Study of (e, 2e) process on potassium at 6 eV–60 eV above threshold in a second-order Born approximation*

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The standard distorted wave Born approximation (DWBA) method has been extended to second-order Born amplitude in order to describe the multiple interactions between the projectile and the atomic target. Second-order DWBA calculations have been preformed to investigate the triple differential cross sections (TDCS) of coplanar doubly symmetric (e, 2e) collisions for the alkali target potassium at excess energies of 6 eV–60 eV. Compared with the previous first-order DWBA calculations, the present theoretical model improves the degree of agreement with experiments, especially for the backward scattering angle region of TDCS. This indicates that the present second-order Born term is capable of giving a reasonable correction to the DWBA model in studying coplanar symmetric (e, 2e) problems in low and intermediate energy ranges.

Keywords: second-order Born approximation, (e, 2e) collisions, potassium, triple differential cross section

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1. Introduction

The single ionization of atoms and molecules by electron impact, namely the (e, 2e) reaction, has attracted continuous interest over several decades. The triple differential cross sections (TDCS) of the (e, 2e) reaction give a comprehensive picture of collision dynamics.[1] In the past decade, impressive progress has been made in theoretical predictions of TDCS in the electron impact ionization of hydrogen and helium by using several non-perturbative approaches, such as exterior complex scaling (ECS),[2] convergent close-coupling (CCC),[3] time-dependent close-coupling (TDCC),[4] and B-spline R-matrix (BSR).[5] As the problems of simple targets are considered to be nearly solved, more attention has been paid to understanding the ionization of complex targets.

Recently, Murray[6] reported a comprehensive set of experimental TDCS for coplanar symmetric (e, 2e) collisions for alkali metal (Na and K) and alkali earth metal (Mg and Ca) targets over a wide range of energies, which provided a challenge for the theories of the ionization processes. Subsequently, theoretical work on K in the same geometry was preformed based on the first-order distorted wave Born approximation (DWBA) with various corrections such as post-collision interaction (PCI), polarization potential, and static exchange potential.[7−10] The PCI effect was included through the angle-dependent effective charge model[7] or a Gamow factor.[9,10] The polarization potential was introduced as a function of the electron density parameter.[8,10] Either the spin averaged static exchange potential (SASEP)[8,10] or the modified semiclassical exchange potential (MSCEP)[9] was employed to consider the electron exchange effect of the target. These modified first-order DWBA calculations showed reasonable improvement for the agreement with the experimental measurements compared with the standard DWBA calculation. However, significant discrepancies remain between theory and experiment. One possible reason for these discrepancies may be that the higher order effects in the projectile-target interaction are missing in these DWBA calculations, which was highly recommended to be included in the future investigations.[7,8,10]

We recently extended the standard DWBA method by treating the projectile-target interactions

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up to the second-order Born amplitude to study the (e, 2e) process of Ar,[11] and a reasonable agreement with the experiment was obtained. In this paper, we have preformed second-order DWBA calculations of TDCS at energies of 6 eV–60 eV above the threshold of potassium. The goal of the present work is to investigate the second-order effect for the sensitivity of theoretical predictions in coplanar symmetric (e, 2e) collisions for potassium. A brief outline of the present theoretical model is presented in the following section.

2. Formalism and calculation details

An (e, 2e) reaction is determined by the energy conservation condition

$$E_0 = E_1 + E_2 + I, \tag{1}$$

where E_0, E_1, and E_2 are the incident, scattered, and ejected electron energies (with momenta $\boldsymbol{k}_0$, $\boldsymbol{k}_1$, and $\boldsymbol{k}_2$, as well as scattering and ejection angles of θ_1 and θ_2), respectively, and I is the ionization potential of the ionized orbital (for K(4s) = 4.34 eV). The momentum transfer is $\boldsymbol{K} = \boldsymbol{k}_0 - \boldsymbol{k}_1$.

In the present second-order Born approximation, the TDCS for the (e, 2e) process on a target may be written as

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_2} = (2\pi)^4\frac{k_1k_2}{k_0}\sum_{av}|f_{\mathrm{B1}} + f_{\mathrm{B2}}|^2, \tag{2}$$

where the first- and second-order terms f_{B1} and f_{B2} are given by

$$f_{\mathrm{B1}} = \langle\chi^{(-)}(\boldsymbol{k}_1)\chi^{(-)}(\boldsymbol{k}_2)|V|\phi_{\mathrm{i}}\chi^{(+)}(\boldsymbol{k}_0)\rangle, \tag{3}$$

and

$$f_{\mathrm{B2}} = \langle\chi^{(-)}(\boldsymbol{k}_1)\chi^{(-)}(\boldsymbol{k}_2)|VG_0^+V|\phi_{\mathrm{i}}\chi^{(+)}(\boldsymbol{k}_0)\rangle, \tag{4}$$

here $V = 1/|\boldsymbol{r}_1 - \boldsymbol{r}_2|$ represents the interaction potential between the incident electron and the target, ϕ_{i} represents the initial state of the target, $\chi^{(+)}$ and $\chi^{(-)}$ represent the distorted wave functions of the incident electron and two outgoing electrons, respectively. G_0^+ is the Green's function

$$G_0^+ = \frac{1}{E_0^+ - H + \mathrm{i}\varepsilon}. \tag{5}$$

The expression of the first-order term has been introduced in detail by McCarthy[12] and will not be repeated here for brevity. One should note that the distorted wave functions in the present model are calculated by using the exchange potential of Furness and McCarthy[13] as modified by Riley and Truhlar[14] which is given by

$$\begin{aligned} V_E(r) = {} & 0.5[E_0 - V_D(r) - \{[E_0 - V_D(r)]^2 \\ & + 4\pi\rho(r)\}^{1/2}], \end{aligned} \tag{6}$$

where $\rho(r)$ is the electron density, and $V_D(r)$ is the direct distorting potential obtained from a Hartree–Fock calculation of the target radial orbital $u_{nl}(r)$ by

$$V_D(r) = \sum_{nl} N_{nl}\int \mathrm{d}r'[u_{nl}(r')]^2/r_>, \tag{7}$$

where $r_>$ is the greater of r and r', and N_{nl} is the number of electrons in each orbital nl.

By inserting a set of intermediate states $|\phi_j\rangle$ whose eigenenergies are ε_j and using the condition $T|\boldsymbol{k}_0\rangle = V|\chi^{(+)}(\boldsymbol{k}_0)\rangle$, the present second-order term f_{B2} can be rewritten as

$$\begin{aligned} f_{\mathrm{B2}} = {} & \sum_j \int \mathrm{d}\boldsymbol{q}\langle\chi^{(-)}(\boldsymbol{k}_1)\chi^{(-)}(\boldsymbol{k}_2)|V|\phi_j\boldsymbol{q}\rangle \\ & \times \frac{1}{E_0^+ - \varepsilon_j - \frac{1}{2}q^2 + \mathrm{i}\varepsilon}\langle\boldsymbol{q}\phi_j|T|\phi_{\mathrm{i}}\boldsymbol{k}_0\rangle. \end{aligned} \tag{8}$$

Define

$$\frac{1}{2}k_j^2 = E_0^+ - \varepsilon_j \tag{9}$$

and use the principal-value integral to solve the equation of the second-order term. Numerically, the q integration is replaced by an N-fold quadrature sum with weights w_n and coordinates q_n, $n = 1, \ldots, N$. The equation becomes a set of algebraic equations which can be written in terms of new coordinates x_{jn} in which the on- and off-shell notations are combined

$$x_{jn} = \begin{cases} k_j, & n = 1 \\ q_{n-1}, & n = 2, \ldots, N+1. \end{cases} \tag{10}$$

Then equation (8) can be expressed as

$$\begin{aligned} f_{\mathrm{B2}} = {} & \sum_j \sum_{n=1}^{N+1} W_{jn}\langle\chi^{(-)}(\boldsymbol{k}_1)\chi^{(-)}(\boldsymbol{k}_2)| \\ & \times V|\phi_j\boldsymbol{x}_{jn}\rangle\langle\boldsymbol{x}_{jn}\phi_j|T|\phi_{\mathrm{i}}\boldsymbol{k}_0\rangle, \end{aligned} \tag{11}$$

where the superweights W_{jn} are

$$W_{jn} = \begin{cases} x_{jn}^2 w_{n-1} \left[\dfrac{1}{2}(k_j^2 - x_{jn}^2)\right]^{-1}, & n = 2, \ldots, N+1, \\ -k_j^2 \displaystyle\sum_{n'=2}^{N+1} w_{n'-1} \left[\dfrac{1}{2}(k_j^2 - x_{jn'}^2\right]^{-1} - \mathrm{i}\pi k_j, & n = 1. \end{cases} \tag{12}$$

To simplify the calculation, we only keep the first term of W_{jn} (i.e. W_{j1}) in Eq. (11), which is very similar to the simplified Green's function (SG) approximation introduced by Reid *et al.*[15,16] In the SG approximation, only the imaginary part of the Green's function was kept in the second-order term. It was proved to be reasonably good for direct ionization processes by Chen and Madison.[17] In the present calculations, the first term of Eq. (11) can be obtained in the same way as f_{B1} by replacing the distorted wavefunction of $\chi^{(+)}(\boldsymbol{k}_0)$ by the plane wavefunction of $\boldsymbol{x}_{j1}$. The second term of Eq. (11) is the T-matrix elements of electron–atom scattering, which can be calculated by solving the coupled integral equations of the coupled-channel optical (CCO) model. Theoretical details of the CCO model for electron scattering from atoms can be found in Ref. [18].

In the present calculation, all the states of potassium are represented by single configuration wave functions which are obtained from the Hartree–Fock calculation, and we treat atomic K as a frozen core plus a valence electron in its initial orbital. The initial state of K is in ground state when calculating the first-order term. In the CCO calculations of the T-matrix in the second-order term, the eight lowest orbitals for K are included in P space for sufficient convergence. They are 4s, 5s, 6s, 4p, 5p, 6p, and 3d, 4d. Two of them, including 4s and 4p, are considered as intermediate states ϕ_j in the calculations of f_{B2}, since they are expected to make dominant contributions to the scattering amplitudes. The optical potential in Q space that describes the continuum is not included in the present calculation. The numbers of partial waves, which have been carefully checked to keep the calculation convergent, are up to 90, 80, and 80 for incident, scattered, and ejected electrons, respectively.

3. Results and discussion

In this paper, we have calculated the TDCS of coplanar symmetric (e, 2e) collisions for potassium at energies of two outgoing electrons fixed at $E_1 = E_2 = 3$ eV, 5 eV, 7.5 eV, 10 eV, 15 eV, 20 eV, 25 eV, and 30 eV. The second-order DWBA model, labeled DWB2 below, is employed in the present calculation. In Fig. 1 we display the present DWB2 calculations (solid curve) of coplanar symmetric (e, 2e) processes for K (4s), along with experimental data of Murray[6] (solid circles) as well as previous first-order DWBA calculations of Khajuria *et al.* with MSCEP and PCI[9] (dotted curve; not available for E_1 (E_2) at 10 eV and 20 eV) and Purohit *et al.* with polarization potential and PCI[10] (dashed curve). All the results are normalized to unity at their maximum points, respectively, and are presented on a logarithmic scale for the convenience of comparison.

As shown in Figs. 1(a)–1(c) for E_1 (E_2) at 3, 5, and 7.5 eV, respectively, all the DWBA calculations fail to reproduce the positions of the experimental forward peaks at $\theta \sim 50°$. It is very interesting that the first-order calculations of Khajuria *et al.* with MSCEP and PCI give a shift towards a large angle, which is opposite to the other two DWBA results, and show additional bumps at angles near 30°. Since Purohit *et al.*[10] also included the PCI effect in their calculation, these should be attributed to the modification of the exchange potential in calculating the distorted wave functions. Good agreements are obtained when comparing the present DWB2 results with experimental data at $\theta \sim 70°$–$110°$. Especially, the present DWB2 model is very successful in reproducing the dips of experimental TDCS at $\theta \sim 100°$, and gives backward peaks at $\theta \sim 115°$, which is very close to the experiment. In Fig. 1(d) for $E_1 = E_2 = 10$ eV, the DWBA calculations give good agreement with experimental data. Only small discrepancies are observed when comparing between first- and second-order results. The present DWB2 model predicts a dip at $\theta \sim 100°$, which is 5° smaller than in experiment and calculations of Purohit *et al.* However, the dip of the present DWB2 prediction is 40% deeper than the first-order results, which is in coincidence with the experiment in magnitude. Figures 1(e) and 1(f) plot the cases of $E_1 = E_2 = 15$ eV and 20 eV, respectively. The experimental TDCS display narrower forward scattering peaks and get flatter in the backward angle region than the above cases. All the DWBA calculations reproduce forward peaks very well, but fail to describe the flat shapes of TDCS backwards. However, the present DWB2 model still predicts the same positions of inflexion point, dip, and backward peaks

at 65°, 95°, and 120°, respectively, as experiment in Fig. 1(e). For higher energies of E_1 (E_2) at 25 eV and 30 eV in Figs. 1(g) and 1(h), the present DWB2 calculations show satisfactory agreement with experimental data, especially in the backward angle region, both in shape and magnitude. Clear double dip features are predicted in the angle region of $\theta \sim 80°$–$120°$ by the present DWB2 model, which is the same as the trend of experimental TDCS. The first-order calculations of Purohit *et al.*[10] also predict these features, but show higher value in magnitude and a little shift towards a large angle.

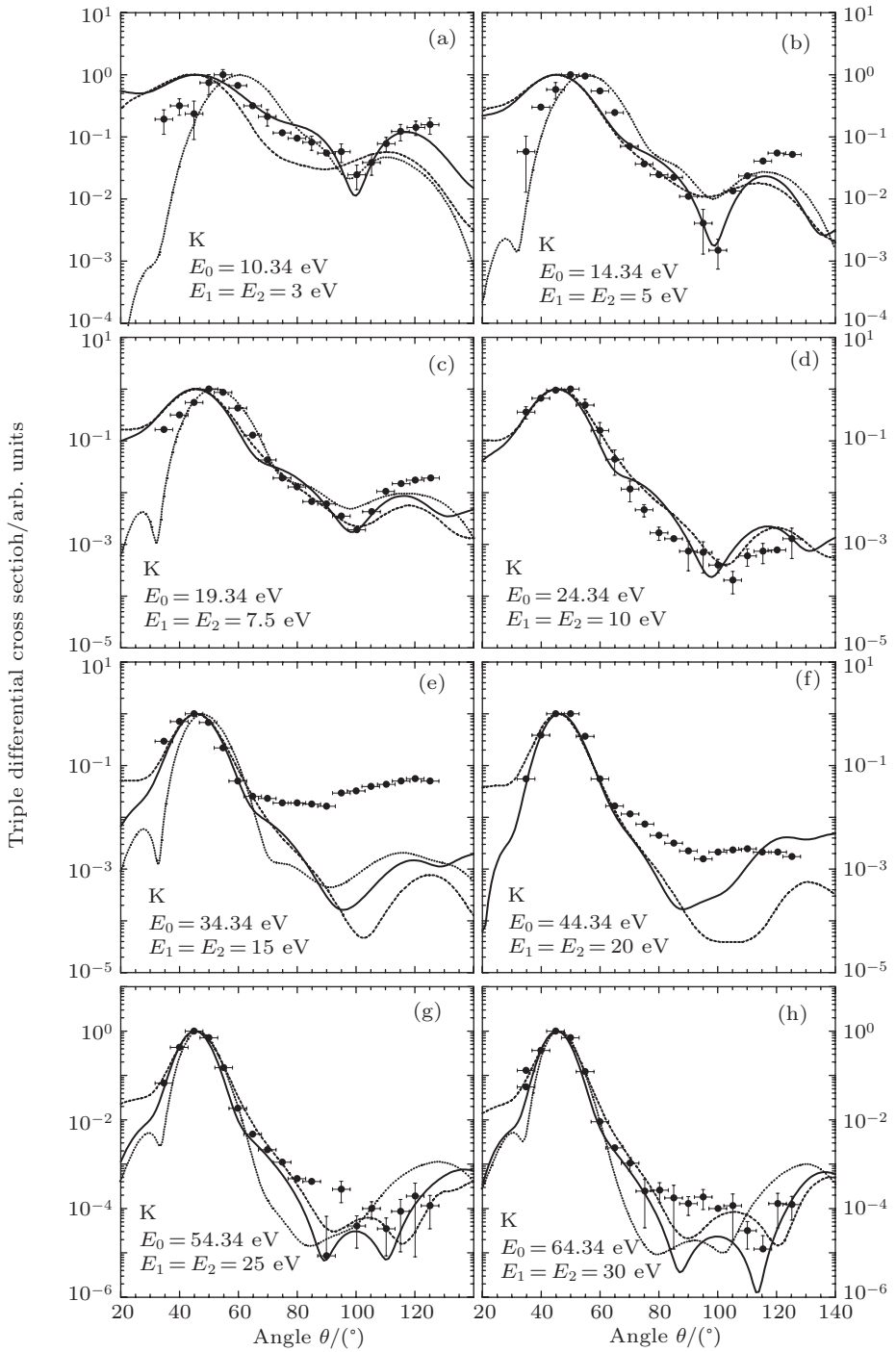


Fig. 1. TDCS of coplanar symmetric (e, 2e) for K (4s) as a function of the scattering angle at $E_1 = E_2 = 3$ eV (a), 5 eV (b), 7.5 eV (c), 10 eV (d), 15 eV (e), 20 eV (f), 25 eV (g), and 30 eV (h). All the theoretical and experimental data have been normalized to unity at their maximum points, respectively. Solid circles: experimental data of Murray,[6] solid curve: present DWB2 calculation; dotted curve: DWBA calculation of Khajuria *et al.* with MSCEP and PCI,[9] dashed curve: DWBA calculation of Purohit *et al.* with polarization potential and PCI.[10]

4. Conclusion

As discussed above, the inclusion of the second-order Born term in the present DWB2 model improves the agreement between DWBA calculations and experimental measurements of coplanar symmetric (e, 2e) collisions for potassium, especially for the backward scattering angle region. This proves that the present second-order term gives a correct description of multi projectile-target interactions, and provides a reasonable correction to the theory, at least in the present cases. However, discrepancies still exist especially for low incident energies. This might be due to a more complex structure of K (4s), which is possibly influenced by the open 3d shell in the electron scattering processes, and a more accurate description of K (4s) target is suggested in future theoretical investigations. Furthermore, the effect of PCI and proper choice of exchange potential should also be important according to the previous first-order DWBA investigations.[7−10] Therefore, the inclusion of these corrections and more intermediate states as well as some unknown effects up to the second-order term will be considered in our future DWB2 research.

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