

The Triple Differential Cross Sections for Electron Impact Ionization of Metastable 3s State Hydrogen Atoms with Exchange Effect

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Abstract

A final state wave function of multiple scattering theory developed by Das and seal is utilized in the present study to calculate the triple differential cross sections (TDCS) for the ionization of metastable 3S state hydrogen atoms at incident electron energy of 250 eV with the exchange effects in the asymmetric coplanar geometry for various kinematic conditions. Our present calculation results are compared with the available hydrogenic ground state experimental data and other existing theoretical results. A good qualitative agreement is shown with those of compared results of the present study specifically with hydrogenic ground state experimental data and metastable 2S and 2P state with exchange effect results. These new results offer an extensive scope for experimental verification in such ionization process.

Keywords

Electron, Cross Sections, Ionization, Scattering

1. Introduction

Bethe [1] was first introduced the theoretical non-relativistic studies for the atomic ionization problems. The triple differential cross-section (TDCS) in electron hydrogen atom ionization collision has become increasingly interesting over the last four to five decades both theoretically and experimentally for relativistic [2]-[9] as well as for non-relativistic energies [10]-[21]. Triple differential cross-section (TDCS), measured in (e, 2e) coincidence experiment investigated first by Ehrhardt *et al.* [22] and Amaldi *et al.* [23]. After that many researchers have been successfully investigated such experiments in a large extent for ioniza-

tion process theoretically both in ground state [16] [24]-[32] and metastable state [33]-[43] of atomic hydrogen by electron and positron impact.

The first theoretical calculation of direct scattering amplitude of the TDCS for the coplanar asymmetric ionization of hydrogenic metastable 2S-state by electrons was calculated by Vučić *et al.* [20] in the coplanar asymmetric geometry. The present study of triple differential cross-section (TDCS) for ionization of metastable 3S state hydrogen atoms by electron exchange were never studied experimentally and theoretically. A few theoretical calculations for the TDCS of metastable 2S and 2P [45]-[50] state hydrogen atoms by electron exchange are observed. The theoretical results of Del *et al.* [21], BBK model [34], and the absolute data [15] for the ionization of hydrogen atoms by electrons from ground state have been considered in the present work for comparison.

The purpose of our present work is to calculate the triple differential cross sections (TDCS) for the electron impact ionization of hydrogen atoms in the metastable 3S state for coplanar asymmetric geometry with exchange effects. The present results give an interesting good qualitative fitness with the hydrogenic ground state ionization experimental data and some other hydrogenic ground state theoretical results as well as hydrogenic metastable 2S state and 2P state results. The new observation created a new dimension in this field of research.

2. Theory

We have considered here the direct and exchange amplitude of the T-matrix element. The T-matrix element for ionization of hydrogen atoms by electrons [17] can be written as,

$$T_{fi} = \langle \Psi_f^{(-)}(\bar{r}_1, \bar{r}_2) | V_i(\bar{r}_1, \bar{r}_2) | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \quad (1)$$

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

$$V_i(\bar{r}_1, \bar{r}_2) = \frac{1}{r_{12}} - \frac{Z}{r_2} \quad (2)$$

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,

$$\Phi_i(\bar{r}_1, \bar{r}_2) = \frac{e^{i\bar{p}_2 \cdot \bar{r}_2}}{(2\pi)^{3/2}} \varphi_{3s}(\bar{r}_1) = \frac{e^{i\bar{p}_2 \cdot \bar{r}_2}}{(2\pi)^{3/2}} \cdot \frac{1}{81\sqrt{3}\pi} (27 - 18r_1 + 2r_1^2) e^{-\lambda_1 r_1} \quad (3)$$

where

$$\varphi_{3s}(\bar{r}_1) = \frac{1}{81\sqrt{3}\pi} (27 - 18r_1 + 2r_1^2) e^{-\lambda_1 r_1} \quad (4)$$

and

$$\lambda_1 = 1/3$$

Equation (4) is the hydrogenic 3S-state wave function, \bar{p}_i 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,

$$\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2) = N(\bar{p}_1, \bar{p}_2) \left[\phi_{\bar{p}_1}^{(-)}(\bar{r}_1) e^{i\bar{p}_2 \cdot \bar{r}_2} + \phi_{\bar{p}_2}^{(-)}(\bar{r}_2) e^{i\bar{p}_1 \cdot \bar{r}_1} + \phi_{\bar{p}}^{(-)}(\bar{r}) e^{i\bar{p} \cdot \bar{R}} - 2e^{i\bar{p}_1 \cdot \bar{r}_1 + i\bar{p}_2 \cdot \bar{r}_2} \right] / (2\pi)^3 \quad (5)$$

where

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

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

$$\begin{aligned} |N(\bar{p}_1, \bar{p}_2)|^{-2} = & \left| 7 - 2[\lambda_1 + \lambda_2 + \lambda_3] - \left[\frac{2}{\lambda_1} + \frac{2}{\lambda_2} + \frac{2}{\lambda_3} \right] \right. \\ & \left. + \left[\frac{\lambda_1}{\lambda_2} + \frac{\lambda_1}{\lambda_3} + \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{\lambda_3} + \frac{\lambda_3}{\lambda_1} + \frac{\lambda_3}{\lambda_2} \right] \right| \end{aligned} \quad (6)$$

here

$$\lambda_1 = e^{\frac{\pi\alpha_1}{2}} \Gamma(1 - i\alpha_1), \quad \alpha_1 = \frac{1}{P_1}$$

$$\lambda_2 = e^{\frac{\pi\alpha_2}{2}} \Gamma(1 - i\alpha_2), \quad \alpha_2 = \frac{1}{P_2}$$

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

The normalization constant $N(\bar{p}_1, \bar{p}_2)$ is calculated numerically using Equation (6) and the approximated value of $N(\bar{p}_1, \bar{p}_2)$ is 1.

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

$$\phi_{\bar{q}}^{(-)}(\bar{r}) = e^{\frac{\pi\alpha}{2}} \Gamma(1 + i\alpha) e^{i\bar{q} \cdot \bar{r}} {}_1F_1(-i\alpha, 1, -i[qr + \bar{q} \cdot \bar{r}])$$

For the electron impact ionization the parameters α_1 , α_2 and α are given below

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

Equation (1) becomes,

$$T_{fi} = N(\bar{p}_1, \bar{p}_2) [T_B + T_{B'} + T_i - 2T_{PB}] \quad (7)$$

where

$$T_B = \langle \Phi_{\bar{p}_1}^{(-)}(\bar{r}_1) e^{i\bar{p}_2 \cdot \bar{r}_2} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \quad (8)$$

$$T_{B'} = \langle \Phi_{\bar{p}_2}^{(-)}(\bar{r}_2) e^{i\bar{p}_1 \cdot \bar{r}_1} | V_i | \Phi_i(\bar{r}_1, \bar{r}_2) \rangle \quad (9)$$

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

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

The direct scattering amplitude $f(\bar{p}_1, \bar{p}_2)$ is determined from

$$f(\bar{p}_1, \bar{p}_2) = -(2\pi)^2 T_{fi} \quad (12)$$

The exchange scattering amplitude is then approximated by

$$g(\bar{p}_1, \bar{p}_2) = f(\bar{p}_2, \bar{p}_1) \quad (13)$$

After analytical calculations using Lewis Integral [44], the triple differential cross-sections (TDCS) with exchange effects is finally takes the following form,

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{p_1 p_2}{p_i} \left[\frac{3}{4} |f - g|^2 + \frac{1}{4} |f + g|^2 \right] \quad (14)$$

Here E_1 is the energy of the ejected electron. Hence, in our present study we have calculated the TDCS with exchange effects, given by the Equation (14) using computer programming language.

3. Results and Discussions

We have discussed here in this section the ionization of metastable 3S state hydrogen atoms by electrons with exchange effect. The triple differential cross-sections (TDCS) at $E_i = 250$ eV incident energy with the ejected electron energy of 5 eV is calculated. The results of exchange effects are displayed by the **Figure 1** ($\theta_2 = 3^\circ$), **Figure 2** ($\theta_2 = 15^\circ$), **Figure 3** ($\theta_2 = 25^\circ$), **Figure 4** ($\theta_2 = 5^\circ$), **Figure 5** ($\theta_2 = 7^\circ$), **Figure 6** ($\theta_2 = 9^\circ$), **Figure 7** ($\theta_2 = 11^\circ$), **Figure 8** ($\theta_2 = 15^\circ$) and **Figure 9** ($\theta_2 = 20^\circ$). We consider here the incident electron energy is $E_i = 250$ eV for some varied ejected angles (θ_1) and for a fixed scattering angle (θ_2). The ejection angle θ_1 varies from 0° to 360° . We consider here the recoil regions of the following figures from $\theta_1(0^\circ - 150^\circ)$ and $\phi = 0^\circ$ on other hand the binary region is from $\theta_1(150^\circ - 360^\circ)$ and $\phi = 180^\circ$.

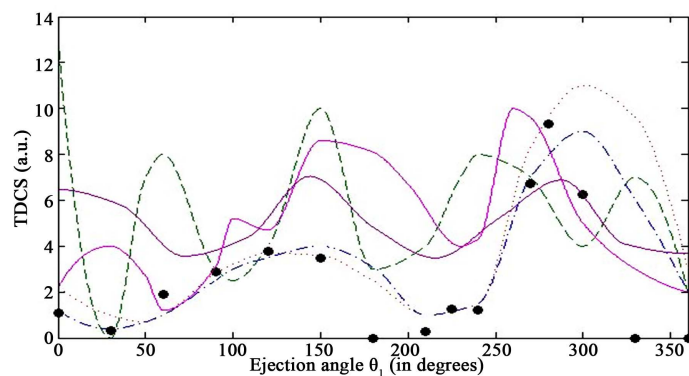


Figure 1. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_2 = 3^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV. Theory: Full filled double curve reflects the present calculation of 3S state with exchange effect. Full single curve represent the first born 3S state result [48]. Dash curve shows the second born 2P state result [47]. Short dash curve focuses hydrogenic ground state second born result [21]; Dash-dotted curve shows hydrogenic ground state BBK model [34] and filled round shows hydrogenic ground state experiments [15].

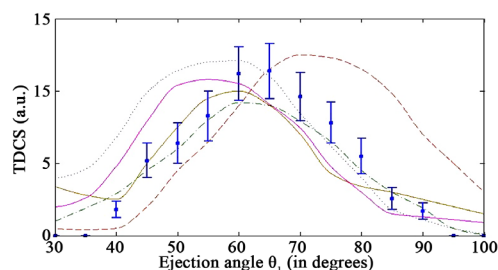


Figure 2. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_2 = 15^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 50$ eV. Theory: Full curve (m) reflects the present calculation of 3S state with exchange effect. Full single curve (red) represent the first born 3S state result [48]. Dash curve shows the second born 2P state result [47]. Short dash curve focuses hydrogenic ground state second born result [21]; Dash-dotted curve shows hydrogenic ground state BBK model [34], dash-dotted curve reflects the second born 2S-state result [38] and square shows hydrogenic ground state experiments [15].

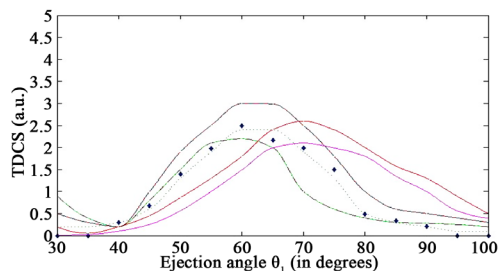


Figure 3. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact for $\theta_2 = 25^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 50$ eV. Theory: Full curve (m) reflects the present calculation of 3S state with exchange effect. Full single curve (red) represent the first born 3S state result [48]. Dash curve shows the second born 2P state result [47]. Short dash curve focuses hydrogenic ground state second born result [21]; Dash-dotted curve shows hydrogenic ground state BBK model [34], dash-dotted curve reflects the second born 2S-state result [38] and square shows hydrogenic ground state experiments [15].

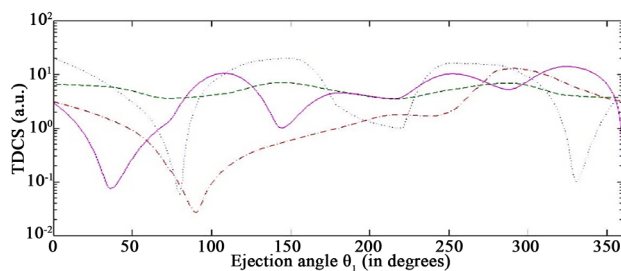


Figure 4. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact with exchange effects for $\theta_2 = 5^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV. Theory: Full curve reflects the present calculation. Dash curve represent the first born 3S-state result [48]. Short dash curve shows the second born 2P-state result [47]. Dash-dot curve exhibits the hydrogenic 2S-state result [38].

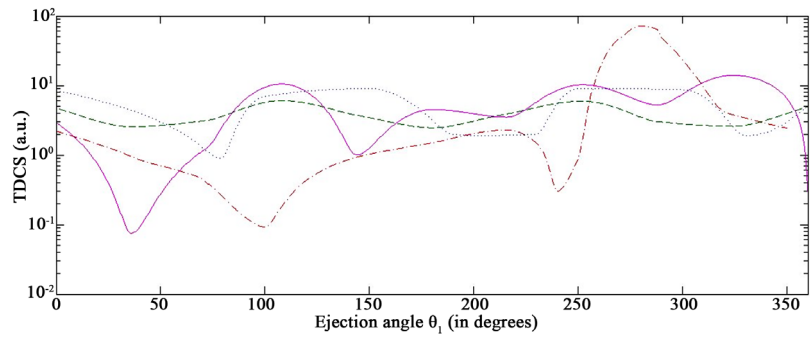


Figure 5. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact with exchange effects for $\theta_2 = 7^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV . Theory: Full curve reflects the present calculation. Dash curve represent the first born 3S-state result [48]. Short dash curve shows the second born 2P-state result [47]. Dash-dot curve exhibits the hydrogenic 2S-state result [38].

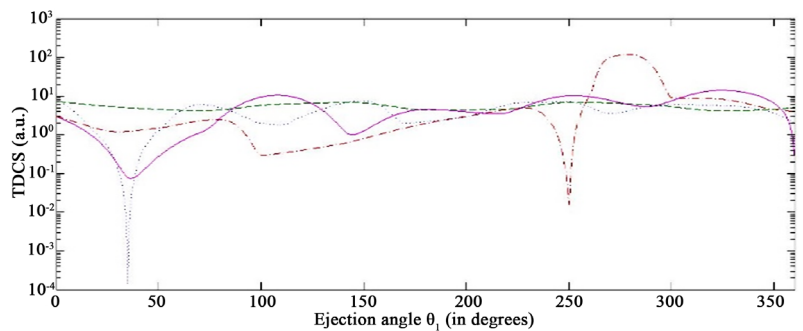


Figure 6. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact with exchange effects for $\theta_2 = 9^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV . Theory: Full curve reflects the present calculation. Dash curve represent the first born 3S-state result [48]. Short dash curve shows the second born 2P-state result [47]. Dash-dot curve exhibits the hydrogenic 2S-state result [38].

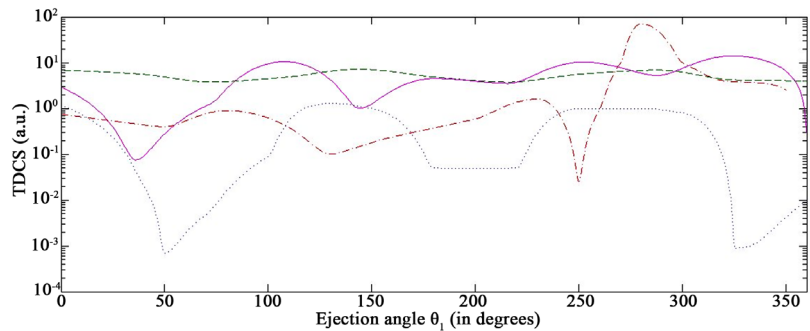


Figure 7. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact with exchange effects for $\theta_2 = 11^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV . Theory: Full curve reflects the present calculation. Dash curve represent the first born 3S-state result [48]. Short dash curve shows the second born 2P-state result [47]. Dash-dot curve exhibits the hydrogenic 2S-state result [38].

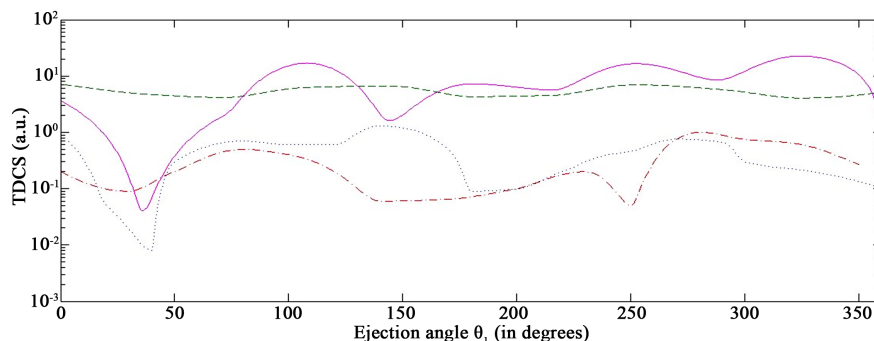


Figure 8. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact with exchange effects for $\theta_2 = 15^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV. Theory: Full curve reflects the present calculation. Dash curve represent the first born 3S-state result [48]. Short dash curve shows the second born 2P-state result [47]. Dash-dot curve exhibits the hydrogenic 2S-state result [38].

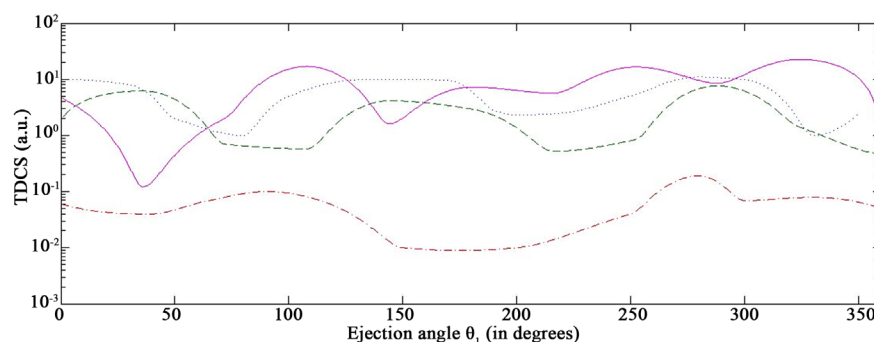


Figure 9. Triple differential cross sections (TDCS) for ionization of atomic hydrogen by 250 eV electron impact with exchange effects for $\theta_2 = 20^\circ$ vary against the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV. Theory: Full curve reflects the present calculation. Dash curve represent the first born 3S-state result [48]. Short dash curve shows the second born 2P-state result [47]. Dash-dot curve exhibits the hydrogenic 2S-state result [38].

Electron-hydrogen ionization from ground state theoretical results of Dal *et al.* [21], the BBK model of Brauner *et al.* [34] and the experimental results of Ehrhardt *et al.* [15] are presented here for comparisons. The earlier works of hydrogenic 2S-state [38] ionization results. The recent works on hydrogenic 2P-state [47] ionization results are also exhibited here for comparison with our present work. We have considered here the triple differential cross-sections (TDCS) with exchange effects for the ionization of metastable 3S-state hydrogen atoms by electrons for the incident electron energy of $E_i = 250$ eV and ejected electron energies $E_1 = 5$ eV and 50 eV. The final continuum state of the present work shows a similar but shifted amplitude in the recoil lobe position as the earlier result of hydrogenic ground state second born approximation [21].

In **Table 1** we figure a comparison data for our present result of triple differential cross sections for ionization of hydrogenic 3S state by electron impact with exchange effects with the 2P state exchange results.

Table 1. Triple differential cross sections (TDCS) for ionization of atomic hydrogen atoms by electron impact with exchange effects are obtained by Equation (14) at metastable 3S-state. The incident energy is 250 eV, the scattering angle is $\theta_2 = 9^\circ$ and the ejected electron energy is $E_1 = 5$ eV. In **Table 1** B1 (2P): is the compared 2P state exchange results and B2 (3S): is the present results.

Ejected angles (θ_1)	B1 (2P)	B2(3S)
0	5.6923	1.1151
36	3.625	5.0858
72	1.46154	0.0752
108	6.4231	5.0380
144	6.8077	5.0135
180	8.3077	7.2945
216	6.6077	6.1394
252	7.19231	5.1394
288	7.7769	10.0288
324	5.15	5.0395
360	5.38462	0.0250

In **Figure 1** we consider the ejected electron energy $E_1 = 5$ eV with a fixed scattering angle $\theta_2 = 3^\circ$ and the incident electron energy is 250 eV. It is exciting to observe that our present results show a good qualitative agreement with the compared results of present first born result [48], the hydrogenic ground state result of BBK model [34], the second born approximation [21], the experimental data [15] and the second born experiment of 2P-state [47] exchange effects results. Our present result shows a fall in the recoil region and two prominent peaks in binary region.

We consider for **Figure 2** the ejected electron energy $E_i = 250$ eV, scattered electron energy $E_1 = 50$ eV and scattered angle $\theta_2 = 15^\circ$. We also consider the ejected electron angle θ_1 from 30° to 100° . In this figure our present results gives small magnitude compared with the previous theoretical results [21] [38] [47] [48] and shows a good qualitative similarity with the experimental results [15] [34].

In a similar way **Figure 3** shows us the 3S metastable state with exchange effects for ejected electron energy $E_i = 250$ eV, scattered electron energy $E_1 = 50$ eV and scattered angle $\theta_2 = 25^\circ$. As we increase our scattering angle (θ_2) the peak of our present study shows a smaller magnitude with hydrogenic ground state second born results [21].

From **Figures 4-9** we compared the present exchange effects results with previous theoretical results like 2P and 2S metastable states [38] [47]. We also include here the present first Born result [48]. The scattering angle varies from $\theta_2 = 5^\circ$ (**Figure 4**), $\theta_2 = 7^\circ$ (**Figure 5**), $\theta_2 = 9^\circ$ (**Figure 6**), $\theta_2 = 11^\circ$ (**Figure 7**), $\theta_2 = 15^\circ$ (**Figure 8**), $\theta_2 = 20^\circ$ (**Figure 9**) in the fixed incident energy

$E_i = 250$ eV, ejected energy $E_1 = 5$ eV and the ejected electron angle is vary from ($\theta_1 = 0^\circ$ to 360°).

Figure 4 and **Figure 5** our present result shows a good agreement of our present result with 2S-state metastable exchange results [38]. The figure displayed a deep lobed peak structure which shows a good qualitative similarity with the compared results [38] [47] [48].

When we increase our scattering angle in **Figure 6** our present result and the present first Born result remains same and give a good qualitative agreement with the compared 2P state exchange result [47].

In **Figure 7** our present TDCS exchange curve shows a very interesting result. It exhibits two falls in recoil region whereas the compared 2S state exchange result [38] there is only one fall in the recoil region. The result shows a bit different from 2P state exchange result [47].

In the **Figure 8** and **Figure 9** the magnitude of the present results smaller than the present first Born results [48]. The characteristic features of the cross section curves of the present calculation shows a good improvement comparing with the previous results as the scattering angles are increasing.

The present result of 3S-state exchange effects gives a good qualitative improvement comparing with the previous 2S and 2P state exchange effect results. The present result also show a similar conduct with the hydrogenic ground state result [21] in the binary region. Moreover there needs more experimental works in this field for further investigation.

Finally, the scattering mechanism for the ionization of metastable 3S state with exchange effects for 250 eV incident electron energy is presented here in this study. The scattered electrons are described by a plane wave in the first Born term of Equation (5) whereas the ejected electrons are defined by a Coulomb wave. In the second term of the Equation (5) the scattered electrons are defined by the Coulomb wave while the ejected electrons are defined by the plane wave. The projectile electron interaction appeared in the third term shows almost similar behavior in the final channel wave function. The fourth term represents two plane waves for both ejected and scattered particles. The above results gives us a strong view of peaks both in recoil region and binary region. We can conclude that the present peak values gives us a good agreement with our compared experimental results as well as the theoretical results. In Our present study the measurements of peak values gives us the encouragement for further research in this field of interest. Moreover it needs more experimental works in this field for further investigation.

4. Conclusion

Our present calculation on the triple differential cross sections for ionization of atomic hydrogen by electron impact with exchange effects in metastable 3S-state exposes a thinkable additional structure of the cross-section curves for small momentum transfer in the ionization of the hydrogen atoms. The final state

wave function $\psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$ of Das and Seal gives a good qualitative result with the hydrogenic ground state experiment as well as with the BBK model of ground state hydrogen atoms. For good qualitative agreement, the present study are very encouraging for the future experiments which may play a vital role to give interesting and significant results in this field of research.

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