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The effect of dynamical screening on helium (e, 2e) fully differential cross-sections*

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This paper presents the fully differential cross sections (FDCS) for 102eV electron impact single ionization of helium for both the coplanar and perpendicular plane asymmetric geometries within the framework of dynamically screened three-Coulomb-wave theory. Comparisons are made with the experimental data and those of the three-Coulomb wave function model and second-order distorted-wave Born method. The angular distribution and relative heights of the present FDCS is found to be in very good agreement with the experimental data in the perpendicular plane geometry. It is shown that dynamical screening effects are significant in this geometry. Three-body coupling is expected to be weak in the coplanar geometry, although the precise absolute value of the cross section is still sensitive to the interaction details.

Keywords: fully differential cross sections, screening effects, perpendicular plane geometry
PACC: 3480D, 3450H

1. Introduction

Experimental results for the electron impact ionization of helium have shown that the problem once believed to be solved is still not fully understood. These experiments, performed on a cold-target-recoil-ion-momentum spectrometer apparatus,[1] measured fully differential cross sections (FDCS) 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 large discrepancies out of the scattering plane. Very recently, experiments performed by Schulz *et al*[2] and Dürr *et al*[3,4] found significant out-of-plane cross sections for 102 eV electron impact ionization of helium. The data are compared with various theoretical predictions from a three-Coulomb (3C) wave-function model,[5−7] the non-perturbative convergent close-coupling model[8] as well as from the first-order and second-order distorted-wave (DWB2).[9−14] The 3C wave function nicely reproduces the magnitudes and the angular positions of the binary and recoil lobes in the coplanar geometry. However, it fails drastically to reproduce the position and shape of the peak structures in contrast to experiment in the perpendicular plane asymmetric geometry.

In this work, we adopt the idea of Ref.[15] to calculate the FDCS for 102 eV electron impact single ionization of helium by means of the modified 3C model proposed by Chen *et al*. Our goal is to assess if this model is able to reproduce the experimental data with reasonable success. The FDCS are calculated at a different scattering angle θ_1 (8°, 10°, 15°, 20°) and fixed energies of ejected electron ($E_2 = 10$ eV, 5 eV) in both the coplanar and perpendicular plane asymmetric geometries. Results are compared with the experimental data and the theoretical 3C and DWB2 results. The qualitative agreement of the present results with the experiment is better than that of 3C, particularly in respect to maxima close to the angle of the ejected electron $\theta_2 = 70°$ and 290°. Atomic units (a. u.) are used unless otherwise specified.

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2. Theory

The transition matrix element reads

$$T_{\rm fi} = \langle \Psi_{\rm f}^{-} | V_{\rm i} | \Psi_{\rm i}^{+} \rangle. \quad (1)$$

Here $\Psi_{\rm i}^{+}$ and $\Psi_{\rm f}^{-}$ are the wavefunction of the initial and final state of the entire collision system (target + projectile), and $V_{\rm i}$ represents the interaction between the incident electron and the target.

The final state $\Psi_{\rm f}^{-}$ should be an eigenfunction of the full Hamiltonian with boundary conditions describing one bound and two outgoing electrons. It consists of the two outgoing electrons and the ground-state wavefunction of the hydrogen-like ion,

$$\Psi_{\rm f}^{-}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \phi_{\rm 3C}(\boldsymbol{r}_1, \boldsymbol{r}_2)\phi_{\rm ion}(\boldsymbol{r}_3). \quad (2)$$

$\phi_{\rm f}(\boldsymbol{r}_1, \boldsymbol{r}_2)$ will be described by the 3C wavefunction in its general form

$$\begin{aligned} &\phi_{\rm 3C}(\boldsymbol{r}_1, \boldsymbol{r}_2) \\ &= (2\pi)^{-3} \exp({\rm i}\boldsymbol{k}_1 \cdot \boldsymbol{r}_1) \exp({\rm i}\boldsymbol{k}_2 \cdot \boldsymbol{r}_2) \\ &\quad \times \prod_j N_{j1}F_1[{\rm i}\alpha_j; 1; -{\rm i}(k_j r_j + \boldsymbol{k}_j \cdot \boldsymbol{r}_j)], \end{aligned} \quad (3)$$

here, N_j, $j \in \{1, 2, 12\}$, are normalization constants which can be given by

$$N_j = \exp(\alpha_j \pi/2)\Gamma(1 - {\rm i}\alpha_j).$$

where α_j $(j = 1, 2, 12)$ are Sommerfeld parameters[5] $\alpha_1 = 1/k_1$, $\alpha_2 = 1/k_2$, $\alpha_{12} = -1/2k_{12}$, with $\boldsymbol{k}_{12} = (\boldsymbol{k}_1 - \boldsymbol{k}_2)/2$.

However, the Sommerfeld parameter is a measure of the strength of the Coulomb interaction between charged particles and the strength of the interaction of any two particles by the presence of the third particle, the modification of the strength of a particular two-body Coulomb interaction depends on the momenta of the two particles relative to the third one, which represents a dynamic screening (DS) of the three two-body Coulomb interactions.[15–17] The modified Sommerfeld parameters are given by Ref.[15],

$$\beta_1 = \frac{-Z_{\rm eff} + \dfrac{k_1}{4k_{12}}(\sin^2\theta)\left(1 - \dfrac{|\,\boldsymbol{k}_1 - \boldsymbol{k}_2\,|}{4k_{12}}\right)}{k_1}, \quad (4)$$

$$\beta_2 = \frac{-Z_{\rm eff} + \dfrac{k_2}{4k_{12}}(\sin^2\theta)\left(1 - \dfrac{|\,\boldsymbol{k}_1 - \boldsymbol{k}_2\,|}{4k_{12}}\right)}{k_2}, \quad (5)$$

$$\beta_{12} = \frac{1 - (\sin^2\theta)\left(1 - \dfrac{|\,\boldsymbol{k}_1 - \boldsymbol{k}_2\,|}{4k_{12}}\right)}{2k_{12}}. \quad (6)$$

The inter-electronic relative angle θ is given by $\theta = (\cos^{-1}\hat{\boldsymbol{k}}_1 \cdot \hat{\boldsymbol{k}}_2)/2$. The effective charge $Z_{\rm eff} = Z - 5/16$.

The calculations have been done in both the coplanar and perpendicular plane asymmetric energy-sharing geometries, which have been carried out numerically following the method described in our earlier work[18] with necessary modifications.

3. Results and discussions

The FDCS for electron impact ionization of helium for both the coplanar and perpendicular plane asymmetric geometries at an incident energy of 102 eV have been calculated, which correspond to the recent measurements of Ref.[3]. For comparing conveniently with other data, the DS3C results have been normalized for the best visual fit of the experiments, and the subsequent multiplicative factor is shown in the figure caption to preserve the information on the relative magnitude of the different theoretical predictions.

The present DS3C results and those of DWB2 together with the experimental data for four angles of the fast electron and two energies of the slow electron are illustrated in Figs.1 and 2. In order to see the influence of three-body effects, we also made calculations by using the 3C wave function for comparison.

For emission in the scattering plane, the cross sections show well-known binary and recoil lobe structure, the qualitative feature of the experimental FDCS is quite well described by the theories except for some quantitative discrepancies in the recoil peak. The peak position is shifted towards smaller ejection angles in the 3C angular distribution. Near the binary peak, the DWB2 calculations are bigger than experimental results for $\theta_1 = 15°$ and $20°$. Some improved agreement with the data is achieved with the DS3C calculation (after normalization of the experiments) to the extent that the binary peak is shifted to larger angles with respect to the 3C results and the binary peak is decreased with respect to the DWB2 results for $\theta_1 = 15°$ and $20°$. The DS3C calculation provides much better shape agreement with the experiment.However, the absolute magnitude is off by as much as a factor of 1–3. We remark that the present results confirm the analysis made in Ref.[19] in which three-body coupling primarily affects the magnitude of the FDCS rather than its shape. This is readily concluded by comparing the 3C with DS3C results since, in the former case, three-body coupling is neglected, whereas the merit of the DS3C is the inclusion of this coupling.

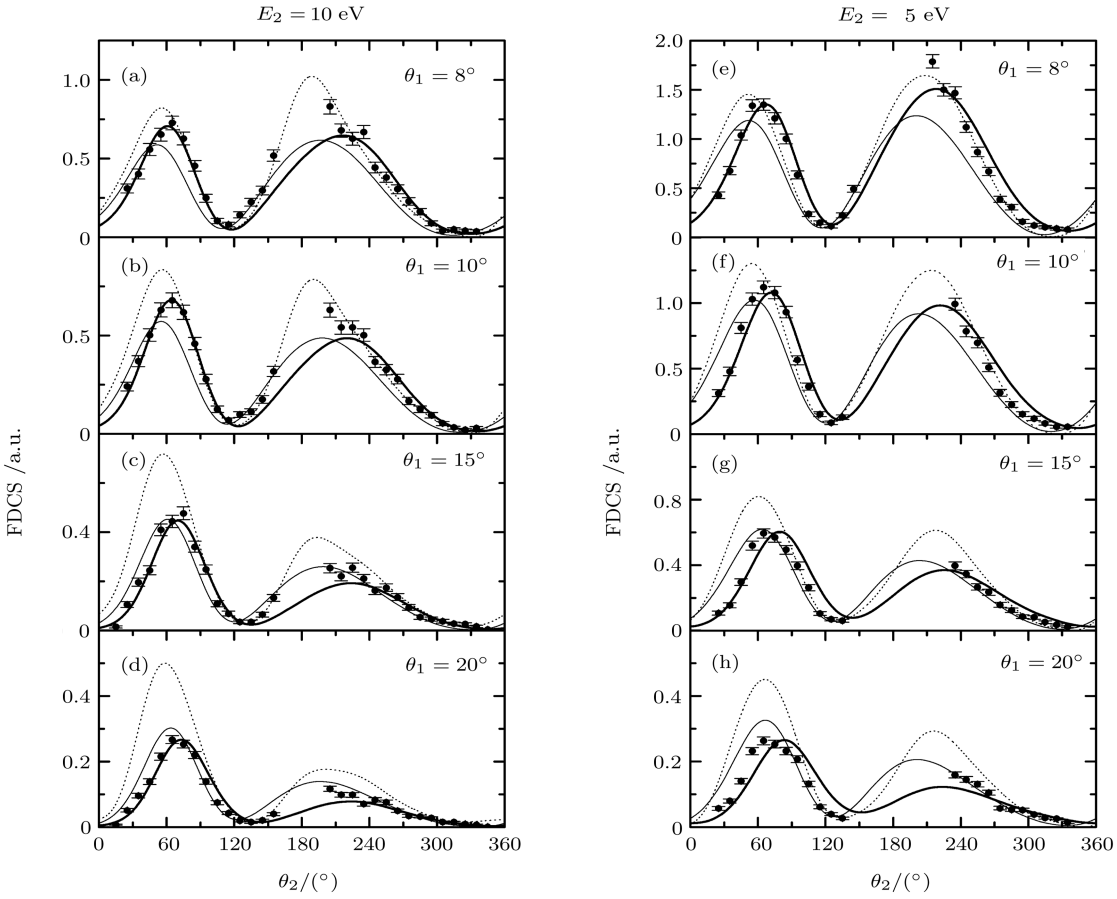


Fig.1. The TDCS for electron impact ionization of helium at an incident electron energy of 102 eV in the coplanar asymmetric geometry for ejected electron energies of 10 eV (left column) and 5 eV (right column) and fixed scattering angles for the faster electron of 8°, 10°, 15°, 20°. The black solid line represents the DS3C result, and the dotted line represents the DWB2,[14] the grey solid line represents the 3C result, the points are absolute experimental data from Dürr *et al.*[3] The DS3C results have been multiplied by 2.04 (a), 1.88 (b), 1.33 (c), 1.0 (d), 2.86 (e), 2.33 (f), 1.79 (g) and 1.08 (h), respectively.

In Fig.2, we show the same comparison for the perpendicular asymmetric geometry. For this geometry the observed cross section reveals distinct features and exhibits maxima close to $\theta_2 = 70°$ and 290° with respect to the incoming projectile direction for both energies $E_2 = 10$ eV and 5 eV, they strongly increase relative to the recoil lobe for increasing scattering angles.

In the left column of Fig.2, results for a fixed ejected energy of 10 eV are shown. The 3C model underestimates the recoil peak close to $\theta_2 = 180°$ for small momentum transfer, or, equivalently, for a small scattering angle. For larger momentum transfers, the out-of-plane peaks appearing around $\theta_2 = 70°$ and 290° are well reproduced by the DS3C (after normalization of the experiments) and DWB2 model, while the 3C completely fails in this angular region. In contrast, the DS3C nicely reproduces the cross section in the perpendicular plane, including the angular positions and relative heights. Strong differences between DS3C and 3C resulting from DS can be observed.

For the lower ejected electron energy $E_2 = 5$ eV, it is very encouraging to see that the DS3C calculations (after normalization of the experiments) show the improvement over the 3C results and are in excellent agreement with the experimental measurements for $\theta_1 = 8°$, 10°, 15°, but do not do as well for the largest momentum transfer case $\theta_1 = 20°$. The reason may be traced to the fact that the original DS3C model is preferable for small momentum transfer. On the other hand, the results of the DWB2 model are generally in good agreement with the experiment. However, at electron ejection angles close to $\theta_2 < 60°$ ($> 320°$) our results are nearer to the experimental data than that of DWB2.

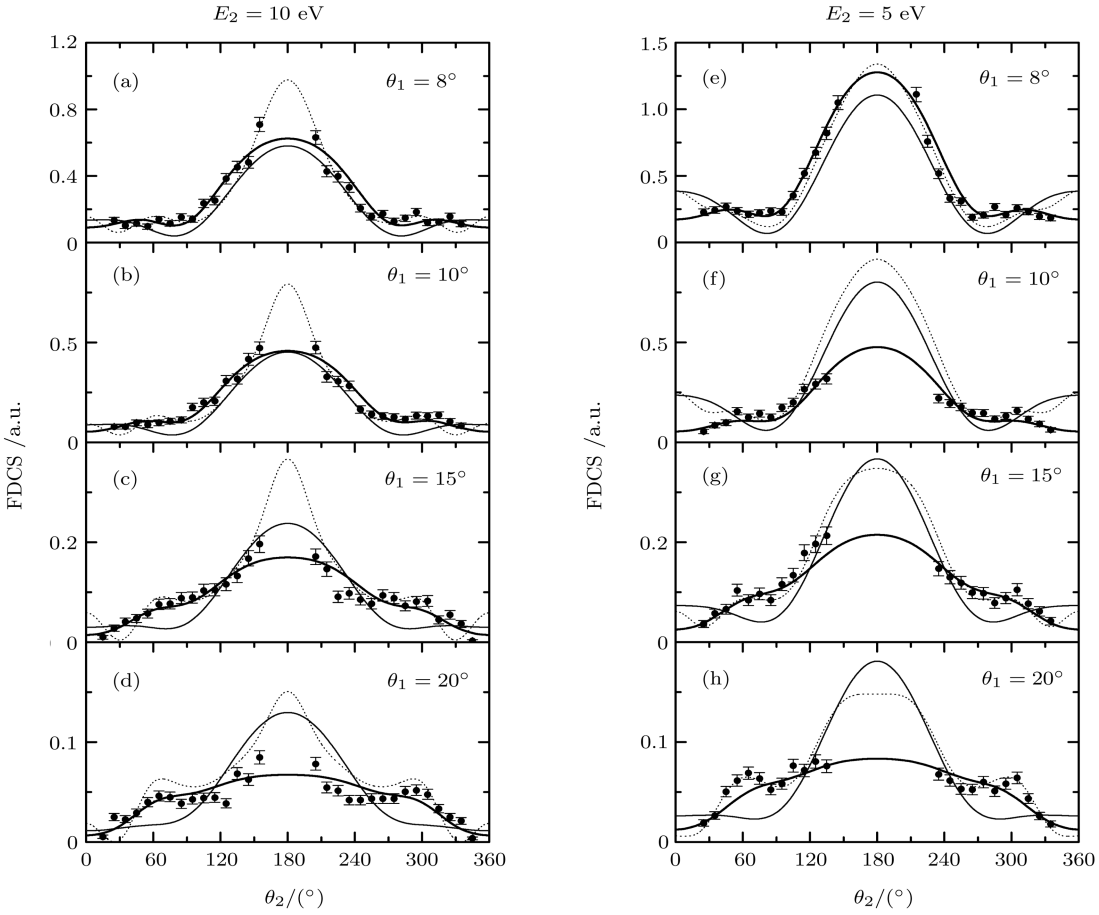


Fig.2. Same as Fig.1 for perpendicular plane asymmetric geometry. The DS3C results have been multiplied by 2.56 (a), 2.5 (b), 1.89 (c), 1.43 (d), 3.3(e), 1.75(f), 1.69(g) and 1.2(h), respectively.

In conclusion, we performed the DS3C calculations for 102 eV electron impact ionization of helium at different scattering angles θ_1 (8°, 10°, 15°, 20°) and fixed energies of ejected electron (E_2 = 10 eV, 5 eV) for both the coplanar and perpendicular plane asymmetric geometries . Comparisons of the predictions from several state-of-the-art theoretical approaches with experimental data reveal that three-body coupling is weak in the coplanar geometry, although the precise absolute value of the cross section is still sensitive to the details of the interaction. For emission in the perpendicular plane, the DS3C result shows improvement over the 3C in obtaining better angular distribution and relative height of the present FDCS in comparison with experiment, which supports our conclusion that the peak structures of the present FDCS are to a large extent due to the DS effects. But it also shows that the description of these effects is still rather incomplete. In addition to account for these effects in the description of the projectile, achieving quantitative agreement requires the use of highly sophisticated wave functions for the initial bound state and ejected-electron-residual-ion interaction.

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