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Theoretical calculation of the triple differential cross sections of the 2p orbital of argon in a coplanar highly asymmetric (e, 2e) reaction

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The triple differential cross sections of the 2p electron of argon in a coplanar highly asymmetric geometry have been calculated with the modified distorted wave Born approximation (DWBA) and the target Hartree–Fock approximation methods. The damping polarization of the semi-classical short-range potentials and the M_{ee} factor are included in the distorting potentials of the modified DWBA. Theoretical results are compared with a recent experiment. The dynamic mechanism of inner shell ionization in a coplanar highly asymmetric geometry (e, 2e) reaction are also discussed.

Keywords: (e, 2e) reaction, coplanar highly asymmetric geometry, distorted wave Born approximation
PACC: 3480D, 3450H

1. Introduction

The (e, 2e) reaction is one of the most subtle atomic processes, which provides many interesting phenomena of the three-body final states in a wide kinematic region.[1,2] The long range of the Coulomb force in the (e, 2e) reaction forbids free motion of particles even at an infinite inter-particle separation because the final state consists of a three-body continuum state whose wavefunction remains a correlated effect for one another even at a macroscopic distance.[3,4] So it is very difficult to carry out a theoretical study of the several particle problems in the (e, 2e) reaction. The theoretical description of collisions[5,6] depends sensitively on different aspects for the different kinematic regions in the (e, 2e) reaction. The triple differential cross section (TDCS), where the energies and momentum of all the three electrons are detected in the experiment, is capable of revealing a rich variety of information for evaluating the dynamic mechanism of the (e, 2e) reaction. Recently, Taouil *et al*[7] reported on the TDCS of the 2p electron of the argon (e, 2e) reaction in a coplanar highly non-symmetry geometry. In their experiments, the energies of the ejected electrons are 7 and 10 eV, but the energies of the fast scattered electrons are 8000 and 5360 eV, respectively. The results of the theoretical calculation with the distorted wave Born approximation (DWBA) method are not in good agreement with their experimental data. The deviations between the theoretical calculation and experiments may result from the significant distortion of the ejected electron wave due to increasing interaction with the core and correlation between the outgoing electrons and the remaining target electrons in the outer orbits. This implies that there are some other mechanisms that have not been otherwise treated in the coplanar highly non-symmetry geometry (e, 2e) reaction before. So accurate theoretical calculations are necessary in order to understand the interaction and collision processes correctly. In this paper, we have added the damping polarization of the semiclassical short-range potentials[8,9] and the M_{ee} factor[10] to the distorting potentials to investigate the dynamic process in the coplanar highly non-symmetry (e, 2e) reaction. The results of theoretical calculations with this modified DWBA method are compared with the measured differential cross section.

2. Theory

We consider the problem of two-electron (with

subscripts f and s) interaction with inert cores ν_f and ν_s which are distorting potentials in the coplanar highly non-symmetry (e, 2e) reaction. They have the long-range form of attractive Coulomb potentials. The corresponding kinetic energies of the two final outgoing electrons are E_f and E_s, and the corresponding momenta are $\boldsymbol{k}_f$ and $\boldsymbol{k}_s$; whereas the energy of incident electrons is E_0 and the corresponding momentum is $\boldsymbol{k}_0$. The TDCS is (in atomic units, $\eta = m_e = c = 1$)[11]

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_f \mathrm{d}\Omega_s \mathrm{d}E_0} = (2\pi)^4 \frac{k_f k_s}{k_0} \sum_{\mathrm{av}} |\langle \boldsymbol{k}_f \boldsymbol{k}_s | T | \alpha \boldsymbol{k}_0 \rangle|^2, \quad (1)$$

where the notation $\sum_{\mathrm{av}}$ represents the sum over final states and the average over initial magnetic and spine degenerate states. α is the bound state of target atoms with separation energy ε_α. The T matrix of the DWBA is

$$\begin{aligned} &\langle \boldsymbol{k}_f \boldsymbol{k}_s | T | \alpha \boldsymbol{k}_0 \rangle \\ =&\langle M_{\mathrm{ee}} \chi^{(-)}(\boldsymbol{k}_f) \chi^{(-)}(\boldsymbol{k}_s) | \nu_{fs} | \alpha \chi^{(+)}(\boldsymbol{k}_0) \rangle, \end{aligned} \quad (2)$$

where ν_{fs} is the electron–electron interaction potential. The element of the electron–electron T matrix is half off shell with energy E corresponding to the final-state relative momentum. In the DWBA, this is accounted for by a suitable potential, in which the motion of the external electron is represented by elastic scattering functions. $|\chi^{(+)}(\boldsymbol{k}_0)\rangle, |\chi^{(-)}(\boldsymbol{k}_f)\rangle$ and $|\chi^{(-)}(\boldsymbol{k}_s)\rangle$ are the distorted waves at different asymptotic conditions. The superscripts '+' and '–' refer to the incident and outgoing waves, respectively. M_{ee} is a factor introduced by Ward and Macek[12]

$$M_{\mathrm{ee}} = N_{\mathrm{ee}} |{}_1F_1[-\mathrm{i}\nu_{fs}, 1, -\mathrm{i}(k_{fs} r_{fs} + \boldsymbol{k}_{fs} \cdot \boldsymbol{r}_{fs})]|^2, \quad (3)$$

where ${}_1F_1(a, b, x)$ is Kummer's confluence hypergeometric function. N_{ee}, the Gamov factor, is intimately related to the normalization of the Coulomb function in the zero energy limit. It plays an interesting role in the Brauner–Briggs–Klar approximation,[13] and is defined as

$$N_{\mathrm{ee}} = \frac{\gamma}{\mathrm{e}^\gamma - 1}, \quad \text{with} \quad \gamma = \frac{2\pi}{|\boldsymbol{k}_f - \boldsymbol{k}_s|}. \quad (4)$$

The distorted waves are described by the following scattering equation

$$[E - K_0 - U_0 - H_s] |\alpha \chi^{(+)}(\boldsymbol{k}_0)\rangle = 0, \quad (5)$$

$$[E - K_f - U_f - K_s - \nu_s - V_{\mathrm{p}}^{\mathrm{d}}] |\chi^{(-)}(\boldsymbol{k}_f) \chi^{(-)}(\boldsymbol{k}_s)\rangle = 0, \quad (6)$$

where K is the kinetic energy, and U and ν are the static-exchange potentials.[11] We have included the exchange of the outgoing electrons by using a spin-averaged model which includes a combination of the direct distorted potentials and the spin-averaged local static-exchange potential $U_f(\nu_s)$, compatible with the possible asymptotic states. The semiclassical potential $V_{\mathrm{p}}^{\mathrm{d}}$ provides a simple procedure for the short-range damping of all the long-range adiabatic terms which asymptotically lead to the polarization forces.[14] It is

$$V_{\mathrm{p}}^{\mathrm{d}} = \frac{\int_0^r \rho(r)^2 r^{2l+2} \mathrm{d}r}{\int_0^\infty \rho(r)^2 r^{2l+2} \mathrm{d}r} V_{\mathrm{p}}, \quad (7)$$

where $\rho(r)$ is the electron density of the atom. V_{p} takes the form described in Ref.[14]

$$\begin{aligned} V_{\mathrm{p}} =& -\frac{9}{2y^4}\left[1 - \frac{1}{3}\mathrm{e}^{-2y}\left(1 + 2y + y^2 + \frac{20}{3}y^3 + \frac{4}{3}y^4\right)\right. \\ &\left. - \frac{2}{3}\mathrm{e}^{-4y}(1 + y^4)\right], \\ y =& \left(\frac{9r}{2\alpha_{\mathrm{p}}}\right)^{1/4}, \end{aligned} \quad (8)$$

where α_{p} is the atomic dipole polarizability.

3. Results and discussion

In this paper we calculate the TDCS of the 2p electron of argon in a coplanar highly asymmetric geometry with the DWBA and the modified DWBA methods. The energies of the ejected electrons are 7 and 10 eV, and the energies of the scattered electrons are 8000 and 5360 eV. The azimuthal angles ϕ of the two detected electrons are ϕ_f=0° and ϕ_s=0°, 180°; the recoil momenta are K=0.75 a.u. and K=0.5 a.u.; the polar angles of the fast electron are settled at θ_f=1.5° and θ_f=0.5°. The variable parameter is the polar angle θ_s of the ejected electron, which is scanned from 0° to 360°. The normalized wavefunction of the target is approximated by the Hartree–Fock (HF) 'independent-electron' orbital model of Bunge *et al.*[16]

The TDCS for ionization from the 2p orbital at 8256 eV incident energy is presented in Fig.1. The theoretical results calculated using the modified DWBA and THFA methods are compared with the experimental data in Ref.[6]. In general, the TDCS in the coplanar highly asymmetric (e, 2e) reaction has two electron peaks:[17] the binary electron peak which corresponds to the direct ionization by the incident electron with the bound electron collisions, and the recoil

electron peak which corresponds to the indirect ionization produced from electrons ejected by the electron–atom collisions. We can see from Fig.1 that the TDCS calculated theoretically with the modified DWBA not only predicts the position of the double electron peaks at about 60° and 230°, but also predicts the rate of the maximum magnitudes of the two electron peak amplitudes 1.4:1. This is better than that calculated with the DWBA method in which the position and the magnitude of the double peaks are almost symmetric. However, the theoretical results calculated with the modified DWBA have not yet predicted the complicated structures of the double peaks in the experimental data of Taouil *et al.* The main difference between the theory and the experiments are obvious. One reason may be the treatment of the atomic structure with the 'independent-electron' model and the single configuration approximation of the HF method. Another reason may be that the influence of the distorted potential created by the target in this work is stronger for the inner-shell ionization in a coplanar highly asymmetric geometry. Because the binding energy of the argon (2p) shell is 249 eV (fine-structure averaged), the distorted potential of the slow electron in the coplanar high asymmetry is not sufficient to predict accurately the TDCS along with the significant post-collision interaction (PCI)[18] for inner ionization of the (e, 2e) reaction.[19]

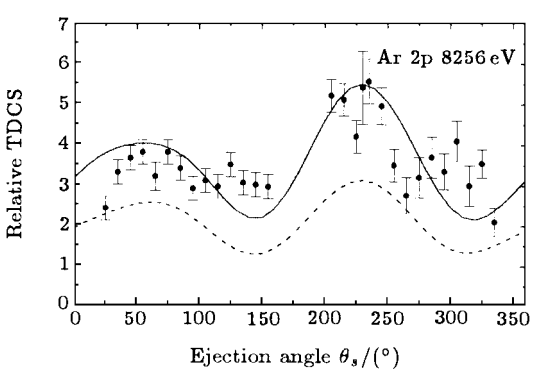


Fig.1. Relative TDCS for the Ar(2p) ionization in a coplanar highly asymmetric geometry: E_0=8256 eV, E_s=7 eV, θ_f=1.5°. The solid curve: the present MDWBA; solid circle: the error bars and the dashed curve by the DWBA calculation are those quoted from Ref.[6].

Figure 2 gives the TDCS for ionization of the 2p electron of argon at a 5720 eV incident energy. The energy of the ejected electron is 10 eV. The scattered angle of fast electrons is 0.5°, different from the scattered angle 1.5° in Fig.1. It is obvious that the profiles of the TDCS are very similar to those in Fig.1. The calculated results also predict the ratio of the maximum magnitudes of the double peaks to be 1.3:1. The large difference in this situation is that the positions of the double peaks are not predicted accurately by the theoretical calculation. There is about 25° deviation between the theoretically calculated result and the experimental data. The data of the TDCS with the small scattering angle in the experiment are sensitive to the theoretical model, which give a stringent test of the theory.[18]

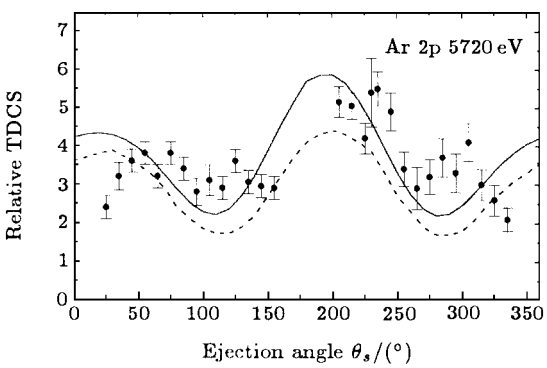


Fig.2. Relative TDCS for the Ar(2p) ionization: E_0=5720 eV, E_s=10 eV, θ_f=0.5°. The solid curve, the dashed curve, the experiment data and the error bar are as in Fig.1.

In conclusion, the effects of the Gamow factor M_{ee} and the short-range damping of polarization give some angular behaviour of the TDCS at low energy. It represents partially the final-state electron–electron interaction in the coplanar high asymmetry. The single configuration approximation of the HF states does not reflect the complicated double-peak structure of the TDCS in which it might come from the effects of PCI

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