Fully differential cross sections for C^{6+} single ionization of helium*

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The three-Coulomb-wave (3C) model is applied to study the single ionization of helium by 2 MeV/amu C^{6+} impact. Fully differential cross sections (FDCS) are calculated in the scattering plane and the results are compared with experimental data and other theoretical predictions. It is shown that the 3C results of the recoil peak are in very good agreement with experimental observations, and variation of the position of the binary peak with increasing momentum transfer also conforms better to the experimental results. Furthermore, the contributions of different scattering amplitudes are discussed. It turns out that the cross sections are strongly influenced by the interference of these amplitudes.

Keywords: ion–atom impact ionization, fully differential cross section, three-Coulomb wave function

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1. Introduction

Studies on ion–atom collisions has been a field of intense activity in atomic physics. In spite of decades of extensive research, even single ionization processes occurring in charged particle–atom collisions have not been completely understood.[1,2] In particular, the heavy-particle-impact single ionization of helium has attracted much attention. Recently, Fischer *et al.*[3] measured the fully differential cross sections (FDCS) for single ionization of helium by 2 MeV/amu C^{6+} impact. They compared their data with the continuum distorted wave-eikonal initial state (CDW-EIS) calculations in the scattering plane. Subsequently, the experimental data were compared with theoretical predictions from an even better approach called three-body distorted wave-eikonal initial state (3DW-EIS) developed by Foster *et al.*[4] It turned out that the 3DW-EIS results were in better agreement with experimental measurements than the CDW-EIS results for nearly every kinematical condition. However, even for this sophisticated theory, the agreement between experiment and theory does not lead to the expected accuracy, particularly for large momentum transfer and low ejected electron energy. A recently developed coupled pseudostate (CP) approximation by McGovern *et al.*[5] was applied to calculate the FDCS for single ionization of helium by C^{6+} projectiles at the same incident energy. However, there are still some discrepancies between the CP theory and experiment. Accordingly, further theoretical analysis and calculations seem appropriate and interesting.

In this work, we use the three-Coulomb (3C) wave method, which has been extensively applied in the fields of electron–atom[6] and ion–atom collisions,[7,8] to calculate the FDCS for single ionization of helium by 2 MeV/amu C^{6+} impact in the scattering plane. In the present model, the initial state is represented as a product of the plane wave for the projectile and the Hartree Fock (HF) ground-state wave function of helium. The final state is approximated as a product of the He^+ ground-state wave function for a passive electron and the three-Coulomb wave. It should be noted that, unlike the 3DW model, this model includes the passive electron in the channel wave function and in the perturbation (details are given in the next section). The aim of this article is to compare the 3C cross sections with the corresponding experimental results, and to assess the ability of the present method to reproduce the peak structure of the experimental data. It makes a significant difference whether the projectile interacts with a He^+ ion or with the He^{2+}

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nucleus and the passive electron separately. The theoretical approach to be used will be described in Section 2. In Section 3, the 3C results are discussed and the good agreement of the present results with experiment is obtained. In particular, the importance of interference effects in determining the shape of the FDCS is demonstrated. Moreover, the physical origin of the features in the FDCS is explained. In Section 4, conclusions are drawn. Atomic units are used throughout the paper unless otherwise stated.

2. Theoretical treatments

In this section, we briefly sketch the theoretical model. Here we consider single ionization of helium by the impact of C^{6+} with incident momentum $\boldsymbol{K}_\mathrm{i}$ relative to the atomic center of mass. The $\boldsymbol{K}_\mathrm{P}$ and $\boldsymbol{k}_\mathrm{T}$ are the momenta of scattered projectile and ejected electron, respectively, with respect to the center of mass of target ion (He^+). The FDCS in the center-of-mass (CM) system is given by[9,10]

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_\mathrm{p}\mathrm{d}\Omega_\mathrm{e}\mathrm{d}E_\mathrm{e}} = N_\mathrm{e}(2\pi)^4\mu_\mathrm{Te}\mu_\mathrm{P,He}^2\frac{K_\mathrm{P}k_\mathrm{T}}{K_\mathrm{i}}|T_\mathrm{fi}|^2, \quad (1)$$

where N_e is the number of electrons in the atomic shell, $\mathrm{d}\Omega_\mathrm{p}$ and $\mathrm{d}\Omega_\mathrm{e}$ denote the differential solid angles with respect to $\boldsymbol{K}_\mathrm{i}$ for the scattered projectile and ejected electron, respectively, and $\mathrm{d}E_\mathrm{e}$ represents the energy interval of the ejected electron. The reduced masses are given by

$$\mu_\mathrm{Te} = \frac{M_\mathrm{T}+1}{M_\mathrm{T}+2}, \quad \mu_\mathrm{P,He} = \frac{M_\mathrm{P}(M_\mathrm{T}+2)}{M_\mathrm{P}+M_\mathrm{T}+2}, \quad (2)$$

where μ_Te is the reduced mass of the ionized electron–target ion subsystem, $\mu_\mathrm{P,He}$ is the reduced mass of the projectile–atom system, M_T is the mass of the target nucleus, and M_P is the mass of the projectile. The electron mass is numerically unity in atomic units.

The T-matrix element is defined as

$$T_\mathrm{fi} = \langle\Psi_\mathrm{f}^-(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{r}_\mathrm{P},\boldsymbol{R}_\mathrm{P})|V_\mathrm{i}|\Phi_i^+(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{R}_\mathrm{P})\rangle, \quad (3)$$

where $\boldsymbol{r}_\mathrm{P}$ and $\boldsymbol{r}_\mathrm{T}$ represent the coordinates of the ionized electron with respect to the projectile and target ion, respectively, $\boldsymbol{R}_\mathrm{p}$ is the position of the projectile relative to the atomic center of mass, and $\boldsymbol{r}_1$ is the coordinate of the passive electron relative to the target nucleus.

The initial state Φ_i^+ is expressed as

$$\begin{aligned}\Phi_\mathrm{i}^+(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{R}_\mathrm{P}) &= \left(\frac{1}{2\pi}\right)^{3/2}\exp(\mathrm{i}\boldsymbol{K}_\mathrm{i}\cdot\boldsymbol{R}_\mathrm{P})\phi_\mathrm{i}(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T}). \quad (4)\end{aligned}$$

For the bound-state wave function ϕ_i, we choose the analytical fitting to the Hartree-Fock (HF) wave function given by Byron and Joachain[11]

$$\phi_\mathrm{i}(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T}) = U(\boldsymbol{r}_1)U(\boldsymbol{r}_\mathrm{T}), \quad (5)$$

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 $\beta = 2.61$.

Perturbation corresponding to the initial state is given by

$$\begin{aligned}V_\mathrm{i} &= V_\mathrm{PT} + V_\mathrm{Pe} + V_\mathrm{Pe_1} \\ &= \frac{Z_\mathrm{P}Z_\mathrm{T}}{R} - \frac{Z_\mathrm{P}}{r_\mathrm{P}} - \frac{Z_\mathrm{P}}{|\,\boldsymbol{R}-\boldsymbol{r}_1\,|}, \quad (6)\end{aligned}$$

where Z_P and Z_T are the charges of the projectile and target nucleus, respectively. Hence, Eq. (3) may be rewritten as

$$\begin{aligned}T_\mathrm{fi} &= T_\mathrm{PT} + T_\mathrm{Pe} + T_\mathrm{Pe_1} \\ &= \langle\Psi_\mathrm{f}^-|V_\mathrm{PT}|\Phi_\mathrm{i}^+\rangle + \langle\Psi_\mathrm{f}^-|V_\mathrm{Pe}|\Phi_\mathrm{i}^+\rangle \\ &\quad + \langle\Psi_\mathrm{f}^-|V_\mathrm{Pe_1}|\Phi_\mathrm{i}^+\rangle. \quad (7)\end{aligned}$$

Here T_PT, T_Pe, and $T_\mathrm{Pe_1}$ stem from the interaction of the incoming projectile with the target nucleus, the ejected electron, and passive electron, respectively.

The final state wave function Ψ_f^- is approximated as

$$\Psi_\mathrm{f}^-(\boldsymbol{r}_1,\boldsymbol{r}_\mathrm{T},\boldsymbol{r}_\mathrm{P},\boldsymbol{R}_\mathrm{P}) = \phi_\mathrm{f}(\boldsymbol{r}_1)\Psi_\mathrm{3C}^-(\boldsymbol{r}_\mathrm{T},\boldsymbol{r}_\mathrm{P},\boldsymbol{R}_\mathrm{P}), \quad (8)$$

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 the three Coulomb wave Ψ_3C^- can be expressed as[6]

$$\begin{aligned}\Psi_\mathrm{3C}^- &= C\exp(\mathrm{i}\boldsymbol{k}_\mathrm{T}\cdot\boldsymbol{r}_\mathrm{T})\exp(\mathrm{i}\boldsymbol{K}_\mathrm{P}\cdot\boldsymbol{R}_\mathrm{P}) \\ &\quad \times {}_1\mathrm{F}_1(\mathrm{i}\alpha_\mathrm{Te};1;-\mathrm{i}(k_\mathrm{T}r_\mathrm{T}+\boldsymbol{k}_\mathrm{T}\cdot\boldsymbol{r}_\mathrm{T})) \\ &\quad \times {}_1\mathrm{F}_1(\mathrm{i}\alpha_\mathrm{PT};1;-\mathrm{i}(K_\mathrm{P}R_\mathrm{P}+\boldsymbol{K}_\mathrm{P}\cdot\boldsymbol{R}_\mathrm{P})) \\ &\quad \times {}_1\mathrm{F}_1(i\alpha_\mathrm{Pe};1;-\mathrm{i}(k_\mathrm{P}r_\mathrm{P}+\boldsymbol{k}_\mathrm{P}\cdot\boldsymbol{r}_\mathrm{P})), \quad (9)\end{aligned}$$

where $\boldsymbol{k}_\mathrm{P} = (1-\gamma)\boldsymbol{k}_\mathrm{T} - (\delta(1-\gamma)+\gamma)\boldsymbol{K}_\mathrm{P}$ ($\gamma = (M_\mathrm{P}+1)^{-1}$, $\delta = (M_\mathrm{T}+1)^{-1}$), ${}_1\mathrm{F}_1$ is the confluent hypergeometric function, and C is a normalization factor given by

$$\begin{aligned}C &= (2\pi)^{-3}\Gamma(1-\mathrm{i}\alpha_\mathrm{PT})\Gamma(1-\mathrm{i}\alpha_\mathrm{Pe})\Gamma(1-\mathrm{i}\alpha_\mathrm{Te}) \\ &\quad \times \exp(-\pi\alpha_\mathrm{PT}/2 - \pi\alpha_\mathrm{Pe}/2 - \pi\alpha_\mathrm{Te}/2), \quad (10)\end{aligned}$$

where Γ is the gamma function. The form of the dynamical Sommerfeld parameters α_PT, α_Pe, and α_Te are

$$\alpha_\mathrm{PT} = \frac{\mu_\mathrm{PT}Z_\mathrm{P}Z_\infty}{K_\mathrm{P}}, \quad \alpha_\mathrm{Pe} = \frac{\mu_\mathrm{Pe}Z_\mathrm{P}}{k_\mathrm{P}},$$

$$\alpha_{\rm Te} = \frac{\mu_{\rm Te} Z_\infty}{k_{\rm T}}, \tag{11}$$

where $\mu_{\rm PT}$ and $\mu_{\rm Pe}$ are the reduced masses of the projectile–target ion subsystem and projectile–ionized electron subsystem, respectively, and Z_∞ is the charge of the target ion. An uncertain point of this model represents the use of the asymptotic charge $Z_\infty = 1$.

The wave function in Eq. (9) approximates the three-body final state as three two-body subsystems and accounts for multiple scattering within these subsystems to infinite order. It is notable that in Eq. (9) all three two-body interactions are treated on an equal footing.

It is worth noting that in the 3DW approximation, helium atom is treated as a hydrogenlike atom, so the projectile–passive electron interaction is not considered in the perturbation. The description of the final-state wave function for the ejected electron is also different. In the 3C calculations, the wave function for the ejected electron is a Coulomb wave. Whereas in the 3DW approximation, it is a numerical solution of the HF Schrödinger equation. If an eikonal phase is taken into account in the initial state, the 3DW approximation becomes the 3DW-EIS model (see Ref. [4] for a detailed discussion).

The nine-dimensional integral (Eq. 3) can be reduced analytically, without any further approximation, to a two-dimensional integral on the real parameters[12] which has to be carried out numerically.

3. Results and discussion

In order to check the accuracy of the 3C model, we have computed the FDCS, using Eq. (1), for C^{6+} impact ionization of helium at an incident energy of 2 MeV/amu in the coplanar geometry, which corresponds to the recent measurements.[3] The results are displayed in Figs. 1–3. The 3DW-EIS[4] and the CP theoretical results[5] are also provided for comparison. Although all the formulae are given for the CM system, the cross sections in Figs. 1–3 are presented for the laboratory system. The conversion from CM to laboratory is given by a constant factor of 16[8] for the present FDCS.

In all cases, we notice a double-peak structure in the angular distributions. The larger peak is normally called the binary peak and the smaller peak is called the recoil peak. Before we proceed with analyzing the dynamical origin of these structures, it is advantageous to study the classical kinematical properties of the collisions that are common to all dynamical models. In Figs. 1–3, the 3C results (solid line), the 3DW-EIS calculations (dashed line), and the CP theoretical results (dotted line) are all in reasonably good agreement with experiment. However, the 3C results are in much better agreement with experiment than the 3DW-EIS and CP results for the recoil peak. For the cases of smaller momentum transfer $q = 0.45$ a.u. and $q = 0.65$ a.u., it is clearly seen that the binary peak is somewhat shifted toward larger ejection angles, in contrast to the experimental data. However, the shift of the binary peak systematically decreases with increasing q. For larger $q = 1.0$ a.u. and $q = 1.5$ a.u., the 3C results are in quite good agreement with experiment both in shape and magnitude except for the case of $E_{\rm e} = 10$ eV where the 3C calculations overestimate the binary peak of the experiment. For the 3DW-EIS and CP results, a disagreement with experiment relative to the 3C results is seen to the extent that the recoil peak is reduced for all cases. On the other hand, the 3C theory fails to give the correct magnitudes of the experiment around the ejected electron angle $\theta_{\rm e} = 0°$ (or $\theta_{\rm e} = 360°$) especially for smaller q. This trend is also observed in the 3DW-EIS and

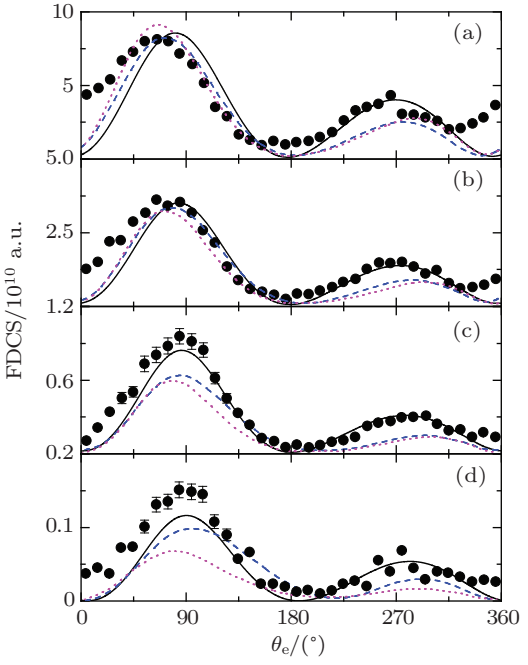


Fig. 1. (colour online) Fully differential cross sections in the scattering plane for 2 MeV/amu C^{6+} single ionization of helium. The ejected electron energy is 1.0 eV and the momentum transfers are (a) 0.45, (b) 0.65, (c) 1.0, and (d) 1.5 a.u., respectively. The angle $\theta_{\rm e}$ is the emission angle of the electron. The solid circles represent the experimental measurements.[3] The 3C (solid), 3DW-EIS[4] (dashed), and CP (dotted) results are also shown.

CP theories. Here we see very reasonable agreement between the three theories. In view of this, we are inclined to suggest that it may not be the theory that is at fault. According to McGovern *et al.*,[5] this discrepancy between theories and experiment implies that the ejected electron is dragged behind the outgoing C^{6+} to a greater extent than predicted by theory (i.e., a larger postcollisional interaction (PCI)).

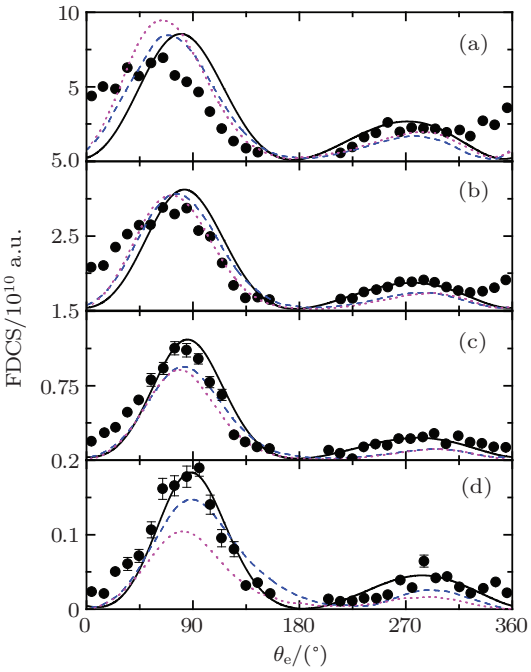


Fig. 2. (colour online) Same as Fig. 1 except that the ejected electron energy is 4.0 eV.

From the preceding discussion, it is obvious that in the 3C calculations the position of the binary peak gets better with increasing q for each of the ejected electron energies, especially for the cases of lower ejected electron energies and larger momentum transfers, and the 3C results are in better agreement with experiment than the 3DW-EIS results. Maybe the differences in the theories lead to the discrepancies in the calculated results. From Eq. (6), it can be seen that in the present calculations the perturbation contains all the interactions between the projectile and target atom (i.e., the sum of the projectile–target nucleus, projectile–ejected electron, and projectile–passive electron interactions). However, the 3DW-EIS model does not consider the projectile–passive electron interaction. The other discrepancy is that in Eq. (8), the present 3C calculations treat the final state as a four-body model which contains the wave function for the passive electron and the three-Coulomb wave, whereas the 3DW-EIS model uses a three-body final-state wave function much like that in Eq. (9). Furthermore, although the 3DW-EIS approach contains the eikonal-initial-state (EIS) approximation, it seems that the initial-state interactions have almost no effect on the calculation.[4] These differences may improve the agreement between the present results and the experiment.

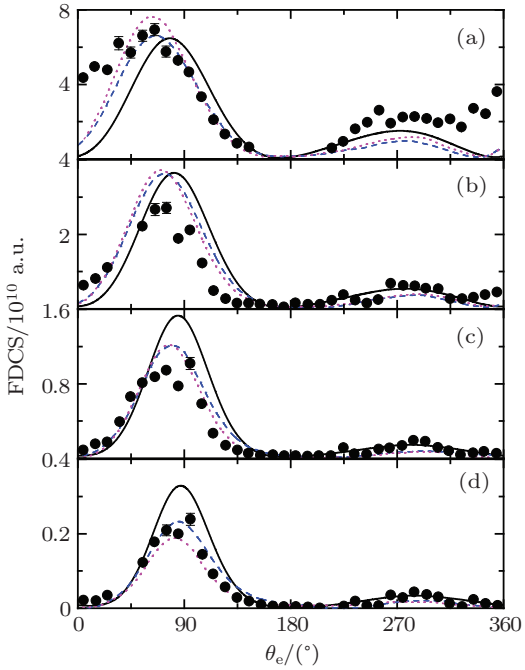


Fig. 3. (colour online) Same as Fig. 1 except that the ejected electron energy is 10.0 eV.

To explore the physical origin of the peak structure in the FDCS, we examine the contributions of different scattering amplitudes to the cross section for the case of ejected electron energy of 1.0 eV and momentum transfer of 0.45 a.u. From Fig. 4, the major individual incoherent contribution to the cross section around the binary region comes from the scattering amplitude $T_{\rm PT}$. This is different from the case of electron-impact ionization (see Refs. [12]–[14] and references therein). Furthermore, the partial cross sections arising from $T_{\rm PT}$ and $T_{\rm Pe}$ have the same peak position. However, a destructive interference of $T_{\rm PT}$ and $T_{\rm Pe}$ leads to a cross section much smaller than the incoherent two amplitudes. Furthermore, the interference also makes the position of the binary peak shift toward larger angles relative to the peak of the incoherent two amplitudes. When $T_{\rm Pe_1}$ is switched on, the interference effect of the three scattering amplitudes (see Eq. (7)) makes this peak shift toward smaller angles and makes the magnitudes smaller than that of the peak due to interference of $T_{\rm PT}$ and $T_{\rm Pe}$, which approaches the experimental data at larger q. However,

for the highest ejected electron energy and larger q, the 3C results overestimate the binary peak of the experiment. The failure of the 3C model predicting the binary peak of the experiment might have been traced back to an inappropriate weighting of the amplitudes $T_{\rm PT}$, $T_{\rm Pe}$, and $T_{\rm Pe_1}$.

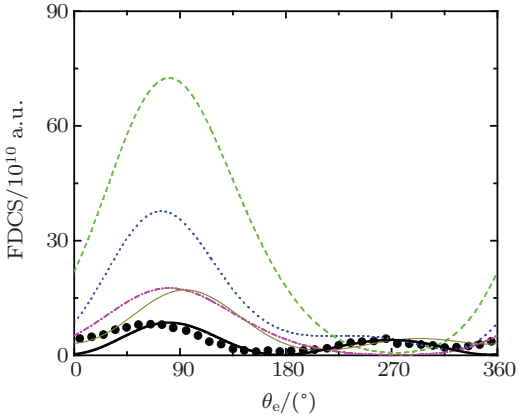


Fig. 4. (colour online) Fully differential cross sections in the scattering plane for 2 MeV/amu C^{6+} single ionization of helium. The ejected electron energy is 1.0 eV and the momentum transfer is 0.45 a.u. The incoherent contributions to the FDCS (thick solid curve) of the scattering amplitudes $T_{\rm PT}$ (dashed curve), $T_{\rm Pe}$ (dotted curve), $T_{\rm Pe_1}$ (dash-dotted curve), and the coherent sum of $T_{\rm PT}$ and $T_{\rm Pe}$ (light solid curve).

In order to observe distinctly the contributions of various scattering amplitudes to the recoil peak, in Fig. 5 we independently display the FDCS with the ejected electron angle ranging from 180° to 360°. From Fig. 5, it seems that the dominant incoherent contribution to the cross section around the recoil peak comes from the scattering amplitude $T_{\rm Pe}$. Just as the case of the binary peak, this is also different from electron-impact ionization. Moreover, it is evidently seen that all the three partial cross sections arising from $T_{\rm PT}$, $T_{\rm Pe}$, and $T_{\rm Pe_1}$ do not show the recoil peak structure. The main point is that the partial cross section arising from $T_{\rm Pe}$ would not give a distinct recoil peak, but merely a shoulder on the cross section. However, the cross section originating from interference between $T_{\rm PT}$ and $T_{\rm Pe}$ reveals a distinct peak. When $T_{\rm Pe_1}$ is switched on, the interference of the three amplitudes not only makes the peak shift toward smaller angles but also makes the magnitudes of the peak smaller than that of the peak due to interference between $T_{\rm PT}$ and $T_{\rm Pe}$. It demonstrates that the shape of the recoil peak mainly depends on the interference between $T_{\rm PT}$ and $T_{\rm Pe}$, and the coherent contribution of the amplitude $T_{\rm Pe_1}$ has influenced the position and magnitudes of the peak. Thus, the amplitude $T_{\rm Pe_1}$ cannot be neglected in the calculation. It is worth noting that the partial cross sections from $T_{\rm PT}$, $T_{\rm Pe}$, and $T_{\rm Pe_1}$ all exhibit a rising trend around $\theta_{\rm e} = 0°$ (or $\theta_{\rm e} = 360°$), whereas the new feature is that an extremely small or even vanishing cross section arises from a destructive interference of $T_{\rm PT}$, $T_{\rm Pe}$, and $T_{\rm Pe_1}$. As mentioned above, the structure of the FDCS is determined by the interference pattern by weighting these amplitudes differently.

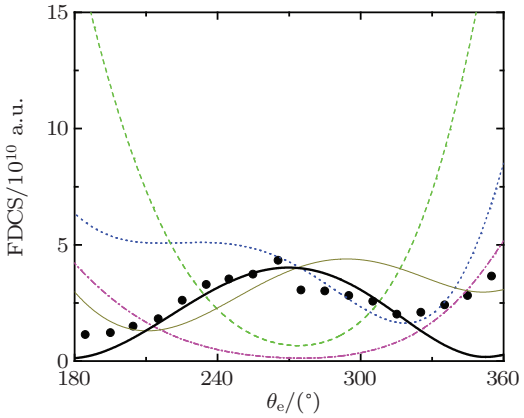


Fig. 5. (colour online) Same as Fig. 4 except that the ejected electron angle is from 180° to 360°.

4. Conclusion

We have carried out the 3C calculations of FDCS for the single ionization of helium by 2 MeV/amu C^{6+} impact in the scattering plane. We note a satisfactory, although not perfect, agreement of the 3C calculations with experimental findings. The 3C results are in very good agreement with experiment in the recoil peak for all the cases, and the variation of positions of the binary peak with increasing momentum transfer gains better agreement with experiment for each ejected electron energy. More importantly, the 3C results are in better agreement with the experiment than the 3DW-EIS and CP theoretical results for the cases of lower ejected electron energies and larger momentum transfers. We also examined the contributions of various scattering amplitudes to the FDCS, which indicates that the cross sections are strongly influenced by the interference by weighting these amplitudes differently. In addition, the coherent contributions of amplitude $T_{\rm Pe_1}$ influence the position and magnitudes of the peak, so the projectile–passive electron interaction cannot be neglected in the calculation. However, the agreement between experiment

and theory is still not as good as expected. Particularly for smaller momentum transfer, the position of the binary peak is shifted toward larger angles. Consequently, the present approach still neglects some important physical effects. For example, the dynamical correlation during the collision[15] or polarization of the helium atom[16] is responsible for the observed behavior, and further theoretical work is needed. This is also our future work to be done.

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