Electron Impact Ionization of Metastable 3S-State Hydrogen Atoms by Electrons in Coplanar Geometry

Sunil Dhar[1], Tania Noor[2, *], Farhana Shirin Chowdhury[3]

[1]Department of Mathematics, Chittagong University of Engineering and Technology, Chittagong, Bangladesh
[2]Department of Mathematics, Premier University, Chittagong, Bangladesh
[3]Department of Computer Science and Engineering, Premier University, Chittagong, Bangladesh

Email address:
sdhar@cuet.ac.bd (S. Dhar), taniatima@gmail.com (T. Noor), fshirin2007@gmail.com (F. S. Chowdhury)

To cite this article:
Sunil Dhar, Tania Noor, Farhana Shirin Chowdhury. Electron Impact Ionization of Metastable 3S-State Hydrogen Atoms by Electrons in Coplanar Geometry. *American Journal of Modern Physics.* Vol. 4, No. 6, 2015, pp. 261-266. doi: 10.11648/j.ajmp.20150406.11

Abstract: In this work we have calculated first born triple differential cross sections (TDCS) for ionization of metastable 3S-state hydrogen atoms by electrons. In this study the final state wave function is described by a multiple scattering theory for ionization of hydrogen atoms by electrons. Results show qualitative agreement with other existing theoretical results for ionization of hydrogen atoms from metastable 2S-state and 2P-state. There are no other available results for ionization of hydrogen atoms from metastable 3S-state. The present result offers an extensive scope for experimental verifications in such ionization process.

Keywords: Electron, Cross Sections, Ionization, Scattering

1. Introduction

Electron impact ionization by charged particles has been known for nearly about five decades. Quantitative measurements, mostly of total ionization cross sections, have been performed in 19th century [1]. In 20th century good quality of works have been done both theoretically and experimentally in triple differential cross sections (TDCS) for relativistic [2-11] as well as for non-relativistic energies [12-24] relative to the multiple scattering theory. Ionization of hydrogen atoms by electrons is the fundamental study of ionization problems. The availability of experimental and theoretical works on ionization of hydrogen atoms makes it gradually interesting. But at present the investigation of ionization from metastable states of hydrogen atoms by charged particles also motivating research in this field and expecting that very soon we may access available experimental data in this field.

The (e, 2e) coincidence measurements in electron impact ionization of light atoms to the study of coplanar asymmetric geometries where the scattered electron are fast and forward while the ejected electron is slow was published theoretically by Ehrhardt [15-16] but in quantum mechanical way it was first treated by Bethe [17]. The e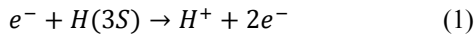xperimental results of (e, 2e) measurements were widely used to explore the ionization process both in ground state [18, 19] and in metastable [20-24] states of atomic hydrogen. BBK theory of Brauner et al. [7] gives qualitatively good results on ionization of hydrogen atoms by electrons and positrons considering at intermediate to high energy level henceforth Das and Seal [19] gives better quantitative results. Ionization of metastable 2s-state hydrogen atom by electron impact [21] and by symmetric scattering in electron and positron impact [12] reveals new features in the cross section curves. Recently ionization of metastable 2P-state hydrogen atom in the coplanar geometry [26] and in coplanar asymmetric geometry [27] gives a new dimension in this field of interest. For ionization of hydrogen atoms by electrons from metastable 3S-state there are no such theoretical and experimental results on triple differential cross section. Theoretical calculations of Dhar [20] and Das and Dhar [21] open up the possibilities of investigating the metastable 3S-state hydrogen atoms by electrons at intermediate and high energy level.

We have calculated the first born triple differential cross sections (TDCS) for ionization of metastable 3S-state hydrogen atoms by 250 eV incident energy following a multiple scattering theory of Das and Seal [19]. It should be recalled that the wave function for multiple scattering theory is designed here for two electrons are moving in a coulomb

field. We obtained very interesting results for triple differential cross sections (TDCS) for ionization of metastable 3S - state hydrogen atoms by electrons at various kinematic conditions applying the multiple scattering theory of Das and Seal [19].

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 about single ionization process of the following type

$$e^- + H(3S) \rightarrow H^+ + 2e^- \qquad (1)$$

Where 3S denotes the metastable state of the target, has been obtained in the coplanar geometry by analyzing triple differential cross sections (TDCS) measured in (e, 2e) coincidence experiments. Here (e, 2e) is that kind of experiment where the ejected electron is detected in coincidence with the scattered electron. It is very well known in [16]. TDCS is a measure of the probability that in an (e, 2e) reaction an incident electron of momentum $\overline{p_1}$ and energy E_1 will produce on collision with the target two electrons having energies E_1 and E_2 and momentum $\overline{p_1}$ and $\overline{p_2}$, emitted respectively into the solid angles $d\Omega_1$ and $d\Omega_2$ centered about the directions (θ_1, Φ_1) and (θ_2, Φ_2).

TDCS is usually denoted by the symbol $\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1}$. For unpolarized incident electrons and and targets, it is a function of the quantities E_i, E_1 or E_2, θ_1, θ_2 and $\Phi = \Phi_1 - \Phi_2$. The multiple scattering theory of ionization of hydrogen atoms by electrons is described in detail in [19]. The T-matrix element for ionization of hydrogen atoms by electrons [19] is given by

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

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

$$V_i(\bar{r}_1, \bar{r}_2) = \frac{1}{r_{12}} - \frac{Z}{r_2} \qquad (3)$$

For hydrogen atom nuclear charge (Z) = 1, r_1 and r_2 are the distance of the two electrons from the nucleus and r_{12} is the distance between the two electrons. The initial channel unperturbed wave function is,

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

$$= \frac{e^{i.\bar{p}_i.\bar{r}_2}}{(3\pi)^{3/2}} \cdot \frac{1}{81\sqrt{3\pi}} (27 - 18\bar{r}_1 + 2\bar{r}_1^2) e^{-\lambda_1 r_1} \qquad (4)$$

Where

$$\varphi_{3S}(\bar{r}_1) = \frac{1}{81\sqrt{3\pi}} (27 - 18\bar{r}_1 + 2\bar{r}_1^2) e^{-\lambda_1 r_1} \qquad (5)$$

and

$$\lambda_1 = 1/3$$

Equation (5) is the hydrogenic 3S-state wave function, $\bar{p}_1$ is the incident electron momentum, $\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$ is the final three-particle scattering state wave function with the electrons being in the continuum with momenta $\bar{p}_1$, $\bar{p}_2$. Co-ordinates of the two electrons taken to be $\bar{r}_1$ and $\bar{r}_2$.

Here $\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$ is approximate wave function and is given by [19]

$$\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2) = N(\overline{p_1}, \overline{p_2})\left[\phi_{\overline{p_1}}^{(-)}(\bar{r}_1)e^{i\overline{p_2}.\overline{r_2}} + \phi_{\overline{p_2}}^{(-)}(\bar{r}_2)e^{i\overline{p_1}.\overline{r_1}} + \phi_{\bar{p}}^{(-)}(\bar{r})e^{i\bar{P}.\bar{R}} - 2e^{i\overline{p_1}.\overline{r_1}+i\overline{p_2}.\overline{r_2}}\right]/(3\pi)^3 \qquad (6)$$

Where

$$\bar{r} = \frac{\overline{r_1}-\overline{r_2}}{2}, \bar{R} = (\bar{r}_1 + \bar{r}_2)/2, \bar{p} = (\overline{p_2} - \overline{p_1}), \bar{P} = \overline{p_2} + \overline{p_1}$$

Now applying equations (3), (4), (5) and (6) in equation (2) we get,

$$T_{fi} = T_B + T_{B'} + T_i - 2T_{PB} \qquad (7)$$

Where

$$T_B = \langle \Phi_{\bar{p}_1}^{(-)}(\overline{r_1})e^{i\bar{p}_2.r_2} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \qquad (8)$$

$$T_{B'} = \langle \Phi_{p2}^{(-)}(\overline{r_2}) e^{i\bar{p}_1.r_1} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \qquad (9)$$

$$T_i = \langle \Phi_{\bar{p}}^{(-)}(\bar{r})e^{i.\bar{P}.\bar{R}} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \qquad (10)$$

$$T_{PB} = \langle e^{i\bar{p}_1.\bar{r}_1+i\bar{p}_2.\bar{r}_2} | V_i | \Phi_1(\bar{r}_1, \bar{r}_2) \rangle \qquad (11)$$

Here equation (7) is called first born term that can be written as

$$T_B = \frac{1}{81(3\pi)^2} \langle \Phi_{\bar{p}_1}^{(-)}(\overline{r_1})e^{i\bar{p}_2.r_2} \left| \frac{1}{r_{12}} - \frac{1}{r_2} \right| e^{i.\bar{p}_i.\bar{r}_2}(27 - 18r_1 + 2r_1^2)e^{-\lambda_1.r_1} \rangle \qquad (12)$$

After analytical calculations using Lewis integral [28],

$$T_{B1} = \frac{16\sqrt{2}\exp(\frac{\pi\alpha_1}{2})[(1-i\alpha_1)(\overline{t^2}-\overline{p_1}.\bar{t}-i\alpha_1\overline{p_1}.\bar{t})\exp(i\alpha_1 ln\vartheta)}{3^{\frac{5}{2}}t^2\{\overline{t^2}-(i+\overline{p_1})^2\}\{1+(\bar{t}-\overline{p_1})^2\}^2} \qquad (13)$$

Where

$$\vartheta = \frac{1+(\bar{t}-\overline{p_1})^2}{t^2-(i+\overline{p_1})^2}$$

With

$$\bar{t} = \bar{p}_i - \overline{p_2}$$

We have computed the above born equation numerically using Computer language programming. The First Born triple differential cross sections is finally calculated by

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{p_1 p_2}{p_i} |T_{fi}|^2 \qquad (14)$$

Where E_1 is the energy of the ejected electron. In our present work we have calculated and computed the TDCS of equation (14).

3. Results and Discussion

In this segment we explore the ionization of atomic hydrogen at metastable 3S-state by electrons. We compared the result with the measured values of 2S-state first born results [20] and with the previous 2P-state first born results [26].We have calculated the first born triple differential cross sections (TDCS) for ionization process at high incident energy $E_i = 250$ eV where the ejected angles (θ_1) varies and the scattered angles (θ_2) are fixed. Our first born calculations are presented in fig.1 to fig.6 for 250 eV incident electron energy. The scattering angles are $\theta_2 = 5^0$ (fig. 1), 7^0 (fig. 2), 9^0 (fig. 3), 11^0 (fig. 4), 15^0 (fig. 5) and 25^0 (fig. 6) and the ejected angle θ_1 varies from 0^0 to 360^0. The results are compared here with the results of hydrogenic 2S-state [20] and Dhar and Nahar [26] 2P- state first born calculations. We consider $\emptyset = 0^0$ as recoil position and $\emptyset = 180^0$ as binary position of the present calculations.

In the first born result of the present calculation we designed the triple differential cross sections (TDCS) for the ionization of metastable 2S- state hydrogen atoms by electrons for the incident energy $E_i = 250$ eV , ejected electron energies $E_1 = 5$ eV for the scattering angles θ_2 existing in the given figures. In the recoil position of the present first born result there is a solid minimum whereas at the binary position the result shows the peak value. The

present first born result is very close to the previous measurement of 2S- state hydrogen atoms first born results almost for all scattering angles.

In the present result fig. 1 shows one clearly peaked structure in both recoil and binary region whereas the hydrogenic 2S- state shows the similar and the 2P-state first born result shows two peaks in both recoil and binary region.

In fig.2 the present TDCS result shows a clear pictures of peaks whereas 2S and 2P state shows almost the same result. In fig.3 the hydrogenic 2S, 2P and 3S state shows almost similar positions. In fig.4 and fig.5 the binary region of 2S and 3S state shows a good peak than the 2P -state. For 25^0 scattering angle the present first born result shows its maximum peak value from the previous values of 2S and 2P states [20, 26] results.

Lastly, we observed that the peak position both in binary and recoil region the present results are very close to the compared result [20] almost for all scattering angles. At some point the result is different from the compared result [26] which happened due to the changes in the atomic position. For increasing scattering angles the present result shows good and interesting peaks.

Here a table: 1 of comparison results for ionization of hydrogenic 2S-state and 3S-state atoms by electrons is given.
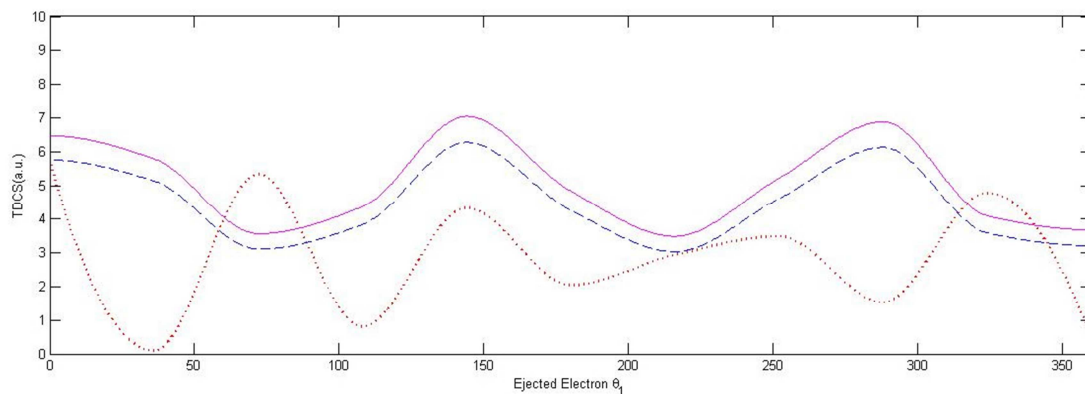

Fig. 1. Triple-differential cross sections (TDCS) for ionization of atomic hydrogen by 250eV electron impact for scattering angle $\theta_2 = 5^0$ vary against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5eV$. Theory: full curve: Present first born result, dash curve: 2S-state first born result [20] and dotted curve: 2P-state first born result [26].
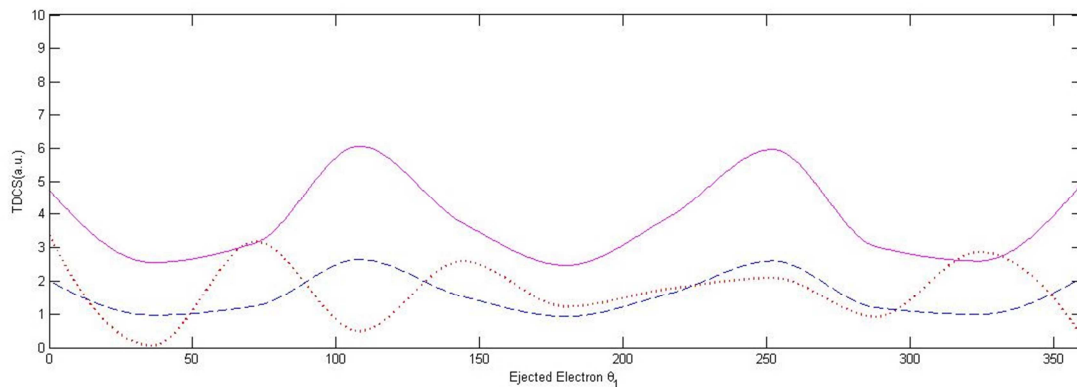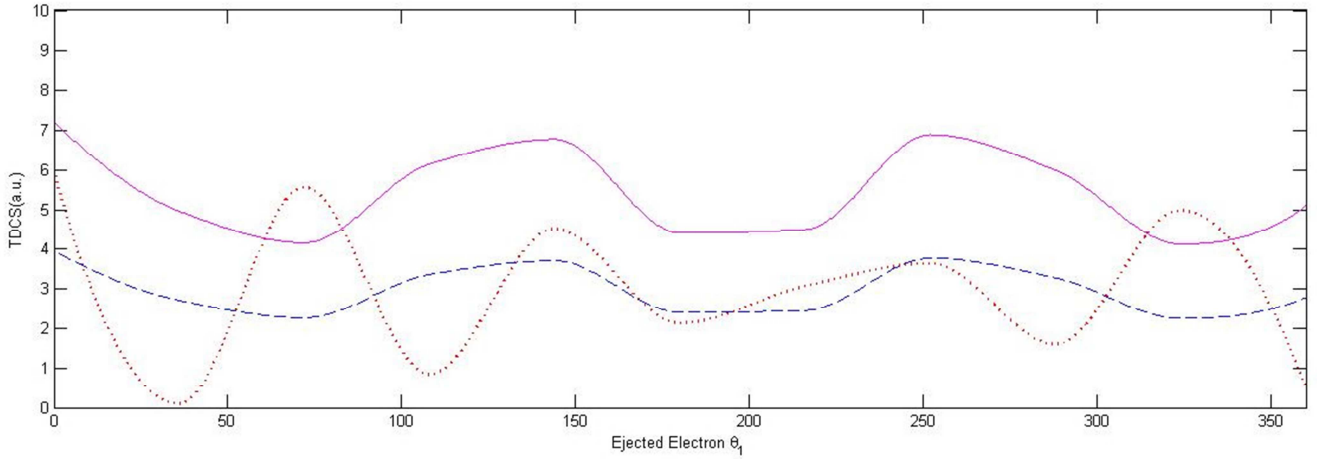

Fig. 2. Triple-differential cross sections (TDCS) for ionization of atomic hydrogen by 250eV electron impact for scattering angle $\theta_2 = 7^0$ vary against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is$E_1 = 5eV$. Theory: full curve: Present first born result, dash curve: 2S-state first born result [20] and dotted curve: 2P-state first born result [26].

Fig. 3. *Triple-differential cross sections (TDCS) for ionization of atomic hydrogen by 250eV electron impact for scattering angle $\theta_2 = 9^0$ vary against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5eV$. Theory: full curve: Present first born result, dash curve: 2S-state first born result [20] and dotted curve: 2P-state first born result [26].*

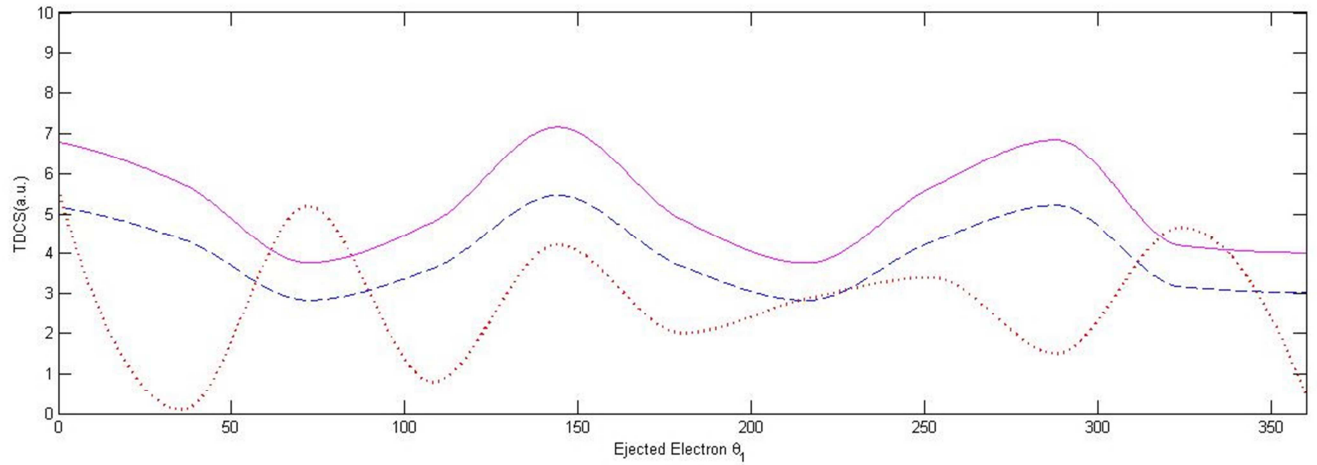**Fig. 4.** *Triple-differential cross sections (TDCS) for ionization of atomic hydrogen by 250eV electron impact for scattering angle $\theta_2 = 11^0$ vary against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5eV$. Theory: full curve: Present first born result, dash curve: 2S-state first born result [20] and dotted curve: 2P-state first born result [26].*
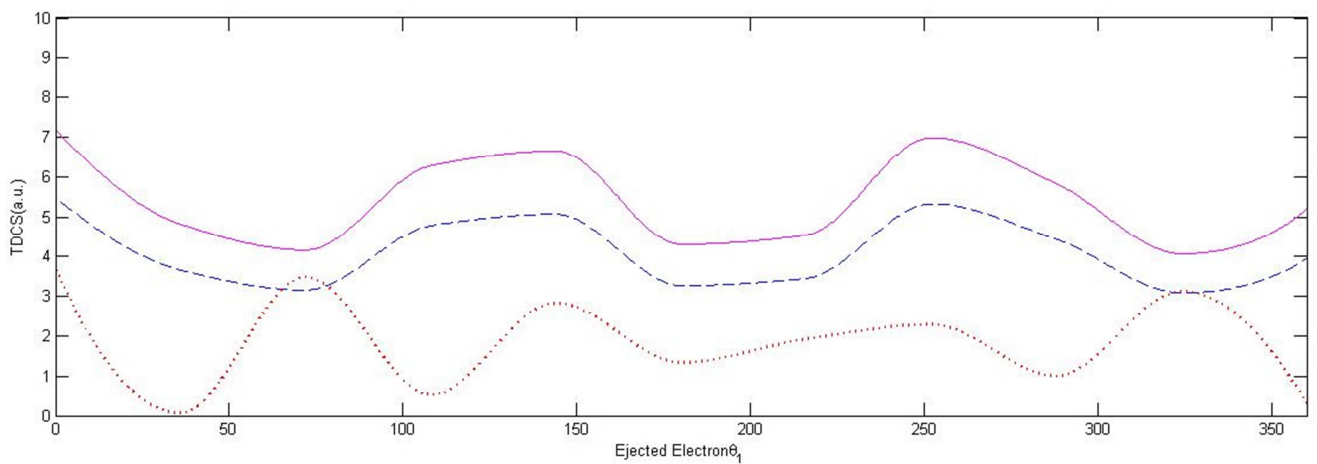

Fig. 5. *Triple-differential cross sections (TDCS) for ionization of atomic hydrogen by 250eV electron impact for scattering angle $\theta_2 = 15^0$ vary against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5eV$. Theory: full curve: Present first born result, dash curve: 2S-state first born result [20] and dotted curve: 2P-state first born result [26].*
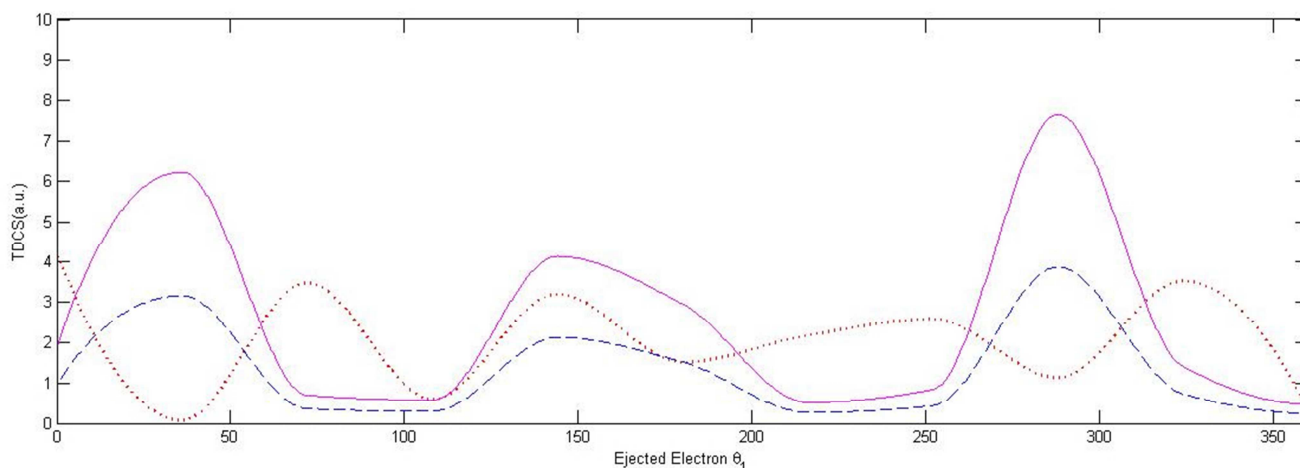
Fig. 6. *Triple-differential cross sections (TDCS) for ionization of atomic hydrogen by 250eV electron impact for scattering angle $\theta_2 = 25^0$ vary against the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is$E_1 = 5eV$. Theory: full curve: Present first born result, dash curve: 2S-state first born result [20] and dotted curve: 2P-state first born result [26].*

Table 1. *Triple differential cross sections (TDCS) for ionization of atomic hydrogen atoms by electron impact at metastable 3S-state are obtained by using equation (14). The incident energy is 250eV, the scattering angle is $\theta_2 = 9^0$ and the ejected electron energy is $E_1 = 5eV$. In the given table B1(3S): is the present 3S-state first born results and B1(2S): is the compared 2S-state first born results.*

Ejected angles(θ_1)	B1(2S)	B1(3S)
0	3.8461	5.6175
36	2.6382	3.8662
72	2.2079	3.2424
108	3.2756	4.7899
144	3.6140	5.2803
180	2.3431	3.4386
216	2.3873	3.5025
252	3.6768	5.3713
288	3.1916	4.6682
324	2.1905	3.2172
360	2.7073	3.9663

4. Conclusion

In this study we have calculated the triple differential cross sections (TDCS) for ionization of hydrogen atoms by electrons in the metastable 3S- state following the multiple scattering theory of Das and Seal. The present results show a very interesting binary peak features. Our present results show similar peaks almost at all scattering angles with the previous measurements of 2S-state. Whereas at binary peak region the present result shows a good agreement with the previous first born result of 2P-state. The present binary peak magnitude are smaller than the compared 2S- state and 2P-state first born results. The present calculation following the multiple scattering theory of Das and Seal provides a significant contribution in the field of metastable 3S-state ionization problems. For judgement of the present works experimental study in the relevant field will be needed. Thus the further calculations at other kinematic conditions will be interesting.

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