

# Double differential cross-sections for ionization of metastable 2P-state hydrogen atoms by electrons at intermediate energies with exchange effects

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## Abstract:

## Introduction

This paper aims to measure the double differential cross-sections (DDCS) for the ionization of metastable 2P-state hydrogen atoms with exchange effects in various kinematic conditions. The incident energies used were 150eV and 250 eV. Ejected electron energies  $E_1 = 4\text{eV}$ ,  $E_1=10\text{eV}$ ,  $E_1=20\text{eV}$ ,  $E_1=30\text{eV}$  and  $E_1=50\text{eV}$  are used for incident energy 150eV and ejected electron energies  $E_1= 4\text{eV}$ ,  $E_1=10\text{eV}$ ,  $E_1=20\text{eV}$ ,  $E_1=50\text{eV}$  and  $E_1=80\text{eV}$  are used for incident energy 250eV. The present calculations are performed using the multiple scattering theory of Das and Seal.

## Result and Discussion

Double differential cross sections were obtained from the triple differential cross sections. The present calculations are compared with the hydrogenic ground-state experimental data, theoretical results, and DDCS first Born results. Discrepancies have been found between the present results and those measurements and theoretical results and also qualitative agreement with those of compared theories.

## Conclusion

The exchange effect results give an enormous prospect for experimental outcomes in the field of ionization problems. We are expecting that the present study makes more significant contribution to the study of atomic scattering problems using the multiple scattering theories. In the future calculations, other kinematic conditions or other atomic species will also be interesting and significant.

**Keywords:** Cross-section, Ionization, Metastable-state, Exchange effects.

## 1. Introduction:

Atomic ionization of hydrogen atoms by electrons is the most fundamental and simplest ionization problem. Though many theoretical calculations of cross section for ionization of hydrogen atoms in the ground state [1-13] and metastable state [14-26] at various incident energies and under different kinematic

conditions are exist, so that's why experimental study regarding this field is very important to justify the theoretical results. The first theoretical study on double differential cross-sections (DDCS) is based on the plane-wave Born approximation operated by Massey & Mohr [3] and McCarrol [27] which was performed at very high energies. After a long time, experimental measurements of doubly differential cross sections (DDCS) in angle and energy had been executed by Shyn [28-33] as well as by group of scholars [34-36] at also higher energies. Consequently, Shyn [32] presented experimental measurements in which the DDCS of secondary electrons ejected from atomic hydrogen have been measured by electron impact over the angular range of  $12^0$  to  $156^0$  and the intermediate incident energy. The theoretical studies on double differential cross-sections (DDCS) is based on Born approximation was performed by Das [9], Das and Seal [10] & [11] at intermediate energies for ionization of hydrogen atoms by electron and developed a multiple scattering theory. The present calculation is done by using the multiple scattering theory of Das [9], Das and Seal [10] & [11].

Metastable 2P 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. A number of excited atoms are accumulated in the metastable state. A metastable state may thus be considered as a kind of temporary energy trap or a somewhat stable intermediate stage of a system, the energy of which may be lost in discrete amounts. In quantum mechanical terms, transitions from the metastable states are less probable than the allowed transitions from other excited states. As an atom has a finite number of protons and neutrons, it will generally emit particles until it gets to a point where its half-life is so long that it is effectively stable. The decay of particles is commonly expressed in terms of half-life, decay constant or lifetime. The excited state of an atom will have an intrinsic lifetime due to radioactive decay. The lifetime of the excited state is given by [37]

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

Where  $A_{ij}$  is the Einstein coefficient. Strong atomic transitions have  $A_{ij}$  of  $10^8-10^9 \text{ S}^{-1}$ , and so lifetimes are 1–10 ns. Lifetime can be shortened by collisions or stimulated emission. The lifetime of the hydrogen atom in metastable 2P-state is  $1.6 \times 10^{-9} \text{ S}^{-1}$ . These are sorted from the experiments [38, 39].

The DDCS for the ionization of metastable 2P-state hydrogen atoms by electrons at intermediate energies with exchange effects were never studied before theoretically and experimentally according to our knowledge. We found that a few theoretical calculations for the TDCS of metastable 2P, 3P, 3S, and 3D [25, 40-42] state hydrogen atoms by electron exchange effects are noticed. Most of the experimental investigations on the DDCS concentrated on the ground-state electron hydrogen ionization collisions. Therefore, hydrogenic ground state experimental results for ionization of metastable 2P state hydrogen atoms by electrons will be valuable and will add a new aspect to the significant study of this field of research.

## 2. Theory:

In the present study, the considerations are the direct and exchange amplitude of the T- matrix element. The direct Transition matrix element for ionization of hydrogen atoms by electrons [18], may be written as,

$$T_{\beta} = \langle \Psi^{(-)}(r_1, r_2) | V_i(r_1, r_2) | \Phi(r_1, r_2) \rangle \tag{1}$$

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

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

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

The initial channel unperturbed wave function is given by

$$\Phi(\bar{r}_1, \bar{r}_2) = \frac{1}{(2\pi)^{3/2}} 2P(r_1)$$

Where the hydrogenic 2P-state wave function is

$$\phi_{2P}(\bar{r}_1) = \frac{r_1}{\sqrt{2\pi}} \cos\theta e^{-\frac{r_1}{2}} \tag{3}$$

Here  $\lambda = \frac{1}{\gamma}$  and  $\phi_{2P}(\bar{r}_1)$  is the hydrogenic 2P-state wave function and  $\Psi^{(-)}(\bar{r}_1, \bar{r}_2)$  is the

final three-particle scattering state wave function [11] and co-ordinates of the two electrons are  $\bar{r}_1$  and  $\bar{r}_2$  respectively.

Here the multiple scattering state wave function [11]  $\Psi^{(-)}$  is given by

$$\Psi^{(-)}(\bar{r}_1, \bar{r}_2) = N(p_1, p_2) \left[ \psi^{(-)}(\bar{r}_1) e^{i\vec{p}_1 \cdot \bar{r}_1} + \psi^{(-)}(\bar{r}_2) e^{i\vec{p}_2 \cdot \bar{r}_2} + \psi^{(-)}(\bar{r}_1) e^{i\vec{p}_1 \cdot \bar{r}_2} - \gamma e^{i\vec{p}_1 \cdot \bar{r}_1 + i\vec{p}_2 \cdot \bar{r}_2} \right] / (\gamma\pi)^3$$

Here

$N(p_1, p_2)$  and  $\psi^{(-)}(\bar{r}_q)$  are computed in Dhar et al [25]

Now equation (1) can be written in following form

$$T_{\beta} = T_B + T_B' + T_i - 2T_{PB} \tag{5}$$

For first Born approximation is  $T_B$  and can be written as

$$T_B = \langle \phi_{p_1}^{(-)}(\mathbf{r}_1) e^{i\mathbf{p}_1 \cdot \mathbf{r}_1} | V_i | \Phi_i(\mathbf{r}_1, \mathbf{r}_2) \rangle \tag{6}$$

and other terms of equation (5) can also be written as

$$T'_B = \langle \phi_{p_2}^{(-)}(\mathbf{r}_2) e^{i\mathbf{p}_2 \cdot \mathbf{r}_2} | V_i | \Phi_i(\mathbf{r}_1, \mathbf{r}_2) \rangle, \tag{7}$$

$$T_i = \langle \phi_i^{(-)}(\mathbf{r}_i) e^{i\mathbf{p}_i \cdot \mathbf{r}_i} | V_i | \Phi_i(\mathbf{r}_1, \mathbf{r}_2) \rangle, \tag{8}$$

$$T_{PB} = \langle \phi_{p_1, p_2}^{(-)}(\mathbf{r}_1, \mathbf{r}_2) e^{i\mathbf{p}_1 \cdot \mathbf{r}_1 + i\mathbf{p}_2 \cdot \mathbf{r}_2} | V_i | \Phi_i(\mathbf{r}_1, \mathbf{r}_2) \rangle \tag{9}$$

The terms  $T_B, T'_B, T_i, T_{PB}$  are calculated analytically following Dhar et al [25]. The direct

scattering amplitude is then calculated in the form

$$\left( \begin{matrix} \vec{p}_1 \\ \vec{p}_2 \end{matrix} \right) = - (2\pi)^2 T_{f, p_1, p_2} \tag{10}$$

and the exchange amplitude calculated by following approximation

$$\left( \begin{matrix} \vec{g} \\ \vec{f} \end{matrix} \right)_{p_1, p_2} = \left( \begin{matrix} \vec{f} \\ \vec{g} \end{matrix} \right)_{p_1, p_2} \tag{11}$$

After analytical calculation, the expressions  $T_B, T'_B, T_i, T_{PB}$  have been calculated

numerically following Lewis integral [43] and Gaussian quadrature formula and TDCS

is obtained in the following expression

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{p_1 p_2}{p_i} \left[ \frac{3}{4} |f - g|^2 + \frac{1}{4} |f + g|^2 \right] \tag{12}$$

After integration of TDCS results of exchange effects of equation (12), we obtained the

DDCS results by following equation

$$\frac{d^2\sigma}{d\Omega_1 d\Omega_2} = \frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} \tag{13}$$

Therefore, in our present calculation of DDCS exchange effects have been calculated using the computer programming language MATLAB, given by equation (13).

### 3. Results and Discussions:

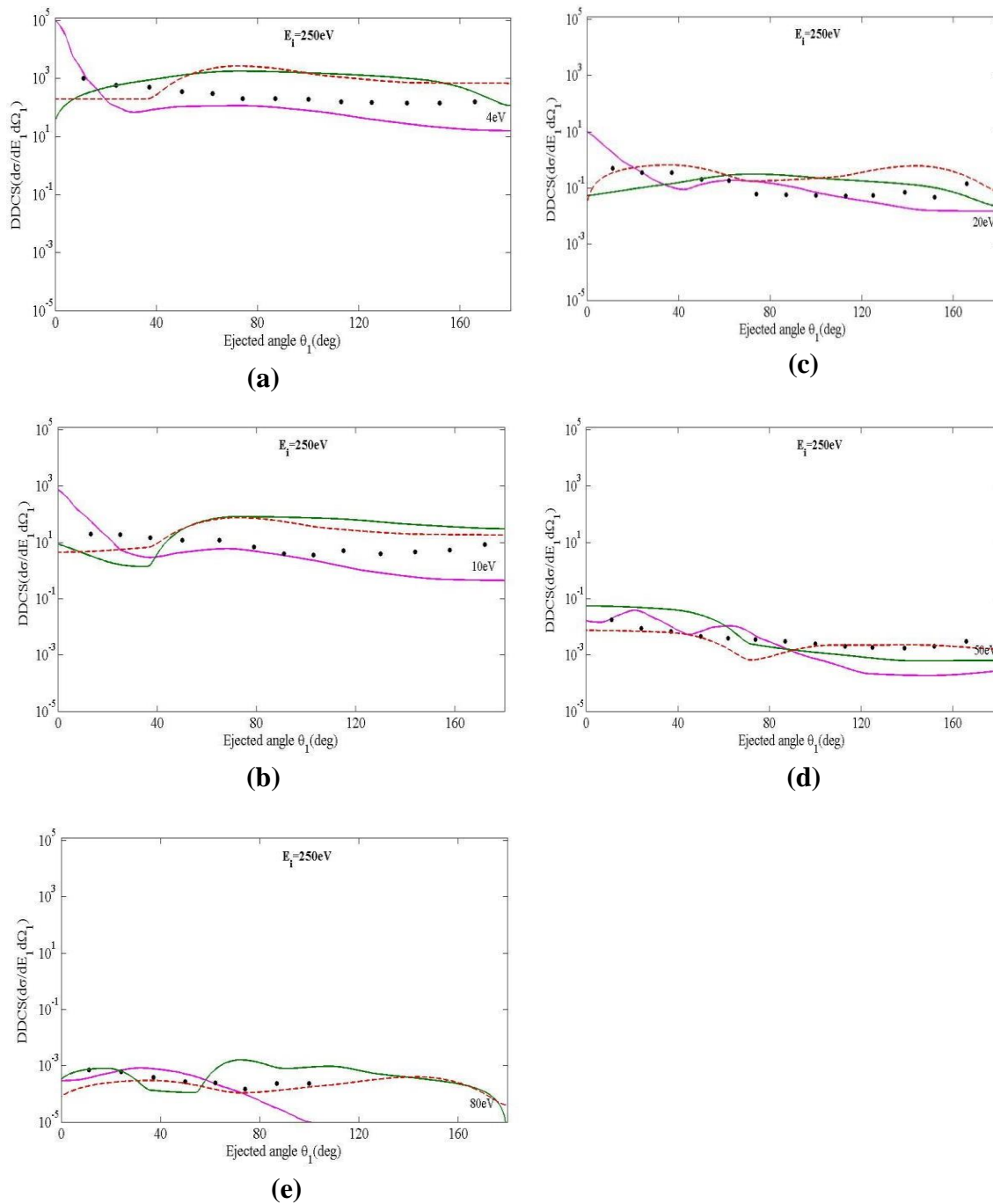
Double differential cross sections (DDCS) are calculated here for the ionization of the metastable 2P state hydrogen atoms by electrons at high incident energy with exchange effect.  $E_i = 250\text{eV}$  (Fig.1), for ejected electron energies  $E_1 = 4\text{eV}$ ,  $E_1 = 10\text{eV}$ ,  $E_1 = 20\text{eV}$ ,  $E_1 = 50\text{eV}$  and  $E_1 = 80\text{eV}$  and at intermediate incident energy  $E_i = 150\text{eV}$  (Fig.2), for ejected electron energies  $E_1 = 4\text{eV}$ ,  $E_1 = 10\text{eV}$ ,  $E_1 = 20\text{eV}$ ,  $E_1 = 30\text{eV}$  and  $E_1 = 50\text{eV}$ . The ejected angle  $\theta_1$  varies from  $0^\circ$  to  $180^\circ$  considered as horizontal axis where DDCS as vertical axis in all figures and the scattered angle  $\theta_2$  varies from  $0^\circ$  to  $100^\circ$ .

Ionization of hydrogen atoms by electrons from the ground state experimental results of Shyn [33], computational result of Das and Seal [12] and first Born results are presented here for comparison. The final state scattering wave function  $\Psi^{(-)}(r, r)$  is the continuum state of the atomic hydrogen. When the contribution of the final continuum state is considered in the ionization of meta-stable 2P state hydrogen atoms by electrons, it shows a reasonable qualitative agreement between the theoretical and hydrogenic ground state experimental results.

In the present DDCS exchange results, the amplitude is substantially large compared to other amplitudes, such as present first Born. However, near the forward and backward direction, there are considerable differences. This implies that near the peak, the projectile electron interactions are most important in the final channel. So we can say that the present results play a significant role in the ionization of atomic hydrogen for intermediate energies.

Firstly, in Fig.1 (a) for incident electron energy  $E_i = 250\text{eV}$  and ejected electron energy  $E_1 = 4\text{eV}$ , the present exchange result shows a broad peak at a whole range of ejected angle  $\theta_1 = 0^\circ$  to  $180^\circ$  which passes closely with the first Born result but shows a reverse pattern with both Das and Seal [12] and Shyn [33]. But at lower angle of  $\theta_1 = 40^\circ$  the present result shows good understanding with the compared results.

After considering the incident electron energy  $E_i = 250\text{eV}$  and ejected electron energy  $E_1 = 10\text{eV}$  in Fig.1(b), it is noticed that the present DDCS result and first Born result are almost similar. Also our observation is that the present DDCS result of metastable 2P- state and Das and Seal [12] show same peak pattern and disappear slowly at  $\theta_1$  increasing after  $40^\circ$  and at the same angles the result of Shyn [33] exhibits reverse shape. Also the present result moves higher than both [12] and [33] at higher  $\theta_1$  values but at lower angle present calculation shows opposite shape with both compared results.



**Fig-1:** DDCS for the ionization of atomic hydrogen by 250 eV electron impact as a function of the ejected electron angle  $\theta_1$  relative to the incident electron direction. The ejected electron energies are 4eV, 10eV, 20eV, 50eV and 80eV. Theory: Dotted curve represents hydrogenic ground-state experimental result [1], continuous curves (purple) represent hydrogenic ground-state results [2], red-dashed curves presents first Born results and continuous curves (green) represent the present results of metastable 2Pstate.

Next after taking the incident electron energy  $E_i=250\text{eV}$  and ejected electron energy  $E_1= 20\text{eV}$  in Fig.1(c), the present calculation proceeds below at lower angle  $\theta_1$  of  $40^\circ$  and upper at higher angle of  $40^\circ$  than both compared results whereas the first Born result advances closely through the present and other compared results making two broad peaks at smaller and larger angles which very significant. It is also noticed that

present metastable-2P state results exist closely to compared ground state theoretical and experimental results at angle between  $40^{\circ}$  to  $100^{\circ}$

If the incident energy  $E_i=250\text{eV}$  and ejected electron energy  $E_1=50\text{eV}$  are considered in Fig.1(d), it is observed that the present exchange result shows similar shape at lower angle of  $\theta_1=80^{\circ}$  but reverse shape at higher value of  $\theta_1$ . On the other side the present calculation expresses good agreement with the hydrogenic ground state theoretical result Das and Seal [12] than other results.

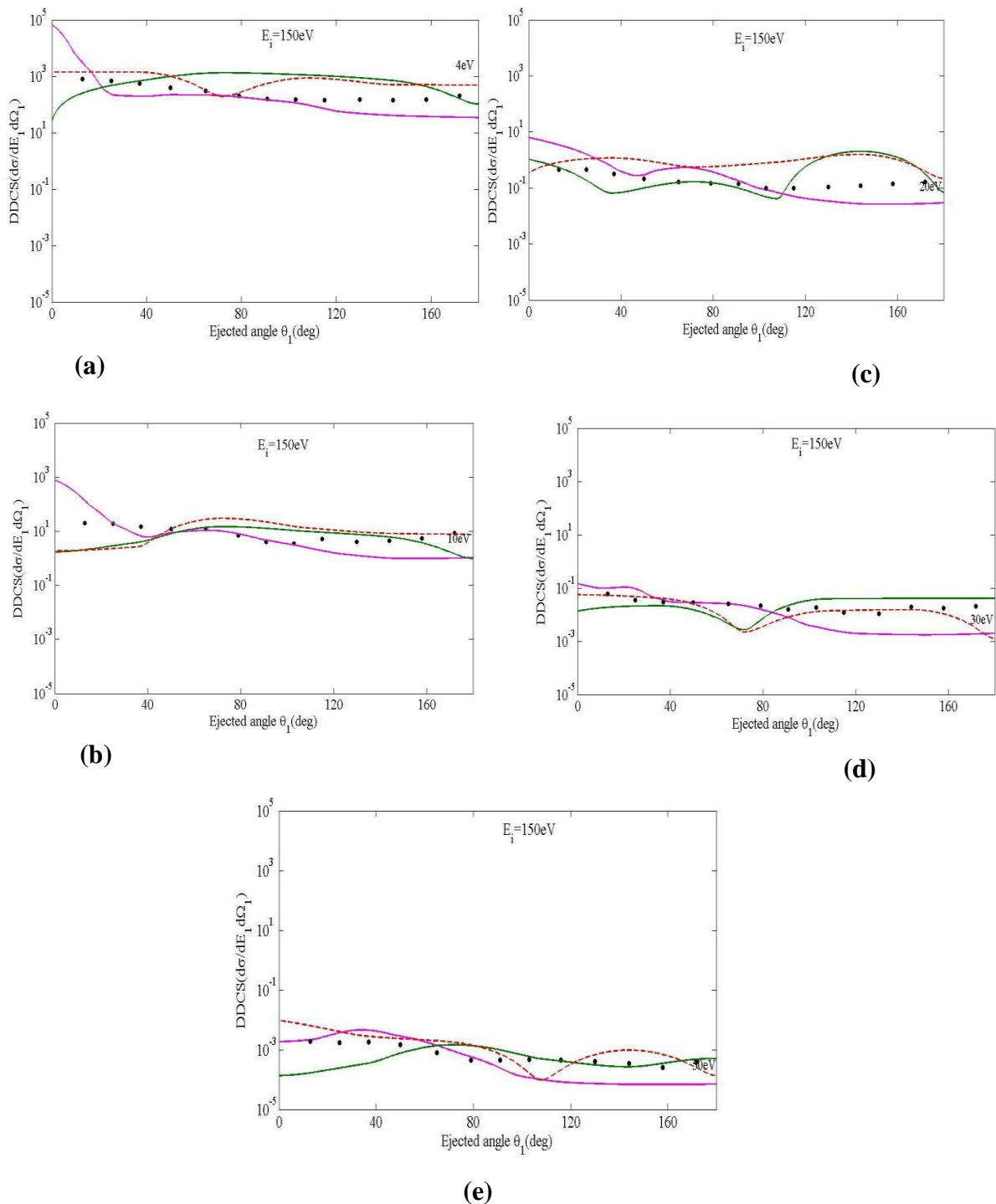
If we increase the incident energy  $E_i=250\text{eV}$  and ejected electron energy  $E_1=80\text{eV}$  in Fig.1(e), the present first Born result and hydrogenic ground state results exhibit similar behavior in shape but present DDCS exchange calculation show opposite pattern over the whole range of ejected angle, because of the electron–electron two-body kinematic and the electron–nucleus final-state interaction which gives rise to the peak-shaped structure of the present result for electrons ejected with 250eV energy using electron impact.

Now let us consider the next case for the incident energy  $E_i=150\text{eV}$  and different ejected angles like 4eV, 10eV, 20eV, 30eV & 50eV in the Fig.2 (a, b, c, d, e) in this section.

Firstly for the incident energy  $E_i=150\text{eV}$  and  $E_1=4\text{eV}$  in Fig.2 (a), we observe that the present result and the first Born results almost similar except the lower peak at  $\theta_1=80^{\circ}$ . We also notice that lower peak position of the present first Born result is closer to the results for the ionization of ground state hydrogen atoms by electrons than the present DDCS exchange calculation. [ comment required for opposite trend] When we increase the ejected electron energy to  $E_1=10\text{eV}$  of the incident energy  $E_i=150\text{eV}$  in Fig.2 (b), the first Born and present results are exactly identical and overestimated with Das and Seal [12] over the ejected angular range. It is interestingly noticed that the present calculation is comparatively nearby the ground state theoretical result. So the present DDCS exchange result is the best fit with theoretical data [12].

The present and the hydrogenic ground state theoretical results are fairly similar in shape for ejected angle up to  $110^{\circ}$ , while experimental data [33] is comparatively closed to the present result for the incident energy  $E_i=150\text{eV}$  and  $E_1=20\text{eV}$  in Fig.2 (c). After greater values of  $\theta_1=110^{\circ}$ , creating a peak the present result goes closely with the present first Born data.





**Fig-2:** DDCS with exchange effects for the ionization of atomic hydrogen at  $E_i=150\text{eV}$  as a function of the ejected electron angle  $\theta_1$  relative to the incident electron direction. The ejected electron energies are considered as 4eV, 10eV, 20eV, 30eV and 50eV. **Theory:** Dotted curves represent hydrogenic ground-state experimental results of Shyn[1], purple continuous curves represent hydrogenic ground-state results of Das & Seal [2], red-dashed curves presents first Born results and green continuous curves represent results of exchange effects at metastable 2P state.

Next after taking kinematic condition as the incident energy  $E_i=150\text{eV}$  and  $E_1=30\text{eV}$  in Fig.2 (d), the first



Born and present result are almost identical in shape and closed to Das and Seal

[12] at lower angular values and also closed to the experimental data [33] at higher angular values which shows a good qualitative agreement between metastable 2P state results and ground state results.

Finally, in the fig.2 (e) we have increased the ejected energy  $E_1=50eV$ , keeping the incident energy as  $E_i=150eV$ , the present calculation and hydrogenic ground state theoretical result [12] show similar peak pattern with shifted position whereas the present first Born results provide lobe-peak structure. Also we noticed that the present DDCS exchange result is comparatively close to the experimental result of Shyn[33] than present first Born result. We see that the present DDCS results of metastable-2P state with exchange effects exhibit a good qualitative understanding with hydrogenic ground state theoretical and experimental results [12, 33] except  $E_1=4eV$  in the both cases which show a similar pattern. On the other side, the present calculations and the present first Born result both reveal similar attitude in each but opposite behavior with ground state data. However, our present results disagree a little bit overall, an advance calculation of future experimental work is also needed for further verification.

To understand these structures of the DDCS exchange effects results the table -1 and table- 2 are presented here where values of the different ejection angle  $\theta_1$  are shown for different values of the scattering angles  $\theta_2$  for four values of ejected electron energy  $E_1$  in the cases  $E_i=250eV$  and  $E_i=150eV$ .

| $\theta_2$<br>(deg) | $\theta_1$ (deg) | $E_1 = 4eV$ | $E_1 = 20eV$ | $E_1 = 50eV$ | $E_1 = 80eV$ |
|---------------------|------------------|-------------|--------------|--------------|--------------|
|                     |                  | DDCS        | DDCS         | DDCS         | DDCS         |
| 0                   | 0                | 0.0413      | 0.0540       | 0.0564       | 0.0003       |
| 1                   | 36               | 0.8793      | 0.1413       | 0.0430       | 0.0008       |
| 2                   | 72               | 1.8276      | 0.3164       | 0.0025       | 0.0001       |
| 4                   | 108              | 1.4955      | 0.2081       | 0.0011       | 0.0001       |
| 10                  | 144              | 0.9513      | 0.1287       | 0.0006       | 0.0016       |
| 20                  | 180              | 0.1198      | 0.0234       | 0.0007       | 0.0008       |
| 30                  | 216              | 0.3309      | 0.0626       | 0.0005       | 0.0010       |
| 40                  | 252              | 0.4621      | 0.0540       | 0.1475       | 0.0005       |
| 60                  | 288              | 0.3881      | 0.0434       | 0.0871       | 0.0004       |
| 90                  | 324              | 0.1676      | 0.0297       | 0.0021       | 0.0002       |
| 100                 | 360              | 0           | 0            | 0            | 0            |

Table-1: DDCS results for ejected angles  $\theta_1$  corresponding to various scattering angles  $\theta_2$  for four different values of ejected electron energies are  $E_1= 4eV$ ,  $E_1= 20eV$ ,  $E_1= 50eV$  and  $E_1= 80eV$  in ionization of hydrogen atoms for 250eV electron.

| $\theta_2$<br>(deg) | $\theta_1$ (deg) | $E_1 = 4eV$ | $E_1 = 20eV$ | $E_1 = 30eV$ | $E_1 = 50eV$ |
|---------------------|------------------|-------------|--------------|--------------|--------------|
|                     |                  | DDCS        | DDCS         | DDCS         | DDCS         |
| 0                   | 0                | 0.0261      | 1.0780       | 0.0136       | 0.0001       |
| 1                   | 36               | 0.6784      | 0.0669       | 0.0218       | 0.0003       |
| 2                   | 72               | 1.3593      | 0.1701       | 0.0028       | 0.0015       |
| 4                   | 108              | 1.1282      | 0.0419       | 0.0401       | 0.0005       |
| 10                  | 144              | 0.7185      | 2.0925       | 0.0417       | 0.0003       |
| 20                  | 180              | 0.1055      | 0.0725       | 0.0423       | 0.0005       |
| 30                  | 216              | 0.2435      | 2.2561       | 0.0381       | 0.0003       |
| 40                  | 252              | 0.3514      | 0.9428       | 0.0072       | 0.0000       |
| 60                  | 288              | 0.2956      | 1.1458       | 0.0034       | 0.0000       |
| 90                  | 324              | 0.1142      | 0.8745       | 0.0012       | 0.0000       |
| 100                 | 360              | 0           | 0            | 0            | 0            |

Table-2: DDCS results for ejected angles  $\theta_1$  corresponding to various scattering angles  $\theta_2$  for four different values of ejected electron energies are  $E_1= 4eV$ ,  $E_1= 20eV$ ,  $E_1= 30eV$  and  $E_1= 50eV$  in ionization of hydrogen atoms for 150eV electron.

We discussed here the ionization techniques of the outcomes for qualitative understanding. Here, we considered four different scattering amplitudes corresponding to the different terms on the right-hand side of equation (3). The first and the second terms of equation (3) express T-matrix elements corresponding to the amplitude in the first Born approximation. The third term interprets that the projectile first scattered off the bound electron and then scattered an infinite number of times off the massive nucleus through large angles leading to a large enhancement of the DDCS for large scattering angle  $\theta_2$ . The fourth term is a higher-order process and contributes only little. In this study, we have seen that the amplitude is substantially large, in magnitude, compared to other amplitudes, such as first Born. This implies that the projectile–electron interactions are most important in the final channel. It is well known that ionization process can occur due to double binary collisions. The projectile–electron binary collision is described by the first term of eq. (3), i.e. it exists also in simple plane-wave approximation. Another double binary collision leads us to the observation that the projectile (corresponding to the amplitude in the second term of eq. (3)) is first scattered from the nucleus and can be deflected, in principle, into any direction. The final shape and magnitude of the DDCS is determined by the coherent superposition of the two transition matrices of the second and third terms corresponding to eq. (3) described by the same of eq. (5).

**Conclusion:**

The present calculation on the Double differential cross sections (DDCS) for ionization of metastable 2P-state hydrogen atoms by 150eV and 250eV electron impact with exchange effects exposes a thinkable additional structure of the cross-section curves for momentum transfer in the ionization of the hydrogen

atoms. It is noticed that the implementation of the final-state wave function  $\Psi^{(-)}(\mathbf{r}_1, \mathbf{r}_2)$  in this study shows a good qualitative agreement with compared hydrogenic ground state theoretical and experimental data which is very significant and inspiring for the future experimental research in this field.

**Acknowledgements:**

I would like to thank the Simulation Lab of Chittagong University of Engineering and Technology (CUET), Chittagong-4349, Bangladesh, for giving supports to perform the computational works.

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