Chin. Phys. B Vol. 21, No. 7 (2012) 073402

Effect of initial-state target polarization on the single ionization of helium by 1-keV electron impact*

Sun Shi-Yan(孙世艳), Ma Xiao-Yan(马晓艳), Li Xia(李 霞), Miao Xiang-Yang(苗向阳), and Jia Xiang-Fu(贾祥富)†

Center for Molecules Research, School of Physics and Information Engineering, Shanxi Normal University, Linfen 041004, *China*

(Received 8 September 2011; revised manuscript received 5 April 2012)

We report new results of triple differential cross sections for the single ionization of helium by 1-KeV electron impact at the ejection energy of 10 eV. Investigations have been made for both the perpendicular plane and the plane perpendicular to the momentum transfer geometries. The present calculation is based on the three-Coulomb wave function. Here we have also incorporated the effect of target polarization in the initial state. A comparison is made between the present calculation with the results of other theoretical methods and a recent experiment [Dürr M, Dimopoulou C, Najjari B, Dorn A, Bartschat K, Bray I, Fursa D V, Chen Z, Madison D H and Ullrich J 2008 *Phys. Rev.* A **77** 032717]. At an impact energy of 1 KeV, the target polarization is found to induce a substantial change of the cross section for the ionization process. We observe that the effect of target polarization plays a dominant role in deciding the shape of triple differential cross sections.

Keywords: triple differential cross section, target polarization, non-coplanar geometry

PACS: 34.80.Dp **DOI:** 10.1088/1674-1056/21/7/073402

1. Introduction

As a result of the continuous development of the experimental technique known as cold-target recoil-ion momentum spectroscopy (COLTRIMS),[1] the field of atomic ionization by electron impact is enjoying a renewed interest. With this technique, the usually tiny projectile's scattering angle can be indirectly obtained by measuring the momenta of ionized electrons and recoil ions. These experiments measured triple differential cross sections (TDCSs) in the scattering plane, as well as out of the scattering plane. Agreement between experiment and theory in the scattering plane has been good for electron-impact ionization for many years. However, it was surprising to see profound discrepancies out of the scattering plane.[2–5]

Very recently, Dürr *et al.* reported absolute measurements of TDCS for single ionization of helium by 1-keV electron impact in the scattering plane and out of the scattering plane geometries.[6] They have also compared their measured data with predictions from various theoretical models: the three-Coulomb (3C) wave function approach,[7–9] the nonperturbative CCC model[10] based on a close-coupling expansion of the multielectron wave function, a second-order distorted-wave models (DWB2), and a hybrid second-order plane-wave Born approximation for the projectile combined with a convergent R matrix (close-coupling) description of the ejected-electron-residual-ion interaction (PWB2-RMPS) theory.[11–16] They have pointed out that at this high impact energy the agreement between all the theories and experiment is very good for obtaining the scattering plane geometry. In the non-coplanar geometry, the TDCSs predicted by different theories have their own merits in reproducing the experimental results. Dey and Roy[17] applied the Glauber approximation (GA) method incorporating the effect of classical post collision interaction (PCI) to calculate the fully differential cross section (FDCS) for the single ionization of helium by electron impact. The GA results are also in good agreement with the experiment in the scattering plane, but noticeable discrepancies have been observed in the plane perpendicular to it. The effect of PCI is not significant in the kinematics. However, for a momentum transfer of 0.5 a.u., all the theoretical calculations exhibit similar features but fail to reproduce the

*Project supported by the Natural Science Foundation of Shanxi Province of China (Grant Nos. 20051008 and 2010011009), the National Natural Science Foundation of China (Grant No. 11047191), the Key Project of Chinese Ministry of Education (Grant No. 211025), and the Natural Science Foundation for Young Scientists of Shanxi Province, China (Grant No. 2009021005).

†Corresponding author. E-mail: jiaxf@dns.sxnu.edu.cn

measurements in a satisfactory manner. The possible explanation for the lack of the accuracy is that polarization of the target, which should be large, needs to be considered in the entrance channel.[18]

In the present paper, we have introduced the effect of target polarization in the initial state to calculate TDCS for 1-keV electron impact single ionization of helium by means of the 3C model in the perpendicular plane and the plane perpendicular to the momentum transfer. Our goal is to assess if the present results with target polarization (WP) are able to reproduce the experimental data with reasonable success and study the effect of target polarization on the angular distribution of TDCS. Results are compared with the experimental data, our calculations without polarization (WOP), DWB2 results, and CCC results. The present WP results predict side peaks near the ejection angles of 90° and 270° which are in qualitative agreement with experiment.

2. Theoretical treatments

Consider an (e, 2e) collision, in which an incident electron with a momentum of $\boldsymbol{k}_{\mathrm{i}}$ ionizes a helium target initially at rest in its ground state. Both scattered and ejected electrons are detected with momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ with respect to the target nucleus. For high incident energy, the electron exchange effect between incident and bound electrons can safely be neglected. Therefore, the corresponding TDCS is given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_2} = N_e(2\pi)^4\frac{k_1k_2}{k_{\mathrm{i}}}|T_{\mathrm{fi}}|^2, \tag{1}$$

where $N_{\mathrm{e}}(=2)$ is the number of identical electrons in the atomic shell which is ionized, $\mathrm{d}\Omega_1$ and $\mathrm{d}\Omega_2$ denote, respectively, the elements of solid angles for the scattered and ejected electrons, and $\mathrm{d}E_2$ represents the energy interval of the ejected electron. The transition matrix elements T_{fi} are given by

$$T_{\mathrm{fi}} = \langle \Psi_f^- | V | \Psi_{\mathrm{i}}^+ \rangle. \tag{2}$$

The final state Ψ_{f}^- should be an eigenfunction of the full Hamiltonian with boundary conditions describing one bound electron and two outgoing electrons. It consists of two outgoing electrons and the ground-state wave function of the hydrogen-like ion. The final continuum state of the two outgoing electrons is approximated by a product of three two-body Coulomb waves.[7] The variable V represents the interaction between the incident electron and the target. The wave function of the initial state of the entire target and projectile collision system Ψ_{i}^+ can be given by

$$\Psi_{\mathrm{i}}^+(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) = (2\pi)^{-3/2}\exp\left(\mathrm{i}\boldsymbol{k}_{\mathrm{i}}\cdot\boldsymbol{r}_1\right)\psi_{\mathrm{i}}(\boldsymbol{r}_2,\boldsymbol{r}_3), \tag{3}$$

where $\boldsymbol{r}_1$, $\boldsymbol{r}_2$, and $\boldsymbol{r}_3$ are the position vectors of the incident electron and the two helium electrons with respect to the target nucleus, respectively. Furthermore, the ψ_{i} represents the ground-state wave function of a free helium atom. In order to consider the effect of polarization of the target in the initial state on the TDCS, we employ two types of ground-state wave functions[19] of helium atom.

The first wave function, referred to as the WOP function hereafter, was suggested by Gupta and Srivastava.[19] Its expression is given as follows:

$$\psi_{\mathrm{i}}(\boldsymbol{r}_2,\boldsymbol{r}_3) = \sum_{l=0}^{1}\phi_l(r_2)\phi_l(r_3) \times \sum_{m=-1}^{+1} a_{lm}Y_{lm}(\hat{r}_2)Y_{l-m}(\hat{r}_3), \tag{4}$$

$$\phi_0(r) = \phi_{\mathrm{s}}(r) = \sum_{i=1}^{2}\gamma_{\mathrm{i}}\,\mathrm{e}^{-\alpha_{\mathrm{i}}r}, \tag{5}$$

$$\phi_1(r) = \phi_\partial(r) = \sqrt{\frac{4\gamma^5}{3}}r\,\mathrm{e}^{-\gamma r}, \tag{6}$$

where the parameters α_1, α_2, γ_1, γ_2, γ, a_{00}, a_{10}, a_{1-1}, and a_{11} determined variationally are give by

$$\begin{aligned}&\alpha_1 = 1.43878,\ \ \alpha_2 = 2.81, \gamma_1 = 2.84193,\\ &\gamma_2 = 1.89889,\ \ \gamma = 2.51336,\ \ a_{00} = 0.99993,\\ &a_{10} = a_{1-1} = a_{11} = -1.13756\times10^{-2}.\end{aligned} \tag{7}$$

These values correspond to the ground-state binding energy of 77.9003 eV.

Our second wave function, referred to as the WP function, has been proposed by Gupta and Srivastava.[19] Here the parameters in Eq. (7) for the polarized wave function are obtained by variationally minimizing $\langle\psi|H|\psi\rangle/\langle\psi|\psi\rangle$ in this high-energy region. It is assumed that the incident electron is approaching head-on towards the atomic nucleus. The projectile–target electron interaction with the projectile fixed at some distance r_0', is then added to the helium-atom Hamiltonian H_0. Thus we have

$$H = H_0 + \frac{1}{|\boldsymbol{r}_0' - \boldsymbol{r}_2|} + \frac{1}{|\boldsymbol{r}_0' - \boldsymbol{r}_3|}. \tag{8}$$

Thereby some parameters are different from those in Ref. [19] for the high-energy collisions. Their values for $r_0' = 0.46$ a.u. are given as follows:

$$\begin{aligned}&\alpha_1 = 0.806865,\ \ \alpha_2 = 2.81, \gamma_1 = 1.20151,\\ &\gamma_2 = 2.42736,\ \ \gamma = 1.46044,\ \ a_{00} = 0.998787,\\ &a_{10} = -0.081185,\ \ a_{1-1} = a_{11} = -0.001115.\end{aligned} \tag{9}$$

The above values correspond to the ground-state binding energy of 69.7115 eV. The projectile-electron interaction along with the target e–e angular correlation built in the trial wave function essentially push the two p-wave orbits in diametrically opposite orientation in a plane perpendicular to the incident direction. A measure of the effect of target polarization is the change of the ratio a_{10}/a_{11} from unity (unpolarized wave function) to about seventy.

3. Results and discussion

For a detailed investigation of cross sections and a quantitative comparison with theory, we consider the absolute cross section as a function of the emission angle of the ejected electron in the perpendicular plane (see Fig. 1) and the plane perpendicular to the momentum transfer geometries (see Fig. 2). In Figs. 1 and 2, our WP and WOP results are compared with the DWB2, PWB2-RMPS, and CCC calculations, and also absolute experimental results of Dürr *et al.*[6] for 1-keV electron impact single ionization of helium at an ejection energy of 10 eV for the two geometries.

In the plane perpendicular to the scattering plane, the experimental data for all three momentum transfers exhibit a trend of cross section at $\theta_2 = 90°/270°$, and decrease of cross section at $\theta_2 = 180°$. The relative intensity of the out-of-plane enhancement increases with increasing momentum transfer. At a momentum transfer $q = 0.5$ a.u. (see Fig. 1(a)), all the theoretical calculations exhibit similar features but fail to reproduce the experimental data in a satisfactory manner. These models underestimate the magnitude of the cross-section enhancement in the plane perpendicular to the scattering plane. Although our WP results underestimate the momentum transfer at 180° and only show a low hump, the trend of enhancement is qualitatively reproduced. At larger momentum transfers (e.g., at $q = 0.75$ and 1.0 a.u., see Figs. 1(b) and 1(c)), our WOP model undoubtedly fails due to drastic underestimation of the out-of-plane maxima. Not only a quantitative disagreement persists but also the side peaks are completely absent in the WOP results. In contrast, all theories except for the WOP model qualitatively reproduce the side-peak structures. There are no experimental values close to 180°. The trend of the available data points in the vicinity of the acceptance minimums is clear in Figs. 1(b) and 1(c). However, the CCC, DWB2, and PWB2-RMPS calculations predict pronounced cross-section maxima in Fig. 1(b). The WP results including the target polarization contribution not only reproduce the side-peak structure, but also the minimum at 180°, which are in better agreement with experimental data than other theoretical results as shown in Figs. 1(b) and 1(c). This suggests that the target polarization strongly affects the magnitude and peak positions of the TDCS.

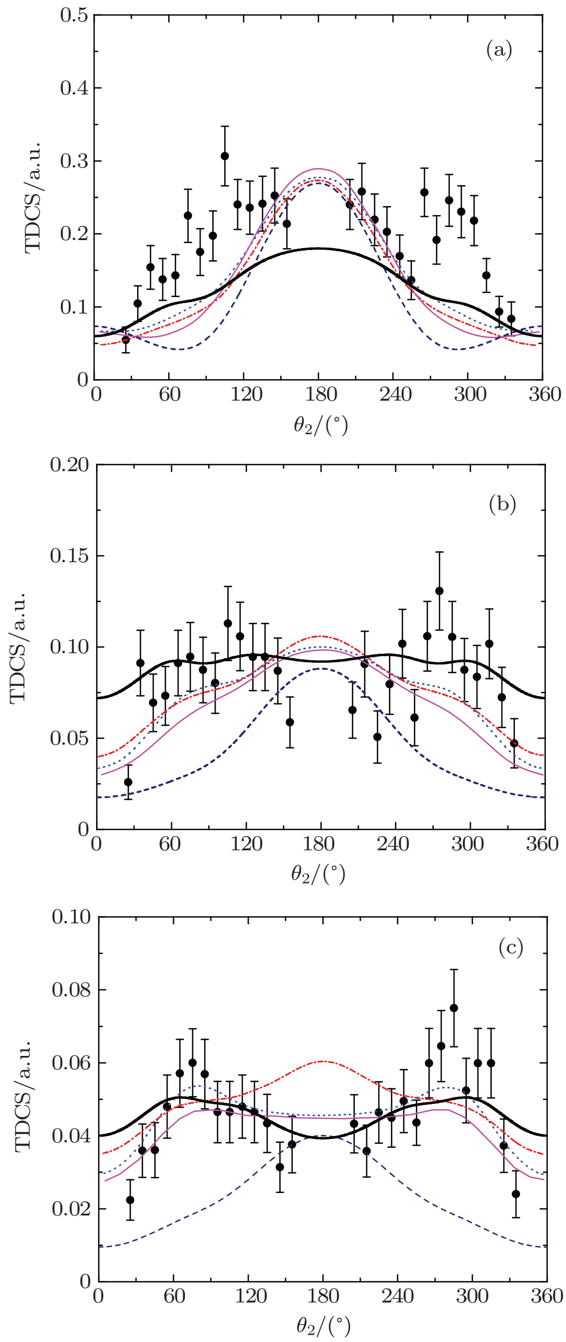

Fig. 1. (colour online) Triple differential cross sections in the plane perpendicular to the scattering plane for 1-keV electron-impact single ionization of helium for an ejected electron energy of $E_2 = 10$ eV and three different momentum transfers of (a) 0.5, (b) 0.75, and (c) 1.0 a.u.. Thick solid lines: WP, dashed lines: WOP, dash-dotted lines: DWB2, dotted lines: PWB2-RMPS, thin solid lines: CCC, solid circles with error bars: experimental data.[6]

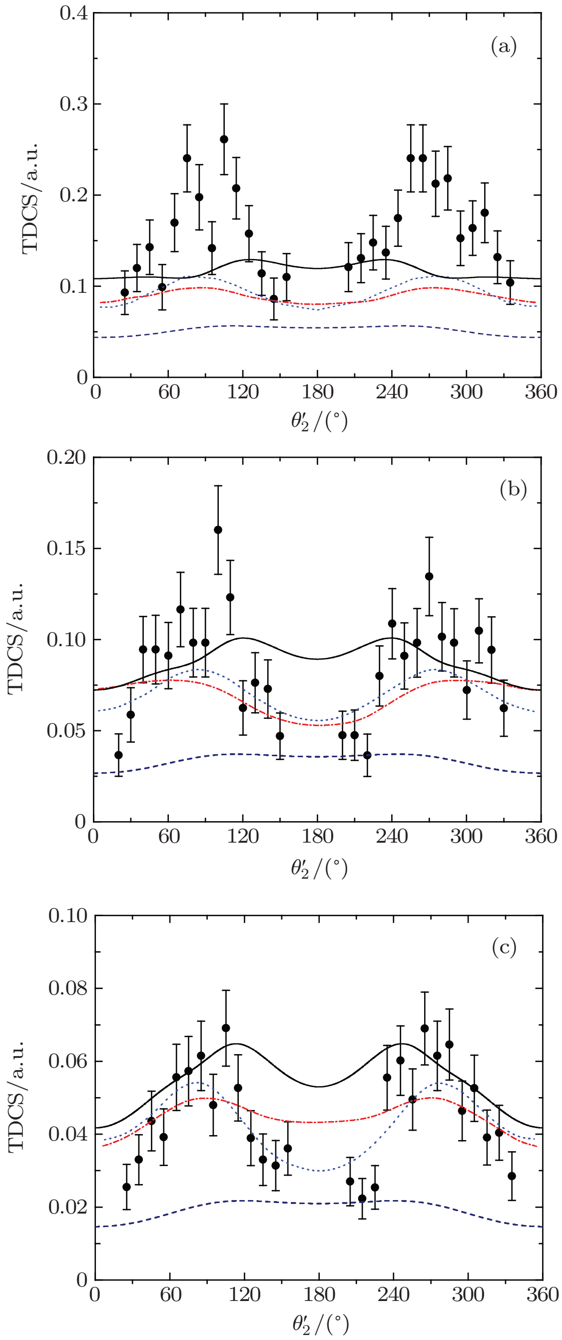

Fig. 2. (colour online) Same as Fig. 1, except that the plane is perpendicular to the momentum transfer vector $\boldsymbol{q}$.

In order to further elucidate the conclusion, we now consider electron emission in the plane perpendicular to the momentum transfer $\boldsymbol{q}$. The resulting cross section is plotted as a function of the emission angle θ_2' in Fig. 2. In the plane perpendicular to $\boldsymbol{q}$, the θ_2' is the angle between the ejected electron momentum and the scattering plane. In this representation, the out-of-plane enhancement results in pronounced maxima at $\theta_2' = 90°/270°$. Also shown in Fig. 2 are the corresponding cross sections predicted by the DWB2, PWB2-RMPS, WP, and WOP results. It should be mentioned here that the CCC results are unavailable only for the geometry till now. From this global comparison of the shapes, the qualitative agreement and the principal shortcomings of the theoretical results can easily be identified. The two second-order models are in excellent agreement with experimental data,[6] although the PWB2-RMPS method comes closest. The WOP model drastically failed out-of-plane, with some improvement over the WOP results achieved by the WP treatment. As mentioned above, the inclusion of the initial-state target polarization leads to the side-peak structures and the intensity at 180°, and thus better agreement with the experimental data for the three momentum transfers than the WOP results. This suggests that the high impact energy is likely to induce quite a large polarization in the target. The approximation is able to reproduce qualitative features seen in the experimental data. The side maxima are apparently seen in these data due to the effect of target polarization in the initial state.

4. Conclusion

Considering the target polarization effects, we have calculated the TDCS for the single ionization of helium by 1-keV electron impact at an ejection energy of 10 eV. In the non-coplanar plane, we find that for all the momentum transfers, the WP results of TDCS apparently lead to the side-peak structure around 90° and 270° and the intensity at 180°, which are in better agreement with experimental data than the WOP results. Therefore, the target polarization contribution is obvious. The present results have shown that the polarization of the target is an important physical parameter in the dynamics of ionization. Unfortunately, some currently unresolved discrepancies still exist for the smallest momentum transfer $q = 0.5$ a.u. and all the results fail to accurately describe the experimental results in a satisfactory manner, although the WP results qualitatively reproduce the angular distribution. The present study suggests that none of the methods discussed here provide an desirable description of the present system. These results favor the hypotheses that ionization events out of the scattering plane are dominated by higher-order processes that are not accurately described even by the DWB2 theory. Fully non-perturbative theories are highly desirable, but such calculations are very demanding and have met serious challenges to date. Hence, improvements to existing perturbative models, e.g., by selecting highly sophisticated wave functions to describe the initial and final channels and the interaction between ejected electrons and residual ions, are worth pursuing in order to achieve quantitative agreement with experimental results. The theoretical work recently published by Kadyrov *et al.*[20] would be very valuable to help theoreticians improve the theoretical description of collision systems of this type.

References

[1] Moshammer R, Ullrich J, Unverzagt M, Schmidt W, Jardin P, Olson R E, Mann R, Dörner R, Mergel V, Buck U and Schmidt-Böcking H 1994 *Phys. Rev. Lett.* **73** 3371

[2] Dürr M, Dimopoulou C, Dorn A, Najjari B, Bray I, Fursa D V, Chen Z J, Madison D H, Bartschat K and Ullrich J 2006 *J. Phys.* B **39** 4097

[3] Schulz M, Moshammer R, Fischer D, Kollmus H, Madison D H, Jones S and Ullrich J 2003 *Nature* **422** 48

[4] Sun S Y, Jia X F, Shi W Q and Li X W 2008 *Acta Phys. Sin.* **57** 3458 (in Chinese)

[5] Sun S Y, Jia X F, Miao X Y, Zhang J F, Xie Y, Li X W and Shi W Q 2009 *Chin. Phys.* B **18** 2744

[6] Dürr M, Dimopoulou C, Dorn A, Najjari B, Bray I, Fursa D V, Chen Z J, Madison D H, Bartschat K and Ullrich J 2008 *Phys. Rev.* A **77** 032717

[7] Brauner M, Briggs J S and Klar H 1989 *J. Phys.* B **22** 2265

[8] Berakdar J 1996 *Phys. Rev.* A **53** 2314

[9] Jones S and Madison D 2000 *Phys. Rev.* A **62** 042701

[10] Bray I 2002 *Phys. Rev. Lett.* **89** 273201

[11] Reid R H G, Bartschat K and Raeker A 1998 *J. Phys.* B **31** 563

[12] Fang Y and Bartschat K 2001 *J. Phys.* B **34** L19

[13] Bellm S, Lower J and Bartschat K 2006 *Phys. Rev. Lett.* **96** 223201

[14] Chen Z J, Madison D H, Whelan C T and Walters H R 2004 *J. Phys.* B **37** 981

[15] Chen Z J and Madison D H 2005 *J. Phys.* B **38** 4195

[16] Chen Z J, Madison D H and Bartschat K 2007 *J. Phys.* B **40** 2333

[17] Dey R and Roy A C 2009 *Nucl. Instr. Meth.* B **267** 2357

[18] Ciappina M F and Cravero W R 2006 *J. Phys.* B **39** 1091

[19] Gupta S and Srivastava M K 1996 *J. Phys.* B **39** 323

[20] Kadyrov A S, Bray I, Mukhamedzhanov A M and Stelbovics A T 2008 *Phys. Rev. Lett.* **101** 230405