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Triple differential cross-sections for the ionization of metastable 2P-state hydrogen atoms by electrons with exchange effects

SUNIL DHAR* and NURUN NAHAR

Department of Mathematics, Chittagong University of Engineering and Technology, Chittagong 4349, Bangladesh
*Corresponding author. E-mail: sdhar03@yahoo.com; sdhar@cuet.ac.bd

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Abstract. In this paper, triple differential cross-sections for the ionization of metastable 2P-state hydrogen atoms by 250 eV electron energy with exchange effects for various kinematic conditions are calculated. Multiple scattering theory proposed by Das and Seal in *Phys. Rev. A* **47**, 2978 (1993) is utilized here. The computational results provide significant peak features that show good qualitative agreement with the hydrogenic ground-state experimental data and theoretical results and the present first Born results. In addition, physical origin of the peaks of the cross-section curves is investigated.

Keywords. Electron; cross-section; ionization; scattering.

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1. Introduction

Atomic ionization of atoms by charged particles plays a significant role in solving problems in atomic physics. Precise calculation of different types of cross-sections, such as single, double and triple differential cross-sections, with varied kinematic conditions show very interesting and challenging problems in many branches of physics, such as astrophysics, plasma physics, fusion technology and many other branches of science. Many new experimental results, especially for the triple differential cross-section (TDCS) [1–5] of the ground-state hydrogen atoms, were pursued which created a new dimension in this field of research.

The theoretical non-relativistic study of the atomic ionization was first introduced by Bethe [6] and then a lot of interesting methods [7–10] were introduced. At present, by analysing TDCS in $(e, 2e)$ coincidence experiments, vast information of single and double ionization are reported in literature. Such experiments were first reported by Ehrhardt *et al* [11] and Amaldi *et al* [12]. After that, many $(e, 2e)$ coincidence measurements [13–17] were carried out. A review of these experiments can be seen in Ehrhardt *et al* [4]. Moreover, many other studies reviewed [18,19] the theory of $(e, 2e)$ reactions. These experiments were successfully applied during the last four decades to investigate the fine details of ionization process both in the ground [20–29] and metastable states [30–41] of hydrogen atoms. The BBK theory of Brauner *et al* [42] focussed its attention on the improvement of the final-state wave function by including the effects of all the long-range Coulomb interactions as well as the electron–electron repulsion. This satisfies the correct boundary condition when the particle separations tend to infinity. The corrected double continuum wave function of Brauner *et al* [42] which was showing results comparable to the second Born, was applied to the ionization of H(2S) and then was displayed by Hafid *et al* [33].

To the best of our knowledge, the TDCS for the ionization of metastable 2P-state hydrogen atoms by electrons with exchange effects were never studied before, both theoretically and experimentally. Most of the theoretical and experimental investigations on the TDCS concentrated on the ground-state electron hydrogen ionization collisions. Only a few theoretical calculations of the TDCS of metastable 2S-state hydrogen atoms were observed. In the present study, we have evaluated the TDCS in the metastable 2P-state hydrogen ionization by electrons with exchange effects at 250 eV electron energy following multiple scattering theory [24]. It is remarkable that the multiple scattering theory was proved very successfully in the study of TDCS results for both ground state [24–26] with exchange effects and metastable 2S-state [34–37] of hydrogen atoms. So, the theoretical results of Das and Seal [24], Dal Cappello *et al* [38], BBK model [42] and the absolute data [4] for the ionization of hydrogen atoms by electrons from the ground state have been considered here for comparison. Accordingly, one of our earlier methods on the hydrogenic 2S-state ionization results [35] is also presented here for comparison.

The aim of our present work is to demonstrate TDCS for the ionization of metastable 2P-state hydrogen atoms using electron impact with exchange effects. This shows interesting qualitative fitness with the hydrogenic ground-state ionization experimental data and some other hydrogenic ground-state theoretical calculations and hydrogenic metastable 2S-state results. Therefore, the present study will provide significant contribution to the future experimental set-up for the ionization of metastable hydrogen atoms by electrons.

2. Theory

In the present study, we have considered the direct and exchange amplitude of the T-matrix element. The T-matrix element for the ionization of hydrogen atoms by electrons [23,24] may be written as

$$T_{\mathrm{fi}} = \langle \Psi_{\mathrm{f}}^{(-)}(\bar{r}_1, \bar{r}_2)\, | V_{\mathrm{i}}(\bar{r}_1, \bar{r}_2) |\, \Phi_{\mathrm{i}}(\bar{r}_1, \bar{r}_2) \rangle, \tag{1}$$

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

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

The nuclear charge of the hydrogen atom 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. Coordinates of the two electrons are taken to be $\bar{r}_1$ and $\bar{r}_2$. The initial channel unperturbed wave function is

$$\Phi_{\mathrm{i}}(\bar{r}_1, \bar{r}_2) = \frac{\mathrm{e}^{i\bar{p}_{\mathrm{i}}\cdot\bar{r}_2}}{(2\pi)^{3/2}}\phi_{2p}(\bar{r}_1) = \frac{\mathrm{e}^{i\bar{p}_{\mathrm{i}}\cdot\bar{r}_2}}{8\sqrt{2}\pi^2} r_1 \cos\theta \mathrm{e}^{-r_1\lambda_1}, \tag{3}$$

where

$$\phi_{2p}(\bar{r}_1) = \sqrt{\frac{1}{32\pi}} r_1 \cos\theta \mathrm{e}^{-r_1/2} = \sqrt{\frac{1}{32\pi}} r_1 \cos\theta \mathrm{e}^{-\lambda_1 r_1}, \quad \left[\lambda_1 = \frac{1}{2}\right]$$

is the hydrogenic 2P-state wave function, $\bar{p}_{\mathrm{i}}$ is the incident electron momentum and $\psi_{\mathrm{f}}^{(-)}(\bar{r}_1, \bar{r}_2)$ is the final three-particle scattering state with the electrons being in the continuum with momenta $\bar{p}_1, \bar{p}_2$. The approximate final-state scattering wave function $\psi_{\mathrm{f}}^{(-)}(\bar{r}_1, \bar{r}_2)$ is given by [23,24]

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

where

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

The normalization constant $N(\bar{p}_1, \bar{p}_2)$ is given by

$$|N(\bar{p}_1,\bar{p}_2)|^{-2} = \Bigg| 7 - 2[\lambda_1 + \lambda_2 + \lambda_3] - \left[\frac{2}{\lambda_1} + \frac{2}{\lambda_2} + \frac{2}{\lambda_3}\right] + \left[\frac{\lambda_1}{\lambda_2} + \frac{\lambda_1}{\lambda_3} + \frac{\lambda_2}{\lambda_1} + \frac{\lambda_2}{\lambda_3} + \frac{\lambda_3}{\lambda_1} + \frac{\lambda_3}{\lambda_2}\right]\Bigg|, \tag{5}$$

where

$$\lambda_1 = \mathrm{e}^{\pi\alpha_1/2}\Gamma(1 - i\alpha_1), \quad \alpha_1 = 1/p_1,$$

$$\lambda_2 = \mathrm{e}^{\pi\alpha_2/2}\Gamma(1 - i\alpha_2), \quad \alpha_2 = 1/p_2,$$

$$\lambda_3 = \mathrm{e}^{\pi\alpha/2}\Gamma(1 - i\alpha), \quad \alpha = -1/p.$$

The normalization constant $N(\bar{p}_1, \bar{p}_2)$ is calculated numerically using eq. (5) for the electron impact and the approximate value of N is nearly 1.

Here, $\phi_{\bar{q}}^{(-)}(\bar{r})$ is the Coulomb wave function which is given by

$$\phi_{\bar{q}}^{(-)}(\bar{r}) = \mathrm{e}^{\pi\alpha/2}\Gamma(1 + i\alpha)\mathrm{e}^{iq\cdot\bar{r}} \times {}_1F_1(-i\alpha, 1, -i[qr + \bar{q}\cdot\bar{r}])$$

where

$$\alpha_1 = \frac{1}{p_1}, \quad \text{for } \bar{q} = \bar{p}_1,$$

$$\alpha_2 = \frac{1}{p_2}, \quad \text{for } \bar{q} = \bar{p}_2$$

and

$$\alpha = -\frac{1}{p}, \quad \text{for } \bar{q} = \bar{p}.$$

Equation (1) then becomes

$$T_{\mathrm{fi}} = T_B + T_{B'} + T_i - 2T_{PB}, \tag{6}$$

where

$$T_B = \left\langle \phi^{(-)}_{\bar{p}_1}(\bar{r}_1)\, \mathrm{e}^{i\bar{p}_2\cdot\bar{r}_2}\, |V_\mathrm{i}|\, \Phi_\mathrm{i}(\bar{r}_1, \bar{r}_2) \right\rangle, \tag{7}$$

$$T_{B'} = \left\langle \phi^{(-)}_{\bar{p}_2}(\bar{r}_2)\, \mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1}\, |V_\mathrm{i}|\, \Phi_\mathrm{i}(\bar{r}_1, \bar{r}_2) \right\rangle, \tag{8}$$

$$T_i = \left\langle \phi^{(-)}_{\bar{p}}(\bar{r})\, \mathrm{e}^{i\bar{P}\cdot\bar{R}}\, |V_\mathrm{i}|\, \Phi_\mathrm{i}(\bar{r}_1, \bar{r}_2) \right\rangle, \tag{9}$$

$$T_{PB} = \left\langle \mathrm{e}^{i\bar{p}_1\cdot\bar{r}_1 + i\bar{p}_2\cdot\bar{r}_2}\, |V_\mathrm{i}|\, \Phi_\mathrm{i}(\bar{r}_1, \bar{r}_2) \right\rangle. \tag{10}$$

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

$$f(\bar{p}_1, \bar{p}_2) = -(2\pi)^2 T_\mathrm{fi}. \tag{11}$$

We also calculated the exchange amplitude by following the approximation

$$g(\bar{p}_1, \bar{p}_2) = f(\bar{p}_2, \bar{p}_1). \tag{12}$$

After analytical calculation, we have evaluated these expressions numerically using Lewis integral [43] and Gaussian quadrature formula. The TDCS is finally given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1 \mathrm{d}\Omega_2 \mathrm{d}E_1} = \frac{p_1 p_2}{p_i}\left[\frac{3}{4}|f-g|^2 + \frac{1}{4}|f+g|^2\right], \tag{13}$$

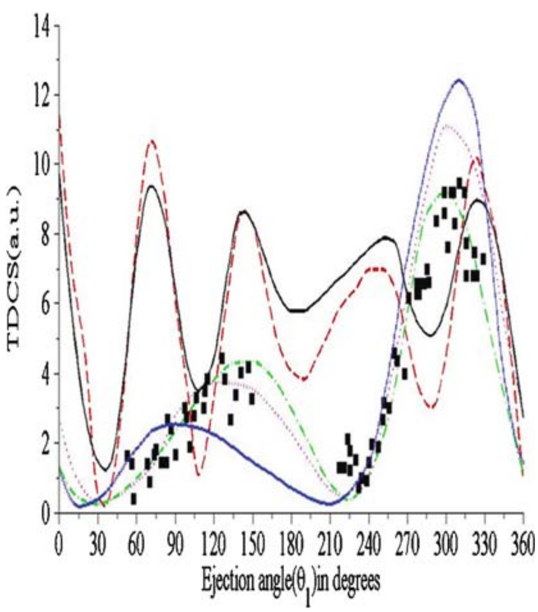

Figure 1. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_2 = 3°$ as a function of the ejected electron θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 5$ eV. Theory: Black curve represents results of 2P hydrogenic state with exchange effects, red dash curve represents first Born result of 2P hydrogenic state, purple short dash curve represents hydrogenic ground-state second Born results [38], green dash–dotted curve represents hydrogenic ground-state BBK model [42], the square represents hydrogenic ground-state experiments [4] and the blue curve represents hydrogenic ground state [24].

where E_1 is the energy of the incident electron. Therefore, in our present calculation we have computed the TDCS, given by eq. (13).

3. Results and discussions

The results for the ionization of metastable 2P-state hydrogen atoms by electrons with exchange effects are displayed in figures 1 ($\theta_2 = 3°$), 2 ($\theta_2 = 15°$), 3 ($\theta_2 = 25°$), 4a ($\theta_2 = 5°$), 4b ($\theta_2 = 7°$), 4c ($\theta_2 = 9°$), 4d ($\theta_2 = 11°$), 4e ($\theta_2 = 15°$) and 4f ($\theta_2 = 20°$). We have presented the TDCS of the present and first Born results at the incident energy $E_\mathrm{i} = 250$ eV for some varied ejected angles (θ_1) and fixed scattering angles (θ_2). θ is considered from 0° to 360°. In all these figures, the region for θ_1 (0°–150°) and $\phi = 0°$, refers to the recoil region, while θ_1 (150°–360°) and $\phi = 180°$, refers to the binary region.

The hydrogenic ground-state theoretical results of Das and Seal [24], Dal Cappello *et al* [38], BBK model of Brauner *et al* [42] and the absolute data of Ehrhardt *et al* [4] and hydrogenic 2S-state ionization results [35] are exhibited for qualitative comparison with our present study. The peak positions, shapes and heights of the reported work provide similar but shifted configura-

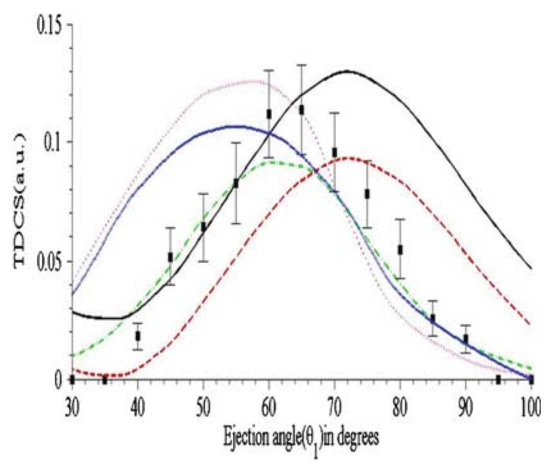

Figure 2. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_2 = 15°$ as a function of the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy is $E_1 = 50$ eV. Theory: Black curve represents results of 2P hydrogenic state with exchange effects, red dash curve represents first Born result of 2P hydrogenic state, purple short dash curve represents hydrogenic ground-state second Born results [38], green dash–dotted curve represents hydrogenic ground-state BBK model [42], the square represents hydrogenic ground-state experiments [4] and blue curve represents hydrogenic ground state [24].

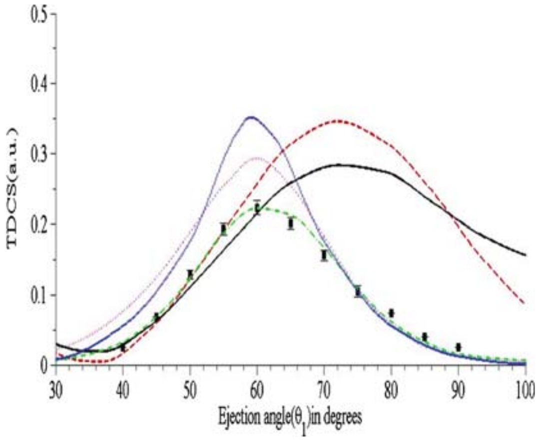

Figure 3. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for $\theta_2 = 25°$ as a function of the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy $E_1 = 50$ eV. Theory: Black curve represents results of 2P hydrogenic state with exchange effects, red dash curve represents first Born result of 2P hydrogenic state, purple short dash curve represents hydrogenic ground-state second Born results [38], green dash–dotted curve represents hydrogenic ground-state BBK model [42], the square represents hydrogenic ground state experiments [4] and blue curve represents hydrogenic ground state [24].

tions with the earlier results of hydrogenic ground-state second Born approximation [38].

Figure 1 depicts the TDCS results with exchange effects for $\theta_2 = 3°$, $E_{\rm i} = 250$ eV and $E_1 = 5$ eV. In this case, we observed that the peak values decreased in the recoil region but increased in the binary region in other reported methods [4,24,38,42]. However, in the binary region, the present peak values are slightly shifted to higher ejection angle with the same magnitude as the experimental hydrogenic ground-state data [4], but exhibit smaller magnitude than other hydrogenic ground-state theoretical calculations [24,38,42], whereas in the recoil region, the peak values of the present results are the highest among all other calculations [4,24,38,42]. We also observed that more than one peak structures exist in both the binary and the recoil regions in the absolute data [4] similar to the present and the first Born results. It is very interesting to notice that the hydrogenic ground-state BBK result [42] and the present results express similar patterns as the hydrogenic ground-state experimental results [4]. But the hydrogenic second Born result [38] shows somewhat different behaviour with the hydrogenic ground-state experimental results [4], because of the electron–electron two-body kinematic and the electron–nucleus final-state interaction which gives rise to the peak-shaped structure in the TDCS for electrons ejected with 250 eV energy using electron impact.

Next we have increased the ejected energy E_1 to 50 eV and the scattering angle θ_2 to 15°, remaining the incident energy $E_{\rm i}$ unaltered as 250 eV. We also have fixed the ejected angle θ_1 from 30° to 100°. The present and the first Born results for the ionization of 2P metastable state hydrogen atoms by electrons with exchange effects, after considering the above kinematic conditions, are shown in figure 2. In this case, the present first Born result exhibits the same peak feature as hydrogenic ground-state results [24,42] except for a slight shift in peak position. Moreover, the present 2P-state hydrogenic results and the ground-state hydrogenic second Born results [38] express exactly the same peak shape as the earlier one. All the peaks of the theoretical results in figure 2 remain either lower or higher than the hydrogenic ground-state measurements [4] which is very significant. Hydrogenic ground-state result of Das and Seal [24] shows good quantitative agreement with the second Born result [38], compared to the experimental data [4]. In addition, the data in [24] coincide with the experimental data of Weigold *et al* [1] in the same kinematic conditions. Thus, we can claim that our present work is in good qualitative agreement with other models for hydrogenic ground state.

Let us consider the next case (figure 3) for $E_{\rm i} = 250$ eV, $E_1 = 50$ eV, $\theta_2 = 20°$ and θ_1 (30°–100°). In this case, we observe that the peak patterns of the present and the first Born results are exactly similar to that of figure 2. But the present peak values were shifted to the higher ejection angles. Therefore, we noticed that the peak positions of the theoretical results [24, 38,42] for the ionization of ground-state hydrogen atoms by electrons are closer to the ground-state experimental results [4] compared to the present and the first Born results. For these kinematic conditions, the hydrogenic ground-state result of Das and Seal [24] best fit with the experimental data of Weigold *et al* [1].

In figures 4a and 4b, the present and the first Born results approach with one lobed structure in the recoil region whereas the 2S-state results [35] provide one deep lobed structure in the same region. However, peaks are almost similar in binary regions in all the cases.

The present and the first Born results exhibit similar peak formation compared to the previous results of hydrogenic 2S-state investigation [35] shown in figure 4c. The peak positions and the peak height of the present and the first Born results are seemed to be identical in the recoil region but the peak height is slightly lower in the binary region than the hydrogenic 2S-state results [35]. On the other hand, the first Born result shows

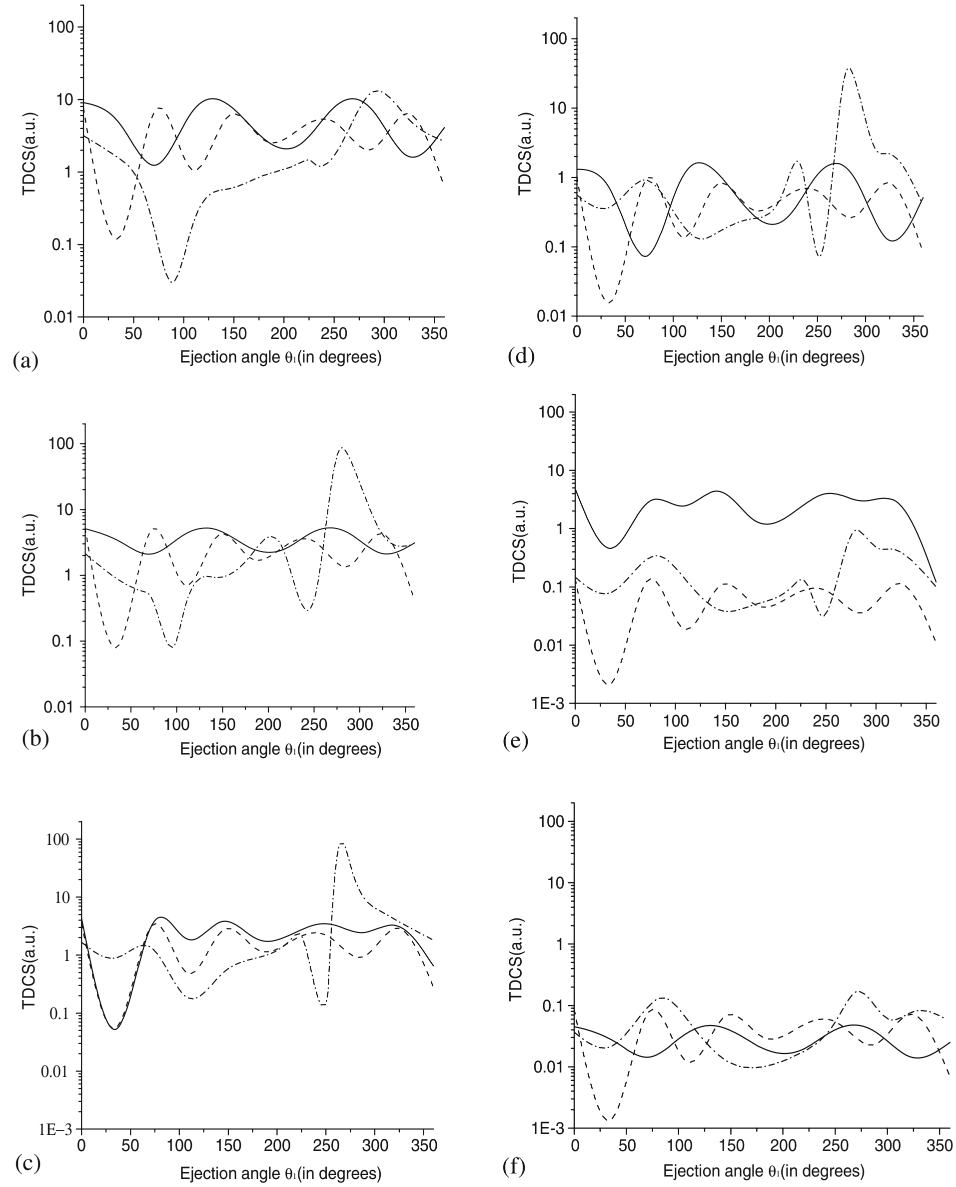

Figure 4. TDCS for the ionization of atomic hydrogen by 250 eV electron impact for (**a**) $\theta_2 = 5°$, (**b**) $\theta_2 = 7°$, (**c**) $\theta_2 = 9°$, (**d**) $\theta_2 = 11°$, (**e**) $\theta_2 = 15°$ and (**f**) $\theta_2 = 20°$ as a function of the ejected electron angle θ_1 relative to the incident electron direction. The ejected electron energy $E_1 = 5$ eV. Solid curve represents results of 2P hydrogenic state with exchange effects, dash curve represents first Born result of 2P hydrogenic state and dash–dotted curve represents hydrogenic 2S-state result [35].

qualitatively better agreement with the hydrogenic 2S results [35] than the present results shown in figure 4d. In contrast to figure 4d, we observe a qualitative enhancement in the TDCS results of the present findings in figure 4e. In this situation, the magnitude of the present binary and recoil peaks are found to be much higher than the corresponding 2S-state ionization [35]. This may be due to the fact that the probability of ionization from the 2P-state is expected to be much higher than that of the corresponding 2S-state. For the same case, the first Born result confirms similar representation of peak positions with 2S-state in both binary and recoil regions. The peak heights decrease slightly for the first Born and increase slightly for the present calculations which are closer to the compared hydrogenic 2S-state results [35]. For higher scattering angle $\theta_2 = 20°$ (figure 4f), the peak values of the present and the first Born results qualitatively agreed in the binary region, but oppositely advanced in the recoil region compared to the hydrogenic metastable 2S-state [35].

The ionization mechanisms of the findings are discussed here for qualitative understanding. Here, we considered four different scattering amplitudes corresponding to the different terms on the right-hand side of eq. (4). The first and the second terms, given by eq. (4), yield 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 TDCS for large scattering angle θ_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 near the peak, 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. (4), 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. (4)) is first scattered from the nucleus and can be deflected, in principle, into any direction. The final shape and magnitude of the TDCS is determined by the coherent superposition of the two transition matrices of the second and third terms corresponding to eq. (4) described by the same of eq. (6).

4. Conclusions

In this paper, the present and the first Born approximation results for the ionization of atomic hydrogen by electron impact with exchange effects in metastable 2P state are investigated theoretically and computationally. We observed that the implementation of the final-state wave function $\psi_{\mathrm{f}}^{(-)}(\bar{r}_1, \bar{r}_2)$ [24] shows good qualitative agreement with hydrogenic ground-state second Born results [38] and the hydrogenic ground-state experiments [4] and also coincides with BBK model [42] of the ground-state hydrogen atoms which is very significant. The present computational findings are encouraging and for future experiments this may play a vital role to provide much interesting and potential results in this area of research. There is more scope for improving this wave function and it can be applicable to various ionization problems.

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