Theoretical analysis on fully differential cross sections for C^{6+} impact ionization of helium*

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Fully differential cross sections (FDCS) are calculated within a four-body model for single ionization of helium by C^{6+} impact at the incident energy of 100 MeV/a.u. (atomic unit). The results are compared with experimental data and other theoretical predictions. It is shown that our results are in very good agreement with experiment for three small momentum transfers in the scattering plane; however, some significant discrepancies are still present at the largest momentum transfer in both the scattering plane and the perpendicular plane. In actuality, the problem has not been explained by the theory during the last decade. Accordingly, the contributions of different scattering amplitudes to FDCS are analyzed. It is found that for the largest momentum transfer the cross section arising from a destructive interference of the three amplitudes is much smaller than the experimental data. However, the cross section due to the constructive interference of two scattering amplitudes between projectile–ionized electron interaction and projectile–passive electron interaction almost approaches the experimental data.

Keywords: ion-impact ionization, fully differential cross section, four-body model, interference effect

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1. Introduction

Although the single ionization of atoms by charged-ion impact has been a fruitful field of study for many decades, the single ionization processes have not been completely understood.[1,2] In particular, for the $C^{6+}+He$ system, the theoretical models were not able to yield a satisfactory description of the measured fully differential cross sections (FDCS).[3,4] As would be expected for a high-energy collision, the shape of the experimental data was in good agreement with theory in the scattering plane. However, the experimental data out of the scattering plane exhibited structure was not well reproduced by theory. So far, none of the published theoretical investigations, both perturbative and non-perturbative, including the first Born approximation (FBA),[5] three-body distorted-wave (3DW),[3,6] correlated continuum wave-eikonal initial state (CCW-EIS),[7] coupled-pseudostate (CP),[5,8] and fully quantum-mechanical convergent close-coupling (CCC) models,[9] have been able to explain the serious discrepancy observed between theory and experiment. Although the time-dependent close-coupling (TDCC) approach[10,11] produced a perpendicular plane FDCS with the positions of the peaks in better agreement with the experiment, the magnitude of the FDCS remained considerably lower than the experiment. Thus, the problem of the theoretical description of FDCS measurements in out-of-plane geometries still remains to be solved. Further theoretical analysis and calculations seem to be appropriate and interesting.

In this paper, we utilize the four-body model to calculate the FDCS for single ionization of helium by 100 MeV/a.u. (atomic unit) C^{6+} impact, both in and out of the scattering plane. A distinct feature of our analysis is that this model includes the passive electron in the wave function and in the perturbation (details are contained in the next section). The aim of this article is to compare the four-body cross sections with the corresponding experimental results and to evaluate the ability of the present method to reproduce the peak structure of the experimental data. It is found that the qualitative agreement of the present results with experiment is obtained. However, at the largest momentum transfer, there is a considerable magnitude discrepancy between our calculations and the measurements. Furthermore, the physical origin of the features to the FDCS is analyzed in detail and conclusions are drawn. Atomic units are used throughout the paper, unless otherwise stated.

2. Theoretical method

In this section single ionization of helium by the impact of C^{6+} with incident momentum $\boldsymbol{K}_\mathrm{i}$ relative to the atomic center of mass is considered. The four-body initial state wave function will be written as the product of a plane wave with momentum $\boldsymbol{K}_\mathrm{i}$ for the projectile and a wave function of helium atom in the ground state

$$\Phi_\mathrm{i}^{+}(\boldsymbol{r}_1,\boldsymbol{r}_T,\boldsymbol{R}_\mathrm{P})=\left(\frac{1}{2\pi}\right)^{3/2}\exp(\mathrm{i}\boldsymbol{K}_\mathrm{i}\cdot\boldsymbol{R}_\mathrm{P})\phi_i(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T}). \quad (1)$$

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In the center-of-mass system, $\boldsymbol{r}_1$ is the coordinate of the passive electron relative to the target nucleus, $\boldsymbol{r}_\mathrm{T}$ represents the coordinate of the ionized electron with respect to the target ion, and $\boldsymbol{R}_\mathrm{p}$ is the position of the projectile relative to the atomic center of mass. For ϕ_i we choose the analytical fitting to the Hartree–Fock (HF) wave function given by Byron and Joachain[12]

$$\phi_i(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T}) = U(\boldsymbol{r}_1)U(\boldsymbol{r}_\mathrm{T}), \tag{2}$$

where $U(\boldsymbol{r}) = (4\pi)^{-1/2}(A\,\mathrm{e}^{-\alpha r} + B\,\mathrm{e}^{-\beta r})$, $A = 2.60505$, $B = 2.08144$, $\alpha = 1.41$, and $\beta = 2.61$.

The wave function Ψ_f^- should be an exact solution of the four-body problem in the final channel, which is represented by a product of the ground-state wave function of He^+ and the three-Coulomb wave Ψ_3C^-

$$\Psi_\mathrm{f}^-(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{R}_\mathrm{P}) = \phi_\mathrm{f}(\boldsymbol{r}_1)\Psi_\mathrm{3C}^-(\boldsymbol{r}_\mathrm{T},\boldsymbol{R}_\mathrm{P}), \tag{3}$$

where $\phi_\mathrm{f}(\boldsymbol{r}_1) = 2^{3/2}\pi^{-1/2}\,\mathrm{e}^{-2r_1}$ is the ground-state wave function of He^+, and Ψ_3C^- can be expressed as[13]

$$\begin{aligned}\Psi_\mathrm{3C}^- =\ & C\exp(\mathrm{i}\boldsymbol{k}_\mathrm{T}\cdot\boldsymbol{r}_\mathrm{T})\exp(\mathrm{i}\boldsymbol{K}_\mathrm{P}\cdot\boldsymbol{R}_\mathrm{P})\\ & \times {}_1\mathrm{F}_1(\mathrm{i}\alpha_\mathrm{Te};1;-\mathrm{i}(k_\mathrm{T}r_\mathrm{T}+\boldsymbol{k}_\mathrm{T}\cdot\boldsymbol{r}_\mathrm{T}))\\ & \times {}_1\mathrm{F}_1(\mathrm{i}\alpha_\mathrm{PT};1;-\mathrm{i}(K_\mathrm{P}R_\mathrm{P}+\boldsymbol{K}_\mathrm{P}\cdot\boldsymbol{R}_\mathrm{P}))\\ & \times {}_1\mathrm{F}_1(\mathrm{i}\alpha_\mathrm{Pe};1;-\mathrm{i}(k_\mathrm{P}r_\mathrm{P}+\boldsymbol{k}_\mathrm{P}\cdot\boldsymbol{r}_\mathrm{P})),\end{aligned} \tag{4}$$

where $\boldsymbol{K}_\mathrm{P}$, $\boldsymbol{k}_\mathrm{T}$ are the momenta of the scattered projectile and ionized electron, respectively, which are both considered with respect to He^+. The $\boldsymbol{r}_\mathrm{P}$ represents the coordinates of the ionized electron with respect to the projectile, and C is a normalization factor given by

$$\begin{aligned}C =\ & (2\pi)^{-3}\Gamma(1-\mathrm{i}\alpha_\mathrm{PT})\Gamma(1-\mathrm{i}\alpha_\mathrm{Pe})\Gamma(1-\mathrm{i}\alpha_\mathrm{Te})\\ & \times\exp(-\pi\alpha_\mathrm{PT}/2-\pi\alpha_\mathrm{Pe}/2-\pi\alpha_\mathrm{Te}/2).\end{aligned} \tag{5}$$

The form of Sommerfeld parameters are

$$\alpha_\mathrm{PT} = \frac{\mu_\mathrm{PT}Z_\mathrm{P}Z_\infty}{K_\mathrm{P}},\quad \alpha_\mathrm{Pe} = -\frac{\mu_\mathrm{Pe}Z_\mathrm{P}}{k_\mathrm{P}},\quad \alpha_\mathrm{Te} = -\frac{\mu_\mathrm{Te}Z_\infty}{k_\mathrm{T}}. \tag{6}$$

Here μ_PT and μ_Pe are the reduced masses of the projectile-target ion subsystem and projectile–ionized electron subsystem, respectively. It is to be noted that in Eq. (4) all three two-body interactions are treated on an equal footing. An uncertain point of this model is the use of the asymptotic charge $Z_\infty = 1$.

The T-matrix element is defined as

$$T_\mathrm{fi} = \langle\Psi_\mathrm{f}^-(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{R}_\mathrm{P})|V_\mathrm{i}|\Phi_\mathrm{i}^+(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{R}_\mathrm{P})\rangle. \tag{7}$$

The perturbation V_i is the projectile–target potential in the initial state, given by

$$V_\mathrm{i} = V_\mathrm{PT}+V_\mathrm{Pe}+V_{\mathrm{Pe}_1} = \frac{Z_\mathrm{P}Z_\mathrm{T}}{R} - \frac{Z_\mathrm{P}}{r_\mathrm{P}} - \frac{Z_\mathrm{P}}{|\,\boldsymbol{R}-\boldsymbol{r}_1\,|}, \tag{8}$$

where V_PT, V_Pe, and V_{Pe_1} are the interaction potential of projectile–target nucleus, projectile–ionized electron, and projectile–passive electron, respectively, Z_P and Z_T are the charges of the projectile and the target nucleus, respectively. R represents the position of the projectile with respect to the target nucleus. Hence, equation (7) may be rewritten as

$$\begin{aligned}T_\mathrm{fi} &= T_\mathrm{PT}+T_\mathrm{Pe}+T_{\mathrm{Pe}_1}\\ &= \langle\Psi_\mathrm{f}^-|V_\mathrm{PT}|\Phi_\mathrm{i}^+\rangle + \langle\Psi_\mathrm{f}^-|V_\mathrm{Pe}|\Phi_\mathrm{i}^+\rangle + \langle\Psi_\mathrm{f}^-|V_{\mathrm{Pe}_1}|\Phi_\mathrm{i}^+\rangle.\end{aligned} \tag{9}$$

In the center-of-mass (CM) system, the FDCS is given by[14,15]

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_\mathrm{p}\,\mathrm{d}\Omega_\mathrm{e}\,\mathrm{d}E_\mathrm{e}} = N_\mathrm{e}(2\pi)^4\mu_\mathrm{Te}\mu_\mathrm{P,He}^2\frac{K_\mathrm{P}k_\mathrm{T}}{K_\mathrm{i}}|T_\mathrm{fi}|^2, \tag{10}$$

where N_e is the number of electrons in the atomic shell, μ_Te is the reduced mass of the ionized electron–target ion subsystem and $\mu_\mathrm{P,He}$ is the reduced mass of the projectile–atom system. The solid angles $\mathrm{d}\Omega_\mathrm{p}$ and $\mathrm{d}\Omega_\mathrm{e}$ represent the scattering direction for the projectile and the ejection direction for the ionized electron, respectively, and $\mathrm{d}E_\mathrm{e}$ represents the energy interval of the ejected electron.

It should be noted that, unlike the 3DW model, this model includes the passive electron in the channel wave function and in the perturbation, and treats the final state as a four-body model which contains the wave function for the passive electron and the three-Coulomb wave. While the 3DW model treats the He target within the one-active-electron approximation, in the 3DW approximation the perturbation only contains the first two items of Eq. (8), and the initial state of the ejected electron is an HF wavefunction and the final state is a static HF wavefunction.

If the projectile–target ion and projectile–ionized electron interactions are switched off ($\alpha_\mathrm{PT} = \alpha_\mathrm{Pe} = 0$), Ψ_3C^- can be transformed into Ψ_1C^-:

$$\begin{aligned}\Psi_\mathrm{1C}^- =\ & N\exp(\mathrm{i}\boldsymbol{k}_\mathrm{T}\cdot\boldsymbol{r}_\mathrm{T})\exp(\mathrm{i}\boldsymbol{K}_\mathrm{P}\cdot\boldsymbol{R}_\mathrm{P})\\ & \times {}_1\mathrm{F}_1(\mathrm{i}\alpha_\mathrm{Te};1;-\mathrm{i}(k_\mathrm{T}r_\mathrm{T}+\boldsymbol{k}_\mathrm{T}\cdot\boldsymbol{r}_\mathrm{T}))\end{aligned} \tag{11}$$

with $N = (2\pi)^{-3}\Gamma(1-\mathrm{i}\alpha_\mathrm{Te})\exp(-\pi\alpha_\mathrm{Te}/2)$. The four-body Coulomb wave final state wave function correspondingly becomes

$$\Psi_\mathrm{f1C}^- = \phi_\mathrm{f}(\boldsymbol{r}_1)\Psi_\mathrm{1C}^-. \tag{12}$$

The present result is the form of the FBA.

The nine-dimensional integral (Eq. (7)) can be reduced analytically, without any further approximation, to a two-dimensional integral on the real parameters[16,19] which has to be carried out numerically.

3. Results and discussion

The FDCS calculation is performed using the four-body model, by Eq. (10), for 100 MeV/a.u. C^{6+} impact ionization of helium both in the scattering plane and the perpendicular plane, which correspond to the measurements.[3,6] The results are displayed in Figs. 1–4 and Figs. 5 and 6, respectively. The FBA and the 3DW theoretical results[3,6] are provided for comparison. In Figs. 7 and 8, we examine the contributions of different scattering amplitudes to the cross section for the largest momentum transfer. In order to make a direct comparison with the laboratory system of experimental measurements, the cross sections in Figs. 1–8 are presented for the laboratory system. The conversion from CM to laboratory is given by a constant factor of 16[3] for the present FDCS.

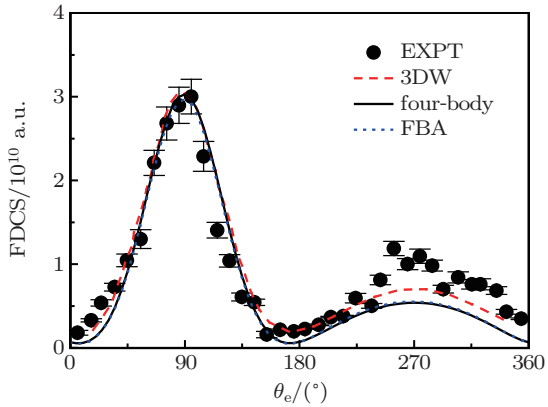


Fig. 1. (color online) FDCS for single ionization of helium by 100 MeV/a.u. C^{6+} in the scattering plane. The electron emission energy $E_e = 6.5$ eV and the momentum transfer $q = 0.75$ a.u. The angle θ_e is the emission angle of the electron. Solid circles: experimental data;[6] solid line: four-body calculation; dashed line: 3DW calculation;[6] dotted line: FBA calculation.

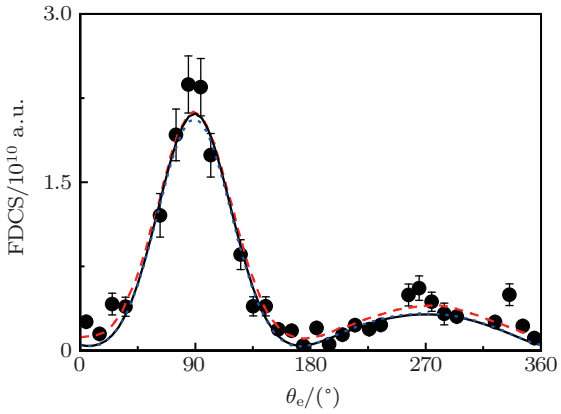


Fig. 2. (color online) The same as Fig. 1, except that the momentum transfer is 0.88 a.u. Besides, the experimental data and the 3DW results are from Ref. [3].

In the scattering plane (Figs. 1–4) the experimental results are basically qualitatively reproduced by the theoretical results. Especially in Figs. 1–3, the four-body, FBA, and 3DW calculations have almost the same results in the binary peak, which are all in reasonably good agreement with the experiment. However, from Fig. 4 for the largest momentum transfer, these theoretical results are about a factor of 2 smaller than the measured data in the binary peak. Although the 3DW results were convolved over experimental uncertainties in energy and momentum transfer, as shown in Ref. [3], the effect of convolution was small, so we do not take it into account in our theoretical results. Furthermore, it is worth noting that the recoil peak decreases rapidly as the momentum transfer increases, and all calculations correctly predict that the recoil peak disappears for the largest momentum transfer. In all cases, we notice that the 3DW results are in better agreement with experiment than the four-body and FBA results. This suggests that the four-body effect is not obvious.

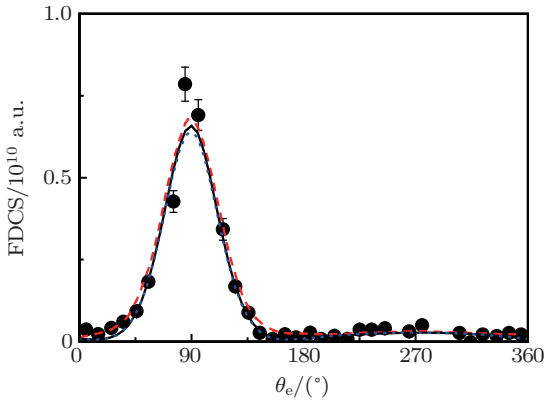


Fig. 3. (color online) The same as in Fig. 2 but for the momentum transfer of 1.43 a.u. and the ejected electron energy of 17.5 eV.

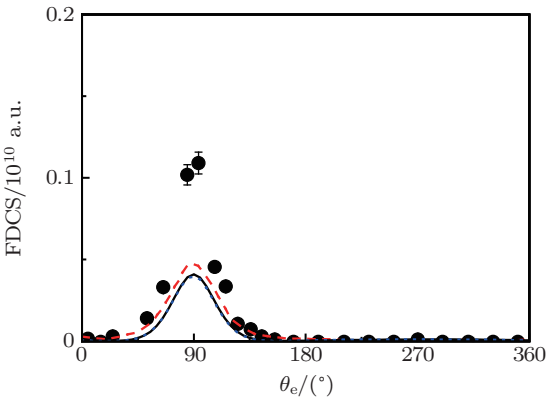


Fig. 4. (color online) The same as in Fig. 2 except that the momentum transfer is 2.65 a.u. and the ejected electron energy is 37.5 eV.

In Figs. 5 and 6, the angular dependence of the perpendicular plane is β_e defined as $\beta_e = \pi/2 - \varphi_e$, φ_e is the azimuthal angle for the ionized electron. As can be seen from Fig. 5, the agreement between experiment and theory is no better than it is in the scattering plane of Fig. 2 where the experimental data have a larger width than theoretical results for the binary peak in the perpendicular plane. In addition, Figure 6 shows a significant difference in magnitude, which is almost the same case as the FDCS for the scattering plane in Fig. 4. It is clear

that the 3DW approximation yields cross sections that show some superiority over the four-body results (see Figs. 5 and 6). Therefore, a similar conclusion within the scattering plane is that the three-body approximation has a better description of the experimental data on the ionization cross section, and the four-body effect does not improve the agreement between the present results and the experiment. In fact, so far, none of the existing theoretical models[7,17] have been able to explain the marked discrepancy observed between experiment and theory. This remains a very challenging task for the theoretical workers.

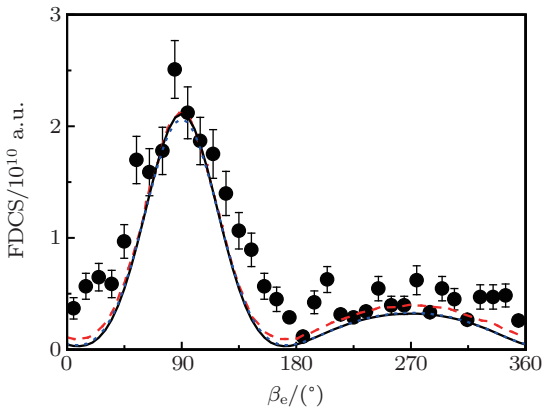


Fig. 5. (color online) The same as in Fig. 2 but the cross section is given in the plane perpendicular to the incident beam direction, containing the momentum transfer q. The angular dependence for the perpendicular plane is β_e.

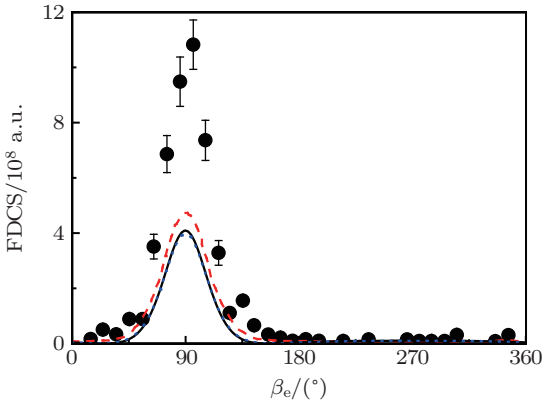


Fig. 6. (color online) The same as Fig. 5 except that the momentum transfer is 2.65 a.u. and the ejected electron energy is 37.5 eV.

To explore the physical origin of the peak structure in the FDCS for the largest momentum transfer in and out of the scattering plane, we examine the contributions of various scattering amplitudes to the FDCS in the present four-body model, as shown in Figs. 7 and 8, respectively.

We can see from Figs. 7 and 8 that the partial cross sections arising from $T_{\rm Pe}$, $T_{\rm PT}$, and $T_{\rm Pe_1}$ have the same peak position. In addition, the largest individual incoherent contribution to the cross section around the binary region comes from the scattering amplitude $T_{\rm Pe}$, followed by amplitude $T_{\rm PT}$, and the smallest contribution is the amplitude $T_{\rm Pe_1}$. Therefore, the structure for the largest momentum transfer observed in the measured FDCS can definitely be attributed to the postcollision interaction (PCI) between the outgoing projectile and the ejected electron.[18] This is different from the case of proton impact ionization (see Ref. [19] and references therein). Furthermore, although the incoherent contribution from the amplitude $T_{\rm Pe_1}$ is the smallest, the major interference contribution to the cross section is from the constructive interference of the scattering amplitudes $T_{\rm Pe}$ and $T_{\rm Pe_1}$. From Figs. 7 and 8, the interference between $T_{\rm Pe}$ and $T_{\rm Pe_1}$ leads to a cross section that almost tends towards an experimental binary peak. This means that the amplitude $T_{\rm Pe_1}$ cannot be neglected in the calculation. One of the reasons for the failure of the 3DW model predicting the observed features in these geometries may be due to the fact that it does not contain the projectile–passive electron interaction. However, when $T_{\rm PT}$ is switched on, the destructive interference of the three scattering amplitudes (see Eq. (9)) makes the magnitudes of this binary peak smaller than the peak of interference of $T_{\rm Pe}$ and $T_{\rm Pe_1}$. This indicates that the role of the internuclear interaction (PT interaction) is unimportant in the observed cross sections, as shown the conclusions made in Ref. [9]. We may safely draw the conclusion that the binary peak of the experiment for the largest momentum transfer in the scattering plane and perpendicular plane mainly arise from an interference effect between the scattering amplitudes $T_{\rm Pe}$ and $T_{\rm Pe_1}$, the coherent contribution of the amplitude $T_{\rm PT}$ only influences the magnitude of the peak. However, in Fig. 5 the measured FDCS seems to appear peak structure for small angle and large angle directions. The theoretical result and further calculation indicate that the theory does not show an experimental additional peak structure, and the results of theoretical analysis are consistent with the above conclusion. In view of this, the failure of the four-body model predicting the peak structures of the experiment for the largest momentum transfer might have been traced back to an inappropriate weighting of the amplitudes $T_{\rm PT}$, $T_{\rm Pe}$, and $T_{\rm Pe_1}$.

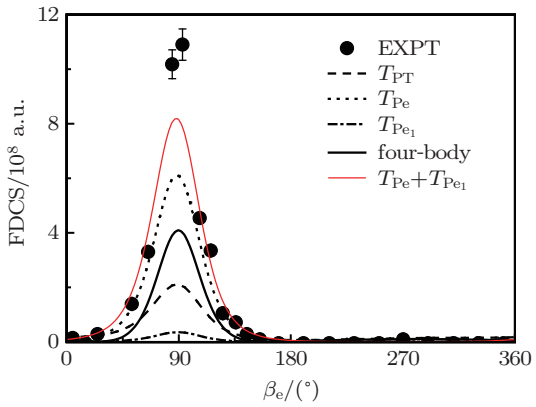


Fig. 7. (color online) The same geometry as in Fig. 4. The thick curve represents the four-body result. The incoherent contributions to the FDCS of the scattering amplitudes $T_{\rm PT}$ (dashed curve), $T_{\rm Pe}$ (dotted curve), $T_{\rm Pe_1}$ (dash–dotted curve), and the coherent sum of $T_{\rm Pe}$ and $T_{\rm Pe_1}$ (light solid curve).

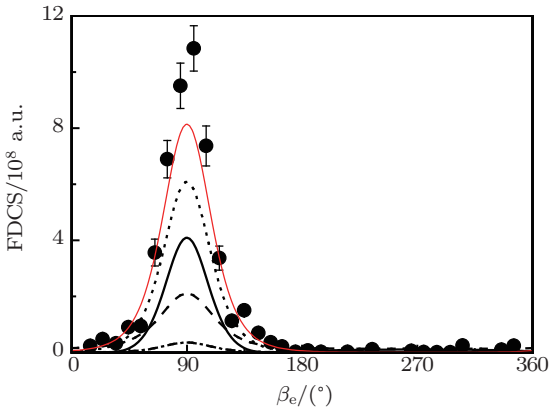


Fig. 8. (color online) The same as in Fig. 7 expect that the cross section is given in the perpendicular plane.

4. Conclusion

We have carried out calculations of FDCS for single ionization of helium by 100 MeV/a.u. C^{6+} projectiles using a four-body theory, both in and out of the scattering plane. It is clearly seen that the four-body results are in good agreement with the absolute experimental data at three small momentum transfers in the scattering plane. However, at the largest momentum transfer in both the scattering plane and the perpendicular plan, the four-body results are much smaller than the experiment in the binary peak. Consequently, in comparison with the 3DW and FBA, the four-body effect is not obvious and does not improve the agreement between the present results and the experiment. We further study the contributions of various scattering amplitudes to FDCS in the present model. It is found that the shape of the structure at the largest momentum transfer in both the scattering and perpendicular planes mainly depends on the coherent sum of $T_{\rm Pe}$ and $T_{\rm Pe_1}$. The $T_{\rm PT}$ interference with two other scattering amplitudes will influence the magnitude of the peak. This indicates that the cross sections are strongly influenced by the interference that is caused by weighting these amplitudes differently. In addition, in our theoretical calculation, the projectile beam is treated as completely coherent. While a recent study[20] indicates that a projectile beam is not coherent in experiment. If the projectile beam is prepared coherently experimentally, the agreement between experiment and theory will be improved. Of course, the validity will need to be further tested by experiment.

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