Second-order Born calculation of coplanar symmetric (e, 2e) process on Mg*

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The second-order distorted wave Born approximation (DWBA) method is employed to investigate the triple differential cross sections (TDCS) of coplanar doubly symmetric (e, 2e) collisions for magnesium at excess energies of 6 eV–20 eV. Comparing with the standard first-order DWBA calculations, the inclusion of the second-order Born term in the scattering amplitude improves the degree of agreement with experiments, especially for backward scattering region of TDCS. This indicates that the present second-order Born term is capable to give a reasonable correction to DWBA model in studying coplanar symmetric (e, 2e) problems of two-valence-electron target in low energy range.

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

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1. Introduction

The (e, 2e) process (i.e. the single ionization of atoms and molecules by electron impact) is one of the most fundamental and attractive problems in atomic and molecular physics.[1–4] Relative cross sections, especially the triple differential cross sections (TDCS), can provide complete information about atomic structure and collision dynamics in the process.[5–9] In the past decade, impressive progress has been made in theoretical predictions of TDCS in the electron impact ionization of H and He by using several non-perturbative approaches, such as exterior complex scaling (ECS),[10] convergent close-coupling (CCC),[11] time-dependent close-coupling (TDCC),[12] and B-spline *R*-matrix (BSR).[13] Since the dynamics of (e, 2e) process for simple targets has been almost fully understood by these state-of-the-art theoretical methods, the focus of research is now shifting to study on the ionization of more complex targets.

Recently, Murray[14] measured a complete set of experimental TDCS for coplanar symmetric (e, 2e) collisions of complex targets which have one- or two-valance electrons in their open shells, such as Na, K, Mg, and Ca. This research provided a challenge to theories, and subsequently a lot of calculations were carried out on the topic. As a well-known theoretical approach in (e, 2e) reaction of complex targets, the distorted wave Born approximation (DWBA) was the most frequently employed method among these theoretical works. Almost all of these DWBA calculations were based on first-order Born amplitude with various corrections to include different kinds of correlations in the (e, 2e) process of target Mg.[15–17] Khajuria *et al.*[15] employed either the spin averaged static exchange potential (SASEP) or the modified semiclassical exchange potential (MSCEP) to consider the electron exchange effect of target in their first-order DWBA model. A Gamow factor was also used to include the post-collision interaction (PCI) effect in the calculation. Then, Hitawala *et al.*[16] carried out the DWBA calculation on Mg (e, 2e) process, which considered the effect of polarization by using a function of electron density parameter. Most recently, Purohit *et al.*[17] modified DWBA method by including the correlation–polarization potential and employing a Ward–Macek factor to take the PCI into account. These modified first-order DWBA calculations showed reasonable improvement in the agreement with the experimental measurements compared with standard DWBA calculation. However, there remain significant discrepancies between theory and experiment at low energies. This may result from the more complicated interactions between projectile and complex target in the collision, which could be introduced by the higher order terms in the DWBA method.

We recently extended the standard DWBA method by treating the projectile–target interactions up to the second-order Born amplitude to improve the description of complicated projectile–target interactions. We investigated the coplanar symmetric (e, 2e) process of one-valence-electron targets Na and K,[18,19] and reasonable agreements with experiment were obtained. Hitawala *et al.*[16] observed in their research that the ratio of forward to backward peak decreased for Mg and Ca in comparison to Na and K, which showed the second-order effects were more involved in the ionization of alkali earth atoms. This motivated us to perform a further investigation on this point. Therefore, in this paper we have carried

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out second-order DWBA calculations of TDCS for excess energies (i.e., incident energy above the ionization potential) at 6, 10, 15, and 20 eV. 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 Mg.

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 Mg(3s) = 7.65 eV). The momentum transfer is $\boldsymbol{K} = \boldsymbol{k}_0 - \boldsymbol{k}_1$.

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

$$\frac{\mathrm{d}^3\sigma}{\mathrm{d}\Omega_1\,\mathrm{d}\Omega_2\,\mathrm{d}E_2} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{\mathrm{av}} |f_{\mathrm{B1}} + f_{\mathrm{B2}}|^2, \tag{2}$$

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

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

and

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

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 target; $\chi^{(+)}$ and $\chi^{(-)}$ represent the distorted wave functions of the incident electron and two outgoing electrons, respectively. G_0^+ is Green's function

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

The expression of f_{B1} and f_{B2} have been described in detail in several earlier publications; for example, Refs. [18] and [19]. Briefly the second-order term f_{B2} is calculated by inserting a set of intermediate states ϕ_j and summing over the product of the direct ionization amplitude and T-matrix elements of electron–atom scattering, which can be calculated by solving the coupled integral equations of the coupled-channel optical (CCO) model.[20]

In the present calculation, the initial state of Mg is in ground state $(3s^2)\ ^1S$ when calculating the first-order term. In the CCO calculations of the T-matrix in the second-order term, 14 lowest discrete channels, including $(3s^2)\ ^1S$, $(3s3p)\ ^3P$, $(3s3p)\ ^1P$, $(3s4s)\ ^3S$, $(3s4s)\ ^1S$, $(3s3d)\ ^1D$, $(3s4p)\ ^3P$, $(3s3d)\ ^3D$, $(3s4p)\ ^1P$, $(3s5s)\ ^3S$, $(3s5s)\ ^1S$, $(3s4d)\ ^1D$, $(3s4d)\ ^3D$, $(3s5p)\ ^1P$, are explicitly coupled in P space for convergence. These states are represented by configuration interaction (CI) wave functions. 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 atomic Mg at energies of two outgoing electrons fixed at $E_1 = E_2 = 3$ eV, 5 eV, 7.5 eV, and 10 eV. Both the first- and second-order DWBA models, labeled DWBA and DWB2, respectively, are employed in the present calculation. The present DWBA model uses the standard spin-average static exchange potential of Furness and McCarthy,[21] which is same as the DWBA (FM) result of Khajuria *et al.*[15] In Fig. 1 we display the present standard DWBA (dotted curve) and DWB2 (solid curve) calculations of coplanar symmetric (e, 2e) processes for Mg(3s), along with the DWBA-PCI result of Khajuria *et al.*[15] (dashed curve), the modified DWBA calculation with polarization potential and PCI corrections (labeled DWBA-pol-PCI below) of Purohit *et al.*[17] (dash–dotted curve) as well as the experimental data of Murray[14] (solid circles). All the results are normalized to unity at $\theta = 45°$, respectively, and are presented on a logarithmic scale for the convenience of comparison.

Figure 1 shows that DWB2 model gives an overall improvement over the standard DWBA, especially for the angles $\theta > 80°$, and gives the best agreement with experimental data among all the modified DWBA calculations. As shown in Fig. 1(a) for E_1 (E_2) at 3 eV, the DWB2 model reproduces the experimental data successfully at $\theta < 85°$. The inclusion of the second-order term raises the cross section in the backward scattering angle region, and gives a more similar shape as experiment than DWBA and DWBA-PCI predictions. This indicates that the projectile–target interactions are more complicated at such a low energy for the two-valence-electron target Mg and the second-order term is capable of effectively improving the description of collision process. The PCI term, on the other hand, makes the curve broader in the forward peak region and does not improve the backward scattering region much. The DWBA-pol-PCI calculation is not available at this energy. In Fig. 1(b) for $E_1 = E_2 = 5$ eV, all of the calculations demonstrate more similar trends to the experimental data than was the case in Fig. 1(a). The DWB2 calculation gives a minimum at $\theta \sim 90°$, which is in best agreement with the experimental measurement, and a maximum at $\theta \sim 110°$, which is a little higher than experimental backward peak in magnitude. We

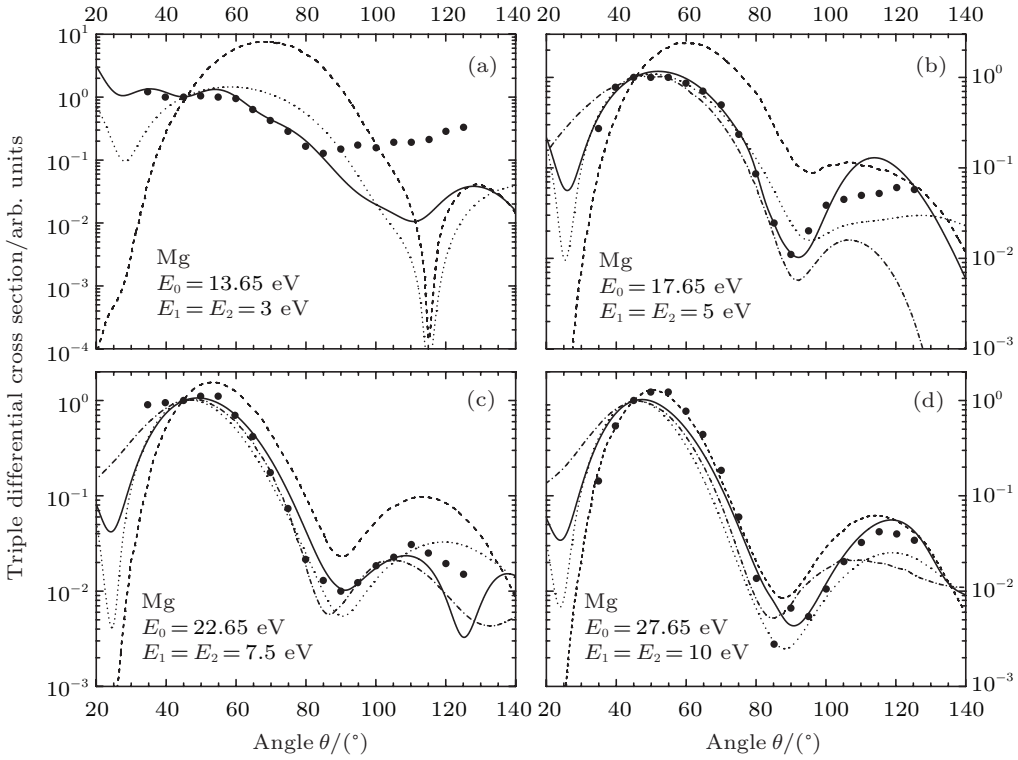


Fig. 1. TDCS of coplanar symmetric (e, 2e) for Mg(3s) as a function of scattering angle at $E_1 = E_2 =$ (a) 3 eV, (b) 5 eV, (c) 7.5 eV, and (d) 10 eV. All the theoretical and experimental data have been normalized to unity at $\theta = 45°$, respectively. Solid circles: experimental data of Murray;[14] solid curve: present DWB2 calculation; dotted curve: present standard DWBA calculation; dashed curve: DWBA calculation with PCI (DWBA-PCI) of Khajuria *et al.*;[15] dash–dotted curve: DWBA calculation with polarization potential and PCI corrections (DWBA-pol-PCI) of Purohit *et al.*[17]

notice that the DWBA-PCI also gives a higher curve than experiment while the DWBA-pol-PCI curve is lower than the others. This probably means that the discrepancy could be attributed to the missing polarization effect in the present DWB2 calculation, which is going to be checked in future investigations. Both figures 1(c) and 1(d) show that the DWB2 model reproduces the qualitative features of the experimental findings. In the case of E_1 (E_2) at 7.5 eV, the inclusion of the second-order term significantly improves the theoretical TDCS at angles from 80° to 120°, especially for the backward peak at $\theta \sim 110°$ where the standard DWBA calculation fails to reproduce its position. The DWBA-PCI result also shows a similar profile as experiment but gives higher peaks. The inclusion of polarization potential and Wark–Macek factor seems to have shifted the backward peak about 15° forwards. In Fig. 1(d) for E_1 (E_2) at 10 eV, only the DWBA-PCI result is in excellent agreement with experimental data for the forward peak at angles near 50°. However, the present DWB2 calculation also gives an improvement over the standard DWBA, and well agrees with the experimental data of Murray[14] at angles from 70° to 130°. The DWBA-pol-PCI result shows a similar shift of backward peak as in Fig. 1(c) when comparing with standard DWBA curve.

As one can see from Fig. 1(a) to Fig. 1(d), the curves of the present DWB2 and DWBA calculations become closer when the excess energy increases, which indicates that the second-order effect is more obvious in the low energy case than that in the high energy case for target Mg. Actually, we also performed calculations for energies of two outgoing electrons at $E_1 = E_2 = 15$ eV, 20 eV, 25 eV, and 30 eV. It is not surprising that the DWB2 and DWBA curves almost coincide with each other in these cases and agree with experimental data. So we omit the figures for these higher energies. However, one could still be given a clue by checking the DWBA (FM) results of Khajuria *et al.* in Fig. 2(e)–2(h) of Ref. [15].

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 Mg, especially for the backward scattering angle region. Murray[14] mentioned that the backward peak was considered to result from elastic scattering into the backward direction of the incident electron from the core, followed by a binary collision with a bound electron. Mg has two valence electrons in its 3s orbital, which makes the interactions between electrons of final states more complicated and indicates an even stronger effect of this multi-scattering process. As a result, the present DWB2 calculation improves the agreement between theoretical prediction and experimental measurement more significantly than in cases that use a one-electron model, such as Na[18] and K,[19] which we have studied before. However, discrepancies

between theory and experiment still exist, which may be due to some missing corrections, such as polarization and PCI in the present DWB2 calculations, as well as some other effects like correlations between electrons of the complex atomic target. Further second-order studies will be preformed with the proper treatment of these corrections.

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