Open Journal of Microphysics, 2024, 14, 67-77
https://www.scirp.org/journal/ojm
ISSN Online: 2162-2469
ISSN Print: 2162-2450

# First Born Double Differential Cross-Section for Ionization of H (3d) by Incident Electron Impact

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**How to cite this paper:** Banerjee, S. and Dhar, S. (2024) First Born Double Differential Cross-Section for Ionization of H (3d) by Incident Electron Impact. *Open Journal of Microphysics*, **14**, 67-77.
https://doi.org/10.4236/ojm.2024.142005

**Received:** February 18, 2024
**Accepted:** May 27, 2024
**Published:** May 30, 2024



## Abstract

Double differential cross section (DDCS) of First-Born approximation is calculated for the ionization of metastable 3d-state hydrogen atoms by electron impact energy at 150 eV and 250 eV. A multiple scattering theory is applied in the present study. The present results are compared with the other related theoretical results for the ionization of hydrogen atoms from different metastable states and ground-state experimental results. The findings demonstrate a strong qualitative agreement with the existing results. The obtained results have an extensive scope for further study of such an ionization process.

## Keywords

Electron, Ionization, Cross-Section, Scattering

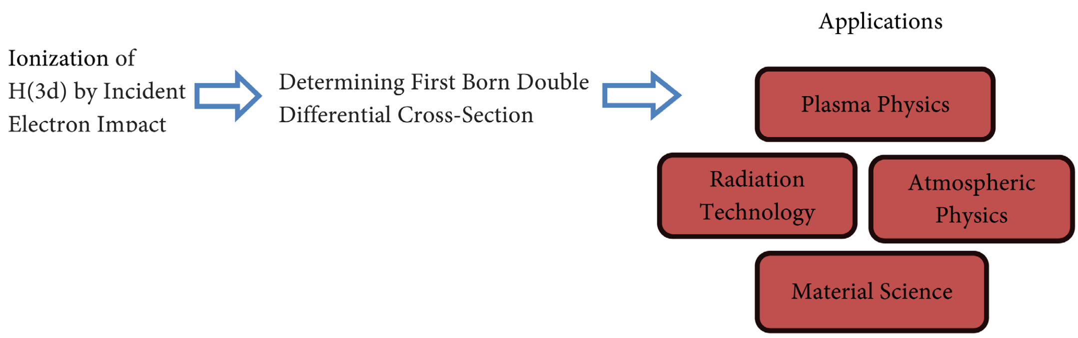
## 1. Introduction

The analysis of multiple ionization of metastable atoms by electrons is in high demand in many experimental fields, particularly astrophysics, plasma physics, radiation physics, and applied mathematics.

The field of electron impact ionization of atoms faces a major challenge in developing a general theoretical framework that accurately predicts ionization cross-sections for many atoms over a practically relevant range of impact energy. Due to its complexity, fully quantum-mechanical treatment of electron impact ionization of atoms is only possible for the simplest cases of hydrogen and helium. To understand the ionization mechanism of the atomic system by electron impact, we used a hydrogen atom target. Hydrogen, the lightest and most abundant substance in the universe, can be ionized by electrons, making it a good candidate for perturbation theory.

The quantum mechanical treatment of ionization by fast particles was first introduced by Bethe [1]. The single and double ionization of hydrogen atoms through electron-atom coincidence experiments, known as (e, 2e) experiments, is a fundamental process. These experiments involve detecting the ejected electron along with the scattered electron. 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]-[11] as well as relativistic [12] [13] [14] [15] energies. Over the past forty years, there has been a growing interest in studying the triple differential cross-section (TDCS) in electron hydrogen atom ionization collisions. For the past fifty years, the ionization of hydrogen atoms by electrons has been studied to understand the process in both the ground state [2] [3] [4] and metastable states [5]-[11] of atomic hydrogen. The study of double differential cross-section (DDCS) for ground-state hydrogen atoms using the (e, 2e) experiment has been widely researched both theoretically and experimentally. Similarly, DDCS for metastable states has also been studied. However, there is currently no literature available on double differential cross-section (DDCS) for the ionization of hydrogenic metastable 3d states.

In this study, we evaluate the double differential cross-section (DDCS) of metastable 3d-state hydrogen atoms by electrons, under various kinematic conditions. We apply the multiple scattering theory of Das and Seal [2]. The results of this study will create a new dimension on the ionization of hydrogenic metastable states. Present results are compared with previous related theories [16] [17] and [18]. The main contributions of the work are given below:




## 2. Theory

Ionization cross-section is the measure of the probability of the ionization process of an atom by electron or molecule.

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. In this theory, we used the multiple scattering theory of Das and Seal [2].

Ionization of atomic hydrogen by electron in the most elaborate form is presently available in the 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 direct T-matrix element for ionization of hydrogen atoms by electrons may be written as [2]

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

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 $V_i\left(\bar{r}_1, \bar{r}_2\right)$ is given by

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

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.

The initial channel unperturbed wave function is

$$\Phi_i\left(\bar{r}_1, \bar{r}_2\right) = \frac{e^{i\bar{p}_i \cdot \bar{r}_2}}{(2\pi)^{3/2}} \varphi_{3d}\left(\bar{r}_1\right) \tag{4}$$

where

$$\varphi_{3d}\left(\bar{r}_1\right) = \frac{1}{81\sqrt{6\pi}} r_1^2 \left(3\cos^2\theta - 1\right) e^{-\frac{r_1}{3}} = \frac{1}{324\sqrt{3\pi^2}} r_1^2 \left(3\cos^2\theta - 1\right) e^{-\lambda_1 r_1} \tag{5}$$

Here $\lambda_1 = \frac{1}{3}$, $\varphi_{3d}\left(\bar{r}_1\right)$ is the hydrogenic 3d-state wave function, and the approximate wave function is given by [2]

$$\begin{aligned} &\Psi_f^{(-)}\left(\bar{r}_1, \bar{r}_2\right) \\ &= N\left(\bar{p}_1, \bar{p}_2\right)\left[\varphi_{\bar{p}_1}^{(-)}\left(\bar{r}_1\right) e^{i\bar{p}_2 \cdot \bar{r}_2} + \varphi_{\bar{p}_2}^{(-)}\left(\bar{r}_2\right) e^{i\bar{p}_1 \cdot \bar{r}_1} + \varphi_{\bar{p}}^{(-)}\left(\bar{r}\right) e^{i\bar{P} \cdot \bar{R}} - 2e^{i\bar{p}_1 \cdot \bar{r}_1 + i\bar{p}_2 \cdot \bar{r}_2}\right] \Big/ (2\pi)^3 \end{aligned} \tag{6}$$

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 triple differential cross section is denoted by the symbol

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1}.$$

and the Coulomb wave function $\varphi_q^{(-)}\left(\bar{r}\right)$ is given by

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

with

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

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

and

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

Now Equation (2) becomes

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

where

$$T_B = \left\langle \varphi_{p_1}^{(-)}\left(\bar{r}_1\right) \mathrm{e}^{i\bar{p}_2\cdot\bar{r}_2} \left|V_i\right| \Phi_i\left(\bar{r}_1, \bar{r}_2\right) \right\rangle \tag{8}$$

$$T_{B'} = \left\langle \varphi_{p_2}^{(-)}\left(\bar{r}_2\right) \mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1} \left|V_i\right| \Phi_i\left(\bar{r}_1, \bar{r}_2\right) \right\rangle \tag{9}$$

$$T_i = \left\langle \varphi_{p}^{(-)}\left(\bar{r}\right) \mathrm{e}^{i\bar{P}\cdot\bar{R}} \left|V_i\right| \Phi_i\left(\bar{r}_1, \bar{r}_2\right) \right\rangle \tag{10}$$

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

Here Equation (8) is called the First Born term and it may be written as

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

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

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

$$T_B = tb_1 + tb_2 \tag{12}$$

where

$$tb_1 = \frac{1}{324\sqrt{3}\pi^2} \int \varphi_{p_1}^{(-)*}\left(\bar{r}_1\right) \mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2} \frac{1}{r_{12}} \mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2} r_1^2 \left(3\cos^2\theta - 1\right) \mathrm{e}^{-\lambda_1 r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \tag{13}$$

$$tb_2 = -\frac{1}{324\sqrt{3}\pi^2} \int \varphi_{p_1}^{(-)*}\left(\bar{r}_1\right) \mathrm{e}^{-i\bar{p}_2\cdot\bar{r}_2} \frac{1}{r_2} \mathrm{e}^{i\bar{p}_i\cdot\bar{r}_2} r_1^2 \left(3\cos^2\theta - 1\right) \mathrm{e}^{-\lambda_1 r_1} \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \tag{14}$$

The terms in Equation (12) have been computed using the First Born approximation.

After analytical calculation by using the Lewis integral [19], The First Born term $T_B$ of Equation (8) is evaluated numerically using the computer language MATLAB. Finally, the triple differential cross-sections for T-Matrix element is given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1 \mathrm{d}\Omega_2 \mathrm{d}E_1} = \frac{p_1 p_2}{p_i} \left|T_{fi}\right|^2 \tag{15}$$

We can use the equation given below to find the DDCS results

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E_1\mathrm{d}\Omega_1} = \int \frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_1}\mathrm{d}\Omega_2 .$$

## 3. Results and Discussions

DDCS are determined here for the ionization of the metastable 3d state hydrogen atoms by electrons at high incident energy $E_i$ = 250 eV (**Figures 1-3**) for

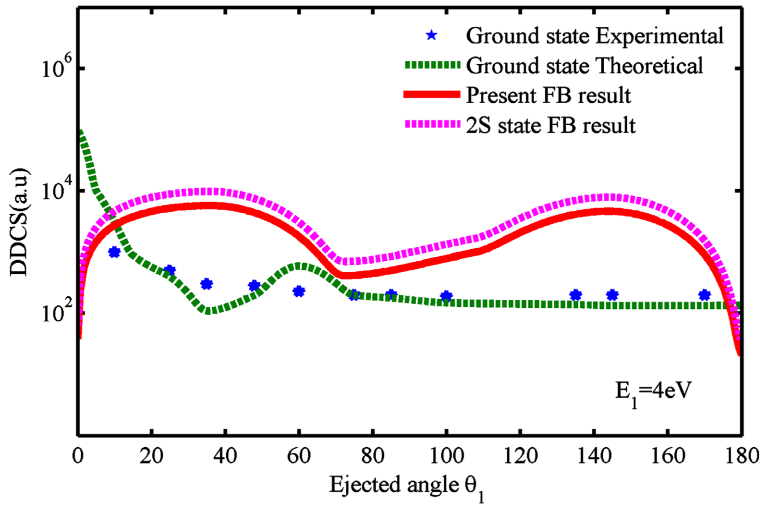



**Figure 1.** Double-differential cross sections (DDCS) versus ejected electron angle $\theta_1$ for electron impact energy $E_i$ = 250 eV, ejected electron energy $E_1$ = 4 eV. Theory: Symbol (Star): Ground state experiment [18], Continuous curve (Red): Present the first born result, dash curve (Green): Ground state theory [16], dash curve (Magenta): 2S-state First born result [17].

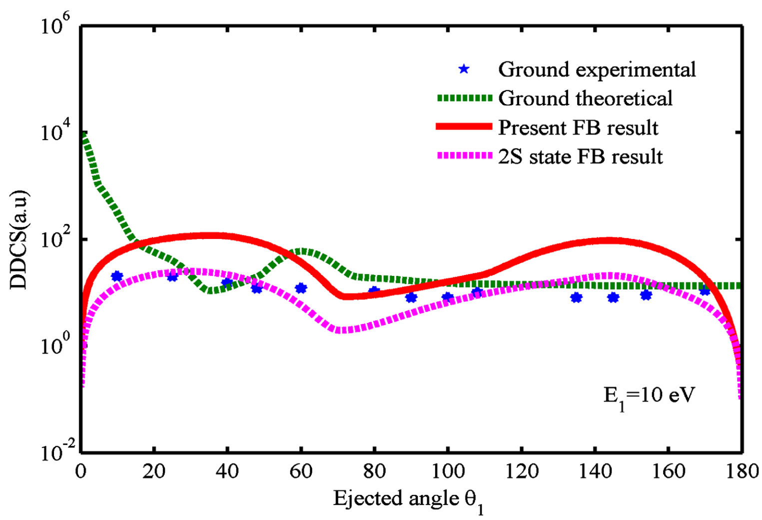



**Figure 2.** Double-differential cross sections (DDCS) versus ejected electron angle $\theta_1$ for electron impact energy $E_i$ = 250 eV, ejected electron energy 10 eV. Theory: Symbol (Star): Ground state experiment [18], Continuous curve (Red): Present the First born result, dash curve (Green): Ground state theory [16], dash curve (Magenta): 2S-state First born result [17].

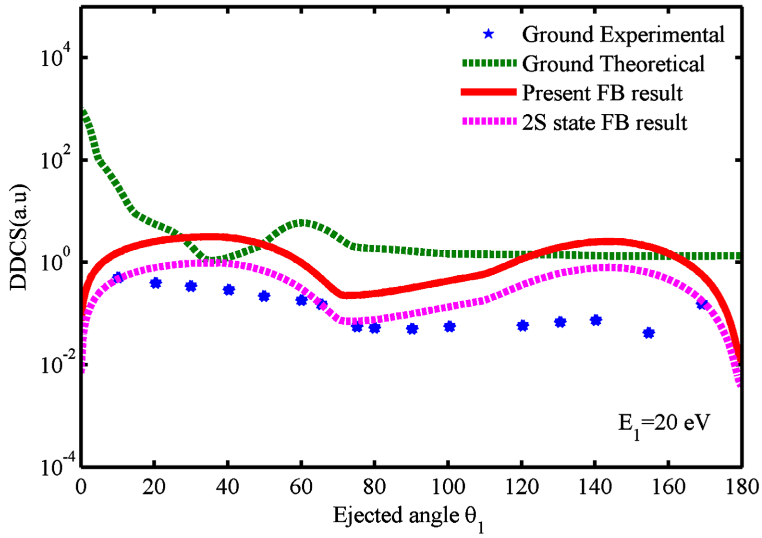



**Figure 3.** Double-differential cross sections (DDCS) versus ejected electron angle $\theta_1$ for electron impact energy $E_i = 250$ eV, ejected electron energy 20 eV. Theory: Symbol (Star): Ground state experiment [18], Continuous curve (Red): Present the First born result, dash curve (Green): Ground state theory [16], dash curve (Magenta): 2S-state First born result [17].

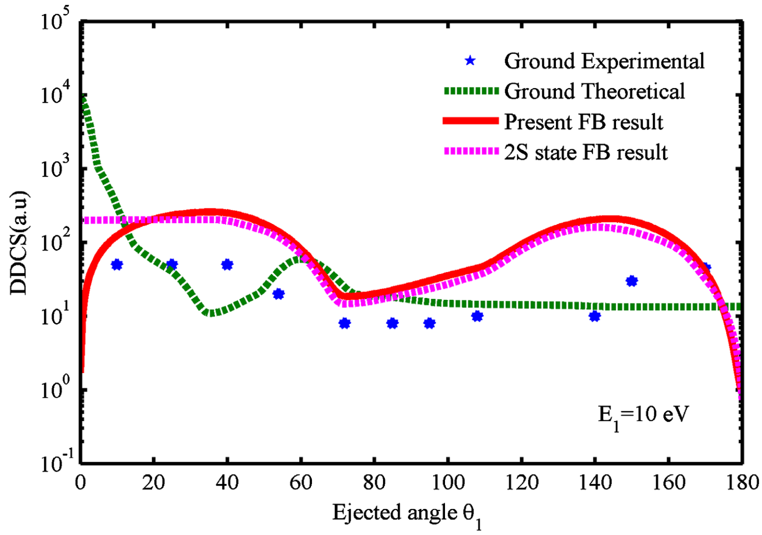



**Figure 4.** Double-differential cross sections (DDCS) versus ejected electron angle $\theta_1$ for electron impact energy $E_i = 150$ eV, ejected electron energy 10 eV. Theory: Symbol (Star): Ground state experiment [18], Continuous curve (Red): Present the First born result, dash curve (Green): Ground state theory [16], dash curve (Magenta): 2S-state First born result [17].

emitted electron energies $E_1 = 4$ eV, 10 eV, and 20 eV. Again, at intermediate incident energy $E_i = 150$ eV (**Figures 4-6**) for emitted electron energies $E_1 = 10$ eV, 20 eV, and 50 eV. The emitted angle $\theta_1$ varies from 0˚ to 180˚ considered as a horizontal axis where DDCS is the vertical axis in all figures and the scattered angle $\theta_2$ varies from 0˚ to 100˚. Ionization of hydrogen atoms by electrons from the ground state experimental results [18] and computational results [16] [17]

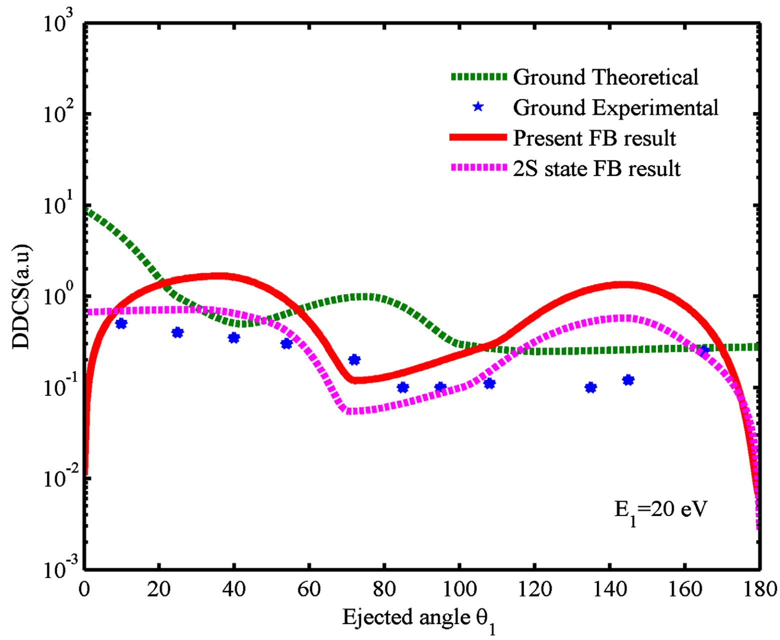



**Figure 5.** Double-differential cross sections (DDCS) versus ejected electron angle $\theta_1$ for electron impact energy $E_i$ = 150 eV, ejected electron energy 20 eV. Theory: Symbol (Star): Ground state experiment [18], Continuous curve (Red): Present the First-born result, dash curve (Green): Ground state theory [16], dash curve (Magenta): 2S-state First born result [17].

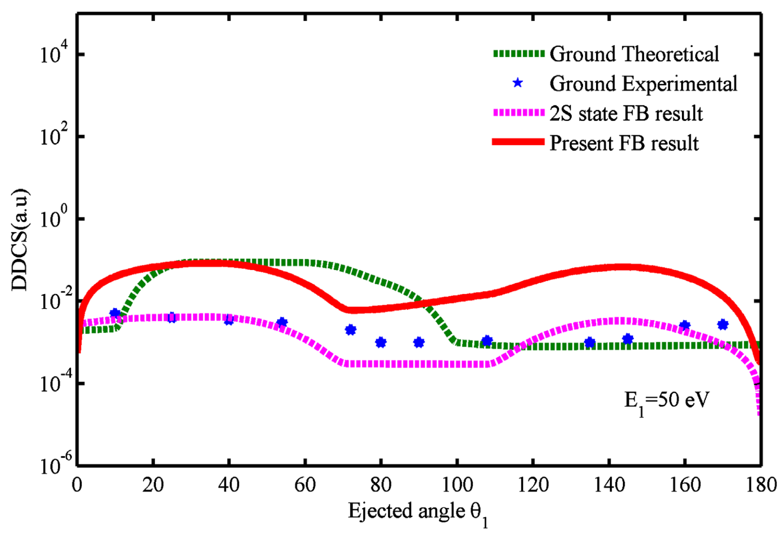



**Figure 6.** Double-differential cross sections (DDCS) versus ejected electron angle $\theta_1$ for electron impact energy $E_i$ = 150 eV, ejected electron energy 50 eV. Theory: Symbol (Star): Ground state experiment [18], Continuous curve (Red): Present the First born result, dash curve (Green): Ground state theory [16], dash curve (Magenta): 2S-state First born result [17].

are presented here for assessment. The final state scattering wave function $\psi_f\left(\overline{r}_1,\overline{r}_2\right)$ is the continuum state of the atomic hydrogen. We consider, $\varphi = 0^\circ$ as a recoil region while $\varphi = 180^\circ$ as a binary region.

For incident energy $E_i$ = 250 eV in **Figure 1**, ejection energy $E_1$ = 4 eV the current the first Born result coincides at $\theta_1 = 10˚$, $\theta_1 = 70˚$, and $\theta_1 = 177˚$ with those ground state results [16]. Furthermore, it is nearer with the ground state experiment results [18] in the ejected electron angle range $\theta_1 = 70˚$ to $\theta_1 = 100˚$.

In **Figure 2**, $E_1 = 10$ eV the current outcome intersect several times with those of ground state result [16] at $\theta_1 = 18˚$, $\theta_1 = 55˚$, $\theta_1 = 100˚$ and $\theta_1 = 170˚$ whereas it crosses three times with the ground state experiment value [18] about at $\theta_1 = 80˚$, $\theta_1 = 90˚$, $\theta_1 = 170˚$ which indicates good assessment. The present and 2S state result [17] show similar shape all entire angular region.

In **Figure 3**, $E_1 = 20$ eV it is seen that the ground state experimental result [18], 2S state result [17] and the current result show similar nature specially in the recoil region. It meets with ground state theoretical result [16] at ejected angles 30˚, 50˚, 120˚, 160˚.

For incident energy $E_i = 150$ eV in **Figure 4**, the present outcome and 2P state result [17] are very close in whole region. Both are intersect with ground state theoretical result [16] at $\theta_1 = 10˚$, $\theta_1 = 60˚$, $\theta_1 = 80˚$ and $\theta_1 = 170˚$ whereas they are nearer to the angular region 50˚ to 110˚ and intersect at an ejected angle about 170˚ with ground state experimental result [18].

Let us consider the case of **Figure 5**, the present DDCS result and 2S-state result [17] show a similar shape in the recoil and binary region where they display quite different shapes with ground state theoretical results [16] due to the different metastable states.

At last, we consider ejection energy as $E_1 = 50$ eV, in **Figure 6**, our current DDCS curve and 2S-state metastable state [17] result display almost similar shape with ground state theoretical result [16] in the recoil region but in the binary region show quite dissimilar pattern. Present DDCS results display higher magnitude in both recoil and binary regions than the corresponding compared

**Table 1.** First Born DDCS for ionization of atomic hydrogen atoms by electron impact at metastable 3d-state. The incident energy is 150 eV.

| $\theta_2$ (deg) | $\theta_1$ (deg) | $E_1 = 10$ eV DDCS | $E_1 = 20$ eV DDCS | $E_1 = 50$ eV DDCS |
|---|---|---|---|---|
| 0 | 0 | 1.7153 | 0.0110 | 0.0006 |
| 1 | 36 | 261.9409 | 1.6799 | 0.0856 |
| 2 | 72 | 18.6716 | 0.1197 | 0.0061 |
| 4 | 108 | 45.3698 | 0.2910 | 0.0148 |
| 10 | 144 | 211.6241 | 1.3572 | 0.0691 |
| 20 | 180 | 0.9535 | 0.0061 | 0.0003 |
| 30 | 216 | 298.0039 | 1.9112 | 0.0974 |
| 40 | 252 | 4.7460 | 0.0304 | 0.0016 |
| 60 | 288 | 85.6190 | 0.5491 | 0.0280 |
| 90 | 324 | 155.3813 | 0.9965 | 0.0508 |
| 100 | 360 | 0 | 0 | 0 |

result of with ground state experimental 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. However, it has a shorter lifetime than the stable ground state. The peak structure of the present results shows good qualitative agreement with compared results in the recoil region but shows somewhat disagreement in the binary region. This may have happened due to the change of the hydrogenic metastable states by electrons. It is remarked that the peak structure for both in recoil and binary region, the First-Born results are very close to the 2S-metastable state with different magnitudes for all scattering angles. But in the binary region, the opposite peak patterns of the 2S-mathastable state [10] are much sharper than the corresponding ground state experimental result [18] and 3d-state results. However, the limitation of the theory is that at low energy, the theory of Das and Seal [2] does not give significant results.

Here is a table (please see **Table 1**.) of comparison results for ionization of hydrogenic 3d for incident energy $E_i = 150$ eV is presented.

## 4. Conclusion

In this work, the first Born double differential cross section (DDCS) of the ionization of metastable 3d-state hydrogen atoms by 150 eV and 250 eV electron impact is computed using a multiple scattering theory. The present new computational result makes a significant contribution to the field of metastable state ionization problem. Regrettably, there is currently no experimental data available for comparing the computational results with the experimental findings of DDCS for the ionization of metastable 3d-state hydrogenic atoms. Therefore, it would be very valuable to obtain experimental results for the ionization of metastable 3d-state hydrogenic atoms by electron. The discovery of new results is expected to inspire other theoretical researchers and experimentalists to conduct further research on various ionization cross-sections for different metastable states of hydrogen or other atoms by electrons and positrons impact, to gain a better understanding of atomic scattering problems. It will add a new dimension to the study of the ionization problem. Calculation for other kinematic conditions or other atomic species will also be interesting.

## Acknowledgements

The computational works have been performed in the Simulation Lab of the Department of Mathematics, Chittagong University of Engineering and Technology Chittagong-4349, Bangladesh.

## Conflicts of Interest

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

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