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Coulomb three-body effects in the single ionization of helium by 16MeV O^{7+} impact

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Abstract. Three-Coulomb-wave (3C) model is applied to study the single ionization of helium by 16MeV O^{7+} impact in the scattering plane. Fully differential cross sections (FDCS) is presented for the different momentum transfers. Our theoretical results are compared with the recent experimental data and the results of continuum distorted-wave eikonal-initial-state (CDW-EIS). It is shown that the 3C calculations qualitatively reproduce the experimental peak structure, especially at smaller momentum transfers.

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Key words: Three-Coulomb-wave,single ionization,fully differential cross section

1 Introduction

Single ionization by highly charged particle impact is a particularly suitable reaction for studying ion-atom collisions problem. With the development of the experimental technique known as COLTRIMS (cold target recoil ion momentum spectroscopy) [1], the fully differential cross-sections (FDCS) for single ionization by ion impact became available and providing a very stringent test of the theory. In particular, the heavy charged particle impact single ionization of helium has attracted much attention. Schulz *et al.* [2] and Madison D H *et al.* [3] measured the FDCS for single ionization of helium by 100MeV amu^{-1} C^{6+} . Fischer *et al.* [4] reported absolute experimental measurements for 2MeV amu^{-1} C^{6+} and 3.6MeV amu^{-1} Au^{Q+} (Q = 24, 53) single ionization of helium. Recently, Schulz *et al.* [5] measured the FDCS for target ionization in16MeV O^{7+} + He collisions.

On the theoretical side, a lot of calculations have been carried out for this particular process. For example, the first Born approximation (FBA) [6], the three-body distorted-wave (3DW) [7], the continuum distorted-wave eikonal-initial-state (CDW-EIS) approxi-

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mation [8] and the coupled-pseudostate (CP) approach [9] . Although their results qualitatively reproduced many of the features of the cross section and are in agreement with the experimental results , significant discrepancies can still be noticed.

The three-Coulomb-wave (3C) [10] is well known and have been shown to be capable of predicting the shapes of cross sections for various types of (e, 2e) and positron-impact ionization processes at intermediate and high energies [10-12]. The description was extended to high energy C^{6+} $-$ helium ionization and showed quite good agreement with experimental values at small momentum transfer in the scattering plane [13].

Following the idea of [13], we study the triple differential cross section for single ionization of helium by 16MeV O^{7+} impact in the scattering plane. It is worth noting that this model includes the passive electron in the channel wave function and in the perturbation. It is observed that 3C calculations qualitatively reproduce the experimental peak structure, especially at smaller momentum transfers.

2 Theoretical treatment

Considering single ionization of helium by the impact of O^{7+} with incident momentum $\mathbf{K}_i$ relative to the atomic center of mass. The $\mathbf{K}_P$ and $\mathbf{k}_T$ are the momenta of scattered projectile and ejected electron, respectively. The FDCS in the CM system is given by [11,12]

$$\frac{d^3\sigma}{d\Omega_P d\Omega_e dE_e} = N_e(2\pi)^4 \mu_{Te} \nu_P^2 \frac{K_P k_T}{K_i} |T_{fi}|^2, \tag{1}$$

where N_e is the number of electrons in the atomic shell. $d\Omega_P$ and $d\Omega_e$ denote the differential solid angles with respect to $\mathbf{K}_i$ for the scattered projectile and the ionized electron, respectively. And dE_e represents the energy interval of the ionized electron. μ_{Te} is the reduced mass of the ionized electron-He^+ subsystem and ν_P is the reduced mass of projectile-atom system. The T-matrix is defined as

$$T_{fi} = \langle \Psi_f^-(\mathbf{r}_1,\mathbf{r}_T,\mathbf{R}_P)|V_i|\Phi_i(\mathbf{r}_1,\mathbf{r}_T,\mathbf{R}_P)\rangle, \tag{2}$$

here $\mathbf{r}_T$ represents the coordinate of the ionized electron with respect to the target core. $\mathbf{R}_P$ is the position of the projectile relative to the atomic center of mass, and $\mathbf{r}_1$ is the coordinate of the remaining passive electron relative to the target nucleus. $\mathbf{R}$ is also needed, representing the position of the projectile with respect to the target nucleus.

The initial state wave function Φ_i will be written as the product of a plane wave with momentum $\mathbf{K}_i$ for the projectile and a wave function of helium atom in the ground state

$$\Phi_i = (2\pi)^{-3/2} \exp(i\mathbf{K}_i \cdot \mathbf{R}_P)\phi_i(r_1,r_T). \tag{3}$$

In the present calculation, we have chosen the analytical fit to the Hartree-Fock wave function given by Byron and Joachain [14] to describe $\phi_i(r_1,r_T)$,

$$\phi_i(r_1,r_T) = U(r_1)U(r_T), \quad U(r) = (4\pi)^{-1/2}(A\exp(-\alpha r) + B\exp(-\beta r)) \tag{4}$$

where A=2.60505, B=2.08144, α=1.41, β=2.61.

And the perturbation V_i is the projectile-target potential in the initial channel, i.e. the undiagonalized part of the total interaction in that channel,

$$V_i = \frac{Z_T Z_P}{R} - \frac{Z_P}{r_P} - \frac{Z_P}{|\mathbf{r}_1 - \mathbf{R}|}, \tag{5}$$

here $\mathbf{r}_P$ represents the coordinate of the ionized electron with respect to the projectile. Z_P and Z_T are the charges of the projectile and the target nucleus, respectively.

The final state wave function is represented by a product of the three-Coulomb wave and the ground-state wave function of the hydrogen-like ion

$$\Psi_f^-(\mathbf{r}_1,\mathbf{r}_T,\mathbf{r}_P,\mathbf{R}_P) = \varphi(\mathbf{r}_1)\psi_{3c}^-(\mathbf{r}_T,\mathbf{r}_P,\mathbf{R}_P), \tag{6}$$

where $\psi_{3c}^-(\mathbf{r}_T,\mathbf{r}_P,\mathbf{R}_P)$ can be expressed as [10]

$$\begin{aligned}\psi_{3c}^- = & N\exp(i\mathbf{k}_T\cdot\mathbf{r}_T)\exp(i\mathbf{K}_P\cdot\mathbf{R}_P)\,{}_1F_1(i\alpha_{Te};1;-i(k_T r_T)+\mathbf{k}_T\cdot\mathbf{r}_T)\\ & {}_1F_1(i\alpha_{PT};1;-i(K_P R_P)+\mathbf{K}_P\cdot\mathbf{R}_P)\,{}_1F_1(i\alpha_{Pe};1;-i(k_P r_P)+\mathbf{k}_P\cdot\mathbf{r}_P)\end{aligned} \tag{7}$$

with the normalization factor

$$N = (2\pi)^{-3}\Gamma(1-i\alpha_{Te})\Gamma(1-i\alpha_{PT})\Gamma(1-i\alpha_{Pe})\exp\left(-\frac{1}{2}\pi\alpha_{Te} - \frac{1}{2}\pi\alpha_{PT} - \frac{1}{2}\pi\alpha_{Pe}\right). \tag{8}$$

${}_1F_1$ is the confluent hypergeometric function. The Sommerfeld parameters have the form

$$\alpha_{Te} = \frac{\mu_{Te}Z_\infty}{k_T}, \quad \alpha_{PT} = \frac{\mu_{PT}Z_P Z_\infty}{K_P}, \quad \alpha_{Pe} = -\frac{\mu_{Pe}Z_P}{k_P}, \tag{9}$$

where μ_{PT}, μ_{Pe} are the reduced masses of the projectile target and projectile electron subsystem, respectively. Z_∞ is the charge of the target core.

The wave function Eq. (7) approximates the three-body final state as three two-body subsystems and accounts for multiple scattering within these subsystems to infinite order. It is to be noted that in (7) all three two-body interactions are treated on an equal footing. An uncertain point of this model represents the use of the asymptotic charge Z_∞=1.

3 Results and discussion

In order to check the accuracy of the 3C model, we have computed the FDCS for 16MeV O^{7+} impact ionization of helium and electron ejected into the scattering plane with ejected electron energy of 8 eV, which corresponds to the measurements of Schulz *et al.* [5]. In Figs. 1-3, the experimental results of Schulz *et al.* [5] and theoretical results of the CDW-EIS method [5] have also been provided in the figure for comparison. We present the

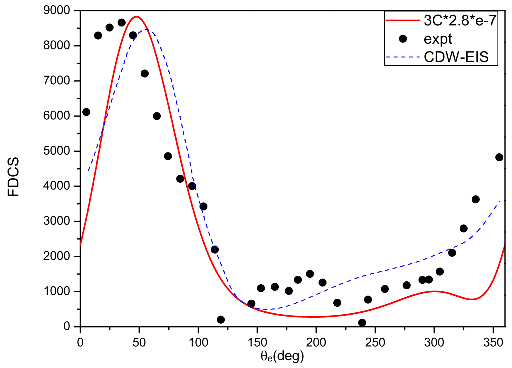

Figure 1: (Color online) FDCS in the scattering plane for 16Mev O^{7+} single ionization of helium with the ejected electron energy is 8 eV. The momentum transfer is 0.5 a.u.. The angle θ_e is the emission angle of the electron. Solid lines: 3C calculations. Dashed lines: CDW-EIS [5]. Solid circles: experimental data [5].

results of theoretical calculations for different momentum transfer values q of 0.5, 1.5 and 4 a.u. in the scattering plane. We have been multiplied a proper factor, to fit them into the same scale as the measurement.

From Figs.1-3 we can see the qualitative features of the experimental FDCS are quite well reproduced by the 3C and CDW-EIS model, though small quantitative discrepancies remain.

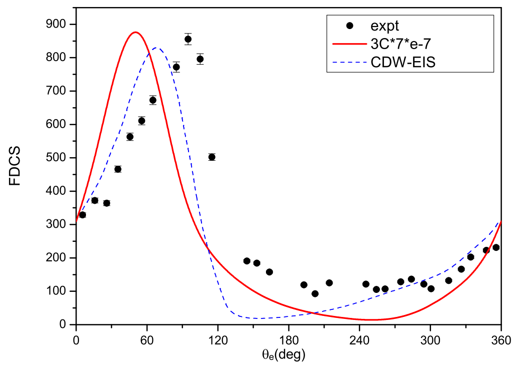

Figure 2: (Color online) Same as fig. 1 except that the momentum transfer is 1.5 a.u..

For small q (see Fig. 1), the binary peak position shifted toward larger ejection angles and the CDW-EIS angular distribution becomes flat in the back-scattering region and fail to reproduce the experimental data in a satisfactory manner. In contrast, the 3C results

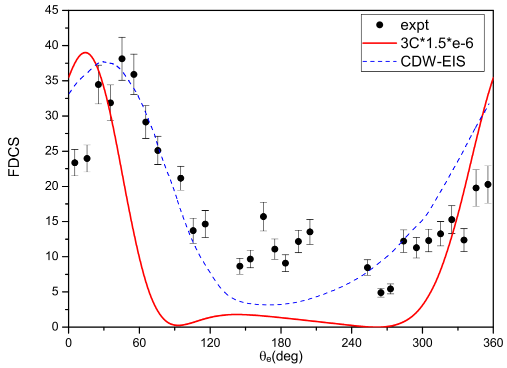

Figure 3: (Color online) Same as fig. 1 except that the momentum transfer is 4 a.u..

predict the forward peak very well and some new peak structures as weak humps and dips in the back-scattering region, which are in better agreement with experiment than the CDW-EIS calculations. For middle q (see Fig. 2), we find that the CDW-EIS results underestimate the magnitude of the binary peak and do not reproduce the experimental trend near $\theta_e = 180^0$. However, it is clearly seen that the 3C result is much better agreement with experiment than the CDW-EIS around about $\theta_e = 180^0$. For large q (see Fig. 3), the 3C results qualitatively indicate such an enhancement as a weak hump, although underestimating the peak at $\theta_e = 180^0$ and in quite good agreement with experiment . On the other hand, the trend of CDW-EIS is exactly opposite and there is a major deviation from the maxima at $\theta_e = 180^0$.

From the preceding discussion, we find that the 3C calculations qualitatively reproduce the forward peak very well and some new peak structures as weak humps and dips in the back-scattering region, which are in better agreement with experiment than the CDW-EIS calculations. Maybe the differences in the theories lead to the discrepancies in the calculated results. Comparing the CDW-EIS and 3C model, in the former case, helium single ionization is regarded as a three-body model (projectile, active electron and residual target), whereas the merit of the 3C model is the four-body (projectile, active and passive electrons, and target nucleus) reaction which contains the wave function for the passive electron and the three-Coulomb wave. Furthermore, in the 3C calculations the perturbation contains all the interactions between the projectile and target atom. However, the CDW-EIS model does not incorporate the PT interaction.

4 Conclusion

We have presented a systematic study of the fully differential single-ionization cross section for electrons emitted into the scattering plane for 16MeV O^{7+} ionization of helium.

We note a satisfactory, although not perfect, agreement of the 3C results with experimental findings.The 3C results are in better agreement with the experimental than the CDW-EIS results. However, there are some discrepancies between the present theory and measurements, so a more definitive explanation needs to be further studied, this is also our future work to be done.

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