**ARTICLE**

# (e, 2e) Investigations of the Simultaneous Ionization and Excitation of Helium to $He^+(n=2)$

Shi-yan Sun, Xiang-fu Jia*

*Centure for research of Molecule Science, School of Physics and Information Engineering, Shanxi Normal University, Linfen 041004, China*

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Three-Coulomb-wave method is employed to treat the process of (e, 2e) simultaneous ionization and excitation to the $n$=2 state of helium, with radial and angular correlated wavefunction of He target. The triple differential cross sections are calculated and analyzed in very asymmetric coplanar geometry at incident energies of 5.50, 1.50 and 0.57 keV. Results are compared with the absolute measurements and the theoretical first and second Born approximation. The present triply differential cross section (TDCS) is found to be in good agreement with experimental data qualitatively. The distinguishing feature noted in TDCS structure is the presence of intense recoil peak that for certain parameters is even larger than the binary peak, an unusual feature for the single-ionization process at high and intermediate energies.

**Key words:** Excitation-ionization, Three-Coulomb-wave model, Triply differential cross section

## I. INTRODUCTION

The well established program of (e, 2e)-ionization experiments on helium has been extended to ionization and simultaneous excitation [1]. In these experiments an atom or a molecule is ionized by electron impact while simultaneously a second electron in the target is promoted to a higher level such that the final state contains an excited ion. Simultaneous ionization-excitation is a highly correlated process, since three electrons change their quantum states as a result of the collision. Electron-impact ionization of helium from the $^1$S ($1s^2$) ground state to the final ionic state $^2$S (2s) or $^2$P (2p) is the simplest ionization excitation process which has attracted wide interest both experimentally and theoretically. The difficulty for experiment is due to the fact that count rates are relatively low when compared to collision processes in which the residual ion is left in the ground state. For theorists, the challenge has been to develop a theory which is capable of explaining these observations. In the last decades, experimental measurements for these processes have been obtained by Dupré *et al.* at 5.50 keV scattered electron energy [2] and Avaldi *et al.* [3] and Stefani *et al.* [4] at 0.57 and 1.50 keV scattered electron energies. Recently, measurements of the simultaneous ionization-excitation processes at lower energies have also been achieved. Rouvellou *et al.* [5], Dogan and Crowe [6], and Bellm *et al.* [7] reported measurements at impact energies of 365.8, 200, and 44 eV, respectively. All the above measurements were performed under highly asymmetric kinematics. The results are in marked contrast with those obtained for direct ionization and show a strong enhancement in the magnitude of the recoil peak relative to that of the binary collision peak.

A number of theoretical studies have been devoted to this problem, such as the second-order plane wave Born (PWB2) calculations of Marchalant *et al.* [8], second-order convergent R-matrix with pseudostates (RMPS) calculations by Fang and Bartschat [9], the second Born model based on the convergent close-coupling (CCC) description of the two-electron final state of Kheifets [10], and B-spline R-matrix approach of Zatsarinny *et al.* [11]. In fact, comparison of earlier theoretical predictions with experimental data shows that the theoretical results are extremely model-dependent.

To our knowledge, three-Coulomb-wave method (3C) calculations to model these results have not yet been published. The aim of the present work is to examine the validity of the 3C approximation for ionization-excitation, in this work, we extend 3C [12] to electron-impact ionization excitation of helium from the ground state to $He^+$ ($n$=2) in the coplanar asymmetric geometry at high and intermediate energies. We have introduced the radial and angular correlated wavefunction in the ground state of the target to calculate such a triply differential cross section (TDCS) for the coplanar, asymmetric energy sharing case by applying the 3C method in the final continuum state of the two electrons and the ion. It should be noted that this final

*Author to whom correspondence should be addressed. E-mail: jiaxf@sxnu.dns.edu.cn, Tel.: +86-357-2051189

 

states are asymptotically an exact solution of the three-body problem [13] and it contains the electron-electron post collision interaction (PCI) effect to all orders of perturbation theory.

## II. THEORY

Consider an incident projectile electron "0" with momentum $\mathbf{k}_0$ colliding with a ground-state helium atom. After an ionizing collision, the projectile has momentum $\mathbf{k}_1$, an electron "2" of momentum $\mathbf{k}_2$ has been ejected from the target and the residual ion with a bound electron "3" is left in the excited state.

$$\mathrm{e}+\mathrm{He}(1\mathrm{s}^2)\rightarrow 2\mathrm{e}+\mathrm{He}^+(n=2) \quad (1)$$

The TDCS for (e, 2e) process on a target as defined in Eq.(1) may be written as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E_2}=2(2\pi)^4\frac{k_1k_2}{k_0}\sum_{l=0}^{n-1}\sum_{m=-l}^{l}|T_{nlm}|^2 \quad (2)$$

$$T_{nlm}=\left\langle\Psi_f{}^-\right|V_i\left|\Psi_i{}^+\right\rangle \quad (3)$$

where, $\mathrm{d}\Omega_1$ and $\mathrm{d}\Omega_2$ are the solid angles of direction of the scattered and the ejected electrons, while $\mathrm{d}E_2$ represents the energy interval of the ejected electron. $T_{nlm}$ is the direct amplitude. $\Psi_i{}^+$ and $\Psi_f{}^-$ are the wave function of the initial and final state of the entire target+projectile collision system, and $V_i$ represents the interaction between the incident electron and the target.

$$V_i=-\frac{2}{r_1}+\frac{1}{r_{12}}+\frac{1}{r_{13}} \quad (4)$$

$$r_{12}=|\mathbf{r}_1-\mathbf{r}_2| \quad (5)$$

$$r_{13}=|\mathbf{r}_1-\mathbf{r}_3| \quad (6)$$

where $\mathbf{r}_1$, $\mathbf{r}_2$ and $\mathbf{r}_3$ are the position vectors of the incident electron, ejected electron and the bound electron of $He^+(n=2)$ with respect to the target nucleus, respectively.

The initial state, which takes into account the incident and the bound electrons, will be written as the product of a plane wave and the ground state wave function of the helium atom,

$$\Psi_i(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=(2\pi)^{-3/2}\mathrm{e}^{i\mathbf{k}_0\mathbf{r}_1}\phi_0(\mathbf{r}_2,\mathbf{r}_3) \quad (7)$$

The helium ground state $\phi_0(\mathbf{r}_2,\mathbf{r}_3)$ is taken from Silverman *et al.* [14]. It contains radial and angular correlations and has the following form:

$$\phi_0=\frac{1}{\sqrt{1+\lambda^2}}\left\{N(\mathrm{e}^{-\alpha r_2-\beta r_3}+\mathrm{e}^{-\alpha r_3-\beta r_2})+\frac{\lambda}{\sqrt{3}}\left(\frac{4}{3}\gamma^5\right)r_2r_3\mathrm{e}^{-\gamma(r_2+r_3)}[Y_{10}(\hat{r}_2)Y_{10}(\hat{r}_3)-Y_{11}(\hat{r}_2)Y_{1-1}(\hat{r}_3)-Y_{1-1}(\hat{r}_2)Y_{11}(\hat{r}_3)]\right\} \quad (8)$$

where constants $\alpha$=2.17621, $\beta$=1.20152, $\gamma$=2.47547, $\lambda$=−0.0617557. The final state $\Psi_f{}^-$ should be an eigenfunction of the full four-body Hamiltonian with boundary conditions describing one bound and two out going electrons. It satisfies equation

$$\left(\hat{H}_0-\frac{1}{r_1}-\frac{1}{r_2}-\frac{1}{r_3}+\frac{1}{r_{12}}-E\right)\Psi_f{}^-(\mathbf{r}_1,\mathbf{r}_2,\mathbf{r}_3)=0 \quad (9)$$

with kinetic energy operator

$$\hat{H}_0=-\frac{1}{2}\nabla_1{}^2-\frac{1}{2}\nabla_2{}^2-\frac{1}{2}\nabla_3{}^2 \quad (10)$$

It consists of two outgoing electrons and a residual ion, the degenerate $n$=2 levels of the $He^+$ ion $\phi_{\mathrm{ion}}(\mathbf{r}_3)$ are just hydrogen-like orbitals. Consequently, there are four possible ways to reach a final state from two terms, $S$ and $P$, in the correlated ground state.

$$\phi_f(\mathbf{r}_3)=\phi_{200}(\mathbf{r}_3)=\sqrt{\frac{1}{\pi}}(1-r_3)\mathrm{e}^{-\lambda_1r_3}=\sqrt{\frac{1}{\pi}}\left(1+\frac{\partial}{\partial\lambda_1}\right)\mathrm{e}^{-\lambda_1r_3} \quad (11)$$

$$\phi_f(\mathbf{r}_3)=\phi_{21m}(\mathbf{r}_3)=\frac{2}{\sqrt{3}}\mathrm{e}^{-\lambda_1r_3}r_3Y_{1m}(\hat{r}_3) \quad (12)$$

The final two outgoing electron continuum state is approximated by a product of three two-body Coulomb wave [12]

$$\Psi_f(\mathbf{r}_1,\mathbf{r}_1,\mathbf{r}_3)=\Psi_{3c}(\mathbf{r}_1,\mathbf{r}_2)\phi_f(\mathbf{r}_3) \quad (13)$$

$$\Psi_{3c}(\mathbf{r}_1,\mathbf{r}_2)=(2\pi)^{-3}\mathrm{e}^{i(\mathbf{k}_1\mathbf{r}_1+\mathbf{k}_2\mathbf{r}_2)}C(\alpha_1,\mathbf{k}_1,\mathbf{r}_1)\cdot C(\alpha_2,\mathbf{k}_2,\mathbf{r}_2)C(\alpha_{12},\mathbf{k}_{12},\mathbf{r}_{12}) \quad (14)$$

$$C(\alpha,\mathbf{k},\mathbf{r})=\Gamma(1-i\alpha)\mathrm{e}^{-1/2\pi\alpha}{}_1F_1\cdot[-i\alpha,1;-i(kr+\mathbf{kr})] \quad (15)$$

here $\mathbf{r}_{12}$=$\mathbf{r}_1$−$\mathbf{r}_2$ is the relative coordinate between the two outgoing electrons and its conjugate momentum $\mathbf{k}_{12}$. ${}_1F_1[a,b,c]$ is the confluent hypergeometric function. $\alpha_j$($j$=1, 2, 12) are the Sommerfeld parameters.

The calculations have been carried out numerically following the method described in our earlier work [15] with necessary modifications. Since the present work deals with the highly asymmetric geometry, the exchange amplitude between the scattered and the ejected electrons may be neglected.

## III. RESULTS AND DISCUSSION

In order to check the accuracy of the 3C model, we have calculated the angle of the fast scattered electron. The TDCS of the simultaneous ionization-excitation processes as a function of the angle of the slow ejected electron for the energy of the fast scattered electron is

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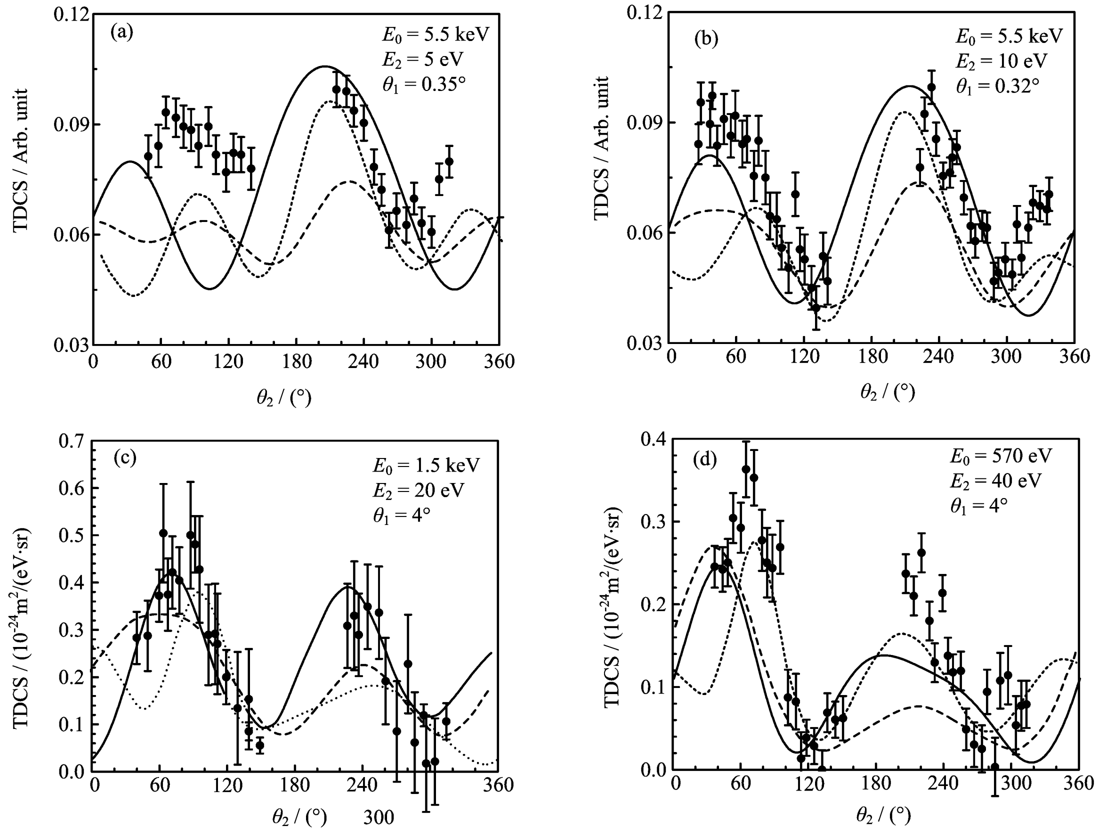


FIG. 1 In-plane angular distribution of the ejected electron for ionization-excitation to the $He^+$ ($n$=2) states. Solid lines, 3C; dotted lines: FBA; dashed lines: SBA; solid circles with error bars: experimental data of Dupré *et al.* [2] in (a) and (b), and experimental data of Stefani *et al.* [4] in (c) and (d). $\theta_1$ is the angle of the fast scattered electron, and $\theta_2$ is the angle of the slow ejected electron.

set at 0.57−5.50 keV in coplanar asymmetric geometry. In Fig.1 our 3C results as compared with experimental results of Dupré *et al.* and Stefani *et al.* and with theoretical results of the first Born approximation (FBA) and the second Born approximation (SBA) [2, 3].

In the case of Fig.1 (a) and (b), the agreement is remarkably good. Our 3C theoretical curve follows the TDCS structure that intense recoil peak is even larger than the binary peak of the experimental data and the magnitude of the cross section is very well reproduced except the position of the binary peak shifting to smaller angles. There is very good agreement between the 3C and SBA calculations and experiment in the recoil peak, and FBA underestimates the cross sections clearly deviating from the experiment. FBA and SBA not only move the binary peak about 25° to larger angles but also change the shape of the angular distributions in the range of the binary peak.

In Fig.1 (c) and (d), at the much lower energies of 1.50 and 0.57 keV, the angular dependence is very similar to the case of ionization only that binary peak is larger than the recoil peak. There is a modest improvement between our results and experiment in the binary peak, but there is considerable disagreement at recoil angles. In the case of Fig.1(c), our 3C calculations increase the magnitude in the binary peak and make the binary peak position shift to smaller angles and these changes improve the agreement with experiment relative to SBA. In the recoil region our 3C calculations display a very much smaller cross section than the experimental data and shift the peak position about 23° to larger angles. For the case of 0.57 keV, our 3C calculations predict similar angular distributions to those of FBA and SBA, the three theoretical results have almost the same binary peak but have lower binary and recoil peaks than the experiment. The results suggest substantial effects of the correlation in the final state at lower energy but are not large enough to materially affect the discrepancy with experiment.

For simultaneous ionization and excitation, it is important to include correlated wavefunction in the ground state of the target as well as in the two-electron continuum wavefunction of the final state. The addition of correlation between the outgoing electrons increases the cross section and provides a noticeable qualitative improvement in the agreement between experiment and theory at higher energies. For the lower energies, there are substantial effects of the correlation in the final

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state but not large enough to materially affect the discrepancy with experiment. In contrast, the initial-state wavefunction used in the present work does include both the radial and angular correlations, we believe that the simple uncoupled wavefunction is primarily responsible for the discrepancies between the present calculations and experiment.

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