Double ionization of helium by ion impact: second Born order treatment at the fully differential level

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Abstract. In this work, a theoretical study of the double ionization of He by ion impact at the fully differential level is presented. Emphasis is made in the role played by the projectile in the double emission process depending on its charge and the amount of momentum transferred to the target. A Born-CDW model including a second-order term in the projectile charge is introduced and evaluated within an on-shell treatment. We find that emission geometries for which the second-order term dominates lead to asymmetric structures around the momentum transfer direction, a typical characteristic of higher order transitions.

1. Introduction

Three collision mechanisms have been identified as responsible of the atomic double ionization (DI) at intermediate to large impact energies. In the two-step-1 (TS1) mechanism, the projectile interacts with only one of the target electrons which subsequently ejects the other via the electron-electron interaction. In the shake-off (SO) mechanism, the second electron relaxes from an ionic bound state to the continuum, following a sudden removal of the primary electron. The third mechanism, usually referred to as two-step-2 (TS2), considers that electrons are sequentially removed by the projectile. In this sense, the TS1 and SO mechanisms involve only one interaction of the projectile with a single electron and can therefore be described as first order terms in a perturbative expansion of the scattering amplitude in the projectile charge Z_P. In contrast, the TS2 mechanism involves two successive projectile-electron interactions and its description requires a second-order term in Z_P. At very high impact energies the SO mechanism dominates the DI process and an accurate description of the initial state correlation is needed, provided the large asymmetry in the electron emission energies. As the impact energy decreases and the scattering event duration increases, emission energies can be less asymmetric, and the electron-electron interaction gains relevance throughout the whole process, and the probability of a double emission mediated by the projectile at all times increases. In this sense, none of these mechanisms is expected to solely dominate the DI at intermediate impact energies. It is clear then that from a theoretical perspective a coherent treatment of them should be proposed at the transition amplitude level.

In this work, we focus on DI processes in ion-helium collisions at an impact energy of 500 keV/amu. At this impact energy the competition among the different mechanisms is expected to be

large. Fully differential cross sections are calculated and analyzed for different projectile charges and momentum transfers. Atomic units are used unless otherwise stated.

2. Theoretical Model

In the present Born-continuum distorted waves (CDW) treatment, the transition amplitude up to second order reads:

$$T_{fi} = T_{fi}^{(1)} + T_{fi}^{(2)}$$

The first order term is given by the First Born Approximation (FBA), in which the projectile is considered as a plane wave in either the initial and final channels:

$$T_{fi}^{FBA}(\vec{k_1}, \vec{k_2}, \vec{\Omega}) = \langle \chi_f | V_i | \chi_i \rangle$$
$$V_i = \frac{Z_P Z_T}{R} - \frac{Z_P}{|\vec{R} - \vec{r_1}|} - \frac{Z_P}{|\vec{R} - \vec{r_2}|}$$

We evaluate this FBA term with a distorted wave method in which both target electrons are explicitly considered [1,2]. The final wave function is given by a 3C model with the dynamical screening scheme proposed by Berakdar and Briggs [3]. This model considers infinite collisions between the components of the target. Hence, it accounts for the SO and TS1 mechanisms.

For the second-order term, we consider the on-shell second Born approximation that we have recently introduced [4], and that accounts for the TS2 mechanisms:

$$T_{fi}^{(TS2)}(\vec{k_1}, \vec{k_2}, \Omega) = \int d\vec{\Omega}_n \langle \chi_f | W_f | \xi_1 \rangle \langle \xi_1 | W_i | \chi_i \rangle$$

The single ionization amplitudes are evaluated within the CDW-EIS approximation and the corresponding perturbations are given by,

$$W_i = \frac{-\nabla_{r_P}^2}{2\mu_P} + \nabla_{r_P} \cdot \nabla_{r_T}$$
$$W_f = -\nabla_{r_P} \cdot \nabla_{r_T}$$

In this study, only one single intermediate state is considered in which one electron is bound to the parent ion while the other is emitted to the continuum with its final momentum.

3. Results

In figure 1 we show the fully differential cross section calculated by means of the FBA at an impact energy of 500 keV for proton impact. The momentum transferred by the projectile Q = 3 a.u.. Electrons are emitted in the scattering plane with equal energies of 10 eV each. Electrons polar angles are measured counter clockwise from the projectile incidence direction. The projectile final momentum is chosen such that the momentum transfer vector lies in the first quadrant. Structures are symmetric with respect to the momentum transfer direction ($\theta_Q = 74°$). Results for other projectiles look identical provided that the FBA transition amplitude only retains the projectile charge information via a Z_P factor. Hence, the only expected change would be that of absolute magnitudes which scale with Z_P^2.
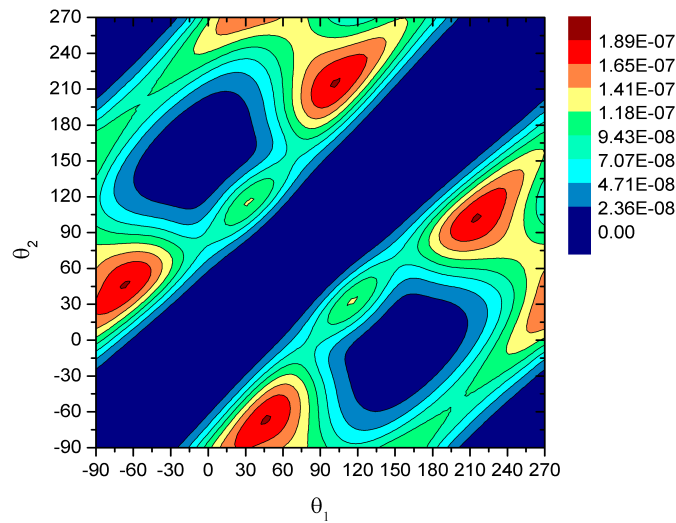
Figure 1: FDCS calculated with FBA of DI of He by proton impact.

In figure 2, we show the fully differential cross sections obtained for the coherent sum of the first and second-order terms of the transition amplitude. In this case, the three collision mechanisms (SO, TS1 and TS2) are incorporated in our theoretical description. The Ward and Macek correlation factor [5] is included in the TS2 term to avoid the unphysical picture of two electrons being emitted hand-in-hand. Three projectiles are considered: proton, He^{2+} and C^{6+}. We now note that the inclusion of the second-order term breaks the symmetry around the momentum transfer direction. This behavior is further highlighted in figure 3 where selected cuts of figures 2 a)-c) are presented. Each cross section has been divided in this case by Z_P^2 to help elucidate how structures deviate from the FBA results. The emission angle of one of the electrons is set as $\theta_1 = 30°$. If the TS1 mechanism were the dominating one, the other electron would be expected to be departing at a relative angle close to 90° which in this case would correspond to $\theta_2 = 120°$ or $-60°$. The former case can be related to a passive parent ion which plays a spectator role during the second electron removal, while the latter would indicate a recoiling parent ion that strongly mediates the double emission process.
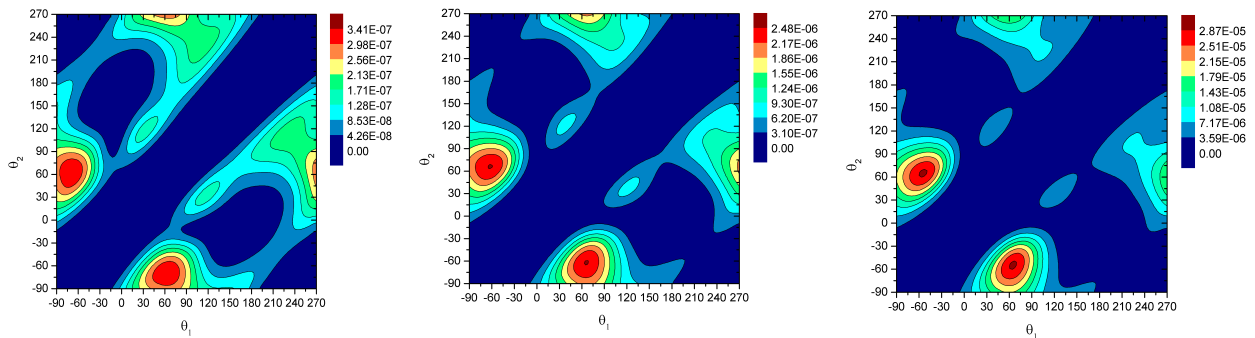

Figure 2: Coherent sum of first and second order for DI of He by proton (a), He^{2+}(b) and C^{6+} (c) impact. The considered impact energy are of 500 keV/amu, the momentum transferred is $Q = 3$ a.u., and the electrons are emitted with 10 eV.
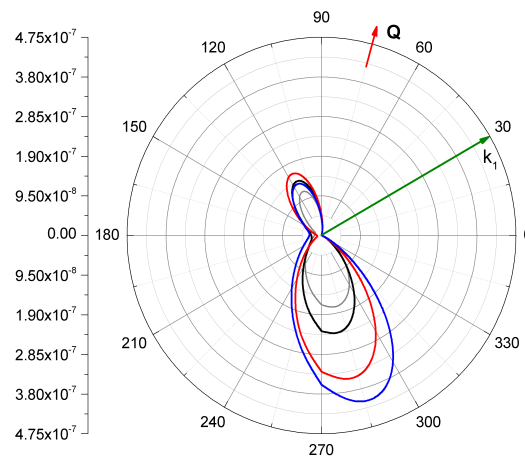
Figure 3: Selected cut of
figure 3 for one electron emitted at 30 degrees. DI of He by proton (black line), He^{2+} (red line) and C^{6+} (blue line) impact. FBA (gray line) The considered momentum transferred is Q = 3 a.u.

From figure 3, we note that the ratio among both lobes changes according to the projectile charge. The lobe located at about -75° drastically increases with projectile charge clearly indicating that the electrons tend to be emitted in the direction of the receding projectile. Moreover, a more subtle shift of this structure towards the projectile direction can also be noticed.

4. Conclusions

Fully differential cross sections for the double ionization of He by ion impact have been theoretically studied by means of a distorted wave model that incorporates the SO, TS1 and TS2 mechanisms. A second-order Born term evaluated on-shell has been introduced to coherently add the TS2 mechanism to the first order term which already contains information on the SO and TS1 mechanisms. From our results we infer that the most visible effect introduced by the second-order term is the rupture of symmetry of the FDCS structures around the momentum transfer direction.

References
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