ARTICLE

Fully Differential Cross Sections for Single Ionization of Helium by Au^{Q+} Impact

Li-li Feng, Shi-yan Sun, Qiao-qiao Duan, Xiang-fu Jia*

School of Physics and Information Engineering, Shanxi Normal University, Linfen 041004, China

(Dated: Received on March 7, 2015; Accepted on May 18, 2015)

We present fully differential cross sections (FDCS) within three-body distorted wave (3DW) for the single ionization of He by 3.6 MeV/amu Au^{Q+} (Q=24, 53) ions. By comparing our calculations with experimental data and other theoretical predictions, we find the cross sections are strongly influenced by highly charged projectile, ejected electron would be "pulled" along in the forward direction. However, all of the theoretical approaches can not display experimental unique forward peak structures in the FDCS.

Key words: Highly charged ions, Fully differential cross section, Three-body distorted wave

I. INTRODUCTION

The study of electron emission spectra in ion-atom collisions has been a field of intense activity for years. However, single ionization processes occurring in atoms by the impact of highly charged particles have not been completely understood [1−5]. During the last decade, investigations on differential single ionization of He by Au^{Q+} (Q=24, 53) projectiles have been reported where the projectile interaction with the He target was much strong [2, 3, 6−9]. These experimental measurements present a substantial challenge to theory, in principle, as they can show up significant discrepancies which can be hidden in less differential cross sections [10]. Nonetheless, the theoretical interpretation of the experimental results can not be satisfactory both in shape and magnitude. The continuum-distorted-wave-eikonal-initial-state approach (CDW-EIS) [1], the three distorted-wave-eikonal-initial-state method (3DW-EIS) [4], the coupled-pseudostate approximation (CP) [10], have not been able to obtain reasonable agreement with the measurements. These unexpected findings may be due to lacking some physical effects that are important for highly charged ions. Accordingly, further other theoretical analysis and calculations seem appropriate and interesting.

Three-body distorted wave (3DW) is well known and has been shown to be capable of predicting the shapes of cross sections at intermediate and high energies of ion-impact ionization processes qualitatively [1, 2, 4]. Recently, 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 [11, 12].

In this work, we will apply the 3DW model to analyze the fully differential cross sections (FDCS) for the single ionization of helium by Au^{Q+} (Q=24, 53) impact at the incident energy of 3.6 MeV/amu. Compared with the corresponding experimental results, the ability of the present method to reproduce the peak structure of the experimental data is assessed.

II. THEORY

Single ionization of helium in the ground state by the impact of Au^{Q+} with incident momentum $\mathbf{K}_i$ relative to the atomic center of mass is considered. In the center-of-mass (CM) system, the T-matrix element is defined as

$$T_{fi} = \langle \psi_f^-(\mathbf{r}_1, \mathbf{r}_\mathrm{T}, \mathbf{R}_\mathrm{P}) | V_i | \Phi_i^+(\mathbf{r}_1, \mathbf{r}_\mathrm{T}, \mathbf{R}_\mathrm{P}) \rangle \quad (1)$$

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

The initial state Φ_i^+ is represented as a product of a plane wave for the projectile and a wave function of helium atom in the ground state

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

For the ground state wave function ϕ_i, we choose the analytical fitting to the Hartree-Fock (HF) wave function given by Byron and Joachain [13],

$$\phi_i(\mathbf{r}_1, \mathbf{r}_\mathrm{T}) = U(\mathbf{r}_1) U(\mathbf{r}_\mathrm{T}) \quad (3)$$

$$U(\mathbf{r}) = (4\pi)^{-1/2} (A\mathrm{e}^{-\alpha r} + B\mathrm{e}^{-\beta r}) \quad (4)$$

*Author to whom correspondence should be addressed. E-mail: amphy0123@163.com, Tel.: +86-357-2051189

DOI:10.1063/1674-0068/28/cjcp1503031

with A=2.60505, B=2.08144, α=1.41, β=2.61 in Eq.(4).

The final state wave function ψ_f^- is approximated by a product of 3DW $\psi_{3\mathrm{DW}}^-$ and the ground-state wave function of He^+,

$$\psi_f^-(\mathbf{r}_1, \mathbf{r}_\mathrm{T}, \mathbf{R}_\mathrm{P}) = \phi_f(\mathbf{r}_1)\psi_{3\mathrm{DW}}^-(\mathbf{r}_\mathrm{T}, \mathbf{R}_\mathrm{P}) \quad (5)$$

$$\phi_f(\mathbf{r}_1) = 2^{3/2}\pi^{-1/2}\mathrm{e}^{-2r_1} \quad (6)$$

$\psi_{3\mathrm{DW}}^-$ can be written as

$$\begin{aligned}\psi_{3\mathrm{DW}}^- = {} & C\exp(i\mathbf{k}_\mathrm{T}\cdot\mathbf{r}_\mathrm{T})\exp(i\mathbf{K}_\mathrm{P}\cdot\mathbf{R}_\mathrm{P})\cdot \\ & {}_1F_1[i\alpha_{Te}; 1; -i(k_\mathrm{T}r_T + \mathbf{k}_\mathrm{T}\cdot\mathbf{r}_\mathrm{T})]\cdot \\ & {}_1F_1[i\alpha_{PT}; 1; -i(K_\mathrm{P}R_\mathrm{P} + \mathbf{K}_\mathrm{P}\cdot\mathbf{R}_\mathrm{P})]\cdot \\ & {}_1F_1[i\alpha_{Pe}; 1; -i(k_\mathrm{P}r_\mathrm{P} + \mathbf{k}_\mathrm{P}\cdot\mathbf{r}_\mathrm{P})] \end{aligned} \quad (7)$$

with the normalization factor

$$\begin{aligned} C = {} & (2\pi)^{-3}\Gamma(1-i\alpha_{PT})\Gamma(1-i\alpha_\mathrm{Pe})\Gamma(1-i\alpha_\mathrm{Te})\cdot \\ & \exp\left(-\frac{1}{2}\pi\alpha_\mathrm{PT} - \frac{1}{2}\pi\alpha_\mathrm{Pe} - \frac{1}{2}\pi\alpha_\mathrm{Te}\right) \end{aligned} \quad (8)$$

where $\mathbf{k}_\mathrm{P}$ and $\mathbf{k}_\mathrm{T}$ are the momenta of scattered projectile and ejected electron, respectively, which are both considered with respect to the center of mass of target ion (He^+),

$$\mathbf{k}_\mathrm{P} = (1-\gamma)\,\mathbf{k}_\mathrm{T} - [\delta(1-\gamma)+\gamma]\mathbf{K}_\mathrm{P} \quad (9)$$

$$\gamma = \frac{1}{M_\mathrm{P}+1}, \quad \delta = \frac{1}{M_\mathrm{T}+1} \quad (10)$$

${}_1F_1$ is the confluent hypergeometric function.

The form of Sommerfeld parameters α_Te, α_PT, α_Pe are

$$\alpha_{Te} = -\frac{\mu_\mathrm{Te}Z_\infty}{k_\mathrm{T}} \quad (11)$$

$$\alpha_\mathrm{PT} = \frac{\mu_\mathrm{PT}Z_\mathrm{P}Z_\infty}{K_\mathrm{P}} \quad (12)$$

$$\alpha_\mathrm{Pe} = -\frac{\mu_\mathrm{Pe}Z_\mathrm{P}}{k_\mathrm{P}} \quad (13)$$

where μ_PT and μ_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_∞=1.

If the final channel projectile-target ion interaction is switched off (α_PT=0), Eq.(5) can be expressed as:

$$\psi_{f_{2\mathrm{C}}}^- = \phi_f(\mathbf{r}_1)\psi_{2\mathrm{C}}^- \quad (14)$$

If both the interaction of the projectile-target ion and interaction of the projectile-ionized electron are neglected (α_{Pe}=α_{PT}=0),

$$\psi_{f_{1\mathrm{C}}}^- = \phi_f(\mathbf{r}_1)\psi_{1\mathrm{C}}^- \quad (15)$$

This is the FBA (first-born-approximation) [14] result.

Perturbation corresponding to the initial state is given by

$$V_i = \frac{Z_\mathrm{T}Z_\mathrm{P}}{R} - \frac{Z_\mathrm{P}}{r_\mathrm{P}} - \frac{Z_\mathrm{P}}{|\mathbf{R}-\mathbf{r}_1|} \quad (16)$$

where $\mathbf{R}$ is the position of the projectile with respect to the target nucleus. Z_P and Z_T are the charges of the projectile and the target nucleus, respectively.

The FDCS in the CM system is given as follows [15, 16]:

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_\mathrm{P}\mathrm{d}\Omega_\mathrm{e}\mathrm{d}E_\mathrm{e}} = N_\mathrm{e}(2\pi)^4\mu_\mathrm{Te}\mu_{\mathrm{P,He}}^2\frac{K_\mathrm{P}k_\mathrm{T}}{K_i}|T_\mathrm{fi}|^2 \quad (17)$$

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.

The nine-dimensional integral (Eq.(1)) can be reduced analytically, to a two-dimensional integral on the real parameters [17, 18] which has to be carried out numerically.

III. RESULTS AND DISCUSSION

To check the accuracy of 3DW, we have investigated the FDCS for single ionization of the helium by the impact of 3.6 MeV/amu Au^{24+} and Au^{53+} ions, with the ejected electron emitted into the scattering plane, which corresponds to the measurements [4]. The results are displayed in Fig.1 and Fig.2, respectively. We compare the FBA, 2C (two-Coulomb-wave) [17], 3DW results with the experimental and 3DW-EIS [4] results. In order to compare conveniently with other data, all of our results have been normalized to put them on the same scale as the experimental data.

From Fig.1 we can see excellent agreement between the FBA and 3DW both in the shape and magnitude. This implies convergence of our results which can describe the collision qualitatively. Binary peak of 2C shifts towards larger ejection angles due to a post-collision interaction (PCI) between the highly charged ion and the ionized electron. With the increase in momentum transfer, 3DW predicts the forward peak very well but there is still small deviation with experimental measurements. All of the theoretical results show the same angular distribution as the experiment and have a shifting of binary peak towards larger ejection angles. Furthermore, the cross sections of all the theories show clear binary peak and distinct recoil peak, but underestimate height of binary peak. It is very delighting to see that the 3DW calculations exhibit the improvement over the 3DW-EIS results and are in excellent agreement with the experimental measurements

DOI:10.1063/1674-0068/28/cjcp1503031

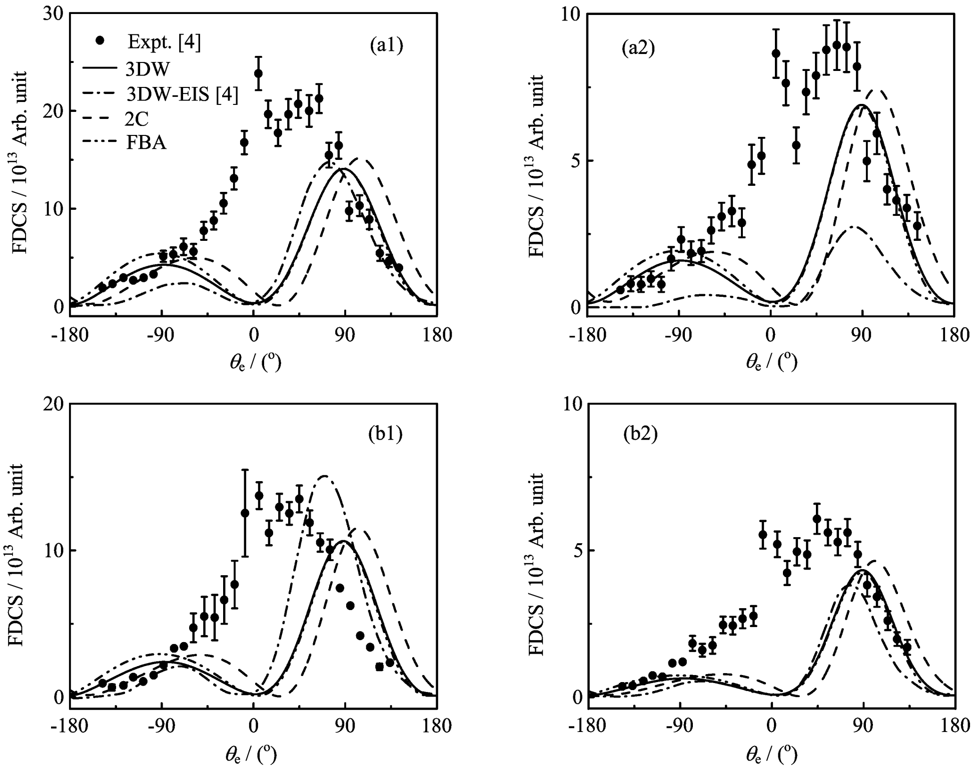

FIG. 1 Fully differential cross sections for 3.6 MeV/amu Au^{24+} impact ionization of helium in the scattering plane. The ejected-electron energy is (a) 4.0 eV and (b) 10 eV, the momentum transfers are (a1, b1) 0.45 a.u. and (a2, b2) 0.65 a.u., respectively. The angle θ_e is the emission angle of the electron.

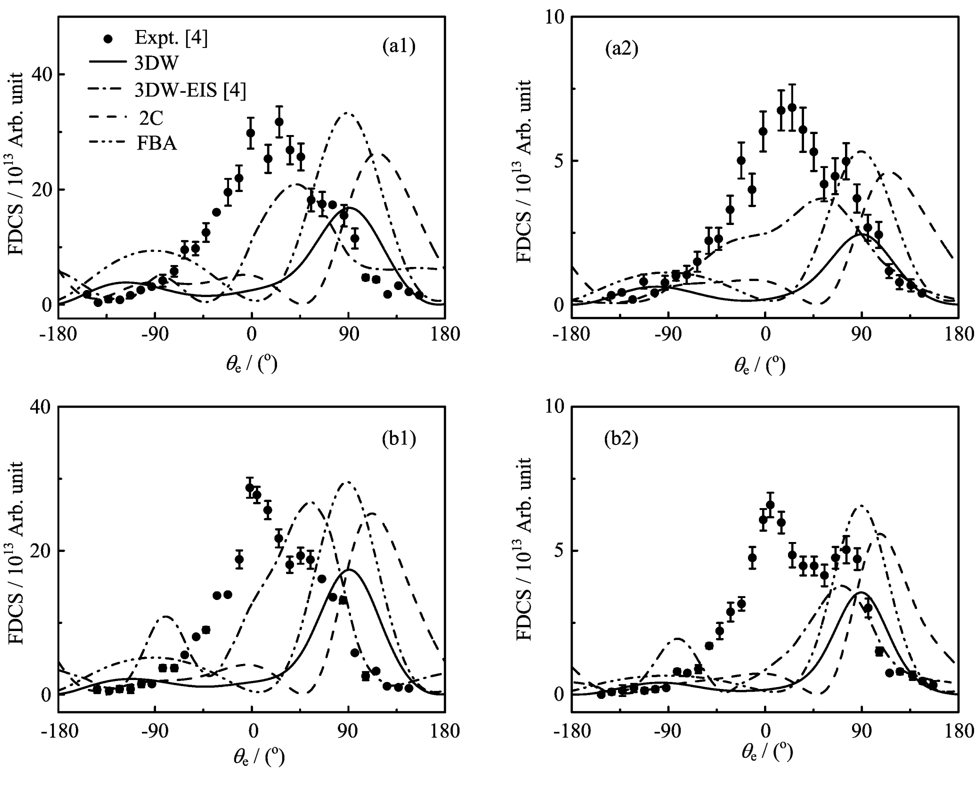

FIG. 2 Fully differential cross sections for 3.6 MeV/amu Au^{53+} impact ionization of helium in the scattering plane. The ejected-electron energy is (a) 4.0 eV and (b) 10 eV, the momentum transfers are (a1, b1) 0.65 a.u. and (a2, b2) 1.0 a.u., respectively. The angle θ_e is the emission angle of the electron.

DOI:10.1063/1674-0068/28/cjcp1503031

in the recoil peak. Experimentally, since the projectile is a positively charged ion, ejected electron is a negatively charged ion, they will be attracted along in the forward direction. Through the comparisons with experimental data, we can see that the 3DW theory does not show its superiority to the 3DW-EIS near the binary peak, neither the 3DW-EIS calculations nor the present results predict a strong peak in the FDCS in the forward direction. The agreement between experiment and these theoretical results is confused that may be due to highly charged projectile.

Figure 2 shows the FDCS for Au^{53+}. As in the Au^{24+} case, the experimental data exhibit a similar structure, the data appear to have a binary peak overlapping a strong forward peak and there is also a shifting of binary peak towards larger ejection angles. For this higher charge state of the projectile, unlike the case of Au^{24+}, there are significant differences observed between the FBA and 3DW where the FBA results overestimate the 3DW results both in the binary peak and recoil peak. Furthermore, the 2C contains some additional structure in addition to the usual binary and recoil peaks in all of cases. The difference between the Au^{24+} and Au^{53+} outcomes is remarkable. The theories are in reasonable agreement for Au^{24+}, but are in dispute with each other for Au^{53+}.

We have presented 3DW results for the single ionization of helium by 3.6 MeV/amu Au^{24+} and Au^{53+} ions. For ionization by Au^{24+} there is a large extent of consensus between FBA and 3DW in the shape and magnitude, therefore we believe that in this case the theory is reliable. However, for Au^{53+} the situation is less satisfactory. We forecast that the failure of the theory stems from highly charged projectile. Consequently, the present approach still neglects some important physical effects, such as the effect of atomic polarization, treatment of projectile-target ion subsystem, and initial state of the projectile [4].

IV. ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China (No.11274215) and the Natural Science Foundation of Shanxi Province, China (No.2010011009).

[1] D. Fischer, R. Moshammer, M. Schulz, A.Voitkiv, and J. Ullrich, J. Phys. B **36**, 3555 (2003).
[2] M. Schulz, R. Moshammer, D. Fischer, and J. Ullrich, J. Phys. B **37**, 4055 (2004).
[3] M. F. Ciappina and W. R. Cravero, J. Phys. B **39**, 1091 (2006).
[4] M. Foster, D. H. Madison, J. L. Peacher, and J. Ullrich, J. Phys. B **37**, 3797 (2004).
[5] R. T. Pedlow, S. F. C. O'Rourke, and D. S. F. Crothers, Phys. Rev. A **72**, 062719 (2005).
[6] R. E. Olson and J. Fiol, Phys. Rev. Lett. **95**, 263203 (2005).
[7] M. Dürr, B. Najjari, M. Schulz, A. Dorn, R. Moshammer, A. B. Voitkiv, and J. Ullrich, Phys. Rev. A **75**, 062708 (2007).
[8] J. Fiol and R. E. Olson, J. Phys. B **37**, 3947 (2004).
[9] V. D. Rodríguez, Nucl. Instrum. Methods B **205**, 498 (2003).
[10] M. McGovern, D. Assafrão, J. R. Mohallem, Colm T. Whelan, and H. R. J. Walter, Phys. Rev. A **81**, 042704 (2010).
[11] X. Y. Fang, R. F. Zhang, H. X. Duan, S. Y. Sun and X. F. Jia, Chin. Phys. B 23, 063404 (2014).
[12] H. X. Duan, S. Y. Sun, X. Y. Fang, R. F. Zhang, and X. F. Jia, Chin. J. Chem. Phys. **27**, 279 (2014).
[13] F. W. Byron and C. J. Joachain, Phys. Rev. **146**, 1 (1966).
[14] H. R. J. Walters and C. T. Whelan, Phys. Rev. A **85**, 062701 (2012).
[15] J. Berakdar, J. S. Briggs, and H. Klar, Z. Phys. D **24**, 351 (1992).
[16] J. Berakdar, J. S. Briggs, and H. Klar, J. Phys. B **26**, 285 (1993).
[17] X. F. Jia, Phys. Rev. A **66**, 062708 (2002).
[18] X. Y. Ma, X. Li, S. Y. Sun, and X. F. Jia, Europhys. Lett. **98**, 53001 (2012).

DOI:10.1063/1674-0068/28/cjcp1503031