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An Analysis of Electron Ionization and Energy Spectrum for 3d-State Hydrogen Atom

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Abstract: The following report presents an extensive theoretical study of the phenomenon of electron-induced ionization of a hydrogen atom. This investigation deals with the ionization of a hydrogen atom in its 3d excited state. This calculation is performed for hydrogen atoms with electron beam energy levels at 250eV and 500 eV. The wave function of the ionized hydrogen atom in the final state is obtained by applying the method of multiple scattering. The spectrum obtained from these calculations reveals many characteristics, and the results of this theoretical study are consistent with those of the hydrogen ground state atom. These results increase the knowledge of the process of electron emission during atomic ionization.

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1. Introduction

The electron impact ionization of an atom is a significant phenomenon wherein an incident electron interacts with an atom and transfers sufficient energy to eject an electron from its orbitals. The phenomenon has several applications in various scientific domains. In radiation physics, it plays a vital role in determining the effects of ionizing radiation on biological systems. In plasma physics, it influences the dynamics of charged particle systems. In astrophysics, it forms a basis for modeling both stars and interstellar regions.

In material science, it assists in comprehending the interaction between electrons and materials [1, 2]. During the past three decades, notable progress has been made in the theoretical and computational approaches to studying electron impact ionization. Studies focused on ionization processes of hydrogen atoms in their simplest form (ground state). Hydrogen is the simplest atomic species that can be employed for validating theoretical models and numerical simulations of ionization cross-sections, kinetic energy distributions of electrons, and other associated properties [3, 4].

Such findings lay a foundation for developing theoretical techniques to analyze other atomic or molecular systems and for comparing them with available experimental data. During the initial investigations of the hydrogen ground state, states like the 3d state have received increased interest due to their significance in the study of complex ionization mechanisms. States like the 3d state have a greater value of angular momentum and larger size, which considerably influence the electron energy spectrum and angular distribution during ionization. Researching the impact of electron-ion collision on ionization of such states gives a better idea about the effects of atomic structure on ionization phenomena. An atomic spectrum is the electromagnetic spectrum radiated or absorbed during a transition of an electron from one energy level to another inside an atom. When an electron shifts energy levels, it either emits or absorbs light at a specific wavelength. It gives valuable information regarding the structure of the atom as well as the behavior of electrons. One important consideration in ionization studies is the triple differential cross-section (TDCS). This shows important details regarding the energy and angle distribution of the released electrons. Computations regarding the triple differential cross-section for several hydrogenic states, such as the metastable 2P and 3P states, have been made under different situations, taking exchange effects into account [5-10]. For instance, the triple differential cross-section of the ionization of atomic H(3p) under different exchange effects and parameters was computed by S. Akter et al. [9] with the Das and Seal [3] theory. Dhar and Nahar [6] did a theoretical study of the energy spectra of the ejected electrons from metastable 2P hydrogen atoms in a unique setup called the coplanar asymmetric geometry. Dhar [11] studied the energy spectra of the particles scattered during the K-shell ionization process of medium to heavy atoms. This occurs due to the interaction of highly energetic relativistic electrons and positrons with these atoms. The computations of Dhar have considered important aspects like exchange processes that consider particle-particle interaction. Multiple scattering theory has traditionally been used to predict the final state wave function of the ionized electron, as it takes into consideration the interaction between the emitted electron and the ion left behind. The technique developed by Das and Seal [3] has proved to provide accurate quantitative results for ionization of hydrogen at intermediate ($5I_0$–$20I_0$) and high ($\gtrsim 20I_0$) energies. The energy spectrum of ejected electrons in hydrogen ionization has also been calculated by J. N. Das and S. Dhar [4]. I. Bray et al. [12] investigated electron-impact excitation and ionization of H-like ions in the ground state (Z = 2–8) across a wide energy range, focusing on spin asymmetry in the cross sections. ML Ranković et al. [13] examined elastic differential cross sections (DCS) of argon atoms by electrons in the intermediate energy range (40–300 eV), while S. N. Nahar et al. [14] studied positron scattering from atoms and molecules.

Non-relativistic studies of the energy spectrum of ejected electrons from the 3d-state hydrogen atom remain limited despite their extensive nature. Das and Seal's theory [3] frequently provides better quantitative results, and the energy spectrum of the ejected electron continues to be of significant theoretical interest. To the best of our knowledge, no comparable experimental investigation exists for the non-relativistic ionization of the 3d hydrogen state, motivating the present study.

2. Mathematical Formation

T-matrix element for ionization of hydrogen atoms by electrons pursuing Das and Seal [3] may be taken as

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

Here, $\overline{\nu_1}$ and $\overline{\nu_2}$ represent the coordinates of the atomic active electron and the incident electron, $(\bar{\mu}_1, \bar{\mu}_2)$ and (E_e, E_s) represent the momenta and energies of the two electrons in the final state and $(\bar{\mu}_i, E_i)$ are the momentum and the energy of the incident electron.

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

$$V_i(\bar{\nu}_1, \bar{\nu}_2) = \frac{1}{\nu_{12}} - \frac{Z}{\nu_2} \tag{2}$$

The nuclear charge of the hydrogen atom is Z=1, ν_1 and ν_2 are the distance of the two electrons from the nucleus and ν_{12} is the distance between two electrons.

The initial channel unperturbed wave function for 3d state are given in the following form

$$\Phi_i(\bar{\nu}_1, \bar{\nu}_2) = \frac{e^{i\bar{\mu}_i.\bar{\nu}_2}}{(2\pi)^{3/2}} \varphi_{3d}(\bar{\nu}_1) \tag{3}$$

Where,

$$\varphi_{3d}(\bar{\nu}_1) = \frac{1}{81\sqrt{6\pi}} \left(\nu_1^2\right)\left(3\cos^2\theta - 1\right) e^{-\lambda_1 \nu_1}$$

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

$$\Psi_f^{(-)}(\bar{\nu}_1, \bar{\nu}_2) = A(\bar{\mu}_1, \bar{\mu}_2)[\phi_{\bar{\mu}_1}^{(-)}(\bar{\nu}_1) e^{i\bar{\mu}_2.\bar{\nu}_2} + \phi_{\bar{\mu}_2}^{(-)}(\bar{\nu}_2) e^{i\bar{\mu}_1\bar{\nu}_1} + \phi_{\bar{\mu}}^{(-)}(\bar{\nu}) e^{i\bar{K}.\bar{R}} - 2e^{i\bar{\mu}_1.\bar{\nu}_1 + i\bar{\mu}_2.\bar{\nu}_2}]/(2\pi)^3 \tag{4}$$

Where

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

$$\bar{\mu} = (\bar{\mu}_2 - \bar{\mu}_1), \; \vec{K} = \bar{\mu}_2 + \bar{\mu}_1,$$

The normalization constant $A(\bar{\mu}_1, \bar{\mu}_2)$ is determined using Das and Seal [3].

The direct scattering amplitude $f(\bar{\mu}_1, \bar{\mu}_2)$ is given by

$$f(\bar{\mu}_1, \bar{\mu}_2) = -(2\pi)^2 T_{fi} \tag{5}$$

The exchange amplitude is obtained from

$$g(\bar{\mu}_1, \bar{\mu}_2) = f(\bar{\mu}_2, \bar{\mu}_1) \tag{6}$$

The triple differential cross-sections for direct T-Matrix element is given by

$$\frac{d^3\sigma}{d\omega_1 d\omega_2 dE_e} = \frac{\mu_1 \mu_2}{\mu_i}\left[\frac{3}{4}|f - g|^2 + \frac{1}{4}|f + g|^2\right] \tag{7}$$

Therefore, Triple Differential cross sections (TDCS) has been determined using computer programming language MATLAB, given by equation (7).

3. Results and Discussions

Figures 1(a) to 1(d) show the calculated triple differential cross-sections (TDCSs) results for electron-impact ionization of the hydrogen 3d state at an incident energy of E_i = 250 eV. Figures 2(a) to 2(c) display the results for E_i = 500 eV. To assess the reliability of our model, we compare the calculated TDCS results with the corresponding ground-state and first Born approximation (FBA) results from Das and Dhar [4], along with the 2p-state results from Dhar and Nahar [6].

In Figure 1(a), our TDCS results demonstrate a smooth variation of cross-section with ejected electron energy (E_e) in the range of $5 \leq E_e \leq 25$ eV. This trend aligns with previous theoretical studies [4,6], confirming the validity of our approach. Specifically, for an emission energy E_e=40 eV, we found from both the results for our excited state as well as the ground-state that there is a pronounced peak in the TDCS values. On the other hand, the 2p-state study [6] reveals a reduction in the cross section at this energy level, implying that ionization from distinct initial states of the atom considerably changes the probability distribution of ionization. Our FBA calculation shows a resemblance to the energy dependence in the ground-state FBA calculations [4]; however, the magnitude of the cross section is smaller since the 3d state is weakly bound.

Figures 1(b) and 1(c) further confirm the similarities between our exchange results and previous studies [4]. Over the full range of ejected energy, our results replicate the main characteristics of the ground-state data. A noticeable peak appears near E_e = 30 eV for both our results and the ground-state results, indicating a favored energy sharing between the scattered and ejected electrons. The 2p-state result [6], however, shows an opposite trend, suggesting that angular momentum and the spatial distribution of the initial bound state greatly affect the energy-sharing process. Our FBA retains the same qualitative profile as the ground-state FBA result [4], but with slightly smaller cross-section amplitude due to reduced overlap between the initial and continuum wave functions for the 3d state.

For ejected energies less than E_e = 50 eV in Figure 1(d), the present results agree very well with those of the ground-state [4], while the 2p-state [6] remains fairly constant in this region. As soon as the ejected electron energies exceed E_e = 60 eV, both present and 2p-state results tend to follow a common trend, whereas the ground-state results become almost flat. It seems likely that higher ejected electron energies minimize the influence of the initial-state structure. The energy dependence of the respective FBA values for the present and ground-state results appears very similar in Figures 1(b) and 1(c).

Table 1 contains the results for the obtained values of TDCS. These results include the current, the ground, and the 2p-state exchange as well as the current and ground FBA calculations. This comparison proves that the current theory is successful in modeling the peculiarities of hydrogen ionization processes discussed in previous research.

In summary, the above findings indicate that there is a marked dependence on the initial state of the electron whether 3d, 2P, or ground state, in determining the energy of ejected electrons. High regions of TDCS are due to constructive interference, while low regions are due to destructive interference. Comparison with previous studies indicates that the model presented here has been able to capture all the major factors involved in electron impact ionization.

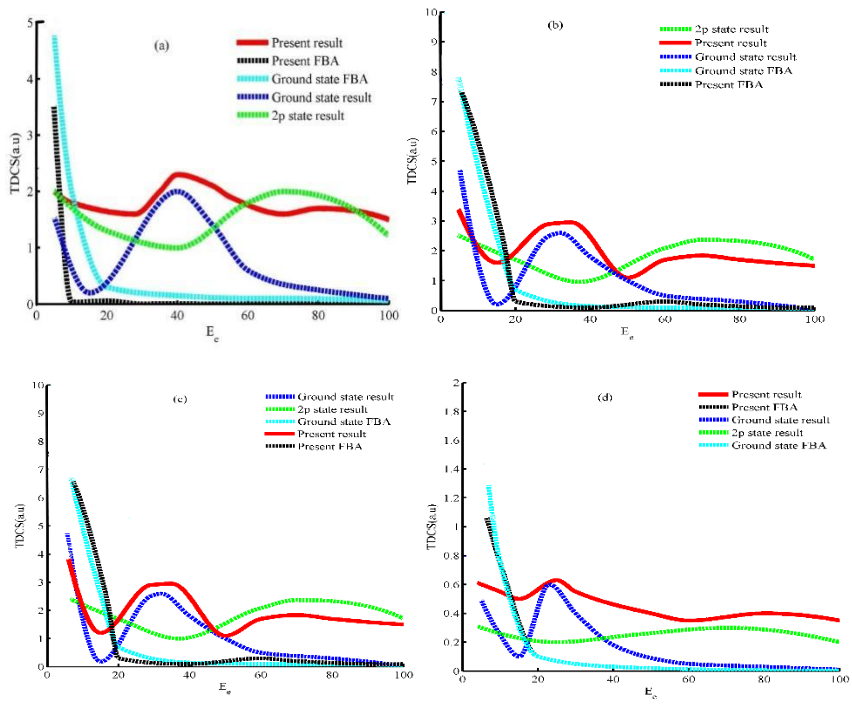

Figure 1: TDCS results for e^-*-H(3d) scattering as a function of the ejected electron energy* E_e *for (a)* $E_i = 250$ eV, $\theta_e = -5^0, \theta_s = 40^0$ (b) $E_i = 250$ eV, $\theta_e = -5^0, \theta_s = 60^0$ and (c) $E_i = 250$eV, $\theta_e = -5^0, \theta_s = 80^0$, (d) $E_i = 250$ eV, $\theta_e = -10^0, \theta_s = 40^0$. *Theory: thick red (-): the present calculations, black dash (-- -): the present FB result, dash green (-- -): 2p state result[6], thick cyan (----): Ground state FB result [4] , blue dash (-- -) : Ground state result [4].*

In Figures 2(a)-2(c), the theoretical values of TDCSs are presented for the ionization process of hydrogen in the 3d state using electrons with the energy E_i = 500 eV. The current work's findings are compared to those for the ground state and 2p-state hydrogen [4,6], along with FBA's values.

From Figure 2(a), in the case where $\theta_e = -5^0, \theta_s = 40^0$ and for the electron energy values of $5 \leq E_e \leq 100$, the current TDCS clearly shows a strong oscillation or wave nature as in Ref. [4] for the ground state. Such an oscillation is attributed to the interference effect between the direct and exchange scattering processes. On the other hand, the calculation on the 2p-state exhibits quite a different character of interference; the result suggests that the nodal structure of the initial wave function has a strong influence on the interference process. An obvious upper peak is observed in the case of both the present calculation and the calculation on the ground state around the ejected electron energy value of 40 eV, whereas, on the contrary, a dip is observed in the case of the 2p-state result. The present FBA curve closely overlaps with the ground-state FBA result [4], confirming the consistency of the theoretical model at high incident energies where exchange effects are relatively small.

For the case of ejected electron energies below E_e = 40 eV in Figure 2(b), the current data points behave similarly to the ground-state calculations [4]. On the other hand, the 2p-state curve tends to be constant, indicating lesser interference effect in this excited state. For the case of E_e > 50 eV, all of the calculated values converge to a constant, showing how the effect becomes small in relation to the exchange contribution of the ejected electron, making the electron behave almost like a plane wave.

On the other hand, in Figure 2(c), a clear peak exists near E_e=30 eV, similar to both the ground-state and current FBA calculations. This peak corresponds to a strong constructive interference between the scattered and ejected waves, indicating an enhanced probability of ionization at that specific energy sharing. However, the 2p-state result [6] exhibits a slightly different profile, likely due to differences in the angular momentum coupling of the initial bound electron. For E_e ≥40 eV, all compared results—including those of Refs. [4,6] and the FBA—tend to flatten, consistent with the general high-energy trend observed in Figure 2(a).

Overall, the TDCS features reveal that for hydrogen in the 3d state, interference and exchange effects are still significant at moderate ejected electron energies, but gradually diminish as E_e increases. The qualitative agreement between the present results and the ground-state findings [4] supports the reliability of the present theoretical model, while the differences observed relative to the 2p state [6] highlight the sensitivity of ionization dynamics to the initial-state angular momentum distribution.

Table 1: For $E_i = 500$ eV, $\theta_e = -5^0, \theta_s = 80^0$, the energy spectrum results of H(3d) electron scattering are distinguished amongst present exchange, ground state exchange, 2P-state exchange, Present FBA, and Ground state FBA results.

E_e	Ground State result	2p State result	Present result	Present FBA	Ground State FBA
5	4.688	1.780	2.240	6.287	5.790
14	0.790	1.705	0.962	1.489	1.913
23	0.450	1.620	1.080	0.3723	0.610
32	0.340	1.410	1.155	0.1501	0.225
41	0.140	1.205	0.802	0.0835	0.094
50	0.118	1.275	0.932	0.0610	0.072
59	0.101	1.430	1.046	0.0432	0.058
68	0.075	1.610	1.082	0.0333	0.049
77	0.055	1.700	1.098	0.0220	0.038
86	0.041	1.646	1.096	0.0134	0.025
95	0.032	1.417	1.071	0.0051	0.012

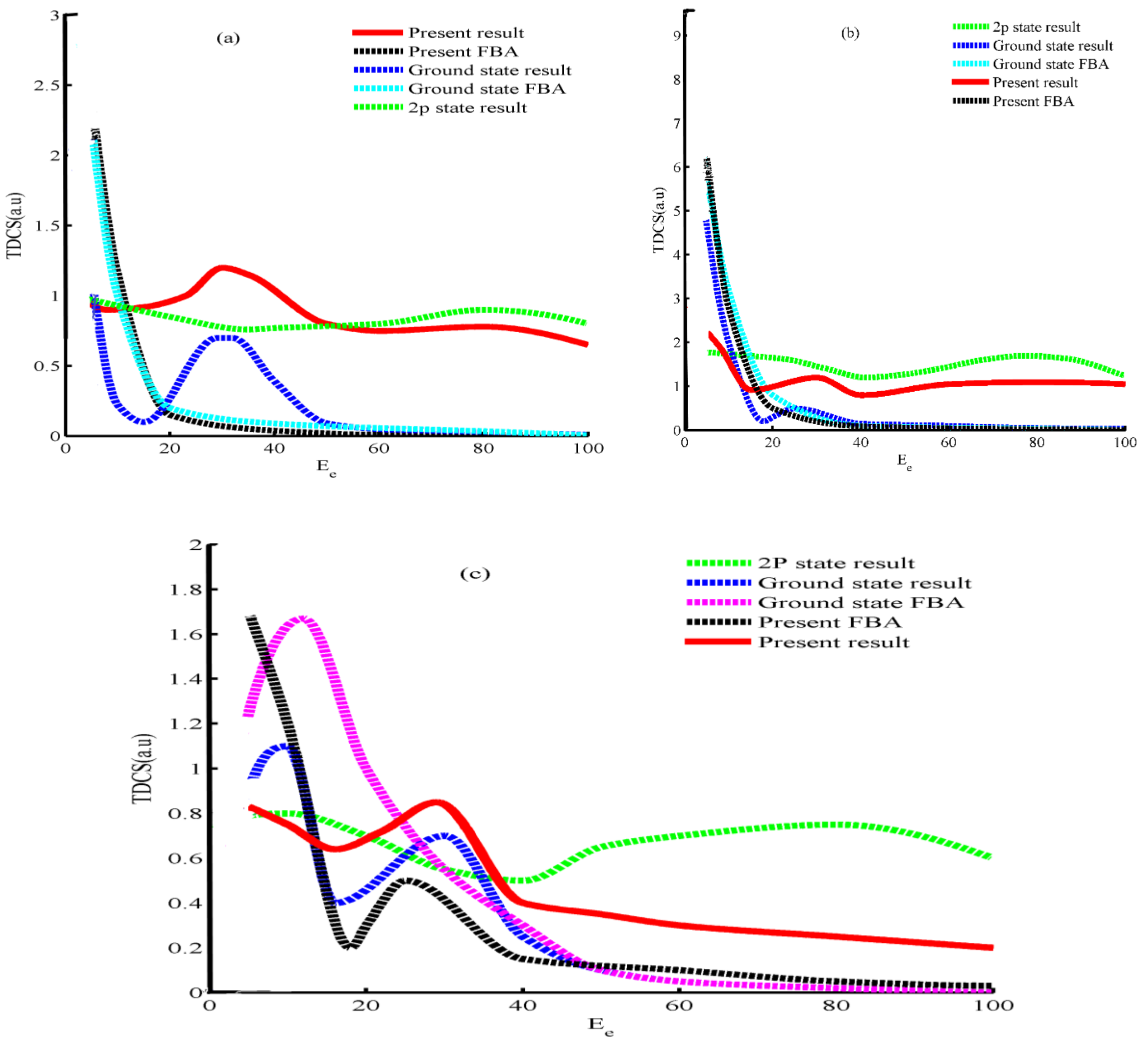

Figure 2: Same as Figure 1 except $E_i = 500\text{eV}$ and (a) $\theta_e = -5^0$, $\theta_s = 40^0$ (b) $\theta_e = -5^0$, $\theta_s = 80^0$ and (c) $\theta_e = -10^0$, $\theta_s = 80^0$.

The obtained TDCS results for the hydrogenic 3d state provide additional insight into electron–atom collision dynamics and contribute to the understanding of ionization mechanisms in excited-state systems. Such results are significant in atomic collision physics because they can be used as benchmark data for testing and improving theoretical models of electron impact ionization. In plasma modeling, excited-state ionization data are useful for describing collision processes, energy transfer mechanisms, and particle distributions in laboratory and astrophysical plasmas. Furthermore, these findings may contribute to astrophysical studies involving stellar atmospheres, interstellar media, and ionized environments where excited hydrogen states play an important role. As there are no experimental data for hydrogen 3d-state ionization at present, the current results on TDCS could be helpful for future experiments in this field. Moreover, the present work may support the extension of theoretical approaches to more complex atomic and molecular collision systems.

4. Conclusions

In this study, we theoretically investigated the energy spectrum of ejected electrons from the ionization of metastable hydrogen atoms in the 3d state. This was done for incident electron energies of 250 eV and 500 eV. We based our calculations on multiple scattering theory and compared the results with existing theoretical data for the hydrogenic ground and 2p states. Since there are no experimental data currently available for the ionization of hydrogen in the 3d state, we cannot directly compare theory and experiment at this time. Future experiments on the ejected-electron energy spectrum for the 3d state would be helpful to confirm and improve our theoretical approach. Our findings show that the ionization dynamics of excited hydrogen states have unique features compared to the ground state, especially in the structure and intensity of the energy spectra. The results have a very significant contribution towards the comprehension of ionization in atoms and also form a platform for future research in this area. It is necessary to conduct experiments to validate the theoretical approaches to understanding the process of electron-impact ionization.

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