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HTML ABSTRACT + LINKS

(e,2e) and (e,3-1e) studies on double processes of He near the Bethe ridge

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Abstract. We report (e,2e) and (e,3-1e) experiments on the double processes of He, i.e. single ionization with simultaneous excitation and double-ionization. The symmetric noncoplanar geometry combined with high incident electron energies has made it possible to study at large momentum transfers. The results are compared with plane wave impulse approximation (PWIA) calculations using He wavefunctions of various levels of sophistication. It is shown that shapes of the momentum dependent (e,2e) and (e,3-1e) cross sections are well reproduced by the PWIA calculations when highly correlated wavefunctions are employed, but noticeable discrepancies between experiment and theory remain in magnitude. The discrepancies are, however, reduced with increasing impact energies, suggesting higher excitation energies may be required to analyze these double processes in terms of the PWIA.

Keywords: (e,2e), (e,3-1e), ionization-excitation, double ionization, electron correlation
PACS: 34.80.Dp

INTRODUCTION

The electron impact single-ionization experiment under the high-energy Bethe ridge conditions is referred to as binary (e,2e) or electron momentum spectroscopy and provides direct information on the one-electron momentum density of the ionized orbital [1]. The key concept in connecting the (e,2e) cross section with the one-electron momentum density is the plane wave impulse approximation (PWIA).

Double processes of the two-electron system He, i.e. single-ionization with simultaneous excitation to n=2 orbital (hereafter called ionization-excitation) and double-ionization, are particularly attractive in view of (e,2e) spectroscopy. Because of the absence of electron correlation in the final ion state, they provide ideal opportunities to examine PWIA as well as electron correlation in the initial target state. As to the ionization-excitation processes of He, the PWIA allows us to probe the one-electron momentum density of excited orbital component involved in the target initial state wavefunction. In the case of double-ionization, the two-electron momentum

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density can be derived by so-called (e,3e) experiments, where all the three outgoing electrons should be detected in coincidence [2,3]. Although direct determination of the two-electron momentum density is not possible, experimentally less demanding (e,3-1e) method, proposed by Popov et al.[4], is very sensitive to electron correlation in the target initial state. In spite of the fundamental importance, however, very few studies have been made on the double processes of He under the kinematics that seek to satisfy the high-energy Bethe ridge conditions [5-10]. Extremely small cross sections of the double processes at large momentum transfer are responsible for the scarcity of such studies.

Under these circumstances, we report (e,2e) and (e,3-1e) experiments on He using a recently developed multichannel (e,2e) spectrometer [9] that features high sensitivity. An impact energy of 2080 eV was used in the symmetric noncoplanar geometry and we have thus achieved a large momentum transfer of 9 a.u., a value that has never been realized so far for study on double-ionization. Thanks to multichannel detectors, primary ionization, where the residual electron remains in the 1s orbital, can also be measured simultaneously with double processes. Comparisons with the primary ionization have made it possible to accurately determine relative intensities of the double processes. Furthermore, measurements at impact energies of 1240 and 4260 eV were also performed in order to examine the incident electron energy dependence of the momentum profiles of the ionization-excitation process. The results are compared with PWIA calculations using various wavefunctions in terms of both shape and absolute magnitude of the cross sections. The present work is the examination of the PWIA for the double processes under the kinematics that are the closest to the high-energy Bethe ridge conditions compared with those employed in the previous (e,2e) and (e,3-1e) studies [5-8].

EXPERIMENTAL METHOD

For electron-impact single-ionization and double-ionization processes of He conservation of linear momentum and energy requires:

$$\boldsymbol{p}_{\mathrm{He+}} = \boldsymbol{p}_0 - \boldsymbol{p}_1 - \boldsymbol{p}_2, \tag{1}$$

$$E_{\mathrm{bind}} = E_0 - E_1 - E_2 \tag{2}$$

and

$$\boldsymbol{p}_{\mathrm{He2+}} + \boldsymbol{p}_3 = \boldsymbol{p}_0 - \boldsymbol{p}_1 - \boldsymbol{p}_2, \tag{3}$$

$$E_3 = E_0 - E_1 - E_2 - \mathrm{IP}^{2+}. \tag{4}$$

Here $\boldsymbol{p}_{\mathrm{j}}$'s and E_{j}'s (j = 0,1,2,3) are momenta and kinetic energies of the incident and outgoing electrons, respectively. $\boldsymbol{p}_{\mathrm{He+}}$ and $\boldsymbol{p}_{\mathrm{He2+}}$ represent the recoil momentum of the residual ion He^{+} and that of He^{2+}, respectively. E_{bind} and IP^{2+} are ionization energy and the double-ionization threshold of He. Since the present experiment involves coincidence detection of two outgoing electrons, $\boldsymbol{p}_{\mathrm{He+}}$ and E_{bind} are fully determined for the (e,2e) processes. On the other hand, for the (e,3-1e) process the obtainable quantities are ($\boldsymbol{p}_{\mathrm{He2+}} + \boldsymbol{p}_3$) and E_3. For the sake of simplicity both $\boldsymbol{p}_{\mathrm{He+}}$ and ($\boldsymbol{p}_{\mathrm{He2+}} + \boldsymbol{p}_3$) are denoted as momentum $\boldsymbol{q}$ here, and in the same sense (e,2e) and (e,3-1e)

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momentum profiles refer to $|\boldsymbol{p}_{He+}|$-dependent (e,2e) cross section and $|\boldsymbol{p}_{He2+} + \boldsymbol{p}_3|$-dependent (e,3-1e) cross section respectively.

In the symmetric noncoplanar geometry, two outgoing electrons having equal energies ($E_1 = E_2$) and polar angles ($\theta_1 = \theta_2 = 45°$) with respect to the incident electron beam axis are detected in coincidence. Then, the magnitude of the momentum q is expressed by

$$q = \sqrt{\left(p_0 - \sqrt{2}\,p_1\right)^2 + \left(\sqrt{2}\,p_1 \sin(\Delta\phi/2)\right)^2}\ , \tag{5}$$

where $\Delta\phi$ (= $\phi_1 - \phi_2 - \pi$) is the out-of-plane azimuthal angle difference between the two outgoing electron detected. If the incident electron energy and momentum are fixed, a given ionization transition can be selected simply by the choice of detection energy ($E_1 = E_2$) and then q can be determined only by $\Delta\phi$. The same is true for (e,3-1e) experiments, if we detect two fast outgoing electrons with equal energies in the symmetric noncoplanar geometry while leaving one slow ejected electron undetected.

In this work, a recently developed multichannel (e,2e) spectrometer has been employed to carry out (e,2e) and (e,3-1e) measurements simultaneously. Details of the spectrometer have been described elsewhere [11].

THEORY

Within the PWIA, the triple differential cross section for (e,2e) process on He is described by

$$\frac{d^3\sigma}{d\Omega_1 d\Omega_2 dE_1} = (2\pi)^4 f_{ee} \frac{p_1 p_2}{p_0} G(q), \tag{6}$$

$$G(q) = \left| \left(\tfrac{1}{2\pi}\right)^{3/2} \sqrt{2} \int \varphi_f^*(\boldsymbol{r}_1) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_2} \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2) d\boldsymbol{r}_1 d\boldsymbol{r}_2 \right|^2 , \tag{7}$$

where $d\Omega_j$ denotes the element of solid angle for the jth outgoing electron and f_{ee} is the half-off-shell Mott scattering cross section [1]. The structure factor $G(q)$ is proportional to the square modulus of the Fourier transform of the overlap between the initial ground state $\Phi(\boldsymbol{r}_1,\boldsymbol{r}_2)$ and the final ion state $\varphi_f(\boldsymbol{r}_1)$. For (e,3-1e) reaction of He, the four-fold differential cross section based on the PWIA model is given by [4]

$$\frac{d^4\sigma}{d\Omega_1 d\Omega_2 dE_1 dE_2} = (2\pi)^4 f_{ee} \frac{p_1 p_2 p_3}{p_0} F(p_3, q), \tag{8}$$

$$F(p_3, q) = \int \left| \left(\tfrac{1}{2\pi}\right)^{3/2} \sqrt{2} \int \varphi_c^*(\boldsymbol{p}_3, \boldsymbol{r}_1) e^{i\boldsymbol{q}\cdot\boldsymbol{r}_2} \Phi(\boldsymbol{r}_1, \boldsymbol{r}_2) d\boldsymbol{r}_1 d\boldsymbol{r}_2 \right|^2 d\Omega_3\ . \tag{9}$$

Here $\varphi_c(\boldsymbol{p}_3,\boldsymbol{r}_1)$ is a Coulomb wave with momentum $\boldsymbol{p}_3$. Eqs.(7) and (8) tell us that within the PWIA the structure factors involved in the cross sections are independent of E_0. Underlying assumptions leading to these equations are that electron energies have to be high enough to describe the incoming and fast two outgoing electrons by plane waves. To make extensive comparisons with experiment, five kinds of models for the He ground state wavefunction have been employed in the present study. The simplest model is the Hartree-Fock (HF) wavefunction [12], in which electron correlation is neglected. Radial correlation is taken into account by the Hylleraas-Eckart-Chandrasehkar (HEC) wavefunction [13]. To examine both radial and angular

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correlations on momentum profiles we have used the following three wavefunctions; a 12-component variation of the Chuluunbaatar, Puzynin and Vinitsky (CPV) wavefunction [14], a configuration interaction (CI) wavefunction of Mitroy et al. [15], and the Bonham and Kohl (BK) wavefunction [16].

RESULTS AND DISCUSSION

Figures 1(a) and (b) show experimental momentum profiles for the primary ionization and ionization-excitation processes. Likewise, the experimental (e,3-1e) momentum profiles at E_3=10 and 20eV are plotted in Figs. 1(c) and (d). Also included in Fig. 1 are the associated PWIA calculations using the HF, HEC, CPV, CI, and BK wavefunctions. Although absolute cross sections can not be determined with the present experiment, relative magnitudes of the individual transitions are maintained. Thus, by normalizing a certain experimental momentum profile to an associated theoretical one, one can place all other experiments on an absolute scale. Here we have chosen the PWIA cross section using the CI wavefunction (PWIA/CI) for the primary ionization as a standard for the normalization procedure. Furthermore, in order to compare the theoretical momentum profiles using different wavefunctions in a common scale, all the calculations are multiplied by scaling factors, which have been obtained so that the area of the theoretical momentum profile for the primary transition is the same as that of the PWIA/CI n=1 momentum profile.

It is immediately clear from Fig. 1(a) that all the PWIA calculations, including HF, are in general agreement with each other and with the experiment. Clearly, there are no noticeable effects of electron correlation in the primary ionization. In contrast, it is evident from Fig. 1(b) that the PWIA calculation using the uncorrelated HF wavefunction shows marked deviation from the experimental momentum profiles. The difference in shape is greatly reduced by taking radial correlation (HEC) or radial and angular correlation (CPV, CI, BK) into account. Although the shape of the experimental momentum profile is reproduced, discrepancies remain in magnitude; calculations always show about 30 % smaller cross sections.

As to the (e,3-1e) momentum profile, HF completely fails to reproduce the observed one, and HEC predicts an order of magnitude smaller cross section. The other three highly correlated wavefunctions result in similar momentum profiles with each other, which are in reasonably good agreement with the experimental ones in terms of shape. However, discrepancies again remain in magnitude; calculated ones underestimate the experimental cross sections by a factor of about 2.4 and 2.9 at E_3=10 and 20eV, respectively.

To see effects of distortion of the electron waves on the observed intensity differences, we have calculated (e,2e) momentum profiles within the distorted-wave Born approximation (DWBA) using the CI wavefunction. It is clear from Fig. 1(b) that the DWBA/CI momentum profile is very similar to the PWIA calculations except for at large momentum and can not explain the observed disagreements between experiment and theory. Thus, the intensity difference can not be attributed to distorted-wave effects.

Two possible sources of the difference in magnitude can be conceived; one is an incomplete description of the target ground-state wavefunction, which has been

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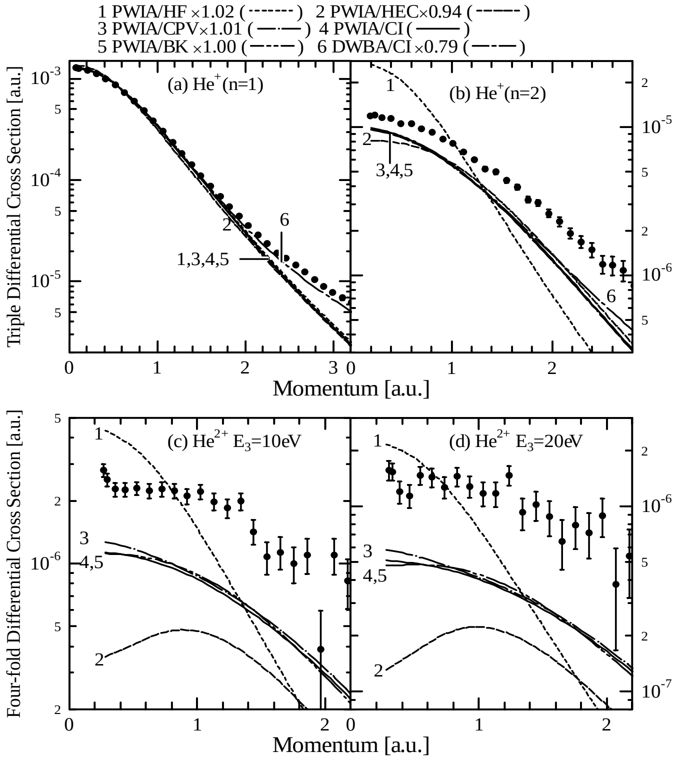

FIGURE 1. Upper panel: comparison of experimental (e,2e) momentum profiles of He for (a) the primary ionization and (b) the ionization-excitation processes and associated theoretical calculations. Lower panel: comparison of experimental (e,3-1e) momentum profiles of He for the doubly ionized He^{2+} with E_3= 10 (c) and 20 eV (d). PWIA calculations are also shown. All the experimental and theoretical momentum profiles are provided as normalized intensities to the PWIA/CI cross sections for the primary transition. For details, see ref. [17].

extensively examined in a separate paper [17]. Another is a failure of the PWIA description of the double processes due to contributions of higher order Born terms, which are not involved in the PWIA model. In what follows we focus our attention on contributions of higher order Born terms for the ionization-excitation process [18].

As mentioned earlier, the structure factor involved in the PWIA cross section should be independent of impact energy (cf. Eqs. (7) and (9)). Hence the validity of the PWIA can be experimentally assessed by a comparison of momentum profiles measured at different impact energies. Figure 2 shows experimental momentum profiles of the ionization-excitation transition at impact energies of 1240, 2080, and 4260eV. In order to compare the momentum profiles at different impact energies, the cross sections have been divided by the kinematical factors. Also illustrated in the figure are the PWIA/CI calculations folded with momentum resolutions of the spectrometer at the energy employed.

The experimental momentum profiles vary considerably with incident electron energy, decrease monotonically with an increase in E_0, and are approaching the PWIA

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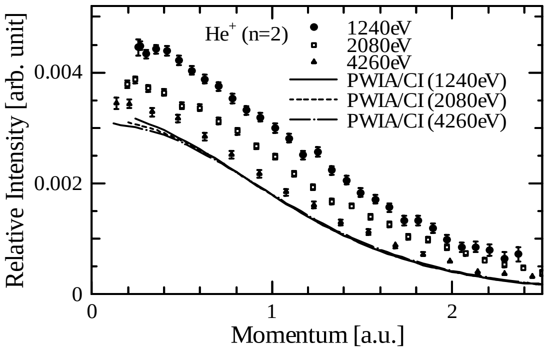

FIGURE 2. Experimental and PWIA/CI momentum profiles of He for the ionization-excitation transition at impact energies of 1240, 2080, and 4260eV. All the momentum profiles are divided by the kinematical factors.

prediction. This suggests that the ionization-excitation experiment should be performed at impact energy of about 5 keV or higher in order to make correct interpretation in terms of PWIA.

In summary, the following conclusions can be drawn from the present findings. First, the primary (e,2e) process of He is very accurately described by PWIA/HF calculation. Second, electron correlation plays a crucial role in ionization-excitation and double ionization processes. Finally, it is suggested that a higher electron impact energy is required than those employed in the present study in order to come to a correct interpretation of the double processes in terms of PWIA.

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