhibit Present First Born results, Dash dotted curve (Green) display 3P-state result [29], Dash curve (Magenta) expose 3S-state result [27] and Dash curve (Blue) demonstrate Hydrogenic ground state Second Born results [16], Dash dotted curve (Blue) reveal Hydrogenic ground state BBK model [11] and Round indicated Hydrogenic ground state experiment [2] (multiplied by 0.00224).

In **Figure 1(c)**, our present result and hydrogenic 3P-state result exits in almost same position with similar peak height. The peak magnitude is the highest among other compared results [2] [11].

In **Figure 2(a)**, our present results show a good agreement with 2S-state [18] and 3S -state [27] metastable results The present TDCS curve display two fall and two peak in recoil region and one fall two peak in binary region while metastable 3S-state result exhibit one fall and one peak in recoil region and one peak in binary region. The present results and 2S-state results show one prominent peak in recoil region.

In **Figure 2(b)**, our present study results exhibit same peak pattern with metastable 3S -state [27] and 2S-state [18] results whereas the present results and metastable 3P –state results [29] show opposite peak pattern at higher ejected angle about $\theta_1 = 288^\circ$.

In **Figure 2(c)**, our present TDCS curve depict a very interesting results. It expressed two falls in recoil region and two peak in binary region. The present result is closer to the 3S-state result [27]. The present result shows a bit different from 3P state results [29].

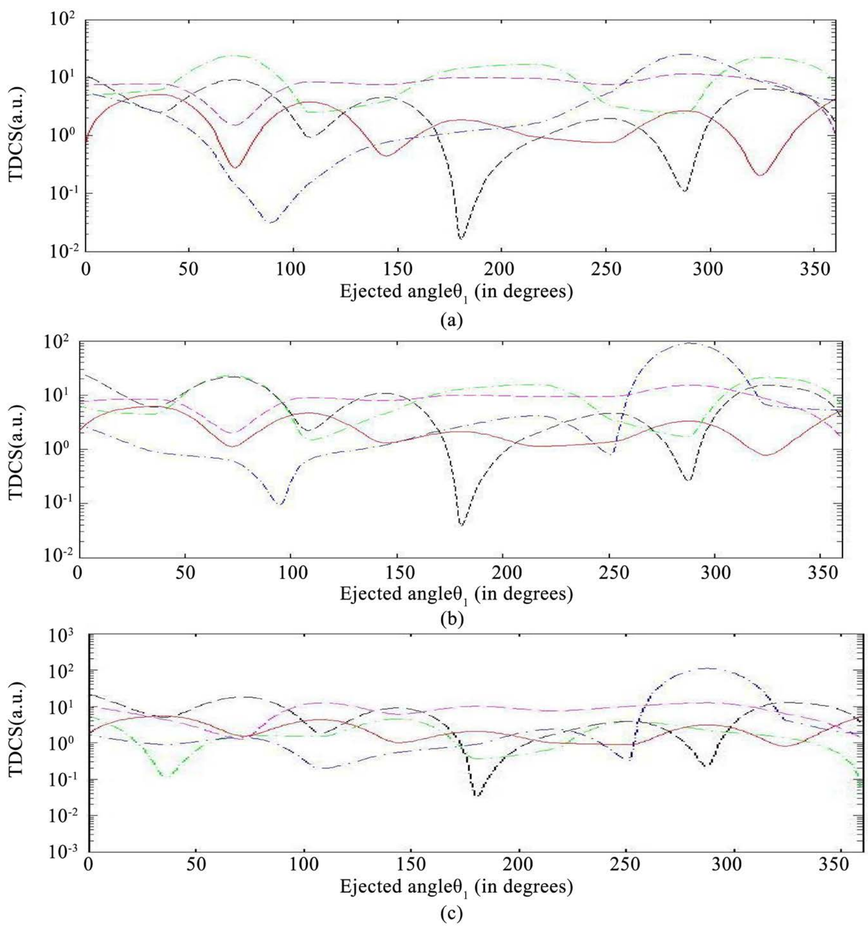

Figure 2. Triple-differential cross sections (TDCS) versus ejected electron angle θ_1 for atomic hydrogen by electron energy $E_i = 250\text{ eV}$ with ejected electron energy with $E_1 = 5\text{ eV}$ and (a) $\theta_2 = 5^\circ$, (b) $\theta_2 = 7^\circ$ (c) $\theta_2 = 9^\circ$. Theory: Continuous curve (Red) illustrate Present result, Dash curve (Black) exhibit Present First Born results, Dash dotted curve (Green) display hydrogenic 3P-state result [29], Dash curve (Magenta) expose hydrogenic3S-state result [27] and Dash dotted curve(Blue) demonstrate hydrogenic 2S-state result [18].

In **Figure 3(a)**, we note that the magnitude of the present and first Born results (black) are lesser than 3S-state [27] and 3P-state [29] results. In this figure, the present result gives a short lobe where 2S-state [18] result show a very sharp peak at ejected angle about 252˚.

In **Figure 3(b)**, the present and first Born results (black) represent similar peak pattern comparing with the 3S-state [27] hydrogenic results whereas the present TDCS curve and first Born curve provide dissimilar peak in the binary region.

In **Figure 3(c)**, the present results and first Born results (black) provide exactly similar behavior as the 3S state [27] results but show a gross difference with the results of 2S-state [18] both in recoil and binary region. The present TDCS curve displays a sharp lobe whereas 2S-state hydrogenic results show a opposite peak at ejected angle near about $\theta_1 = 72^\circ$.

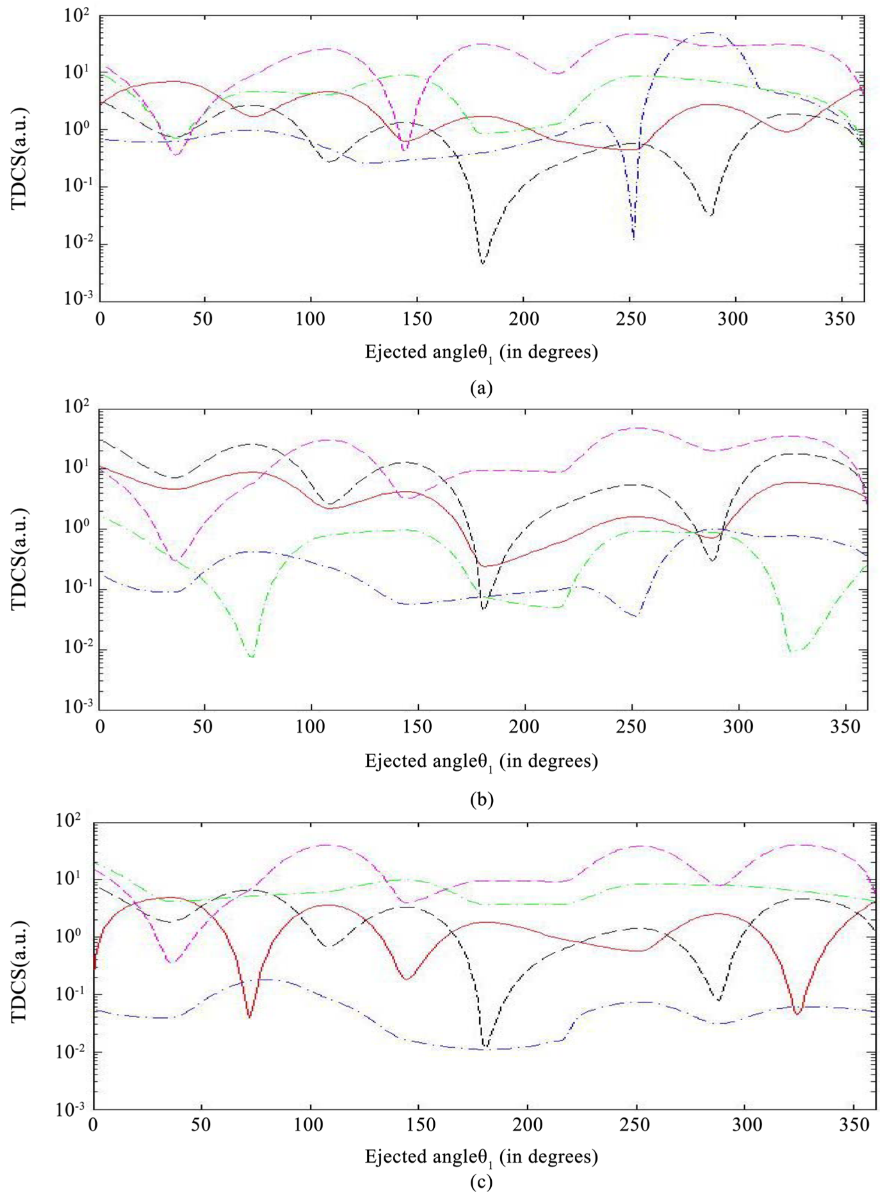

Figure 3. Triple-differential cross sections (TDCS) versus ejected electron angle θ_1 for atomic hydrogen by electron energy $E_i = 250\,\text{eV}$ with ejected electron energy with $E_1 = 5\,\text{eV}$ and (a) $\theta_2 = 11^\circ$, (b) $\theta_2 = 15^\circ$, (c) $\theta_2 = 20^\circ$ Theory: Continuous curve (Red) illustrate Present result, Dash curve (Black) exhibit Present First Born results, Dash dotted curve (Green) display hydrogenic 3P-state result [29], Dash curve (Magenta) expose hydrogenic3S-state result [27] and Dash dotted curve(Blue) demonstrate hydrogenic 2S-state result [18].

Finally, Metastable 3d-state is an excited state of an atom or other system with a longer lifetime than the other excited states. The lifetime of 3d state of hydrogen atom is 2.3×10^{-7}. The lifetime of excited state is given by [35]. However, it has a shorter lifetime than the stable ground state. The peak structure of the present results show good qualitative agreement with compared result in the recoil region but show somewhat disagreement in the binary region. This may be

Table 1. Triple differential cross section (TDCS) for electron impact Ionization of H (3d) by incident electron are distinguished with 3P-state, 3S-state & 2S-state results where the incident energy is 250 eV, the scattering angle is $\theta_2 = 9^\circ$ and the ejected electron energy is $E_1 = 5\ \text{eV}$.

Ejected angle (θ_1)	2S	3S	3P	3d
0	1.6501	5.0059	11.8679	1.6989
36	0.9001	6.2634	0.4252	5.3959
72	1.3875	1.2531	2.1485	1.5032
108	0.1952	7.5195	3.5834	4.3023
144	0.5401	6.2167	9.7624	1.0020
180	0.8989	10.0276	0.3155	2.0506
216	2.3450	9.5268	0.7248	0.9956
252	0.3201	10.0284	8.4297	0.8921
288	110.00	12.5360	5.0455	3.1015
324	4.1569	6.2681	1.7845	0.8012
360	1.7890	1.2506	0.0850	5.4074

happened due to the change of the hydrogenic metastable states ionization by electrons. It is remarked that, the peak pattern of the energy spectrum as obtained from our present study is closer to the compared results [27] [29] in some cases and again sometimes different. It may be happened due to the change of atomic state.

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

4. Conclusion

The present estimation reveals imaginable additional formation of the cross-section curves for intermediate momentum transfer in the ionization of the hydrogen atoms in the hydrogenic metastable 3d-state at 250 eV electron impact energy. It is remarked that, the implementation of the final state wave function of Das and Seal [15] yields good qualitative agreement with hydrogenic ground state as well as metastable 2S-state, 3S-state and 3P-state results for qualitative enhancement. It is a new work. New empirical outcomes for ionization of metastable 3d-state hydrogen atoms by electrons will be valuable and originate a novel dimension in order to perceive the study of ionization problems.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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