Electron Impact Ionization of H(3d) by Incident Electron With Exchange Effects

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Abstract: In the present Study, the triple differential cross sections (TDCS) are estimated for the ionization of metastable 3d-state hydrogen atoms by incident electron at 250 eV with exchange effects for various kinematic condition pursuing a multiple scattering theory. The present calculation 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 exchange effect results give an immense opportunity for experimental trial in the field of ionization problems. **Keywords:** Electron, Ionization, Cross-Section, Scattering.

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I. Introduction

The theoretical non-relativistic studies for the atomic ionization by fast particle was first treated by Bethe [1]. Electron impact ionization by electrons processes are used in a diverse range of fields such as radiation physics, plasma physics as well as astrophysics. In the last three decades significant progress has been made in understanding the atomic physics of electron-atom ionization theoretically hydrogenic ground states [2-14] and hydrogenic metastable states [15-23] and experimentally in ground states [28-30] for non-relativistic energies [2-26] as well as for relativistic energies [27-31].

In the field of electron impact ionization is to develop a general theoretical framework, which will provide an accurate ionization cross sections for many atom over a practically relevant impact energy range. Due to its perplexity, the fully quantum mechanical treatment of atomic ionization by electron is possible for the artless cases of hydrogen atom. In this work, atomic hydrogen is used as target in order to perceive the ionization mechanism of atomic system by electron impact energy.

Hydrogenic metastable 3d state is an excited state which has a relatively long lifetime than the other excited states. A metastable sate has a higher energy than the ground state. The lifetime of excited state is given by [32]

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

where A_{ii} is Einstein A Co-efficient.

The lifetime of metastable 3d state of hydrogen atom is 2.3×10^{-7} s.

The exchange interaction with an exchange energy is a quantum mechanical effect that only occurs between identical particles. The effect is due to the wave function of indistinguishable particles being subject to exchange symmetry ,that is either remaining unchanged or changing sign when two particles are exchanged.

A multiple scattering theory [12] has been applied in the present TDCS calculation in the metastable 3d-state hydrogen atom ionization by 250eV electron energy. Lewis integral [33] has been used in the present study for analytical calculation.

The existent new study results will add a new dimensions on ionization of hydrogenic metastable states. Current results are compared with previous related theories [15],[21] and [23]. In the study of hydrogenic ionization for ground state [2-4,12] and metastable states [15-16,20-23] are played a exigent preamble using the multiple scattering theory of Das and Seal [12]. So, the present results seem to be interesting.

II. Theory

The direct T-matrix element for ionization of hydrogen atoms by electrons, following Das and Seal [12] may be written as

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

Here, $\overline{r_1}$ and $\overline{r_2}$ represent the coordinates of the atomic active electron and the incident electron, $(\overline{p_1}, \overline{p_2})$ and (E_1, E_2) represent the momenta and energies of the two electrons in the final state and $(\overline{p_i}, E_i)$ 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

$$V_{i}(\bar{r}_{1}, \bar{r}_{2}) = \frac{1}{r_{12}} - \frac{Z}{r_{2}}$$
(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.

The initial channel unperturbed wave function is given in the following form

$$\Phi_{i}(\bar{r}_{1},\bar{r}_{2}) = \frac{e^{i\bar{p}_{i},\bar{r}_{2}}}{(2\pi)^{3/2}} \phi_{3d}(\bar{r}_{1}).$$

where

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

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 [12]

$$\Psi_{f}^{(-)}(\bar{r}_{1},\bar{r}_{2}) = N(\bar{p}_{1},\bar{p}_{2}) \left[\phi_{\bar{p}_{1}}^{(-)}(\bar{r}_{1}) e^{i\bar{p}_{2}.\bar{r}_{2}} + \phi_{\bar{p}_{2}}^{(-)}(\bar{r}_{2}) e^{i\bar{p}_{1}.\bar{r}_{1}} + \phi_{\bar{p}}^{(-)}(\bar{r}) e^{i\bar{p}.\bar{R}} - 2e^{i\bar{p}_{1}.\bar{r}_{1}+\tilde{p}_{2}.\bar{r}_{2}} \right] / (2\pi)^{3}$$
(4)

where

$$\begin{split} \overline{r} &= \frac{\overline{r_2} - \overline{r_1}}{2}, \ \overline{R} = \frac{\overline{r_1} + \overline{r_2}}{2}, \\ \overline{p} &= \left(\overline{p_2} - \overline{p_1}\right), \ \overline{P} = \overline{p_2} + \overline{p_1}, \\ \text{The normalization constant } N\left(\overline{p_1}, \overline{p_2}\right) \text{is calculated using Das and Seal [12] and Dhar and Nahar [20].} \\ \text{the Coulomb wave function } \phi_q^{(-)}(\overline{r}) \text{ is used from Das and Seal [12] and Dhar and Nahar [20]} \\ \text{Now equation (1) becomes} \\ T_{fi} &= T_B + T_{B'} + T_i - 2T_{PB} \\ \text{(5)} \\ \text{where} \\ T_B &= \left\langle \phi_{p_1}^{(-)}(\overline{r_1}) \ e^{\overline{ip_2} \cdot \overline{r_2}} |V_i| \Phi_i(\overline{r_1}, \overline{r_2}) \right\rangle \end{split}$$

(6) $T_{B'} = \left\langle \phi_{p_1}^{(-)}(\bar{r}_2) e^{i\bar{p}_1.\bar{r}_1} \middle| V_i \middle| \Phi_i(\bar{r}_1, \bar{r}_2) \right\rangle$ (7)

$$T_{i} = \left\langle \phi_{p}^{(-)}(\bar{r}) e^{i\bar{P}.\bar{R}} |V_{i}| \Phi_{i}(\bar{r}_{1}, \bar{r}_{2}) \right\rangle$$

$$(8)$$

$$T_{PB} = \left\langle e^{i\bar{p}_{1.\bar{\eta}} + i\bar{p}_{2}.\bar{r}_{2}} |V_{i}| \Phi_{i}(\bar{r}_{1}, \bar{r}_{2}) \right\rangle$$

$$(9)$$

The direct scattering amplitude $f(\overline{p}_1, \overline{p}_2)$ is then determined from

$$f(\overline{p}_1,\overline{p}_2) = -(2\pi)^2 T_{fi}.$$

And the exchange scattering amplitude for hydrogen atom is

$$g(\overline{p}_1, \overline{p}_2) = f(\overline{p}_2, \overline{p}_1)$$

Finally using Lewis integral [33], the TDCS with exchange effects is taken the following form

$$\frac{d^{3}\sigma}{d\Omega_{1}d\Omega_{2}dE_{1}} = \frac{p_{1}p_{2}}{p_{i}} \left[\frac{3}{4}\left|f-g\right|^{2} + \frac{1}{4}\left|f+g\right|^{2}\right].$$
(10)

where E_1 is the energy of the incident electron. Right hand side of equation (10) is computed numerically using computer programming language Mat Lab.

III. Results and Discussions

In this section, the ionization of hydrogenic metastable 3d state by electron with exchange effects is discussed here. The existent results are compared with the hydrogenic ground state theoretical results [8,13] and the absolute data [24]. In this study, the ejected angle θ_1 varies from 0° to 360° considered as horizontal axis where scattering angles θ_2 is fixed and referred as vertical axis. The ionization results of hydrogenic metastable 2S state [15], 3S state [21] and 3P state [23] are exhibited here for comparison with our current and first Born results.

The present results of hydrogenic metastable 3d state by electron with exchange effect are designed corresponding to the different scattering angles $\theta_2 = 3^\circ$ Fig. 1(a), 15° Fig. 1(b), 25° Fig. 1(c) for ejected electron energies $E_1 = 50$ eV and the scattering angle $\theta_2 = 5^\circ$ Fig. 2(a), 7° Fig.2(b), 9° Fig.2(c), 11° Fig. 3(a), 15° Fig. 3(b) and 20° Fig. 3(c) for ejected electron energies $E_1 = 5$ eV.

The incident electron energy of $E_i = 250$ is taken here. In all figures, $\theta_1 (0^\circ - 150^\circ)$ and $\phi = 0^\circ$ is

considered as recoil region while $\theta_1 (150^\circ - 360^\circ)$ and $\phi = 180^\circ$ is referred as binary region.

In Fig. 1(a) It is inspiring to notice that, the peak values of present results and first Born results good qualitative agreement with those of the compared results [8,13,24] in the recoil region but show somewhat vary in the binary region. This may be occurred due to the change of the hydrogenic metastable states by electrons. Here the binary peak values of the present and first Born results slightly shifted right about $\theta_1 = 288^{\circ}$. from other compared results.

In Fig. 1(b) The peak magnitude of present and first Born results are inferior than the hydrogenic ground state experimental results [24], hydrogenic ground state Second Born results [13] and hydrogenic metastable 3S-state results[21]. The peak pattern of the present and first born result show nicely identical with hydrogenic 3P-state [23] ionization results but shortly differ with the hydrogenic ground state BBK results [8]. In Fig. 1(c) the peak shape of our present result and hydrogenic 3S state result[21],3P-state result[23] provide similar but shifted configuration with hydrogenic ground state Second Born results [13]. The peak magnitude is the highest from other compared results [8,24].



Fig. 1. Triple-differential cross sections (TDCS) with exchange effects 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 [23], Dotted curve(Magenta) expose 3S-state result [21] and Dash curve(blue) demonstrate Hydrogenic ground state Second Born results [13], Dash dotted curve(blue) reveal Hydrogenic ground state BBK model [8] and Star indicated Hydrogenic ground state experiment [24] (multiplied by 0.00224).



Fig.2. Triple-differential cross sections (TDCS) with exchange effects 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) $\theta_2 = 9^0$. Theory: Continuous curve (red) illustrate Present result, Dash curve(Black) exhibit Present First Born results, Dash curve(Green) display 3P-state result [23], Dotted curve(Magenta) expose 3S-state result [21] and Dash dotted curve(blue) demonstrate 2S-state result [15].



Fig. 3. Triple-differential cross sections (TDCS) with exchange effects versus ejected electron angle θ_1 for atomic hydrogen by electron energy $E_i = 250 \, eV$ with ejected electron energy with $E_1 = 5 eV$ and (a) $\theta_2 = 11^{\circ}$, (b) $\theta_2 = 15^{\circ}$, (c) $\theta_2 = 20^{\circ}$. Theory: Continuous curve (red) illustrate Present result, Dash curve(Black) exhibit Present First Born results, Dash curve(Green) display 3P-state result [23], Dotted curve(Magenta) expose 3S-state result [21] and Dash dotted curve(blue) demonstrate 2S-state result [15].

From Fig. 2(a-c)-Fig. 3(a-c), our present exchange effects results of hydrogenic 3d-state results including first Born results are compared with hydrogenic 2S-state [15], 3S-state [21] and recent works on hydrogenic 3P-state [23].

In Fig. 2(a) the magnitude of our obtained exchange effect results is smaller than compared results [21,23]. In the binary region, the present exchange curve depicts a nice lobed as 2S state [15] and 3P state exchange effect [23] at ejected angle about 288° whereas the first Born curve gives a very sharp peak at ejected angle about 180° .

In Fig. 2(b) current result provide two lobed and two peak in recoil region and two lobed and one peak in binary region. In recoil region, our present TDCS exchange effects curve exhibit prominent peak pattern

with metastable 3S -state [21] and 2S-state [15] results whereas in the binary region the present results show opposite peak shape.

In Fig. 2(c) at ejected angle about 72° . our present TDCS curve with 3S-state result [21] represent a nice peak which are identical while first Born results and 2S-state [15] results and 3S-state result [23] expressed reverse peak.

In **Fig. 2(a-c)**, it is observed that the magnitude of new exchange effect results is lower than other compared results [15,21,23] because of different metastable states of finite lifetime.

In Fig. 3(a). In this figure, the present result give a petty lobe where 2S-state [15] result show long lobe at ejected angle about 288° .

In Fig. 3(b) the present outcomes demonstrate similar peak form with first Born results(black) even though different peak structure with 2S-state [15] and 3P-state [23] hydrogenic exchange effect results. The present TDCS curve and 3S-state [21] hydrogenic results reveal reverse peak shape in the recoil region at

ejected angle about 108° . The present results and first Born results(black) provide exactly similar behavior as the 3S state[21] and 3P-state [23] results but show a gross difference with the results of 2S-state [15] both in binary region.

At last, In **Fig. 3(c)**, we note that the magnitude of the present and first Born results(black) and 3S-state [21] exchange effect results are higher than 2S-state [15] and 3P-state [23] results.

Finally, It is remarked that, the peak pattern of the energy spectrum as obtained from our present study is closer to the compared results [21,23] but somewhere differ from those. It may be occurred due to the change of lifetime of hydrogenic excited states. The lifetime of excited 3d states is usually short due to the high energy.

A table (please see **Table 1**.) of comparison exchange effect results for ionization of hydrogenic 2S-state, 3S-state and 3P-state atoms by electron is provided.

Table 1: Electron Impact Ionization of H(3d) by Incident Electron With Exchange Effects are distinguished with 3P-state, 3S-state & 2S-state results where the incident energy is 250eV, the scattering angle is $\theta_2 = 7^0$ and the ejected electron energy is $E_1 = 5eV$.

Ejected angle(θ_1)	28	38	3P	3d
0	2.7504	5.1015	2.5452	0.3851
36	0.8927	0.0858	0.7910	3.0118
72	0.6123	1.8789	2.6915	0.0961
108	0.6352	15.5059	0.8542	1.7045
144	1.1868	1.0016	2.0015	0.1337
180	2.6014	5.2025	1.1202	0.3521
216	4.1507	5.0001	1.7023	0.0989
252	0.7891	11.5223	2.0024	0.1461
288	90.5301	7.9098	0.8921	0.8592
324	6.5760	25.0001	2.5442	0.0460
360	5.2812	1.8582	0.7025	2.1343

IV. Conclusion

The present estimation reveals imaginable additional formation of the cross-section curves for intermediate momentum transfer in the ionization of the hydrogen atoms in the hydrogenic metastable 3d-state at 250 eV electron impact energy. It is remarked that, the implementation of the flnal state wave function of Das and Seal [12] yields good qualitative agreement with hydrogenic ground state as well as BBK model. New empirical outcomes for ionization of metastable 3d-state hydrogen atoms by electrons will be valuable and originate a novel dimension in order to perceive the study of ionization problems.

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References

- [1]. Bethe H, Zur Theorie des Durchgangs schneller Korpuskularstrahlen durch Materie Annalen der Physik, 1930; 397, 325-400
- [2]. Das J.N, Momentum-Space Analysis of Scattering States with Possible Application to Atomic Ionization, Physical Review A, 1990;42, 1376
- [3]. Das J.N.and Seal S,Symmetric Scattering Ine±-H Ionization Collisions, Pramana, 1993; 40, 253-258

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

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

- [6]. Byron WF, Joachen JC and Piraux B. journal of Physics B: Atomic, Molecule and Optical Physic. 1980; 13, L673
- [7]. Byron WF, Joachain JC, Piraux B. Theory of coplanar asymmetric (e, 2e) reactions in helium. Journal of Physics B: Atomic, Molecular and Optical Physics, 1986; 19, 120
- [8]. Brauner M, Briggs JC and Klar H. Triply-differential cross sections for ionisation of hydrogen atoms by electrons and positrons, Journal of Physics B: Atomic, Molecular and Optical Physics, 1989; 22, 2265
- [9]. Brauner M and Briggs JC. Ionisation to the projectile continuum by positron and electron collisions with neutral atoms, J. Phys. B. At. Mol. Phys. (1986);19, L325
- [10]. Brauner M, Briggs JC and Klar H. Structures in differential cross sections for positron impact ionization of hydrogen, J. Phys. B. At.Mol. Opt. Phys. 1991; 24, 2227
- [11]. Berakder J and Klar H. Structures in triply and doubly differential ionization cross sections of atomic hydrogen J. Phys. B. At. Mol. Opt.Phys. 1993; 26, 3891
- [12]. Das JN and Seal S , Electron-Hydrogen- Atom Ionization Collisions at Intermediate (5I0- 20I0) and High(≥20I0) Energies Physical Review A, 1993;47,2978
- [13]. Dal Capppello C, Haddadou A, Menas F and Roy AC. The second Born approximation for the single and
- double ionization of atoms by electrons and positrons, J. Phys. B: At. Mol.Opt.Phys. 2011; 44, 015204
- [14]. Berakdar J, Engelns A, Klar H. Oriented and Aligned two electron continue. J.Phys B At Mol Opt Phys, 1996;29,1109
- [15]. Dhar S. Electron Impact Ionisation of Metastable 2S-State Hydrogen Atoms ,Australian Journal of Physics, 1996; 49,937
- [16]. Das JN and Dhar S. Symmetric Scattering in Electron and Positron Impact Ionization of Metastable 2S-State Hydrogen Atom, Pramana J.Phys, 1996;47, 263-269.
- [17]. Vučič S, Potvliege RM and Joachain CJ. Second Born Triple-Differential Cross Sections for the Coplanar Asymmetric Ionization of H(2S) by Fast Electrons Physical Review A ,1987; 35, 1446.
- [18]. Qi YY, Ning LN, Wang JG and Qu YZ. Plasma effect on fast-electron-impact ionization from 2p state of hydrogen-like ions. Physics of Plasmas ,2013; 20,123301
- [19]. Dhar S and Nahar N. Electron impact ionization of metastable 2P-state hydrogen atoms in the coplanar geometry, Results in Physics 2015; 5,3-8
- [20]. Dhar S and Nahar N. Triple differential cross-sections for the ionization of metastable 2P-state hydrogen atoms by electrons with exchange effects, Pramana-J. Phys, 2016; 87, 69
- [21]. Dhar S, Noor T. The Triple Differential Cross Sections for Electron Impact Ionization of Metastable 3s State Hydrogen Atoms with Exchange Effect, Open Journal of Microphysics, 2017; 7, 53-65
- [22]. Dhar S, Akter S and Nahar N. First Born Triple Differential cross-section for ionization of H(3P) by electronimpact in the asymmetric coplanar geometry, Open Journal of Microphysics, 2016; 6, 15-23
- [23]. Akter S, Dhar S, Nahar N, Das L C. Ionization of metastable 3P state hydrogen atom by electron with exchange effects, Pramana Journal of physics, 2018; 91,78
- [24]. Ehrhardt H, Knoth G, and Schlemmer P, Jung K. Differential Cross Sections of Direct Single Electron Impact Ionization, Zeitschrift f
 ür Physik D Atoms, Molecules and Clusters, 1986; 1, 3.
- [25]. Ehrhardt H, Knoth G, Schlemmer P and Jung K. Absolute H(e,2e)p cross section measurements: Comparison with first and second order, Physics Letters A ,1985; 110, 92
- [26]. Ehrhardt H, Roder J. In:Whelan CT, Walters HRJ, Coincidence studies of electron and photon impact ionization. Plenum. 1997; p. 1–10.
- [27]. Das JN and Dhar, S. 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, 1998a; 31, 2355.
- [28]. Dhar S. The Energy Spectrum of Scattered Particles in the K-Shell Ionization of Medium Heavy Atoms byRelativistic Electrons and Positrons with Exchange Effects. J. Phys B At Mol Phys, 2008; 41,155204
- [29]. Jones S and Madison DH. Ionization of hydrogen atoms by fast electrons. Phys Rev A, 2000; 62, 042701
- [30]. Das JN and Dhar S. Calculation of Triple Differential Cross-Sections of K-Shell Ionization of Medium-Heavy Atoms by Electrons for Symmetric GeometryPramana J.Phys, 1998; 51, 751.
- [31]. Jones S and Madison DH. Scaling behavior of the fully differential cross section for ionization of hydrogen atom s by the impact of fast elementary charged particles. Phys Rev A, 2002; 65, 052727
- [32]. Tenneyson J, Astronomical Spectroscopy, An Introduction to the Atomic and Molecular Physics of Astronomical Spectra, 2nd edn(World Scientific Publishing,), 2011
- [33]. Lewis RR. Potential scattering of high-energy electrons in second born approximation Physical) Review. 1956; 102, 537.

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