Vol 10 No 4, April 2001
1009-1963/2001/10(04)/0290-05

Chinese Physics

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EXCHANGE AND FINAL CHANNEL SCREENING EFFECTS IN (e, 2e) PROCESSES*

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(Received 7 September 2000)

The DS3C model has been improved by taking into account the final channel screening effects. The triple differential cross sections for electron impact ionization of helium at an incident energy of 40 eV are considered. The results of the present DS3C model are compared with the absolute measurements and those of other theoretical models. It has also been shown in which situation the exchange effects are crucial.

Keywords: (e, 2e), triple differential cross sections, screening effects, exchange effects
PACC: 3480D, 3450H

I. INTRODUCTION

Energy and angle resolved coincidence measurements of two escaping electrons following electron impact ionization of atomic system, so-called (e, 2e) measurements, provide detailed information on the ionization mechanism as well as dynamics of three charged particles moving in the three-body continuum. Recently, there has been considerable experimental and theoretical effort in the study of (e, 2e) processes in the case of the helium target. The understanding of electron impact ionization of helium at high energies may be considered satisfactory. We therefore wish to investigate these processes at the low-energy region.

Substantial theoretical progress has been made recently in the field of electron impact ionization. Since the work of Brauner, Briggs and Klar[1] (BBK) there has been a rapid increase in general interest and variety of theoretical approaches. These include methods evolved from consideration of the three-body boundary conditions[1−5], methods that have apparently inappropriate boundary conditions such as close-coupling[6−8] and distorted-wave[9] approaches, and methods that avoid the need for the three-body boundary conditions using time-dependent[10,11] and time-independent[12] techniques.

The BBK model[1] should be regarded as a significant advance in the theory of (e, 2e) processes, in which a three-Coulomb (3C) product wavefunction that satisfies the asymptotic three-body Schrödinger equation exactly was first used to describe the final state. This 3C wavefunction was quite successful in reproducing the triple differential cross sections (TDCS) for electron impact ionization of hydrogen[1] and helium[13] at high and intermediate energies. However, for low incident energies, the calculated TDCS using the 3C wavefunction are not in agreement with experiment[2]. The major limitation of the BBK model lies in the fact that the dynamic screening of any two-body Coulomb interaction, i.e., the influence on the strength of the interaction of any two particles by the presence of the third one, has not been taken into account. This deficiency was first corrected by Berakdar and Briggs[2] through the introduction of new Sommerfeld parameters for the symmetric case in which the two outgoing electrons have equal energies. We have extended the work of Berakdar and Briggs by formulating the effective Sommerfeld parameters for both symmetric and asymmetric cases[4] and the results turned out to be in quite good agreement with the measurements.[4,14]

However, in both the BBK and the DS3C models, the incident electron is described by a plane wave and the final state continuum electrons are assumed to move in a point Coulomb potential in order to facilitate analytic treatments. Neither of these approximation is accurate for low energies. Recently, the evidence of the initial state correlation effects has been demonstrated by Jones and Madison[15]. In this paper, the DS3C model[4] suggested earlier by us will be improved by taking into account the final channel screening effects for electron impact ionization of he-

*Project supported by the National Natural Science Foundation of China (Grant No. 19634040), the Natural Science Foundation of Anhui Province (Grant No. 99022022) and the Education Foundation of Anhui Province (Grant No. 97JL101).

lium. In addition, the exchange effects will also be demonstrated.

II. THEORY

In this section we briefly sketch the theoretical model. Here we consider a helium target being singly ionized by the impact of an electron with incident momentum $\boldsymbol{k}_0$. The TDCS for the simultaneous detection of two continuum electrons escaping with momenta $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ and emerging into directions defined by solid angles Ω_1 and Ω_2 is given by

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\mathrm{d}\Omega_2\mathrm{d}E} = (2\pi)^4\frac{k_1k_2}{k_0}\left[\frac{3}{4}\mid f(\boldsymbol{k}_1,\boldsymbol{k}_2)-g(\boldsymbol{k}_1,\boldsymbol{k}_2)\mid^2 + \frac{1}{4}\mid f(\boldsymbol{k}_1,\boldsymbol{k}_2)+g(\boldsymbol{k}_1,\boldsymbol{k}_2)\mid^2\right], \quad (1)$$

where $f(\boldsymbol{k}_1,\boldsymbol{k}_2)$ and $g(\boldsymbol{k}_1,\boldsymbol{k}_2)$ are the direct and exchange amplitudes respectively with $f(\boldsymbol{k}_2,\boldsymbol{k}_1) = g(\boldsymbol{k}_1,\boldsymbol{k}_2)$. The direct amplitude is

$$f(\boldsymbol{k}_1,\boldsymbol{k}_2) = < \Psi^-_{\boldsymbol{k}_1,\boldsymbol{k}_2} \mid V_i \mid \Phi_{\boldsymbol{k}_i} > . \quad (2)$$

The transition operator is taken as the projectile–target potential

$$V_i = -\frac{2}{r_1} + \frac{1}{\mid \boldsymbol{r}_1-\boldsymbol{r}_2\mid} + \frac{1}{\mid \boldsymbol{r}_1-\boldsymbol{r}_3\mid}, \quad (3)$$

where the coordinates $\boldsymbol{r}_2$ and $\boldsymbol{r}_3$ refer to the electrons initially bound to helium and $\boldsymbol{r}_1$ denotes the coordinate of the projectile electron with respect to the nucleus. The initial state wavefunction $\Phi_{\boldsymbol{k}_i}$ is a product of an incoming plane wave representing the impinging projectile and a Hartree–Fock type wavefunction given by Byron and Joachain[16] describing the ground state of helium (see Ref.[17] for details). The final state wavefunction $\Psi^-_{\boldsymbol{k}_1,\boldsymbol{k}_2}$ should then be an eigenfunction of the full four-body Hamiltonian with boundary conditions describing one bound and two outgoing electrons, and can be expressed as

$$\Psi^-_{\boldsymbol{k}_1,\boldsymbol{k}_2} = (2\pi)^{-3}\exp(i\boldsymbol{k}_1\cdot\boldsymbol{r}_1 + i\boldsymbol{k}_2\cdot\boldsymbol{r}_2)\psi_f(\boldsymbol{r}_3) \times \prod_j N_j\,{}_1F_1[i\alpha_j;1;-i(k_jr_j+\boldsymbol{k}_j\cdot\boldsymbol{r}_j)], \quad (4)$$

where $j = 1,2,12$, and the momentum $\boldsymbol{k}_{12}$ is defined as $\boldsymbol{k}_{12} = (\boldsymbol{k}_1-\boldsymbol{k}_2)/2$ whereas its conjugate coordinate is given by $\boldsymbol{r}_{12} = \boldsymbol{r}_1 - \boldsymbol{r}_2$. Also, N_j, $j \in \{1,2,12\}$ are normalization constants which can be given by

$$N_j = \exp(\alpha_j\pi/2)\Gamma(1-i\alpha_j). \quad (5)$$

The ground state of He^+ is described by $\psi_f(\boldsymbol{r}_3)$ and α_j, $j \in \{1,2,12\}$ being Sommerfeld parameters. The assumption that the three-body system consists of three spatially-independent two-body systems leads to the representation of the Sommerfeld parameters in the BBK model[1] as $\alpha_1 = -Z/k_1$, $\alpha_2 = -Z/k_2$ and $\alpha_{12} = 1/2k_{12}$ where Z is the charge of residual ion.

However, the Sommerfeld parameter is a measure of the strength of the Coulomb interaction between charged particles, and the strength of interaction of any two particles in the three-body Coulomb system is affected by the presence of the third one. Having recognized this, we suggested the DS3C model[4] to modify the 3C wavefunction by formulating the effective Sommerfeld parameters based on the work of Berakdar and Briggs[2]. Here we cite the explicit functional form of the product charges $Z_j = \alpha_j k_j$, $j \in \{1,2,12\}$ as

$$Z_1 = -Z + \frac{k_1}{4k_{12}}\sin^2\theta\left(1-\frac{\mid k_1-k_2\mid}{4k_{12}}\right) \quad (6)$$

$$Z_2 = -Z + \frac{k_2}{4k_{12}}\sin^2\theta\left(1-\frac{\mid k_1-k_2\mid}{4k_{12}}\right), \quad (7)$$

$$Z_{12} = 1 - \sin^2\theta\left(1-\frac{\mid k_1-k_2\mid}{4k_{12}}\right), \quad (8)$$

where $\theta = (\cos^{-1}\hat{\boldsymbol{k}}_1\cdot\hat{\boldsymbol{k}}_2)/2$. In our earlier works, we take $\boldsymbol{Z}$ in (6) and (7) as 1 for both hydrogen and helium targets.[4] However, it is only correct for hydrogen. For a helium target, the effective charge of the He^+-core seen by the escaping electrons is not exactly 1 because the charge of the nucleus is not completely screened by the bound electron in He^+, especially for slow outgoing electrons. Based on this consideration, we should replace $\boldsymbol{Z}$ in (6) and (7) by $\boldsymbol{Z}^1_{\mathrm{eff}}$ and $\boldsymbol{Z}^2_{\mathrm{eff}}$, respectively. It is reasonable that we demand $\boldsymbol{Z}^i_{\mathrm{eff}}$ $(i = 1,2)$ to go to 1 as the energies of the outgoing electrons tend to infinity in order to satisfy boundary conditions. Here we take the ansatz of Berakdar and Briggs[18] for $\boldsymbol{Z}^i_{\mathrm{eff}}$ as

$$\boldsymbol{Z}^i_{\mathrm{eff}} = 1 + a\exp(-bE_i) \qquad (i = 1,2), \quad (9)$$

where the parameters $a = 0.5052$, $b = 2.5496$ are determined empirically.

In this work, we apply the present improved DS3C model to the calculation of TDCS for electron impact ionization of helium in the asymmetric geometry at low energy. To our knowledge, the lowest incident energy measurements available for helium in the asymmetric geometry are due to Röder *et al.*[19] which provide a rigorous test of the current theories.

III. RESULTS AND DISCUSSION

The TDCS for electron impact ionization of helium at an incident energy of 40 eV in the coplanar asymmetric geometry have been calculated. In figures 1(a), (b), (c) and (d) are shown the present improved DS3C results and those of the original DS3C model compared with the absolute measurements[19] for a fixed ejected energy of 4 eV and scattering angles θ_1 of $-20°$, $-25°$, $-30°$ and $-35°$. The results of the convergent close-coupling (CCC) method[19] and those of the BBK model have also been plotted for comparison. In addition, in order to demonstrate the exchange effects, we compare the corresponding TDCS results of the present improved DS3C model with the cross sections generated singly by the direct and exchange amplitudes in figures 1(a′), (b′), (c′) and (d′).

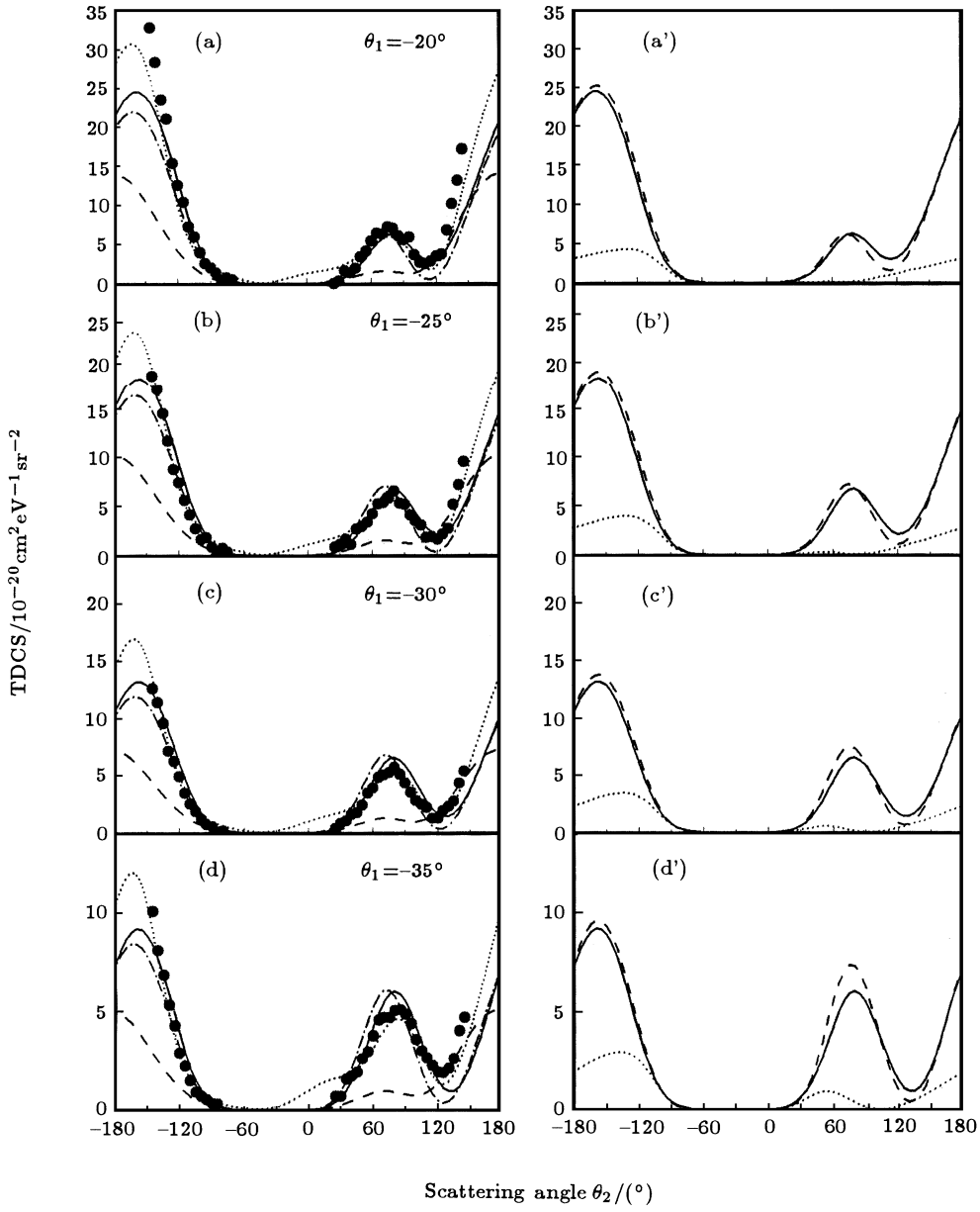


Fig.1. TDCS for electron impact ionization of helium at an incident energy $E_0 = 40$ eV in the coplanar asymmetric geometry for an ejected energy of 4 eV. The scattering angle θ_1 is fixed at (a) $\theta_1 = -20°$, (b) $\theta_1 = -25°$, (c) $\theta_1 = -30°$ and (d) $\theta_1 = -35°$. The circles denote the absolute experimental data of Röder *et al.*[19]; the full and the chain curves correspond to the present improved DS3C model and the original DS3C model, respectively; the dotted curve corresponds to the CCC method of Röder *et al.*[19] and the broken curve corresponds to the BBK model. The cross sections generated singly by the direct (broken curve) and exchange (dotted curve) amplitudes in the improved DS3C model corresponding to the calculations in (a)-(d) are shown in (a′)-(d′) compared with the TDCS results (solid curve).

From figure 1 one may easily deduce that the original DS3C model shows a large improvement over the BBK model in obtaining better magnitudes and shapes of the cross sections compared with the measurements, which has been discussed in our earlier work[14]. Here, we mainly focus on comparing the improved DS3C model with the original one. It can be seen from figure 1 that the improved DS3C model reproduces higher cross sections in the recoil peak whereas it yields slightly lower cross sections in the binary peak than the original DS3C model does, so that good agreement for a small scattering angle (figure 1(a)) of $\theta_1 = -20°$ and excellent agreement for large scattering angles of $\theta_1 = -25°$, $-30°$ and $-35°$ (figures 1(b)–(d)) with the measured cross sections in the recoil peak have been achieved. On the other hand, it should be noted that the location of the binary peak of experiment is exactly predicted by the present improved DS3C model while this position is shifted to a smaller angle by about 10° in the original DS3C model, although the magnitudes generated by both the improved and the original theoretical models are almost the same. In addition, it can be found that the underestimation of the original DS3C model for the cross sections in the dip around $\theta_2 = 120°$ on the right side of the binary peak has also been improved by the present theoretical model.

Since the CCC method developed recently[20] has been widely applied to various problems in atomic physics and has proved to be the most generally successful and reliable method for the description of electron scattering on helium and hydrogen-like targets at all projectile energies, we have illustrated the corresponding CCC results[19] for comparison. It can be seen from figure 1 that the results of the CCC method are generally in very good agreement with experiment and in quite good agreement with the present theory, although small quantitative discrepancies remain. However, it should be noted that we get cross sections identically zero for $\theta_1 = \theta_2$ which is observed in the experiment, whereas with the CCC method Röder *et al.*[19] get a small but nonzero number.

From figure 1(a), it can be seen that for a small scattering angle $\theta_1 = -20°$ the present improved DS3C model still underestimates the cross sections in the recoil peak where both electrons are travelling in the backward direction, whereas the results of the CCC method are in excellent agreement with experiment. This really tests the internal scattering region rather than the boundary conditions. The CCC method works well in the internal region, while the the DS3C works well with correct boundary conditions.

It has been shown in figure 1(a′)–(d′) that the TDCS are due to an interplay of direct and exchange scattering and the separate contributions of direct and exchange amplitudes. However, for the situations considered here, the momentum transfer $\boldsymbol{k} = \boldsymbol{k}_0 - \boldsymbol{k}_1$ is small, and hence the TDCS are mainly contributed by the direct amplitude.[17]

In figure 2 are shown the TDCS for fixed angles of $\theta_2 = 25°$ and 147° of the slow electron. It can be seen that for $\theta_2 = 25°$ the cross sections in the peak region of $-110° < \theta_1 < -40°$ are greatly magnified and the location of the peak is shifted by about 10° in the present improved DS3C model compared with those in the original DS3C model so that the agreement with the experimental measurements could be considered satisfactory. For the case of $\theta_2 = 147°$, the present DS3C model reproduces higher cross sections in the peak around $\theta_1 = 0°$ as well and the agreement with experiment and CCC becomes better. However, it is unfortunate that for the region of $\theta_1 < -120°$ in figure 2(a) the present DS3C yields cross sections that are even smaller, which results in poorer agreement with experiment. This demonstrates that the improved DS3C model should not be considered fully successful.

It has been suggested in our earlier work[14] that the exchange effects between two outgoing electrons cannot be ignored, especially for the case where the scattering angles of slow electrons are fixed. This statement is only correct in one aspect. From figure 2(a′) and (b′) it can be seen that for $\theta_2 = 25°$ the TDCS are mainly contributed by the exchange amplitude whereas for $\theta_2 = 147°$ the contributions from the exchange amplitude can be ignored. The real reason for this is that large cross sections correspond to a small momentum transfer[17]. Even for fixed angles of θ_1, the exchange effects still become more important as the angle of θ_1 increases, which has been demonstrated in figure 2 in Ref.[17]. This is because the cross sections generated singly by the direct amplitude tend to be smaller as the angles of θ_1 become larger and in this case the larger momentum transfer appears. For the case of $\theta_2 = 25°$ in figure 2(a′) the exchange scattering corresponds to $\theta_1 = 25°$ so that the momentum transfer is small, which yields large cross sections. This is why the total TDCS are mainly contributed by the exchange amplitude. On the other hand, for the case of θ_1=147°, the exchange scattering

corresponds to a very large momentum transfer and hence yields cross sections that are very small.

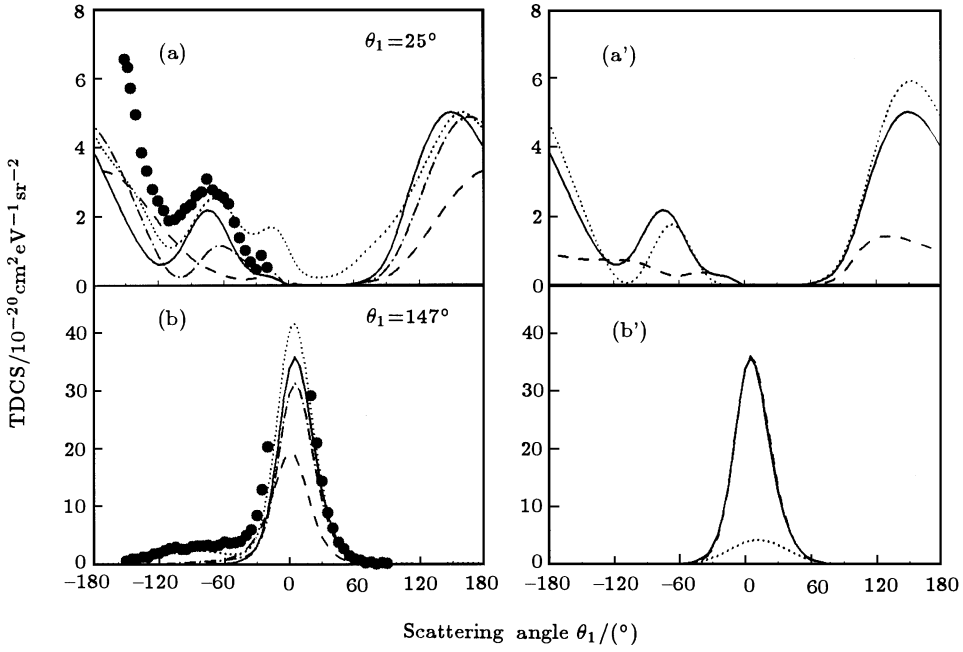


Fig.2. Same as figure 1 but for fixed angles of θ_2.

IV. CONCLUSION

In this work, we have performed a study of electron impact ionization of atomic helium at an incident energy of 40 eV in four kinds of theoretical models. The original DS3C model has been improved by taking into account the final channel screening effects. Generally, the present DS3C calculations result in improved agreement with measured cross sections. In addition, the exchange effects have been considered. It has been shown in which situation the exchange effects are crucial.

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