Dynamic correlation in the electron angular distribution in ionization of helium by ion impact

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Abstract. Single ionization of helium by proton impact is investigated in terms of a four-body distorted wave model. In this approximation both electrons are considered as active, being one of them ionized whereas the other remains in a residual target bound state. The influence of dynamic correlation between electrons is investigated by comparison with a four-body uncorrelated distorted wave model. Double differential cross sections as a function of the emission angle for fixed electron energies and different collision energies are presented.

1. Introduction

The present work deals with single ionization of helium atoms by fast proton impact within a four-body distorted wave model. Originally the three body distorted wave models, like the continuum distorted wave (CDW, [1]) and the continuum distorted wave-eikonal initial state (CDW-EIS, [2]), were developed to investigate ion-atom processes for monoelectronic targets. They were introduced in order to accelerate the convergence of a Born series description. Later an extension of the CDW-EIS description for single ionization of multielectronic targets was made by Fainstein et al. [3]. They reduced the multielectronic case to a monoelectronic treatment within a three-body approximation, being the three bodies considered the projectile, the residual target and the active electron (the one to be ionized as a consequence of the collision). The other electrons, the passive ones, were supposed to remain as frozen in their initial orbitals during the reaction (see [3]). Four-body distorted wave models were also introduced to study single ionization of dielectronic targets [4]. Correct boundary conditions were preserved in both entry and exit channels but only the active electron was considered to be distorted by the projectile. In order to avoid any asymmetry in the description of the target electrons, in a previous work [5], we considered both of them as active electrons in a four-body distorted wave-eikonal initial state formulation (4B-DW-EIS). Both electrons were considered to evolve simultaneously, so that any change in one of them is felt by the other and vice versa, so that they are dynamically correlated. Following reference [5], double differential cross sections for the case of single ionization of He by bare ion impact as a function of the emission angle for fixed ejected electron energies are calculated. The influence of the dynamic electronic correlation is determined by comparison with a four-body dynamically uncorrelated model. This model, called CB-CDW-EIS in [5], treats the
residual target bound electron excitation as in a first Born approximation with correct boundary conditions (Coulomb-Born approximation; CB) and the ionization process as in the CDW-EIS approximation.

2. Theory
Let us consider the impact of a bare ion of nuclear charge $Z_P$ on a dielectronic target of nuclear charge $Z_T$. We describe the reaction within the straight-line version of the impact parameter approximation, where $\vec{R} = \vec{R}_0 + \vec{v}t$, being $\vec{R}$ the internuclear vector, $\vec{v}$ the impact velocity and $t$ the collision time, considering $t = 0$ at the closest distance between the nuclei. The reaction is described from a reference frame fixed to the target nucleus. Both electrons are considered to be active during the collision.

Following a distorted wave formalism, and in order to preserve correct asymptotic conditions (see [5]), the initial and final distorted wavefunctions are chosen as

$$\chi^+_\alpha(x_1, x_2, t) = \varphi_\alpha(x_1, x_2) \mathcal{L}^+_\alpha(s_1, s_2) \times$$

$$\times \exp \left[ -i \frac{Z_P Z_T}{v} \ln \left( vR - \vec{v} \cdot \vec{R} \right) \right] \times$$

$$\times \exp \left( -i E_\alpha t \right)$$

and

$$\chi^-_\alpha(x_1, x_2, t) = \frac{1}{\sqrt{2}} \left( 1 + \mathcal{P}_{12} \right) \left[ \varphi_\beta(x_1, x_2) \mathcal{L}^-_\beta(s_1, s_2) \right] \times$$

$$\times \exp \left[ -i \frac{Z_P Z_T}{v} \ln \left( vR + \vec{v} \cdot \vec{R} \right) \right] \times$$

$$\times \exp \left( -i E_\beta t \right)$$

with $x_j$ and $s_j$ denoting the position vector of the $j$-th electron ($j = 1, 2$) as seen from the target and projectile nuclei, respectively, $\varphi_\alpha$ is the initial two-electron bound wavefunction with atomic energy $E_\alpha$ and $\varphi_\beta$ is a two-electron function with energy $E_\beta$ describing one of the electrons bound and the other in a continuum state of the target and $\mathcal{P}_{12}$ is the commutation operator.

The two-electron distorting initial $\mathcal{L}^+_\alpha$ and final $\mathcal{L}^-_\beta$ functions are given by

$$\mathcal{L}^+_\alpha(s_1, s_2) = \prod_{j=1,2} \mathcal{F}^+_\alpha(s_j) =$$

$$= \prod_{j=1,2} \exp \left[ -i \frac{Z_P}{v} \ln (v s_j + \vec{v} \cdot \vec{s}_j) \right]$$

and

$$\mathcal{L}^-_\beta(s_1, s_2) = \mathcal{F}^-_\beta(s_1) \mathcal{L}^-_\beta(s_2) =$$

$$= N^* \left( \frac{Z_P}{p} \right) _1F_1 \left[ -i \frac{Z_P}{p}, 1, -i (p s_1 + \vec{p} \cdot \vec{s}_1) \right] \times$$

$$\times \exp \left[ i \frac{Z_P}{v} \ln (v s_2 - \vec{v} \cdot \vec{s}_2) \right]$$

where $\vec{p}$ is the linear momentum of the ionized electron with respect to the projectile, $_1F_1$ is the confluent hypergeometric function and $N$ its normalization factor.

For the He case the initial target bound wavefunction was considered within a five-zeta
Roothaan-Hartree-Fock representation (see [6]) in which it is given by the product of one-electron five-functions $\phi_\alpha(x)$

$$\varphi_\alpha(x_1, x_2) = \phi_\alpha(x_1)\phi_\alpha(x_2) \quad (5)$$

The two-electron final wavefunction $\varphi_\beta$ is chosen as

$$\varphi_\beta(x_1, x_2) = \phi_\beta(x_1)\phi_\beta(x_2) =$$

$$= \phi_\beta(x_2) \exp(i\vec{k} \cdot \vec{x}_1)/(2\pi)^{3/2} \times$$

$$\times N^* \left( \frac{Z_T - 1}{k} \right) \times$$

$$\times \ _1 F_1 \left[ -i \left( \frac{Z_T - 1}{k} \right), 1, \ i(kx_1 + \vec{k} \cdot \vec{x}_1) \right] \quad (6)$$

where $\vec{k}$ is the momentum of the ejected electron seen from the target nucleus. In (6), $\phi_\beta$ represents a hydrogenic state corresponding to the residual target. The continuum wavefunction in (6) corresponds to the interaction between the ionized electron and the residual target at large asymptotic separation. We have verified [5] that a possible ionization path in which the projectile impacts on the electron that remains bound to the target while the other one is ejected through a dynamical shake-off mechanism gives negligible contributions to the transition amplitude by comparison with the mechanism of direct interaction of the projectile with the emitted electron.

Thus, for the 4B-DW-EIS approximation the prior version of the scattering amplitude results

$$A^{-}_{\alpha\beta}(\vec{p}) = i \left( \rho v \right)^{2iZ_PZ_T/v} \sqrt{2} \int_{-\infty}^{+\infty} \mathrm{d}t \left[ S^\text{bound}_{\alpha\beta}(\vec{p}, t) a^\text{ion, -}_{\alpha\beta}(\vec{p}, t) \right], \quad (7)$$

where $S^\text{bound}_{\alpha\beta}(\vec{p}, t)$ is a one-electron time dependent overlap integral corresponding to a final bound state, and $a^\text{ion, -}_{\alpha\beta}(\vec{p}, t)$ a one-electron time dependent scattering amplitude corresponding to electron ionization (see [5] for further details). Thus, the excitation channel is populated through a dynamical shake-off mechanism.

A four-body dynamically uncorrelated model can be obtained by a further approximation to the 4B-DW-EIS one using the distortions

$$\mathcal{L}^+_\alpha(\vec{s}_1, R) = \mathcal{E}^+_\alpha(\vec{s}_1) \exp \left[ -i \frac{Z_P}{v} \ln(vR - \vec{v} \cdot \vec{R}) \right] \quad (8)$$

and

$$\mathcal{L}^\text{-}_\beta(\vec{s}_1, R) = \mathcal{F}^-_{\beta}(\vec{s}_1) \exp \left[ \frac{Z_P}{v} \ln(vR + \vec{v} \cdot \vec{R}) \right] \quad (9)$$

This leads to a transition amplitude given by

$$A^{-}_{\alpha\beta}(\vec{p}) = i \left( \rho v \right)^{2iZ_P(Z_T - 1)/v} \sqrt{2} \ S^\text{bound}_{\alpha\beta}(\vec{p})A^\text{ion, -}_{\alpha\beta}(\vec{p}) \quad (10)$$

where now $S_{\alpha\beta}^\text{bound}(\vec{p})$ is the time-independent overlap integral between the initial and final bound states, and $A^\text{ion, -}_{\alpha\beta}(\vec{p})$ is a one-electron transition amplitude given by

$$A^\text{ion, -}_{\alpha\beta}(\vec{p}) = \int_{-\infty}^{+\infty} dt \ a^\text{ion, -}_{\alpha\beta}(\vec{p}, t). \quad (11)$$
3. Results and discussions
Double differential cross sections (DDCS) for single ionization of He calculated with the 4B-DW-EIS and CB-CDW-EIS ([5]) models are shown in figures 1 and 2 for the cases of 1.5 MeV and 4.2 MeV proton impact, respectively. Only the final He$^+$ (1s) state is considered in the calculations which is the dominant channel for the ionization reaction studied. A general good agreement is found between both theoretical models and existing experimental data [7]. 4B-DW-EIS results are normalized according to the procedure given in our previous work [5]. Thus, as there discussed, the difference between both theoretical models will give a lower bound to the contribution of the dynamic electron correlation.

From figures 1 and 2, the influence of dynamic correlation appears to be more important at forward and backward emission angles. In the binary peak region, where the reaction is dominated by the projectile-electron interaction the dynamic correlation seems to play a weaker role. It can be seen that, for the cases presented, the correction introduced by this interaction can be at least 20% for the case of 1.5 MeV proton impact whereas for the 4.2 MeV a correction at least as high as 50% is found.

To the light of these results we can conclude that for this system the dynamic electron correlation may play an important role on the doubly differential angular spectra for single ionization. However, a further systematic study of its importance as a function of the impact and ejected electron energies and on the projectile charge state appears as necessary. This is matter of our present research.

Figure 1. Double differential cross section for single ionization of He by 1.5 MeV proton impact as a function of the emission angle for fixed electron energy of 300 eV (figure a) and 500 eV (figure b). Theory: ——, 4B-DW-EIS calculations; - - - -, CB-CDW-EIS calculations [5]. Experiments: ●, Toburen et al. extracted from [7].
Figure 2. Double differential cross section for single ionization of He by 4.2 MeV proton impact as a function of the emission angle for fixed electron energy of 341 eV (figure a) and 1166 eV (figure b). Theory: ——, 4B-DW-EIS calculations; - - - -, CB-CDW-EIS calculations [5]. Experiments: ●, Stolterfoht et al. extracted from [7].

4. Conclusions
A four-body distorted wave model has been developed and applied to the case of single ionization of He by high energy proton impact. Double differential cross sections have been calculated as a function of the emission angle for a fixed energy of the ionized electron. The comparison of the 4B-DW-EIS results with the ones from CB-CDW-EIS shows that the dynamic electron correlation can give an important contribution on the DDCS. This effect is shown to be more important at forward and backward electron emission.

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