Theoretical calculation of triple differential cross sections for ionization of H(3d) by electron Impact

Sushmita Banerjee*, Sunil Dhar
Department of Mathematics, Chittagong University of Engineering and Technology, Chittagong, Bangladesh
*Corresponding author's Email: sushmita@cuet.ac.bd

ABSTRACT

In the present work, triple differential cross sections (TDCS) are calculated for the ionization of metastable 3d-state hydrogen atoms by electron at 250 eV for various kinematic condition applying a multiple scattering theory. The present new results are very interesting and are compared with the theoretical results of hydrogenic different metastable states as well as the hydrogenic ground state experimental data. Obtained new finding results are in good qualitative agreement with those of compared theories. The present results give an great opportunity for further study of such ionization problems.

Keywords: Electron, Ionization, Cross-Section, Scattering.

1. Introduction:

In high energy ion-atom collisions, ionization is one of the most momentous reaction. Electron impact ionization by charged particles are used in solving problems in isolated range of field like astrophysics, plasma physics , fusion technology, radiation physics etc. The triple differential cross-sections has been attained in ejected electron energy and ejected angles in the electron hydrogen mechanism. The theoretical non-relativistic studies for the atomic ionization by Charged particle was first treated by Bethe [1]. Over the last four decades, the theoretical and experimental study in electron atom ionization collision on different cross sections has become gradually interesting for non-relativistic [2-25] as well as relativistic [26-28] energies. Ionization of the hydrogenenic atom by electron is a good image for perturbation theory because of the existence of empirical consequence. In this context, the electron-electron coincidence experiments called (e,2e) experiments, provide a clear concept of the kinematics of the collisions by giving information about the direction of the scattered and ejected electrons. During the last five decades, Ionization of hydrogen atom by electron have been considered to explore the details of the ionization process both in the ground state [2-13] and metastable states [14-25] of atomic hydrogen.
In the current study, atomic hydrogen is used as target in order to perceive the ionization mechanism of atomic system by electron impact energy. A multiple scattering theory [13] has been applied in the present estimaton of the triple differential cross-sections(TDCS) in the metastable 3d-state hydrogen atom ionization by 250eV electron energy. Lewis integral [29] has been used in the present study for analytical calculation.
The existent new study results will present a new dimensions on ionization of hydrogenic metastable states. current results are compared with previous related theories [16],[24] and [25].

2. Theory:

The direct T-matrix element for ionization of hydrogen atoms by electrons, following Das and Seal [13] may be written as

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

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

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

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.

We have the initial channel unperturbed wave function is

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

Where

$$\phi_{3d}(\bar{r}_1)=\frac{1}{81\sqrt{6\pi}}\left(r_1^{\,2}\right)\left(3\cos^2\theta-1\right)e^{-r_1/3}\quad .$$

$$\Phi_i(\bar{r}_1,\bar{r}_2)=\frac{1}{324\sqrt{3}\pi^2}\left(r_1^{\,2}\right)\left(3\cos^2\theta-1\right)e^{-\lambda_1 r_1} \tag{2}$$

Here $\lambda_1=\frac{1}{3}$, $\phi_{3d}(\bar{r}_1)$ is the hydrogenic 3d-state wave function and $\Psi_f^{(-)}(\bar{r}_1,\bar{r}_2)$ is approximate wave function is given by [13]

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

where

$$\bar{r}=\frac{\bar{r}_2-\bar{r}_1}{2},\ \bar{R}=\frac{\bar{r}_1+\bar{r}_2}{2},$$

$$\bar{p}=(\bar{p}_2-\bar{p}_1),\ \ \bar{P}=\bar{p}_2+\bar{p}_1,$$

The normalization constant $N(\bar{p}_1,\bar{p}_2)$ is calculated using Das and Seal [13] and Dhar and Nahar [22].

the Coulomb wave function $\phi_q^{(-)}(\bar{r})$ is used from Das and Seal [13] and Dhar and Nahar [22]

Now equation (1) becomes

$$T_{fi}=T_B+T_{B'}+T_i-2T_{PB} \tag{4}$$

where

$$T_{\mathbf{B}}=\left\langle\phi_{p_1}^{(-)}(\bar{r}_1)\ e^{i\bar{p}_2\cdot\bar{r}_2}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{5}$$

$$T_{B'}=\left\langle\phi_{p_2}^{(-)}(\bar{r}_2)\ e^{i\bar{p}_1\cdot\bar{r}_1}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{6}$$

$$T_i=\left\langle\phi_p^{(-)}(\bar{r}\ )\ e^{i\bar{P}\cdot\bar{R}}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{7}$$

$$T_{PB}=\left\langle e^{i\bar{p}_1\cdot\bar{r}_1+i\bar{p}_2\cdot\bar{r}_2}\left|V_i\right|\Phi_i(\bar{r}_1,\bar{r}_2)\right\rangle \tag{8}$$

Using the Lewis integral [29], We have evaluated First Born term $T_{\mathbf{B}}$ of equation (5)

Similarly we have calculated analytically the above equations (6),(7) and (8) for second Born results using the Lewis integral [29]. After that we have computed the above equations using Gaussian quadrature formula. Finally the triple differential cross-sections for T-Matrix element is given by

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

3. Results and Discussions:

In this section, We have calculated in this work the triple differential cross-sections(TDCS) at high incident energy $E_i = 250\ eV$ for various ejected angles θ_1 and fixed scattering angles θ_2 . Triple differential cross sections for ionization of metastable 3d-state hydrogen atoms by incident electron are presented at different energies . The existent results are compared with the ionization of hydrogen atoms by electrons from ground state theoretical results of Dal et al.[14], the BBK model of Brauner et al. [10] and the experiment results of Ehrhardt et al.[2]. Also the earlier works on hydrogenic 2S-state [16], 3S-state [24] and recent works on hydrogenic 3P-state [25] ionization results are exhibited here for comparison. The present results of triple differential cross section are presented in the following nine figures where we have designed the electron impact TDCS varying against the angle of ejection (θ_1) of the ejected electron.

In this study, the ejected angle θ_1 varies from 0^o to 360^o considered as horizontal axis where scattering angles θ_2 is fixed and referred as vertical axis. The present results of hydrogenic metastable 3d state by electron are designed corresponding to the different scattering angles $\theta_2 = 3^o$ Fig. 1(a) for ejected electron energies $E_1 = 5eV$,15^o Fig. 1(b), 25^o Fig. 1(c) for ejected electron energies $E_1 = 50\ eV$ considering the ejected angle θ_1 from 30^o to 100^o and the scattering angle $\theta_2 = 5^o$ Fig. 2(a), 7^o Fig. 2(b), 9^o Fig 2(c), 11^o Fig. 2(d) , 15^o Fig. 2(e) and 20^o Figure 2(f) for ejected electron energies $E_1 = 5eV$.

The incident electron energy of $E_i = 250\ eV$ is taken here. In all figures, $\theta_1(0^o - 180^o)$ and $\phi = 0^o$ is considered as recoil region while $\theta_1(180^o - 360^o)$ and $\phi = 180^o$ is referred as binary region.

In Fig. 1(a) the present results shows a qualitative comparison with the present first Born result , the hydrogenic ground state result of BBK model [10] ,the second Born approximation [14], the hydrogenic ground state experimental data [2] , 3S-state results [24] and recent works on hydrogenic 3P-state [25] ionization results. The peak values of present results and first Born results show good qualitative agreement with those of the compared results in the recoil region but show somewhere dissimilar in the binary region. This may be happened due to the change of the hydrogenic metastable states by electrons. Here in the recoil region the peak values of present and first Born and 3P-state results [25] are about double results of the other compared results. The binary peak values of the present results slightly shifted right from other compared results.

In Fig. 1(b), The peak value of present and first Born results are lower than the hydrogenic ground state experimental results [2], hydrogenic metastable 3S-state results[24] and hydrogenic metastable 3P-state results[25]. Also the peak values of current results shifted slightly to the right at higher ejected angle near about $\theta_1 = 72^o$ than other compared results [2],[10] and [14].The peak pattern of the present result shows exactly similar conduct with the hydrogenic ground state BBK results [10] with slight shift.

In Fig. 1(c), Our present result and hydrogenic 3P-state result exits in almost same position with similar peak height. The peak magnitude is the highest among other compared results [10,2].

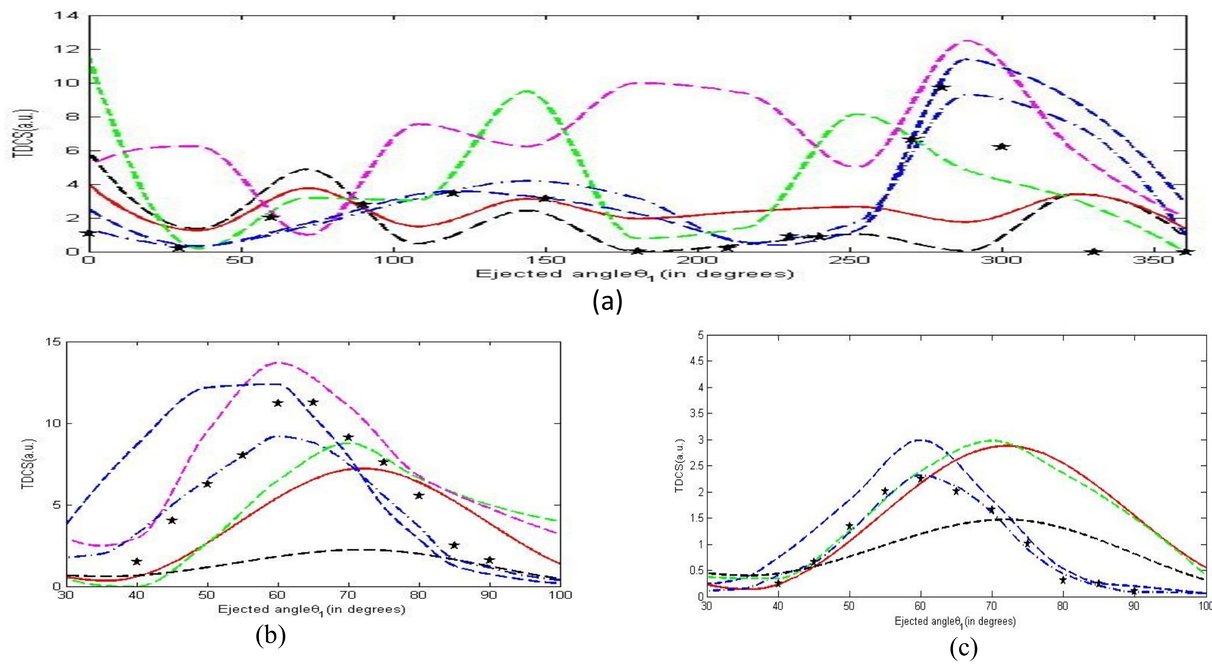

Fig. 1. Triple-differential cross sections (TDCS) with versus ejected electron angle θ_1 for atomic hydrogen by electron energy 250 eV with (a) $E_1 = 5eV$ and $\theta_2 = 3^0$,(b) $E_1 = 50eV$ and $\theta_2 = 15^0$,(c) $E_1 = 50eV$ and $\theta_2 = 25^0$.Theory: Continuous curve (Red) illustrate Present result, Dash curve(Black) exhibit Present First Born results, Dash curve(Green) display 3P-state result [25], Dash curve(Magenta) expose 3S-state result [24] and Dash curve(Blue) demonstrate Hydrogenic ground state Second Born results [14], Dash dotted curve(Blue) reveal Hydrogenic ground state BBK model [10] and Star indicated Hydrogenic ground state experiment [2] (multiplied by 0.00224).

In Fig. 2(a) , our present results show a good agreement with 2S-state [16] and 3S -state [24] metastable results. The present TDCS curve display two fall and two peak in recoil region and one fall two peak in binary region while metastable 3S-state result exhibit one fall and one peak in recoil region and one peak in binary region. The present results and 2S-state results show one prominent peak in recoil region.

In Fig. 2(b), our present study results exhibit same peak pattern with metastable 3S -state [24] and 2S-state [16] results whereas the present results and metastable 3P–state results [25] show opposite peak pattern at higher ejected angle about $\theta_1 = 288^o$

In Fig. 2(c), our present TDCS curve depict a very interesting results. It expressed two falls in recoil region and two peak in binary region . The present result is closer to the 3S-state result [24].The present result shows a bit different from 3P state results[25].

In Fig. 2(d), we note that the magnitude of the present and first Born results are lower than 3S-state [24] and 3P-state [25] results. In this figure, the present result give a short lobe where 2S-state [16] result show a deep lobe at ejected angle about 252^o.

In Fig. 2(e), the magnitude of present and first Born results are increased from 2S state [16] and 3P state[25] results. In the recoil field near about $\theta_1 = 72^o$, the existence outcome and first Born outcome give dull peak whereas 2S state outcome give a nice lobe.

In Fig. 2(f), the present results and first Born results provide exactly similar behavior as the 3S state[24] results in the recoil region but show a gross difference with the results of 3P-state [25] both in recoil and binary region. The present TDCS curve reversely coincide with 2S state results [16] at ejected angle near about $\theta_1 = 72^o$.

Finally, it is remarked that, the peak pattern of the energy spectrum as obtained from our present study is closer to the compared results [24,25] in some cases and again sometimes different. It may be happened due to the change of atomic state.

Here a table (please see Table 1) of comparison results for ionization of hydrogenic 2S-state, 3S-state and 3P-state atoms by electron is presented.

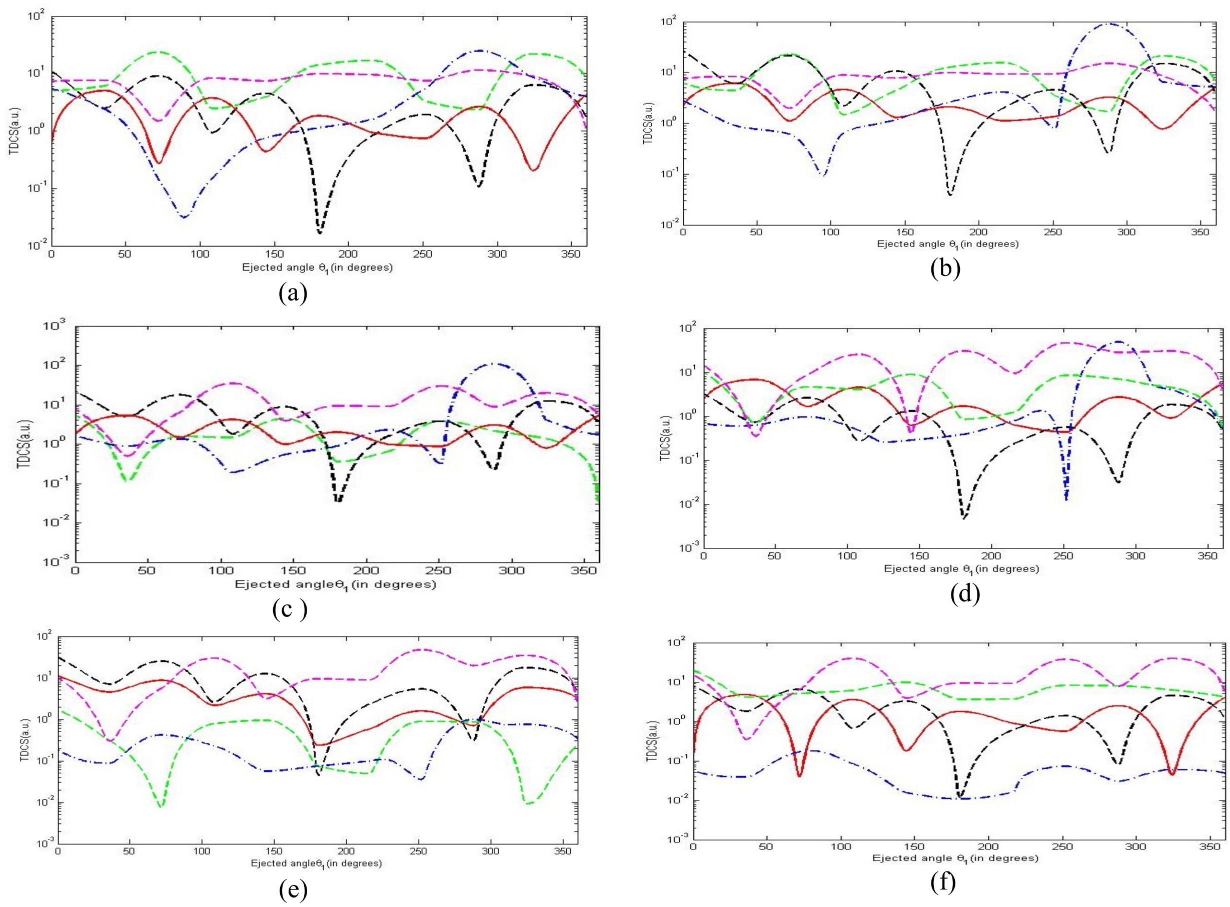

Fig. 2: Triple-differential cross sections (TDCS) versus ejected electron angle θ_1 for atomic hydrogen by electron energy $E_i = 250\ eV$ with ejected electron energy with $E_1 = 5eV$ and (a) $\theta_2 = 5^0$, (b) $\theta_2 = 7^0$ (c) $\theta_2 = 9^0$ (d) $\theta_2 = 11^0$,(e) $\theta_2 = 15^0$,(f) $\theta_2 = 20^0$. Theory: Continuous curve (Red) illustrate Present result, Dash curve(Black) exhibit Present First Born results, Dash curve(Green) display hydrogenic 3P-state result [25], Dash curve(Magenta) expose hydrogenic3S-state result [24] and Dash dotted curve(Blue) demonstrate hydrogenic 2S-state result [16].

Table 1: Triple differential cross section (TDCS) for electron impact Ionization of H(3d) by incident electron are distinguished with 3P-state, 3S-state & 2S-state results where the incident energy is 250eV, the scattering angle is $\theta_2 = 11^0$ and the ejected electron energy is $E_1 = 5eV$.

Ejected angle(θ_1)	2S	3S	3P	3d
0	0.6893	14.5786	9.9526	2.4629
36	0.6312	0.3563	0.7509	6.8799
72	0.9800	8.7532	4.6928	1.6808
108	0.4637	25.5528	4.1025	4.5879
144	0.2895	0.3963	9.0039	0.6282
180	0.3901	30.9523	0.8623	1.7184
216	0.7981	9.5389	1.2522	0.6285
252	1.3501	47.2595	8.6012	0.4408
288	49.5325	28.5003	7.4021	2.7559
324	4.0013	30.6939	4.1513	0.9146
360	0.5321	3.7095	0.5027	5.6182

4. Conclusion:

The present calculation exposes additional possible structure of the cross-section curves for intermediate momentum transfer in the hydrogenic 3d-state ionization at 250 eV impact energy. In the present estimation, the correlated three particle final state wave function of Das and Seal [13] has been followed. New theoretical computational observations for ionization of hydrogenic 3d state by electrons may be generalized for application to the other atom as well as ions and which may play a vital role to provide much interesting and potential results in this field of research.

Acknowledgements:
The computational works are executed in the Simulation Lab of Department of Mathematics, Chittagong University of Engineering and Technology, Chittagong-4349, Bangladesh.

References:

[1] Bethe H , (1930) Zur Theorie des Durchgangs schneller Korpuskularstrahlen durch Materie Annalen der Physik, **397**, 325-400

[2] Ehrhardt H, Knoth G, and Schlemmer P, Jung K, .(1986) Differential Cross Sections of Direct Single Electron Impact Ionization , Zeitschrift für Physik D Atoms, Molecules and Clusters, **1**, 3.

[3] Ehrhardt H, Knoth G , Schlemmer P and Jung K, (1985) Absolute H(e, 2e)p cross section measurements: Comparison with first and second order, Physics Letters A **110**, 92

[4] Das J.N, (1990) Momentum-Space Analysis of Scattering States with Possible Application to Atomic Ionization, Physical Review A, **42**, 1376

[5] Das J.N.and Seal S. (1993) Symmetric Scattering Ine±-H Ionization Collisions, Pramana, **40,** 253-258

[6] Das J.N. and Dhar S. (1999) Energy Spectrum of Ejected Electrons in Ionization of Hydrogen Atoms by Electrons. *Pramana*, **53**, 869-875

[7] Joachain JC and Piraux B. (1986) Comments at. Mol. Phys.,**17** 261

[8] Byron W.F , Joachen J.C and Piraux B. (1980) journal of Physics B: Atomic, Molecule and Optical Physic.**13**, L673

[9] Byron W.F , Joachain J.C, Piraux B. (1986) Theory of coplanar asymmetric (e, 2e) reactions in helium. *Journal of Physics B*: *Atomic*,*Molecular and Optical Physic*s **19**, 120

[10] Brauner M , Briggs J.C and Klar H. (1989) Triply-differential cross sections for ionisation of hydrogen atoms by electrons and positrons , Journal of Physics B: Atomic, Molecular and Optical Physics. **22,**2265

[11] Brauner M and Briggs JC. (1986) Ionisation to the projectile continuum by positron and electron collisions with neutral atoms, J. Phys. B. At. Mol. Phys. **19,** L325

[12] Berakder J and Klar H. (1993) Structures in triply and doubly differential ionization cross sections of atomic hydrogen. J. Phys. B. At. Mol. Opt. Phys. **26,** 3891

[13] Das JN and Seal S . (1993) Electron-Hydrogen Atom Ionization Collisions at Intermediate (5I0-20I0) and High(≳20I0) Energies. Physical Review A, **47**,2978

[14] Dal Capppello C, Haddadou A, Menas F and Roy AC. (2011) The second Born approximation for the single and double ionization of atoms by electrons and positrons , J. Phys. B: At. Mol.Opt.Phys. **44**, 015204

[15] Berakdar J, Engelns A, Klar H. (1996) Oriented and Aligned two electron continue. J.Phys B At Mol Opt Phys,**29**,1109

[16] Dhar S. (1996) Electron Impact Ionisation of Metastable 2S-State Hydrogen Atoms ,Australian Journal of Physics, **49**,937

[17**]** Das JN and Dhar S. (1996) Symmetric Scattering in Electron and Positron Impact Ionization of Metastable 2S-State Hydrogen Atom,Pramana J.Phys, **47**, 263-269

[18] Das, J.N. and Dhar, S. (1998) Calculation of Triple Differential Cross-Sections of K-Shell Ionization of Medium-Heavy Atoms by Electrons for Symmetric Geometry. *Pramana*, **51**, 751-756.

[19] Vučič S, Potvliege RM and Joachain C J. (1987) Second Born Triple-Differential Cross Sections for the Coplanar Asymmetric Ionization of H(2S) by Fast Electrons Physical Review A **35**, 1446.

[20] Qi Y Y, Ning L N, Wang J G and Qu Y Z. (2013) Plasma effect on fast-electron-impact ionization from 2p state of hydrogen-like ions.Physics of Plasmas **20**,123301

[21] Dhar S and Nahar N. (2015) Electron impact ionization of metastable 2P-state hydrogen atoms in the coplanar geometry , *Results in Physics* **5**,3-8

[22] Dhar, S.and Nahar, N.(2016). Triple differential cross-sections for the ionization of metastable 2P-state hydrogen atoms by electrons with exchange effects , Pramana-J. Phys. **87,** 69

[23] Dhar S ,Noor T and Chowdhury FS. (2015) Electron impact ionization of Metastable 3S-state hydrogen atoms by electrons in coplanar geometry, American Journal of Modern Phys., **4(6),** P-261-266

[24] Noor T and Chowdhury F.S. (2016),Calculation of Triple Differential cross sections for the ionization of H(3S) by electron impact, American Journal of Modern Phys., **5(6),** P-162-171

[25] Dhar S, Akter S, Saha A and Nahar N. (2017) Triple differential cross sections for ionization of metastable 3P-state hydrogen atoms by electrons, IOSR journal of applied physics **9**, P: 21-29

[26] Das J. N and Chakraborty. (1985) Atomic inner-shell ionization,Phys. Rev.**A 32**, 176

[27] Das J. N and Dhar, S. (1998a) Energy Spectrum of Scattered Electrons in K-Shell Ionization of Medium to Heavy Atoms by Relativistic Electrons. *Journal of Physics B*: *Atomic*, *Molecular and Optical Physics*, **31**, 2355.

[28] Dhar S. (2008) The Energy Spectrum of Scattered Particles in the K-Shell Ionization of Medium Heavy Atoms by RelativisticElectrons and Positrons with Exchange Effects. J. Phys B At Mol Phys, **41**,155204

[29] Lewis RR.,(1956) Potential scattering of high-energy electrons in second born approximation Physical) Review. **102**, 537.