Open Journal of Microphysics, 2023, 13, 1-13
https://www.scirp.org/journal/ojm
ISSN Online: 2162-2469
ISSN Print: 2162-2450

Double Differential Cross-Section for the Ionization of Hydrogenic 2S Metastable State

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How to cite this paper: Chowdhury, Md.T.H. and Dhar, S. (2023) Double Differential Cross-Section for the Ionization of Hydrogenic 2S Metastable State. *Open Journal of Microphysics*, **13**, 1-13.
https://doi.org/10.4236/ojm.2023.131001

Received: February 1, 2023
Accepted: February 25, 2023
Published: February 28, 2023

Abstract

Double differential cross-sections of first Born estimation for ionization of hydrogenic 2S state by electrons are assessed for various kinematics situations in the asymmetric coplanar geometry. A final state wave function of multiple scattering theory is followed in this study. The present outcomes are compared with those of hydrogenic ground state, 2P state and ground state experimental results. Obtained findings show a good qualitative agreement with existing results.

Keywords

Hydrogen, Ionization, Double Differential Cross-Section, Metastable, Scattering

1. Introduction

Ionization process is one of the most significant reactions in atomic collisions. Much information on ionization dynamics has been obtained by assessing the double differential cross sections (DDCS) for emitted electron energy and emitted angles. Ionization by fast particles was first planned quantum mechanically by Bethe [1]. The application of the multi-parameter detection technique, together with the advancement in computational procedures, has made it likely to implement a whole experimentation in which kinematical parameters (like momentum and energies) of all performing particles are determined. This kind of experiment has been successfully used to investigate the fine details of the ionization process both in the ground state [2]-[11] and metastable state [12]-[21]. In atomic ionization collisions, the DDCS covers facts about the angular and energy distribution of secondary electrons [11]. Here, atomic hydrogen is used as a target in order to perceive the ionization mechanism of atomic system by electron impact energy. The emitted electron is detected in coincidence with the scattered electrons and it is a well-known experiment [22] called (e, 2e) experiments. The ionization of atomic hydrogen by electron influence is of major significance and of rare gas atoms, particularly, the cross-sections acquired with ground state ionization, is considered as benchmark facts and before [23] there is a few data existed for atomic hydrogen, though it is the simplest and the most convenient system for theoretical analysis. DDCS of ionization comprises valued info about both the collision dynamics and the internal structure of atomic or molecular systems. Experimental evaluation angle and energy have been obtained [24] [25] [26] [27] [28] and other groups [29]-[39] for DDCS.

In this work, the DDCS for ionization of hydrogenic metastable 2S state by electron impact at 150 eV and 250 eV energies has been calculated. We use a wave function [10] [11] [12] to calculate the DDCS integrated over the scattering angle. It will be interesting here to use the wave function of metastable 2S state hydrogen atoms by electrons. To the best of our knowledge, the DDCS for the ionization of metastable 2S-state hydrogen atoms by electrons at intermediate and high energies were never studied before experimentally. No theoretical calculations of the DDCS of metastable 2S state hydrogen atoms were observed. Therefore, hydrogenic ground state experimental results for ionization of metastable 2S state hydrogen atoms by electrons will be valuable and our outcomes will add a new dimension to the significant study of this field of research.

2. Theory

The direct Transition matrix element for ionization of hydrogen atoms by electron [27], may be written as,

$$T_{FI} = \left\langle \psi_F^{(-)}\left(\overline{\gamma}_1, \overline{\gamma}_2\right) \middle| V_I\left(\overline{\gamma}_1, \overline{\gamma}_2\right) \middle| \Phi_i\left(\overline{\gamma}_1, \overline{\gamma}_2\right) \right\rangle \tag{1}$$

where the perturbation potential $V_I\left(\overline{\gamma}_1, \overline{\gamma}_2\right)$ is given by

$$V_I\left(\overline{\gamma}_1, \overline{\gamma}_2\right) = \frac{1}{\gamma_{12}} - \frac{1}{\gamma_2} \tag{2}$$

For hydrogen atoms nuclear charge is Ze = 1, γ_1 is the distance of the atomic electron and γ_2 is the distance of projectile electron from the nucleus and γ_{12} is the distance between the two electrons (**Figure 1**).

The initial channel unperturbed wave function is given by

$$\Phi_i\left(\overline{\gamma}_1, \overline{\gamma}_2\right) = \frac{e^{i\overline{p}_i \cdot \overline{\gamma}_2}}{(2\pi)^{\frac{3}{2}}} \phi_{2S}\left(\overline{\gamma}_1\right) \tag{3}$$

where $\phi_{2S}\left(\overline{\gamma}_1\right) = \frac{1}{4\sqrt{2\pi}}\left(2-\gamma_1\right)e^{-\lambda_1\gamma_1}$.

Here $\lambda_1 = \frac{1}{2}$ and $\phi_{2S}\left(\overline{\gamma}_1\right)$ is the hydrogen 2S state wave function and $\psi_F^{(-)}\left(\overline{\gamma}_1, \overline{\gamma}_2\right)$ is the final three particle scattering state wave function [7] and coordinate of the two electrons are $\overline{\gamma}_1$ and $\overline{\gamma}_2$ respectively.

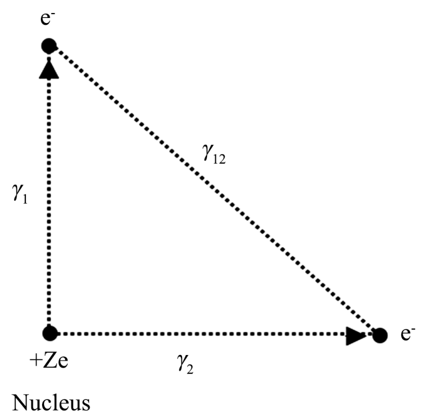


Figure 1. Collision effect amongst two electrons and the nucleus.

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

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

Here $N(\bar{p}_1,\bar{p}_2)$ is normalization constant,

$$\bar{\gamma}=\frac{\bar{\gamma}_1-\bar{\gamma}_2}{2},\ \bar{R}=\frac{\bar{\gamma}_1+\bar{\gamma}_2}{2},\ \bar{p}=\bar{p}_2-\bar{p}_1,\ \bar{P}=\bar{p}_2+\bar{p}_1$$

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

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

$$T_{FI}=T_b+T_b'+T_I-2T_{PB} \tag{5}$$

For first Born estimation equation may be written as

$$\begin{aligned}T_b&=\frac{1}{16\pi^2}\phi_{\bar{p}_1}^{(-)}(\bar{\gamma}_1)e^{i\bar{p}_i\cdot\bar{\gamma}_2}\left|\frac{1}{\gamma_{12}}-\frac{1}{\gamma_2}\right|e^{i\bar{p}_i\cdot\bar{\gamma}_2}(2-\gamma_1)e^{-\lambda_1\gamma_1}\\
&=\frac{1}{16\pi^2}\int\left[\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\left(\frac{1}{\gamma_{12}}-\frac{1}{\gamma_2}\right)e^{i\bar{p}_i\cdot\bar{\gamma}_2}(2-\gamma_1)e^{-\lambda_1\gamma_1}\right]d^3\gamma_1d^3\gamma_2\\
&=\frac{1}{16\pi^2}\int\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_{12}}2e^{i\bar{p}_i\cdot\bar{\gamma}_2}e^{-\lambda_1\gamma_1}d^3\gamma_1d^3\gamma_2\\
&\quad-\frac{1}{16\pi^2}\int\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_2}2e^{i\bar{p}_i\cdot\bar{\gamma}_2}e^{-\lambda_1\gamma_1}d^3\gamma_1d^3\gamma_2\\
&\quad-\frac{1}{16\pi^2}\int\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_{12}}\gamma_1e^{i\bar{p}_i\cdot\bar{\gamma}_2}e^{-\lambda_1\gamma_1}d^3\gamma_1d^3\gamma_2\\
&\quad+\frac{1}{16\pi^2}\int\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_2}\gamma_1e^{i\bar{p}_i\cdot\bar{\gamma}_2}e^{-\lambda_1\gamma_1}d^3\gamma_1d^3\gamma_2\\
&=Tb_1+Tb_2+Tb_3+Tb_4\end{aligned} \tag{6}$$

Here

$$Tb_1=\frac{1}{16\pi^2}\int\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_{12}}2e^{i\bar{p}_i\cdot\bar{\gamma}_2}e^{-\lambda_1\gamma_1}d^3\gamma_1d^3\gamma_2$$

$$Tb_2=-\frac{1}{16\pi^2}\int\phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)e^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_2}2e^{i\bar{p}_i\cdot\bar{\gamma}_2}e^{-\lambda_1\gamma_1}d^3\gamma_1d^3\gamma_2$$

$$Tb_3 = -\frac{1}{16\pi^2}\int \phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)\mathrm{e}^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_{12}}\gamma_1\mathrm{e}^{i\bar{p}_i\cdot\bar{\gamma}_2}\mathrm{e}^{-\lambda_1\gamma_1}\mathrm{d}^3\gamma_1\mathrm{d}^3\gamma_2$$

$$Tb_4 = \frac{1}{16\pi^2}\int \phi_{\bar{p}_1}^{(-)*}(\bar{\gamma}_1)\mathrm{e}^{-i\bar{p}_i\cdot\bar{\gamma}_2}\frac{1}{\gamma_2}\gamma_1\mathrm{e}^{i\bar{p}_i\cdot\bar{\gamma}_2}\mathrm{e}^{-\lambda_1\gamma_1}\mathrm{d}^3\gamma_1\mathrm{d}^3\gamma_2 = \frac{1}{2}\frac{\partial}{\partial\lambda_1}(tb_2)$$

T_b, is the first Born term for TDCS and other terms T'_b, T_I, T_{PB} are calculated in our work of [12]. Afterward, investigative calculation by using the Lewis integral [40], the above terminologies of Equation (6) have been calculated mathematically and the triple differential cross-sections for T-Matrix element is specified by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\mu_1\mathrm{d}\mu_2\mathrm{d}E_1} = \frac{p_1 p_2}{p_i}\left|T_{FI}\right|^2. \tag{7}$$

Later integration of TDCS result [12] of Equation (7), we can acquire the DDCS result using following equation:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}E_1\mathrm{d}\mu_1} = \int \frac{\mathrm{d}^3\sigma}{\mathrm{d}E_1\mathrm{d}\mu_1\mathrm{d}\mu_2}\mathrm{d}\mu_2 \tag{8}$$

Therefore, double differential cross sections (DDCS) have been determined using computer programming language MATLAB, given by Equation (8).

3. Results and Discussion

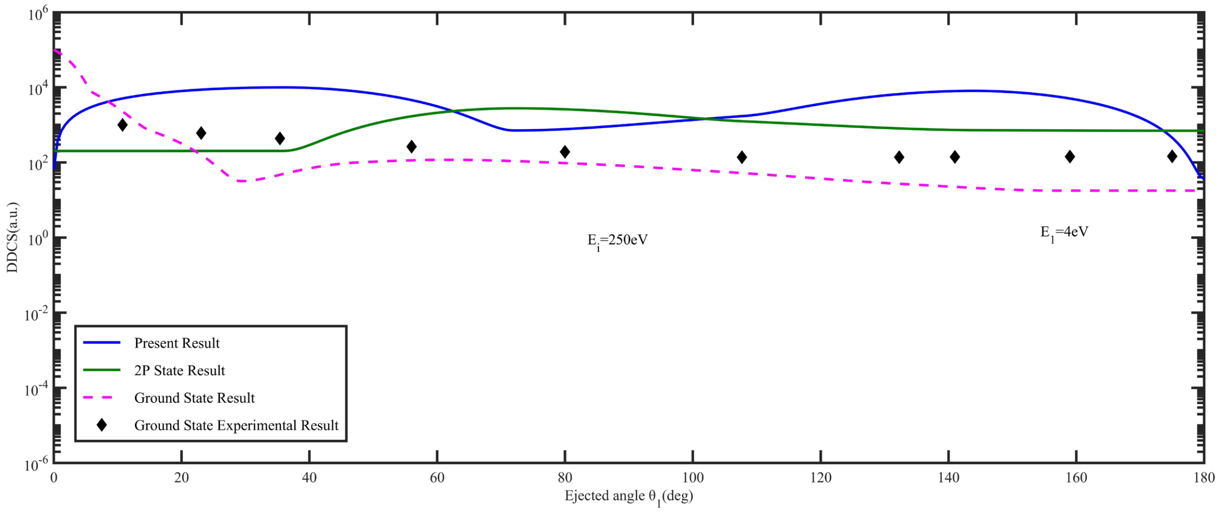
DDCS are determined here for the ionization of the metastable 2S state hydrogen atoms by electrons at high incident energy E_i = 250 eV (**Figure 2**) for emitted electron energies E_1 = 4 eV, 10 eV, 20 eV, 50 eV and 80 eV.

Again, at intermediate incident energy E_i = 150 eV (**Figure 3**), for emitted electron energies E_1 = 4 eV, 10 eV, 20 eV, 30 eV and 50 eV. The emitted angle θ_1 varies from 0˚ to 180˚ considered as horizontal axis where DDCS as vertical axis in all figures and the scattered angle θ_2 varies from 0˚ to 100˚.

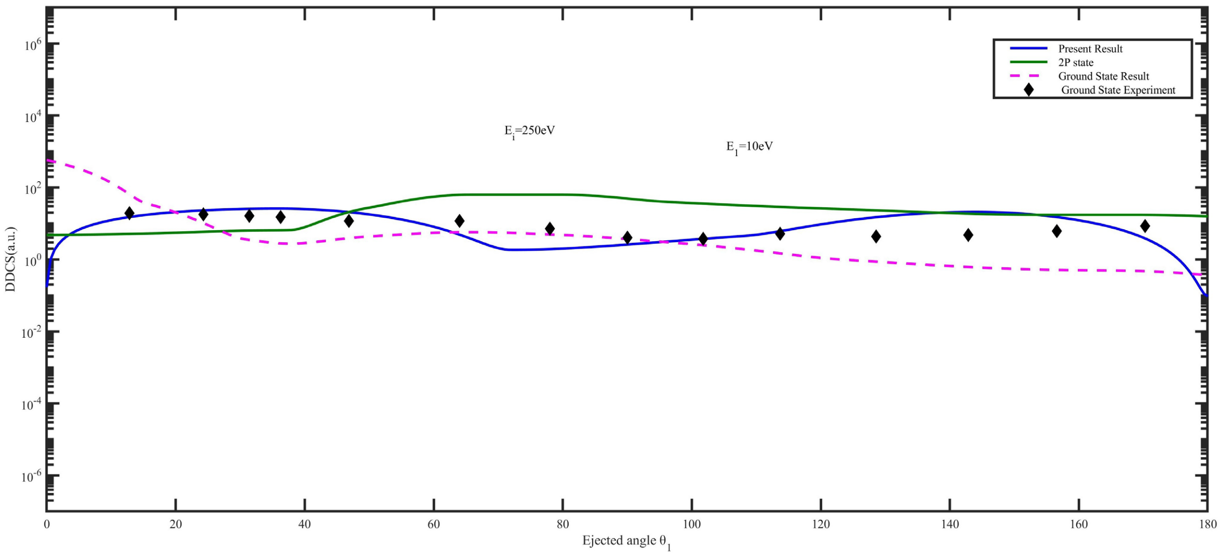
Ionization of hydrogen atoms by electrons from the ground state experimental results [24] and computational results [11] [19] are presented here for assessment. The final state scattering wave function $\psi_F^{(-)}(\bar{\gamma}_1, \bar{\gamma}_2)$ is the continuum state of the atomic hydrogen.

For incident energy E_i = 250 eV in **Figure 2(a)**, ejection energy E_1 = 4 eV the current first Born result overlays at about θ_1 = 10˚ with those of [11], where at higher ejection angle θ_1 lies above those of [11] making a onward peak and lies below closely the experimental values at lesser θ_1, meets at θ_1 = 5˚ and θ_1 = 175˚ correspondingly with those of [24] and meets about θ_1 = 62˚, θ_1 = 100˚ and θ_1 = 173˚ respectively with those of [19].

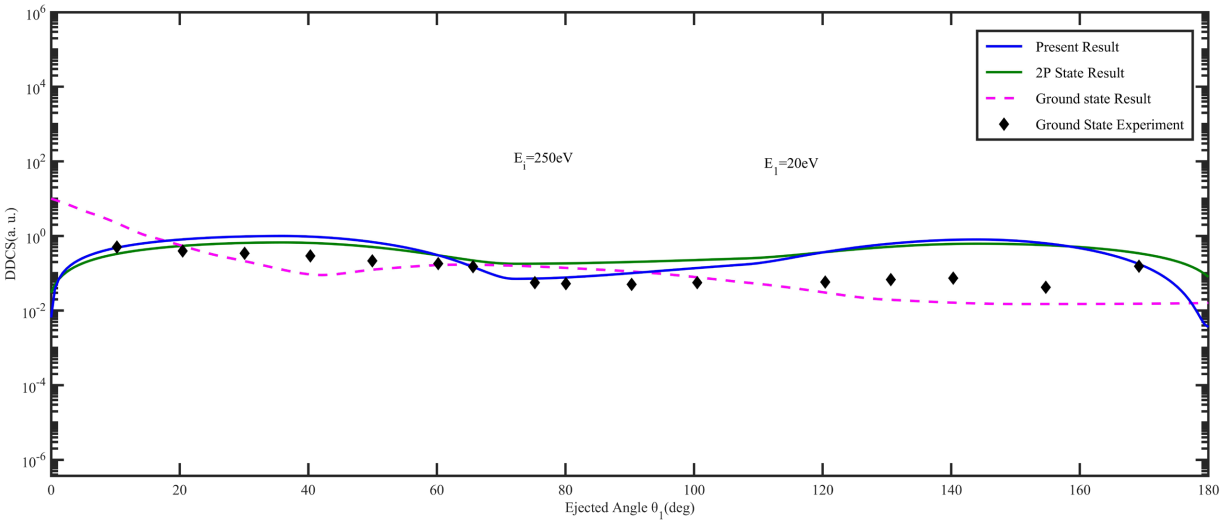
In **Figure 2(b)**, E_1 = 10 eV our result concurs several times at nearly θ_1 = 5˚, θ_1 = 45˚, θ_1 = 138˚ and θ_1 = 155˚ with those of [19], meets almost θ_1 = 20˚, θ_1 = 60˚, θ_1 = 100˚ and θ_1 = 177˚ with those of ground state result [11]. Moreover the curve intersects several times with those of [24] and peak flattens as the energy increases and ultimately disappears which indicates good assessment.


DDCS(a.u.)
Ejected angle θ1(deg)
E_i=250eV
E_1=4eV
Present Result
2P State Result
Ground State Result
Ground State Experimental Result

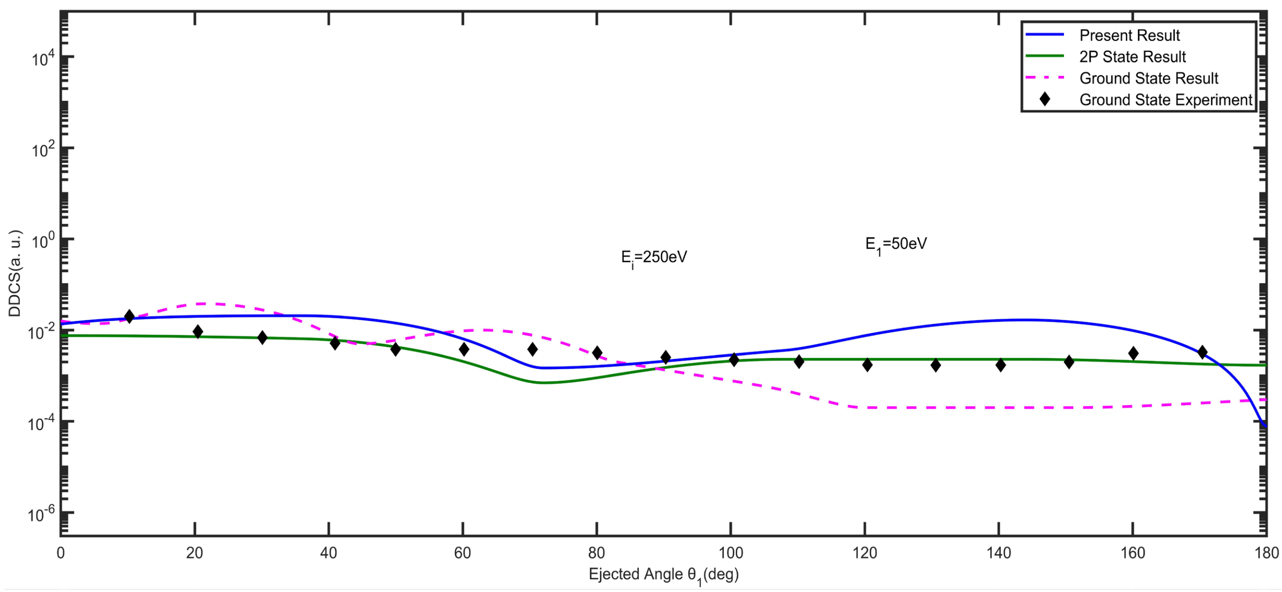
(a)


DDCS(a.u.)
Ejected angle θ1
E_i=250eV
E_1=10eV
Present Result
2P state
Ground State Result
Ground State Experiment

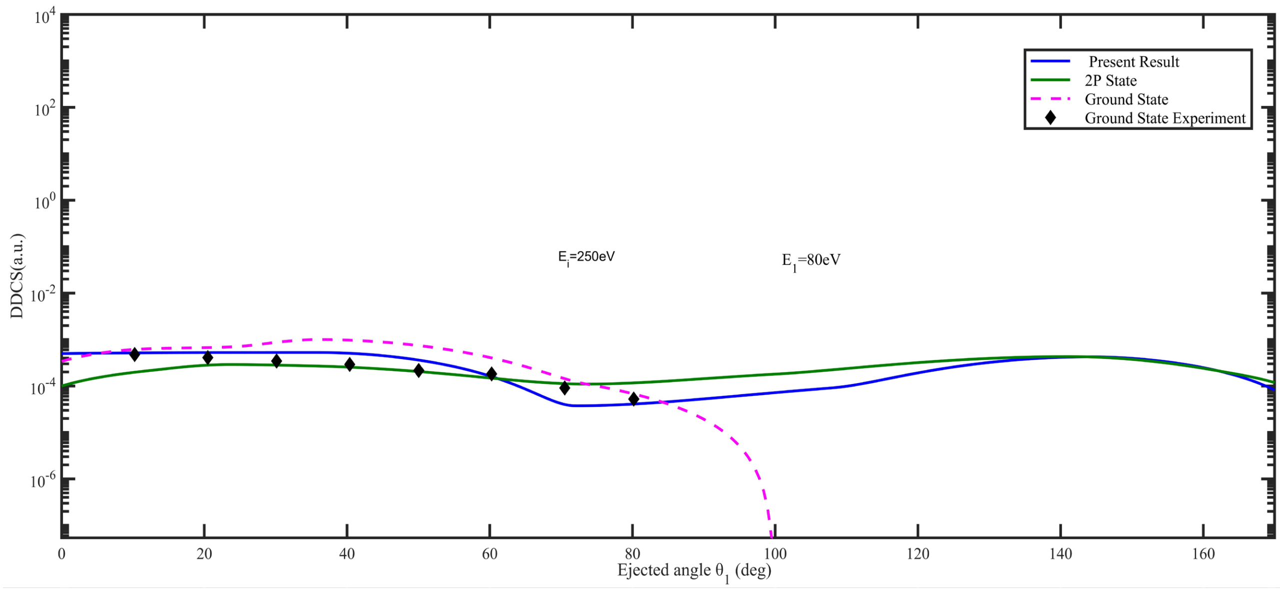
(b)


DDCS(a. u.)
Ejected Angle θ1(deg)
E_i=250eV
E_1=20eV
Present Result
2P State Result
Ground state Result
Ground State Experiment

(c)



(d)

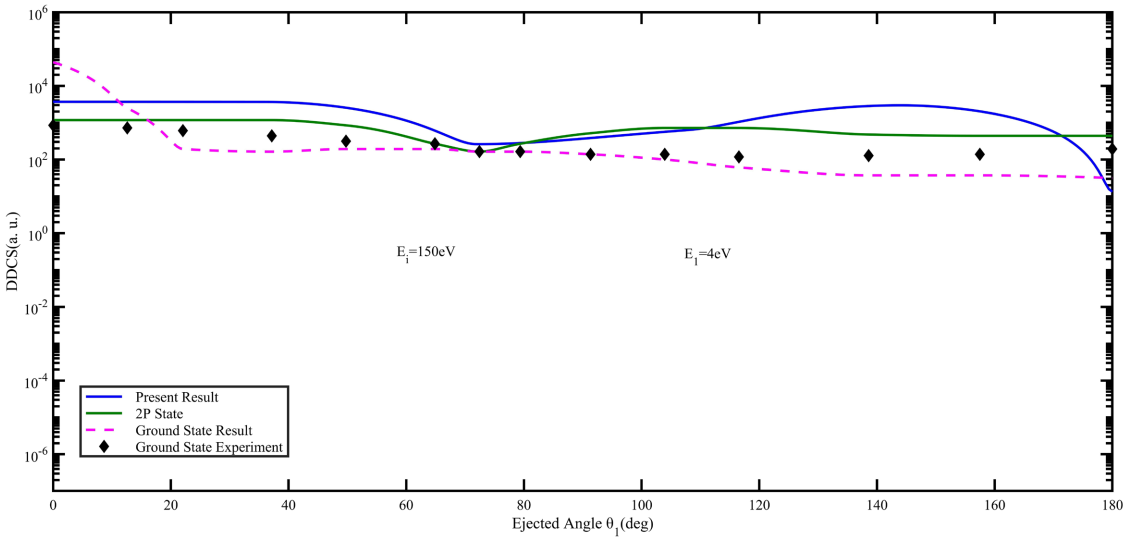


(e)

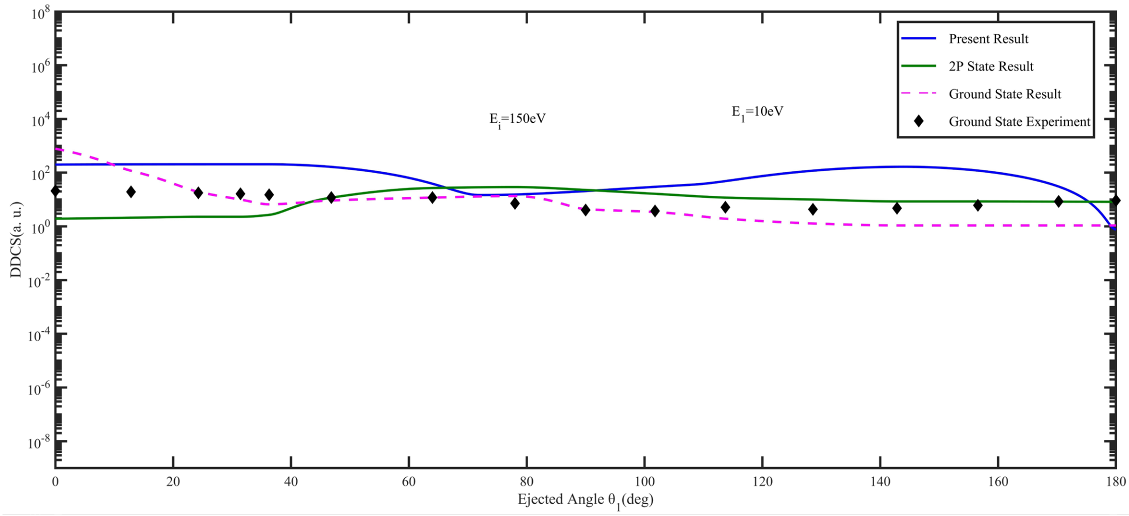
Figure 2. DDCS for the Ionization of atomic hydrogen by 250 eV electron effect as a function of the emitted electron angle θ_1 comparative to the incident electron path. The emitted electron energies are 4 eV, 10 eV, 20 eV, 50 eV, 80 eV respectively. Concept: (◆) curves denote hydrogenic ground-state experimental result [24], (---) denote hydrogenic ground-state results [11], (—) curves illustrate the results of metastable 2P state [19] and (—) denote the present outcomes of metastable 2S state.

In **Figure 2(c)**, E_1 = 20 eV the present outcome displays similar shapes with 2P state [19] as well as at θ_1 = 65˚ and θ_1 = 175˚ like hydrogenic ground state experimental results [24] which shows good qualitative assessment.

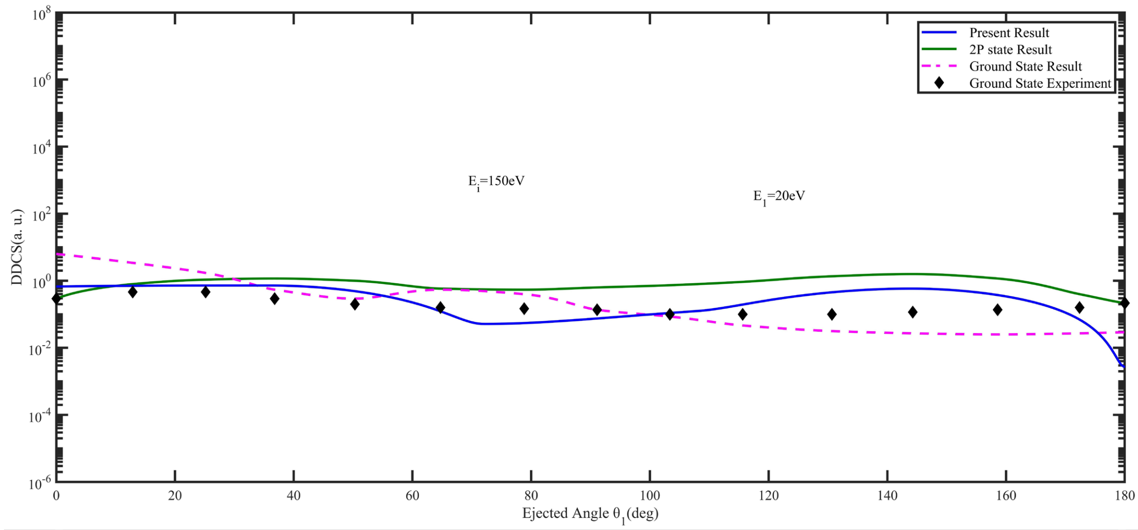
In **Figure 2(d)**, E_1 = 50 eV the current outcome concurs several times with those of ground state result [11] at θ_1 = 18˚, θ_1 = 35˚, θ_1 = 55˚, θ_1 = 80˚ and θ_1 = 176˚, crosses four times with the ground state experiment value [24]. Also, it makes a big peak at higher angle which indicates good assessment.


DDCS(a. u.)
Ejected Angle θ1(deg)
Ei=150eV
E1=4eV
Present Result
2P State
Ground State Result
Ground State Experiment

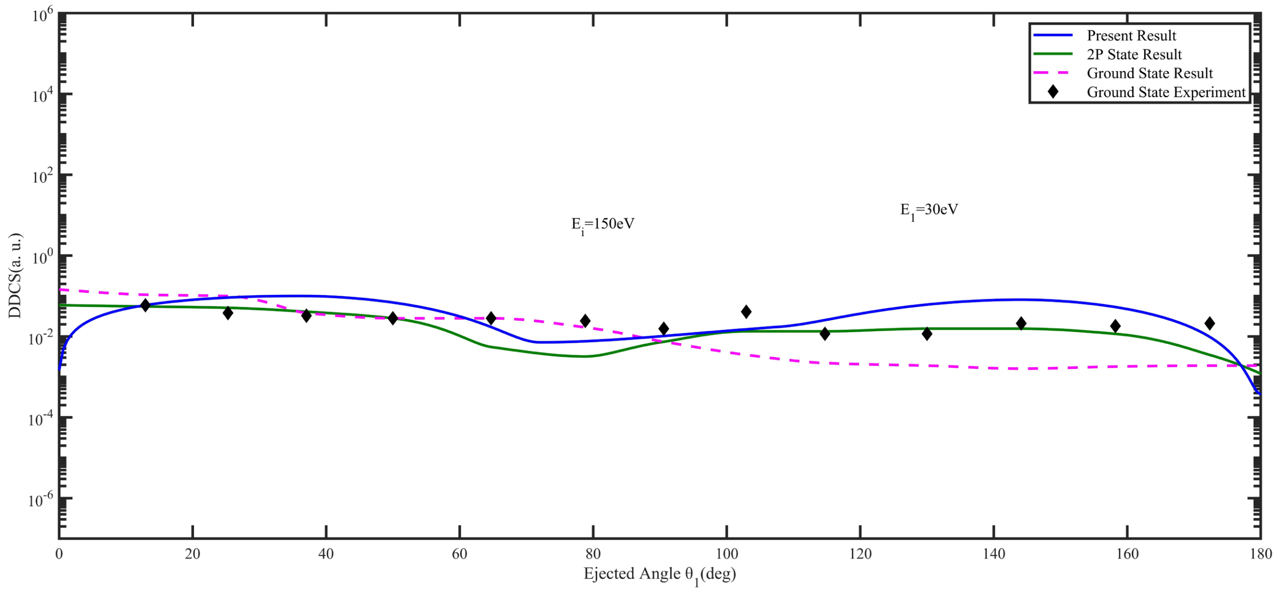
(a)


DDCS(a. u.)
Ejected Angle θ1(deg)
Ei=150eV
E1=10eV
Present Result
2P State Result
Ground State Result
Ground State Experiment

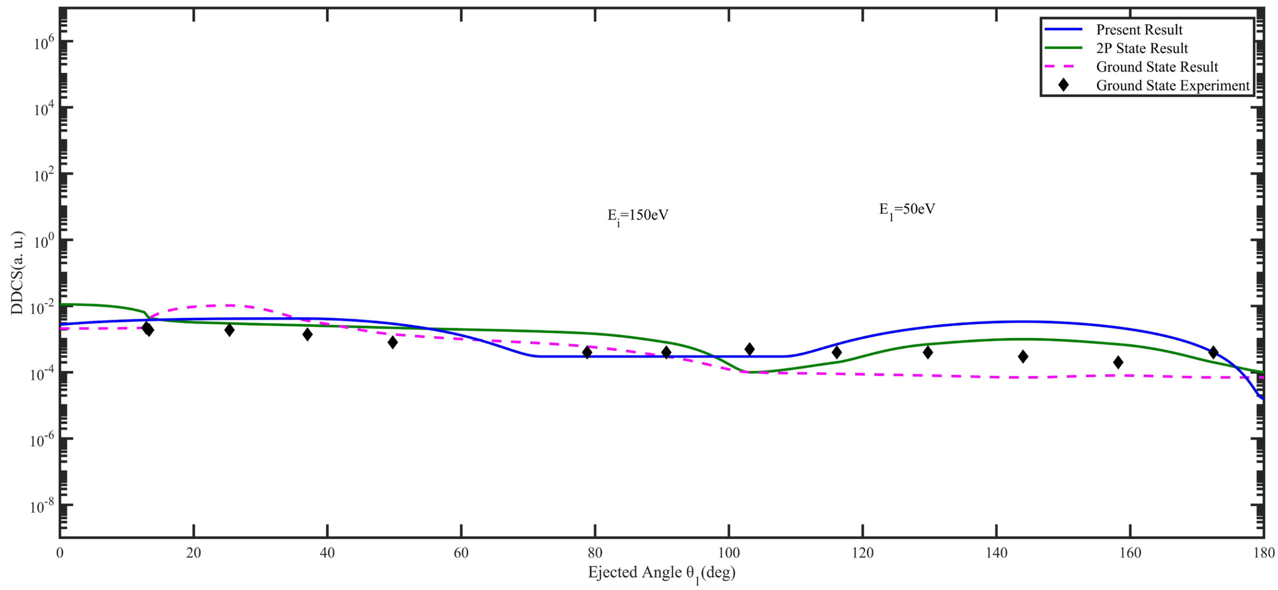
(b)


DDCS(a. u.)
Ejected Angle θ1(deg)
Ei=150eV
E1=20eV
Present Result
2P state Result
Ground State Result
Ground State Experiment

(c)



(d)



(e)

Figure 3. DDCS for the ionization of atomic hydrogen by 150 eV electron effect as a function of the emitted electron angle θ_1 relative to the incident electron direction. The emitted electron energies are 4 eV, 10 eV, 20 eV, 30 eV, 50 eV. Concept: (◆) curves denote hydrogenic ground-state experimental result [24], (---) denote hydrogenic ground-state results [11], (—) denote the results of metastable 2P state [19] and (—) denote the current results of metastable 2S state.

Lastly, in **Figure 2(e)**, E_1 = 80 eV it is seen that the experimental result, the theoretical result, 2P state result and the current result show similar nature in shape at ejection angles up to $\theta_1 = 80^\circ$ and at higher angle, the present outcome and 2P state results [19] displays a peak with big magnitude which indicate the good assessment. It displays a good assessment with the theoretical data as well as hydrogenic ground state experimental results.

For incident energy E_i = 150 eV, in **Figure 3(a)**, ejection energy E_1 = 4 eV, the present outcome meets at about θ_1 = 80˚, θ_1 = 110˚ and θ_1 = 170˚ with those of 2P state outcomes [19], nearby θ_1 = 10˚ and θ_1 = 177˚ concurs ground state results [11], furthermore it is nearer around θ_1 = 70˚ and intersect at θ_1 = 172˚ with the ground state experiment results [24].

In **Figure 3(b)**, E_1 = 10 eV, our curve intersects several times with those of 2P state results [19], relatively closer to the ground state results [11] at lesser angles, lies above to the experimental values. Approximately, θ_1 = 10˚ meets with the ground state results [11], it creates maximum at θ_1 = 150˚ and at higher ejection angle, θ_1 the curve meets with those of ground state results [11].

In **Figure 3(c)**, E_1 = 20 eV our present outcome coincides various times at θ_1 = 32˚, θ_1 = 55˚, θ_1 = 100˚ and θ_1 = 175˚ with those ground state results [11], accordingly passes at θ_1 = 62˚, θ_1 = 100˚ and θ_1 = 165˚ with ground state experiment results [24]. Our result creates a peak at θ_1 = 140˚ and passing nearer to both the experimental and the theoretical results. It displays a good qualitative judgement.

Again considering E_1 = 30 eV in **Figure 3(d)**, the theoretical result forms two peak nearby θ_1 = 40˚, θ_1 = 145˚ and lower deep at about θ_1 = 75˚. Comparison of these present outcomes with ground state results [11], 2P state results [19], and ground state experiment results [24] show a suitable qualitative exhibition.

At last, we consider ejection energy as E_1 = 50 eV, in **Figure 3(e)**, our curve overlay four times at θ_1 = 14˚, θ_1 = 55˚, θ_1 = 97˚ and θ_1 = 177˚ those of [19] and at higher angles between 70˚ to 110˚ a lower deep formed where the experimental curve-runs relatively closer to the current outcome which shows a suitable judgement.

Table 1. DDCS results for emitted angles θ_1 corresponding to various scattering angles θ_2 for four different values of emitted electron energies are E_1 = 4 eV, E_1 = 20 eV, E_1 = 50 eV and E_1 = 80 eV in ionization of hydrogen atoms for 250 eV electron.

θ_2 (deg)	θ_1 (deg)	E_1 = 4 eV	E_1 = 20 eV	E_1 = 50 eV	E_1 = 80 eV
		DDCS	DDCS	DDCS	DDCS
0	0	64.9	0.00652	0.01359	0.000499
1	36	9926.0	0.99705	0.02075	0.000525
2	72	707.4	0.07106	0.00147	0.000037
4	108	1719.1	0.17268	0.00359	0.000091
10	144	8019.1	0.80550	0.01676	0.000424
20	180	36.1	0.00362	0.00007	0.000001
30	216	11292.4	1.13412	0.02361	0.000598
40	252	179.8	0.01806	0.00037	0.000009
60	288	3244.3	0.32588	0.00010	0.006784
90	324	5887.9	0.59143	0.00019	0.012313
100	360	0	0	0	0

It is observed that the present first Born result coincides at $\theta_1 = 60^\circ$ with result once only and similarly concurs two time each at lower and higher ejection angle θ_1 with experimental result of Shyn as well as those of the Roy, Mandal and Sil. We also see that results one may look carefully to the **Table 1** where values of the different ejection angles θ_1 are presented for different values of the scattering angles θ_2 for four values of emitted electron energy E_1, in the case $E_i = 250$ eV.

4. Conclusions

In this study, DDCS for ionization of metastable 2S-state hydrogen atoms by 150 eV and 250 eV electron effect has been estimated.

To understand these configurations of the DDCS, the current calculation applying the multiple scattering theory [11] provides a significant contribution in the field of metastable 2S-state ionization problems. Due to the absence of any experimental data for the DDCS results of the hydrogenic metastable 2S-state ionization process, it is not possible to compare the present computational results with the experimental findings. Therefore, hydrogenic ground state experimental results for ionization of metastable 2S state hydrogen atoms by electrons will be valuable, present computational work gives a significant contribution in the field of ionization problems for further research.

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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