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Double Differential Cross-Sections for Ionization of Metastable 2P State Hydrogen Atoms by Electrons at Intermediate and High Energies

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Abstract

The First Born double differential cross-sections for ionization of metastable 2P state of hydrogen atoms by electrons are calculated at intermediate and high energies100eV, 150eV and 250eV applying a multiple scattering theory. The present new results are compared with hydrogenic ground state experimental measurements and other existing theoretical results. The results show a good qualitative agreement with those of compared result. There is no available experimental data for the ionization of hydrogenic metestable states. So new theoretical and experimental study in this field of ionization will be interesting.

Keywords: *Ionization, Cross-section, Metastable states, Scattering.*

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1. Introduction

Ionization is one of the most important reactions in high energy ion-atom collisions. Much information on ionization dynamics has been obtained by measuring the DDCS in ejected electron energy and ejected angles.A study of atomic ionization by charged particles plays an important role in solving problems in atomic physics, astrophysics, plasma physics, fusion technology and many other branches of science [1]. The DDCS contains information about the angular and energy distribution of secondary electrons in atomic ionization collisions[2].The ionization of atomichydrogen by electron impact is of fundamental importance [3] and of rare gas atoms, particularly, the cross-sections obtained with ground state ionization, is considered as benchmark data. DDCS of ionization, contain valuable information about both the collision dynamics and the internal structure of atomic or molecular systems.Experimental evaluationsin angle and energy have been obtained by Shyn [4-8] and other groups [9-16] for DDCS. On the theoretical side, the best available theoretical calculation of DDCS is based on the plane-wave Born approximation [17-18], which can only be expected to be valid at very high incident energies.

Bethe [19] first calculatedionization by fast particles quantum mechanically. The utilization of the multi-parameter detection technique, together with the progress in computational methods, have made it possible to perform a complete experiment in which kinematical parameters (like momentum and energies) of all acting particles are determined. In such

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calculations, the ejected electron is detected in coincidence with the scattered electrons and it is a well known experiment [20] called (e, 2e) experiments. This kind of experiments have been successfully used during the last four decades to investigate the fine details of the ionization process both in the ground state [21–30] and metastable [31–46] states of atomic Hydrogen. Before Shyn [1], there is no data existed for atomichydrogen, though it is the simplest and the most convenient system for theoretical analysis. In this work, the DDCS for ionization of hydrogenic metastable 2P state by electron impact at100eV, 150eV and 250eVintermediateand highenergieshas been calculated.A wave function[25-27]is used herein thecalculation of the triple differential cross sections (TDCS)in the metastable 2P-state hydrogen atoms by electron following the multiple scattering theory of Das and Seal [25, 26]. It is noted that the multiple scattering wave functionhas been designed for two electrons moving in a coulombfield, which include higher order and correlation effects.We use this wave function to calculate the DDCS integrated over the scattering angle.Itwillbe interesting here to use thewave function in the present studyof DDCS forionization of metastable 2P state hydrogen atoms by electrons.To the best of our knowledge, the DDCS for the ionization of metastable 2P-state hydrogen atoms by electrons at intermediate and high energies were never studied before experimentally. Most of the experimental investigations on the DDCS concentrated on the ground-state electron hydrogen ionization collisions. Only a fewtheoretical calculations of the DDCS of metastable 2S and 2P-state hydrogen atoms were observed. Therefore, hydrogenic ground stateexperimental resultsfor ionization of metastable 2P state hydrogen atoms by electrons will be valuable and will add a new dimension to the significant study of this fieldof research.

2. Theory

The direct Transition matrix element for ionization of hydrogen atoms by electrons [6],may be written as,

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

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.

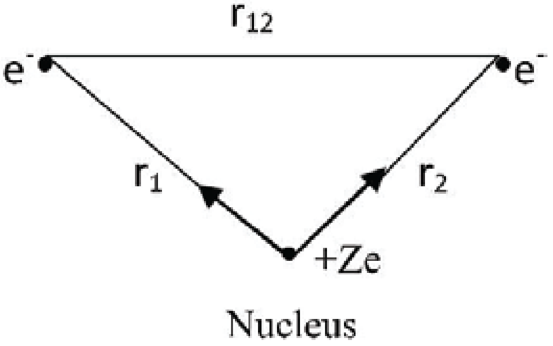


Fig: Interaction between two electrons and the nucleus.

The initial channel unperturbed wave function is given by

$$\Phi_i(\bar{r}_1, \bar{r}_2) = \frac{e^{i\bar{p}_i \cdot \bar{r}_2}}{(2\pi)^{3/2}} \phi_{2P}(\bar{r}_1),$$

where $\phi_{2P}(\bar{r}_1) = \frac{r_1}{4\sqrt{2\pi}} \cos\theta \, e^{-\frac{r_1}{2}}$ (3)

Here $\lambda_1 = \frac{1}{2}$ and $\phi_{2P}(\bar{r}_1)$ is the hydrogenic 2P state wave function and $\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$ is the final three-particle scattering state wave function [25] and co-ordinates of the two electrons are $\bar{r}_1$ and $\bar{r}_2$ respectively.

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

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

Here

$N(\bar{p}_1, \bar{p}_2)$ is normalization constant, $\bar{r} = \frac{\bar{r}_2 - \bar{r}_1}{2}$,

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

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

Now 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 approximation equation may be written as

$$T_B = \frac{1}{16\pi^2} \left\langle \phi_{p_1}^{(-)}(\bar{r}_1) e^{i\bar{p}_2.\bar{r}_2} \left| \frac{1}{r_{12}} - \frac{1}{r_2} \right| e^{i\bar{p}_i.\bar{r}_2} r_1 \cos\theta \; e^{-r_1\lambda_1} \right\rangle$$

$$= \frac{1}{16\pi^2} \int \left[\phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2.\bar{r}_2} \left(\frac{1}{r_{12}} - \frac{1}{r_2} \right) \times e^{i\bar{p}_i.\bar{r}_2} r_1 \cos\theta \; e^{-\lambda_1 r_1} \right] d^3r_1 d^3r_2$$

$$= \frac{1}{16\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2.\bar{r}_2} \frac{1}{r_{12}} e^{i\bar{p}_i.\bar{r}_2} r_1 \cos\theta e^{-\lambda_1 r_1} d^3r_1 d^3r_2$$

$$- \frac{1}{16\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2.\bar{r}_2} \frac{1}{r_2} e^{i\bar{p}_i.\bar{r}_2} r_1 \cos\theta \, e^{-\lambda_1 r_1} d^3r_1 d^3r_2$$

$$\therefore T_{\mathbf{B}} = \mathrm{tb1} + \mathrm{tb2} \tag{6}$$

where

$$\mathrm{tb1} = \frac{1}{16\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2.\bar{r}_2} \frac{r_1}{r_{12}} e^{i\bar{p}_i.\bar{r}_2} \cos\theta \, e^{-\lambda_1 r_1} d^3r_1 d^3r_2$$

and

$$\mathrm{tb2} = -\frac{1}{16\pi^2} \int \phi_{p_1}^{(-)*}(\bar{r}_1) e^{-i\bar{p}_2.\bar{r}_2} \frac{r_1}{r_2} e^{i\bar{p}_i.\bar{r}_2} \cos\theta \, e^{-\lambda_1 r_1} d^3r_1 d^3r_2$$

T_B, is the first Born term for TDCS and other terms T'_B, T_i, T_{PB} are calculated in the our work of Dhar and Nahar [47]. After analytical calculation by using the Lewis integral [48], the above expressions of eq. (6) have been calculated numerically and the triple differential cross-sections for T-Matrix element is given by

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = \frac{p_1 p_2}{p_i} \left| T_{fi} \right|^2 \tag{7}$$

After integration of TDCS results [47] of equation (7), we can obtain the DDCS results using following equation

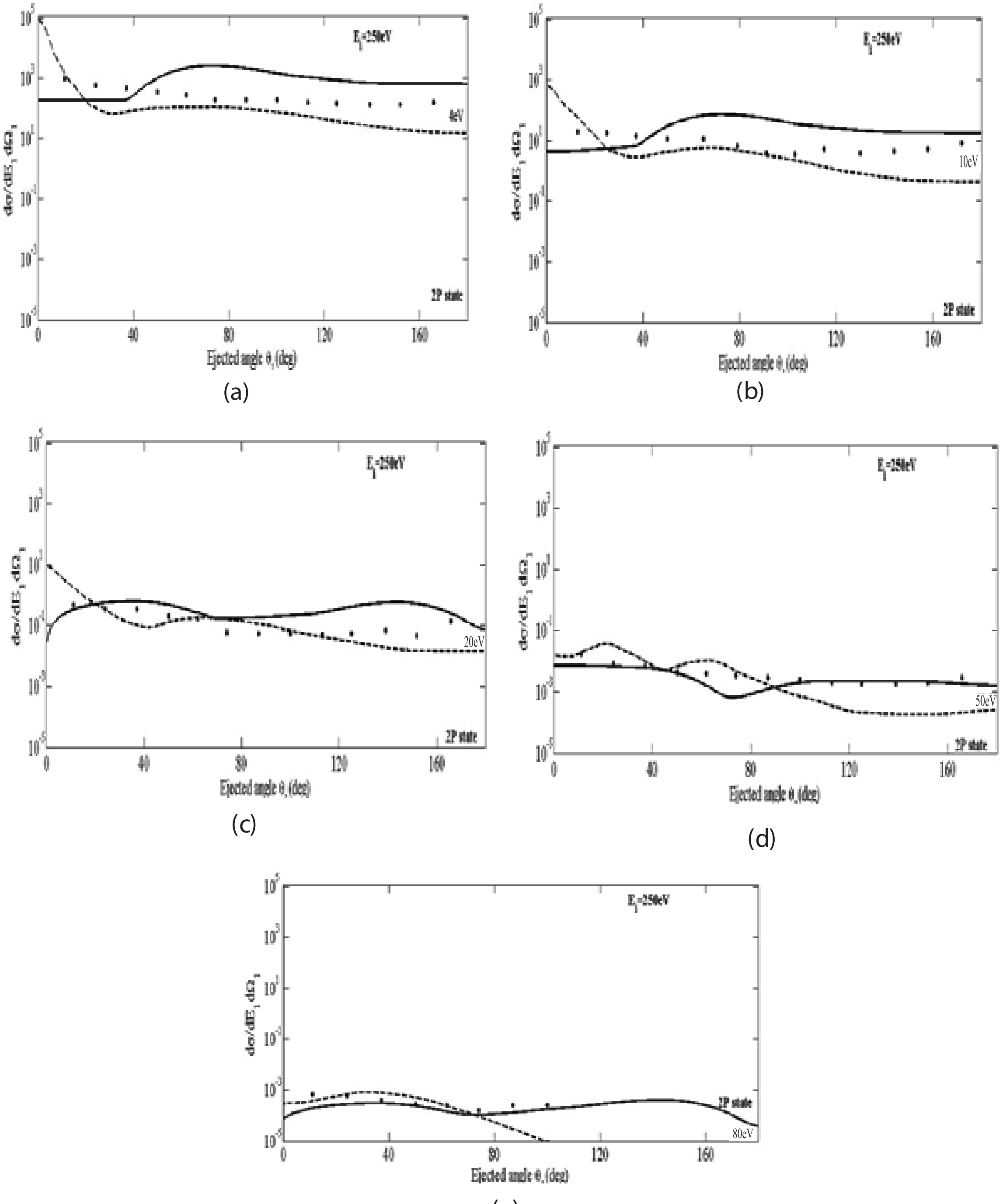
$$\frac{d^2\sigma}{dE_1 d\Omega_1} = \int \frac{d^3\sigma}{dE_1 d\Omega_1 d\Omega_2} d\Omega_2 \tag{8}$$

Therefore, in our present calculation DDCS has been computed using the computer programming language MATLAB, given by equation (8).

3. **Results and Discussion**

In this study, Double differential cross sections (DDCS) are computed here for the ionization of the metastable 2P state hydrogen atoms by electrons at high incident energy E_i=250eV (Fig.1), for ejected electron energies E_1=4eV, 10eV, 20eV 50eV, and 80eV at intermediate incident energy E_i =150eV(Fig. 2), for ejected electron energies E_1=4eV, 10eV, 20eV, 30eV, and 50eV. The ejected angle θ_1 varies from 0^0 to 180^0 considered as horizontal axis where DDCS as vertical axis in all figures and the scattered angle θ_2 varies from 0^0 to 100^0. Ionization of hydrogen atoms by electrons from the ground state experimental results of Shyn [1] and computational result of Das and Seal [2] are presented here for comparison. We also presented a comparison of our result with Roy, Mandal and Sil [3]. The final state scattering wave function

$\Psi_f^{(-)}(\bar{r}_1, \bar{r}_2)$ is the continuum state of the atomic hydrogen. When the contribution of the final continuum state is considered in the ionization of metastable 2P state hydrogen atoms by electrons, it shows a fall of binary lobe amplitude and a rise of recoil lobe amplitude. It is generally observed that for medium values of θ_1, there are reasonable qualitative agreement between the theoretical and hydrogenic ground state experimental results. In the present DDCS results, the amplitude is substantially large, in magnitude, 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 asignificant role in the ionization of atomic hydrogen for intermediate and high energies.



(a) (b)

(c) (d)

(e)

Fig. 1: DDCS for the ionization of atomic hydrogen by250 eV electron impact as a function of the ejected electron angle θ1 relative to the incident electron direction. The ejected electron energies are 4eV, 10eV, 20eV, 50eV and 80eV. Theory: Dotted curves represents hydrogenic ground-state experimental result [1], dashed curves represent hydrogenic ground-state results [2] and continuous curves represent the present results of metastable 2P state.

In Fig.1(a), for incident energy Ei=250eV and E1=4eV, the present first Born resultcoincidesat about θ1=200with those of Das and Seal [2] whereat higher ejection angle θ1lies above those of [2] making a forward peak andlies below closely the experimental values at smaller θ1andoverlapabout atθ1=420with those of Shyn [1]. After increasingejection energy toE1=10eVin Fig.1(b), thepresent resultcoincide at smallerangles thanthose of Das and Seal [2] and of Shyn [1]. At higher ejection angle θ1our curve lies above those of Das and Seal [2] and of Shyn [1] making a forward peak and then peak flattens as the energy increases and ultimately disappears which shows good qualitative agreement.Now takingthe ejection energy E1as 20eVin Fig.1(c)the present result exhibits similar peak patternswith large magnitude atθ1=200 and θ1=740with those of Das and Seal [2] as well as at θ1=150 and θ 1=1700likehydrogenic ground stateexperimental resultswhich shows good qualitative agreement. Next consideringthe ejection energy E1as 50eVin Fig.1(d),the present result overlaped two times at θ1=450 and θ 1=900with the theoretical result at smaller and higher ejected angles. Also thepresent result comparetively closer to thehydrogenic ground stateexperimental result than that of theoretical results creating a lower dip at θ 1=700.Finallytakingejectedenergy E1=80eVin Fig.1(e), it is obserbed that the experimentalresult, the theoretical result, and the present result show simillar nature in shape at smaller ejection angles up to θ1=700and at higher energy the present result show a peak with large magnitude which exhibit the good comparison.

In Fig.-2(a): for incidentenergy E_i=150eV andE_1=4eV, it is observed that the pesent result coincides at about θ_1=$16_0$and θ_1=$70_0$with those of Das and Seal [2] and at higher ejection angle $\theta_1$lies above those of [2] creatinga forward peak which is flatten slowly wherealso coincides at θ_1=70_0 andlies aboveclosely the experimental values at higher angle θ_1. It exhibits a good agreement with the theoretical data as well as hydrogenic ground stateexperimental results.

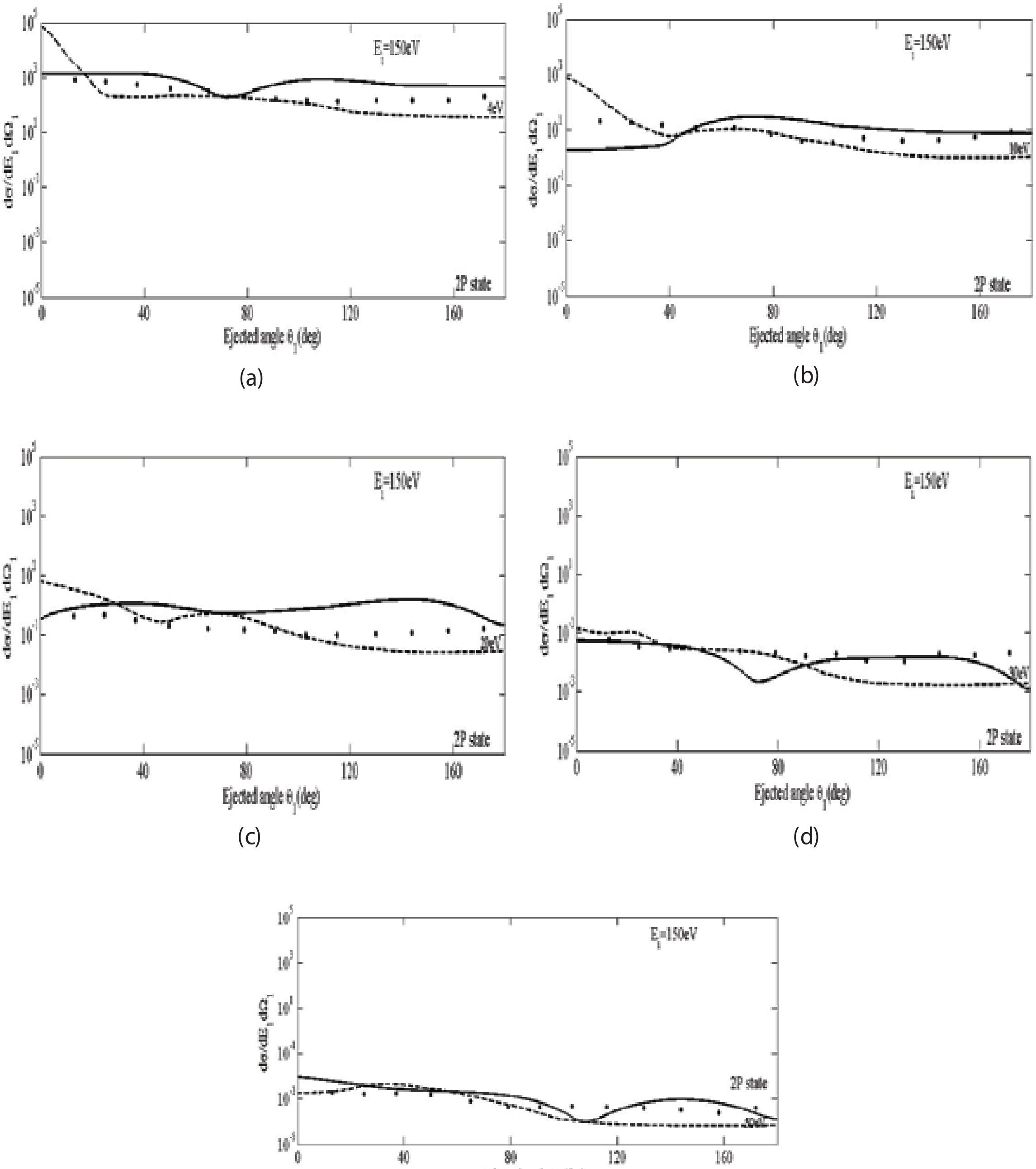
After considering ejection energy E_1 as 10eV in Fig.2(b), our curve lies far below those of Das and Seal [2] at smaller angles and runs comparatively closer to the experimental values. Around $\theta_1 = 70^0$ the present result crosses with those of Das and Seal [2] and of Shyn [1] creating a peak and level slowly at higher ejection angle θ_1. This shows good comparison with both theoretical and experimental values.

Next taking ejection energy E_1=20eV in Fig.2(c), our present result coincides two times at $\theta_1 = 28^0$ and $\theta_1 = 75^0$ with those of Das and Seal [2] as well as a concurrence at $\theta_1 = 98^0$ with Shyn [1] and at ejection angle between 28^0 and 75^0 our result lies those of Das and Seal [2] and at $\theta_1 = 150^0$ a peak created and lying above with the experimental and the theoretical results. It shows that a good qualitative agreement.

After increase the ejection energy E_1=30eV in Fig.2(d), the present result overlaped four times at $\theta_1=32^0$, $\theta_1 = 48^0$, $\theta_1 = 90^0$ and $\theta_1 = 178^0$ with Das and Seal [2] and creating a lower deep at about $\theta_1 = 74^0$ and passes comparatively closer to Shyn [1] from lower angle to higher angle which exhibits a good comparison.

Finally, our consideration of ejection energy as E_1=50eV in Fig.2(e), the theoretical result coincide at $\theta_1 = 25^0$, $\theta_1 = 54^0$ and $\theta_1 = 105^0$ with our result and at higer angles between 105^0 to 180^0 a peak created where the experimental curve runs comparatively closer to the present result which shows a good comparison.

In Fig. 3, the DDCS for ionization of metastable 2P state hydrogen atoms by electrons as a function of ejected angle θ_1 for incident energy E_i=100eV and ejected electron energy E_1=15eV and the experimental data of Shyn , the theoritical curve of Curran and Walters for electron impact at E_1=14eV and the DDCS values of Roy,



(a) (b)

(c) (d)

(e)

Fig.2: DDCS for the ionization of atomic hydrogen by 150 eV electron impact as a function of the ejected electron angle θ1 relative to the incident electron direction. The ejected electron energies are 4eV, 10eV, 20eV, 30eV and 50 eV. Theory: Dotted curves represent hydrogenic ground-state experimental results [1], dashed curves represent hydrogenic ground-state results [2] and continuous curves represent results of metastable 2P state.

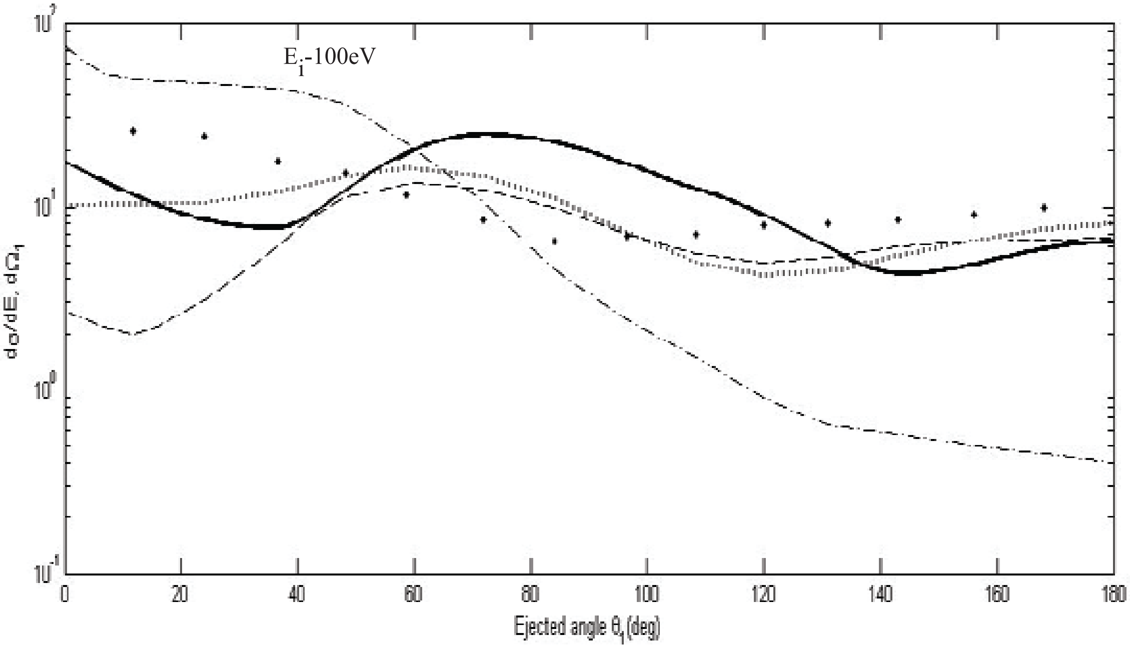


Fig.3: DDCS for the ionization of atomic hydrogen by 100 eV electron impact as a function of the ejected electron angle θ1 relative to the incident electron direction. The ejected electron energy is E1=15eV. Theory: Dotted curve (•) represent hydrogenic ground-state experimental results [1], small dotted curve (·····) represents Curan and Walters[14], E1=14eV, short-broken curve (-·-·-·) represents for positron impact, dashed curve (- - -) presents the Roy, Mandal and Sil[3] and continuous curve(—) represents the present calculation.

Mandal and Sil are also presented here for comparison. It is observed that the present first Born result coincides at θ_1 =60^0 with positron impact 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 ejected electron energy E_1 in the case E_i=250eV.

4. Conclusions

In this work the DDCS for ionization of metastable 2P-state hydrogen atoms by 100 eV, 150 eV and 250 eV electron impact has been calculated. It is noted that when the full wave function isused, then the present results represent qualitative agreement with the available hydrogenic ground state experimental data [1] and those of hydrogenic ground state theoretical models [2] present result meets at ejection angles θ_1=15^0, θ_1=50^0 and θ_1=145^0 and between 15^0 and 50^0 our data lies below whereas between 50^0 and 145^0 overestimate the data of Curran and Walters. Finally presentvalues compare well with the Curran and Walters data as well as the hydrogenic ground state experimental data.

To understand these structures of the DDCS and the present first Born results. The present calculation using the multiple scattering theory of Das and Seal [2] provides a significant contribution in the field of metastable 2P-state ionization problems. Due to the absence ofany experimental data for the DDCS results of the hydrogenic metastable 2P-state ionization process, it is not possible to compare the

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	201.6	0.03	0.0076	0.0831
1	36	202.0	0.67	0.0065	0.3048
2	72	2755.5	0.18	0.0007	0.1108
4	108	1240.0	0.25	0.0023	0.2078
10	144	722.1	0.62	0.0023	0.4088
20	180	697.2	0.08	0.0017	0.0409
30	216	592.2	0.71	0.0050	0.4434
40	252	163.0	0.08	0.0001	0.0483
60	288	98.7	0.37	0.0035	0.2286
90	324	3.7	0.51	0.0009	0.2840
100	360	0	0	0	0

Table-1: DDCS results for ejected angles θ_1 corresponding to various scattering angles θ_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.

present computational results with the experimental findings. Thus for judgment of this work, hydrogenic ground stateexperimental study in the relevant field is needed. Therefore, hydrogenic ground stateexperimental resultsfor ionization of metastable 2P state hydrogen atoms by electrons will be valuable and will add a new dimension to the significant study of this field of research.

Acknowledgements

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