

# Post-collisional effects on single ionization in 75 keV p+He collisions

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## Abstract

We report fully differential cross-section calculations using distorted wave theories for helium single ionization by 75 keV p impact. Comparisons are made with absolute experimental data and we find that good results are obtained in the magnitude without the need for normalization factors. However, discrepancies are quite apparent in the position and shape of the peak structures in the fully differential angular distribution of the ejected electrons. We assess the influence of the internuclear interaction on low-energy electron emission in the scattering plane and in the perpendicular plane. Our continuum distorted wave-eikonal initial state calculations with (without) the internuclear interaction yield better results for the large (small) momentum transfer. We discuss this behaviour as a consequence of active electron screening for low-energy electron emission.

## 1. Introduction

As a result of the continuous development of the experimental technique known as COLTRIMS (cold-target recoil-ion momentum spectroscopy), the field of atomic ionization by ion impact is enjoying a renewed interest [1, 2]. With this technique, the usually tiny projectile's scattering angle can be indirectly obtained by measuring the ionized electron and recoil ion momenta. Consequently, fully differential cross sections (FDCS) for ion impact ionization can now be measured even for fast heavy ion impact, constituting a challenging ground in which different proposed theories can be assessed [3]. First measurements of FDCS were reported in 2001

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by Schulz *et al* [4], for single ionization of helium by  $C^{6+}$ , 100 MeV  $\text{amu}^{-1}$ . Since then, several experiments using other projectiles and energy ranges have been performed (for a recent review see [5]). Fischer *et al* [6] have reported absolute experimental measurements for 2 MeV  $\text{amu}^{-1} C^{6+}$  and 3.6 MeV  $\text{amu}^{-1} Au^{Q+}$  ( $Q = 24, 53$ ) single ionization of helium in the scattering plane (defined by the plane containing the initial and final projectile momenta) for several momentum transfers and ejected electron energies. For Au projectiles, their theoretical calculations using a continuum distorted wave-eikonal initial state (CDW-EIS)-based model showed remarkable differences between experiment and theory, both in absolute magnitude (the theoretical predictions were off by up to two orders of magnitude), and shape (a strong forward peak is observed in the data which is not even qualitatively reproduced by theory).

Recently, kinematically complete experiments were made at intermediate impact energies (75 keV p+He) and for these relatively slow and light projectiles the energy loss and the scattering angle of the projectile can be directly measured. From these data it is possible to obtain all the kinematic variables of the collision problem [7]. Unexpected effects due to higher-order contributions were found from this experiment. In high energy ion impact experiments, the so-called binary peak is usually observed in the direction of the momentum transfer vector  $\mathbf{q}$ , which is defined as the difference between the initial and scattered projectile momentum. However, for highly charged fast projectiles, the binary peak tends to shift forward from  $\mathbf{q}$ 's direction [8] and shift backward for electron impact [9]. This effect can be explained in terms of the post-collision interaction between the outgoing projectile and the ejected electron occurring after the primary ionizing interaction. For intermediate projectile energies, a backward shift instead of a forward shift was observed, which can be explained in terms of the projectile-residual-ion interaction [7]. If this interpretation is correct, this effect should not be observable for fast heavy-ion impact or for slow electron impact [10].

Before COLTRIMS experiments [1], the influence of the internuclear potential in ionization cross sections was often overlooked since double differential ionization cross sections (DDCS) in electron energy and emission angle do not depend (to first order in  $1/M_{T,P}$ ) on this interaction, since it is common to incorporate it only in terms of a phase in the transition amplitude. On the theoretical side, a single ionization process involves the evolution of three charged particles with Coulomb interactions. It is well known that this three-body problem has no known analytical solution. However, the asymptotic form of such solutions, i.e. when the three particles are far apart, was found. One widely used perturbative method which includes the long tail of Coulomb potentials in the wavefunctions at intermediate and high energies is the continuum-distorted-wave (CDW) theory. This scheme was originally introduced by Cheshire [11] to model processes of charge transfer in ion-atom and ion-ion collisions. The CDW formalism was later applied to single ionization for ion-atom collisions by Belkic [12]. Nevertheless, one major deficiency of the CDW ionization theory was a problem associated with the normalization of the initial wavefunction at low impact energies [13]. This weak point was corrected by the CDW-EIS theory first introduced by Crothers and McCann [14]. In such a model, an eikonal phase, derived from the asymptotic limit of the Coulomb distortion, is responsible to account for the electron-projectile interaction in the initial channel. Single differential cross sections (SDCS) and DDCS, using the CDW-EIS theory, have been calculated for single ionization of helium by proton impact in a large range of impact energies, starting at the low to intermediate range (50–100 keV). The success of the theory to reproduce the experimental data has been remarkable (see [15] and references therein). However, for differential cross sections as a function of projectile parameters [16, 17], or recoil ion momentum, it has been shown that the interaction between the projectile and the residual-target-ion (PI interaction) has a large influence depending on the ejected electron energies and momentum transfer values [18–21].

In recent papers, the effects of the inclusion of the internuclear potential (PI interaction) in the FDCS have been studied. Although several ways to account for the PI interaction have been proposed [19, 20, 22], none of them has been completely satisfactory in reproducing the experimental data for the whole range of parameters studied. Taking into account a simple dynamical model for the internuclear effective charge in the semiclassical approach, we were able to reproduce the FDCS for 2 MeV amu<sup>-1</sup> C<sup>6+</sup> single ionization of helium [23].

Due to the steady increase in computational power, it is possible now to treat all the interactions between particles pairs in a single collision process on an ‘equal footing’. One of the latest approaches in this direction is the so-called 3DW-EIS by Foster *et al* [24]. In this model, the PI interaction is taken into account by a Coulomb wavefunction for the final state and an eikonal phase for the initial one. The obtained FDCS is numerically calculated using quadratures. However, even this sophisticated theory is not able to completely reproduce the experimental data available at high and intermediate energies [3].

When even lower impact energies are considered, the role of the PI interaction in FDCS is supposed to increase. In this paper, we present theoretical calculations for 75 keV p single ionization of helium. Our aim is to explore the role of the post-collisional effects and the PI interaction in FDCS for intermediate ion impact ionization by protons within distorted wave theories. We will employ a prior CDW-EIS model and take into account the PI interaction in a semiclassical way. Furthermore, the screening of the passive electron is incorporated using an effective charge for the interaction between the ionized electron and the residual–target–ion. Our aim is to assess if such a simple model is able to reproduce with reasonable success the experimental data. To support this last statement we have made calculations neglecting the PCI effects to show how important is to adequately model these interactions in a single ionization process. In the following section, we briefly recall the incorporation of the PI interaction in our distorted wave formalism. In section 3 we report our results and compare them with available experimental data. Atomic units are used throughout unless otherwise stated.

## 2. Theories

We will consider helium single ionization as a one active electron process and assume that in the final state the ejected electron moves in the combined Coulomb field of the incident ion and the residual target core. Partial screening of the active electron–target interaction due to the ‘passive’ helium electron is modelled by an effective charge as considered within the usual prior CDW-EIS approach.

Distortion of the final electronic state by the projectile is represented by a pure Coulomb function, and by an eikonal phase in the entrance channel [14]. The PI interaction is usually treated as a pure Coulomb interaction between a projectile with charge  $Z_P$  and the ‘true’ target core charge,  $Z_T = 1$ . The PI interaction is then included in the transition amplitude  $a_{if}(\rho)$ , in the eikonal approximation, through its multiplication by a phase factor [25, 26], which for the pure Coulomb internuclear interaction yields [14, 15]

$$a_{if}(\rho) = i(\rho v)^{2iv} a'_{if}(\rho) \quad (1)$$

with  $v = Z_P Z_T / v$ , and where  $\rho$  defines the impact parameter ( $\rho \cdot v = 0$ ).  $a_{if}(\rho)(a'_{if}(\rho))$  is the transition amplitude with (without) the internuclear interaction. Using two-dimensional Fourier transforms it is possible to find a relation between  $a_{if}(\rho)$  and  $T_{if}(\eta)$ , i.e. the transition matrices as a function of the impact parameter  $\rho$  or the transverse component of the momentum transfer  $\eta$  [34]. Consequently, the transition matrices with and without the internuclear

interaction can be written alternatively:

$$T'_{if}(\boldsymbol{\eta}) = \frac{1}{2\pi} \int d\rho e^{i\boldsymbol{\eta}\cdot\rho} a'_{if}(\rho), \quad (2)$$

$$T_{if}(\boldsymbol{\eta}) = \frac{iv^{2iv}}{2\pi} \int d\rho \rho^{2iv} e^{i\boldsymbol{\eta}\cdot\rho} a'_{if}(\rho). \quad (3)$$

Applying the inverse Fourier transform of (2) and replacing in (3), we have

$$T_{if}(\boldsymbol{\eta}) = \frac{iv^{2iv}}{(2\pi)^2} \int d\boldsymbol{\eta}' T'_{if}(\boldsymbol{\eta}') \int d\rho \rho^{2iv} e^{i(\boldsymbol{\eta}-\boldsymbol{\eta}')\cdot\rho}. \quad (4)$$

The integral over impact parameter can be done analytically to obtain [19]

$$T_{if}(\boldsymbol{\eta}) = v \frac{iv^{2iv} (2\pi)^{-iv}}{2^4 \pi^3} \int d\boldsymbol{\eta}' T'_{if}(\boldsymbol{\eta}') |\boldsymbol{\eta} - \boldsymbol{\eta}'|^{-2(1+iv)}. \quad (5)$$

The remaining integral in (5) is evaluated numerically using quadratures. As it is well known, this approximation is valid as long as (i) the projectile suffers very small deflections in the collision and (ii) the velocity of the recoil ion remains small compared to that of the emitted electron. Even at energies as low as 75 keV the momentum transfers studied here correspond to scattering angles of 1 mrad or less so that condition (i) is still fulfilled. Because of the large recoil-ion to electron mass ratio, condition (ii) is always satisfied.

In the centre of mass (CM) frame, the FDCS as a function of the energy and ejection angle of the electron, and direction of the outgoing projectile, is given by [27–29]

$$\frac{d^3\sigma}{dE_k d\Omega_k d\Omega_K} = N_e (2\pi)^4 \mu^2 k \frac{K_f}{K_i} |T_{if}|^2 \delta(E_f - E_i), \quad (6)$$

where  $N_e$  is the number of electrons in the atomic shell,  $\mu$  is the reduced mass of the projectile–target subsystem, and  $K_i$  ( $K_f$ ) is the magnitude of the incident particle initial (final) momentum. The ejected electron's energy and momentum are given by  $E_k$  and  $k$ , respectively. The solid angles  $d\Omega_K$  and  $d\Omega_k$  represent the direction of scattering of the projectile and the ionized electron, respectively. The projectile solid angle  $d\Omega_K = \sin\theta_K d\theta_K d\phi_K$  can be expressed in terms of the momentum transfer  $q$  via the relations  $q \approx K_i \sin\theta_K$  and  $K_i \approx K_f$ , fulfilled for heavy ions projectiles, i.e. small scattering angles.

We use non-orthogonal Jacobi coordinates ( $\mathbf{r}_P$ ,  $\mathbf{r}_T$ ) to describe the collision process. These coordinates represent the position of the active electron with respect to the projectile ( $\mathbf{r}_P$ ) and the target ion ( $\mathbf{r}_T$ ), respectively.  $\mathbf{R}_T$  is also needed, representing the position of the incoming projectile with respect to the CM of the subsystem e–T. If we neglect terms of orders  $1/M_T$  and  $1/M_P$ , where  $M_T$  is the mass of the target ion nucleus and  $M_P$  is the mass of the incident heavy ion, we can write  $\mathbf{R}_T = \mathbf{r}_T - \mathbf{r}_P$ .

Within the prior CDW–EIS model, the transition amplitude can be computed as

$$T_{if}^{\text{CDW-EIS}} = \langle \chi_f^{\text{CDW}} | W_i | \chi_i^{\text{EIS}} \rangle, \quad (7)$$

where the initial (final) state distorted wave  $\chi_i^+$  ( $\chi_f^-$ ) is an approximation to the initial (final) state which satisfies the outgoing-wave (+) (incoming-wave (–)) conditions. For the initial state the asymptotic form of the Coulomb distortion (eikonal phase) is used in the electron–projectile interaction together with a semi-analytical Roothaan–Hartree–Fock description for the initial bound-state wavefunction [30]

$$\chi_i^{\text{EIS}} = (2\pi)^{-3/2} \exp(i\mathbf{K}_i \cdot \mathbf{R}_T) \psi_{1s}(\mathbf{r}_T) \mathcal{E}_v^+(\mathbf{r}_P), \quad (8)$$

where  $\mathcal{E}_v^+(\mathbf{r}_P)$  is

$$\mathcal{E}_v^+(\mathbf{r}_P) = \exp\left(-i\frac{Z_P}{v} \ln(vr_P - \mathbf{v} \cdot \mathbf{r}_P)\right). \quad (9)$$

The final-state wavefunction is cast into the form [14, 31]

$$\chi_f^{-\text{CDW}} = (2\pi)^{-3/2} \exp(i\mathbf{K}_f \cdot \mathbf{R}_T) \chi_T^-(\mathbf{r}_T) C_P^-(\mathbf{r}_P), \quad (10)$$

where  $C_P^-$  represents the Coulomb distortion of the ejected electron wavefunction due to the projectile

$$C_P^-(\mathbf{r}_P) = N(v_P) {}_1F_1(-iv_P, 1, -ik_P r_P - i\mathbf{k}_P \cdot \mathbf{r}_P), \quad (11)$$

where  $v_P = \frac{Z_P}{k_P}$  is the Sommerfeld parameter,  $\mathbf{k}_P$  is the relative momentum of the e-P subsystem and  $N(v_P)$  is the usual Coulomb factor

$$N(v_P) = \Gamma(1 - iv_P) \exp(\pi v_P / 2). \quad (12)$$

On the other hand,

$$\chi_T^-(\mathbf{r}_T) = (2\pi)^{-3/2} \exp(i\mathbf{k}_T \cdot \mathbf{r}_T) N(v_T) {}_1F_1(-iv_T, 1, -ik_T r_T - i\mathbf{k}_T \cdot \mathbf{r}_T) \quad (13)$$

(where  $v_T = \frac{Z_T}{k_T}$  and  $\mathbf{k}_T$  is the relative momentum of the e-T subsystem) is the wavefunction for the ejected electron in the field of the target-residual-ion.

The perturbation potential  $W_i$  in (7) is defined by

$$(H_i - E_i) \chi_i^+ = W_i \chi_i^+, \quad (14)$$

where  $H_i$  is the full electronic initial Hamiltonian (neglecting the total CM motion) and  $E_i$  is the total initial energy of the system in the CM frame.  $W_i$  is composed of two differential operators that can be written as [32]

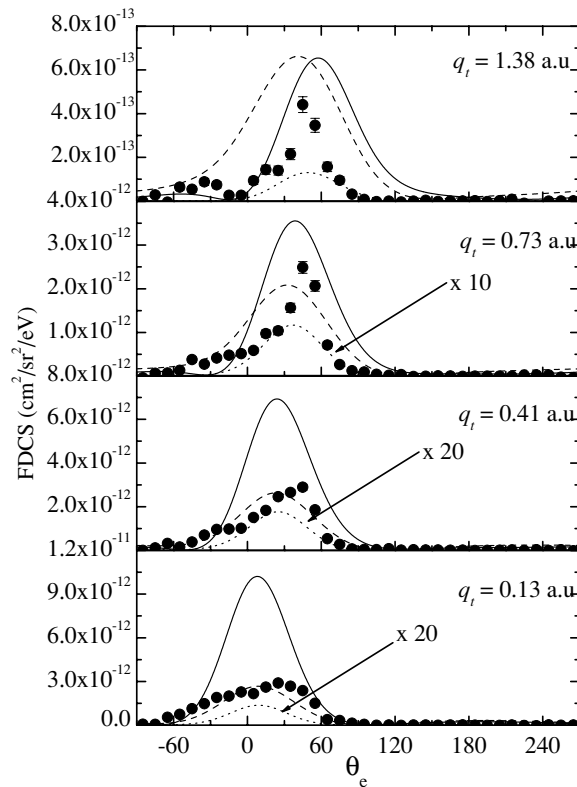
$$W_i = \frac{1}{2} \nabla_{\mathbf{r}_P}^2 - \nabla_{\mathbf{r}_T} \cdot \nabla_{\mathbf{r}_P}. \quad (15)$$

We compute FDSCS, i.e. equation (6), for single ionization of helium by 75 keV of protons, using the prior CDW-EIS scheme (7) together with the semiclassical approach to incorporate the PI interaction. We call this theory CDW-EISPI to distinguish it from the usual CDW-EIS theory where the PI interaction is not accounted for. Our CDW-EISPI model was used before in FDSCS calculations for the ionization of helium by highly charged ions and for the high impact energy range [33]. In this work, we explore and extend the application of the CDW-EISPI model to intermediate energies.

### 3. Results

We present in figure 1 the results for theoretical calculations and their comparison to the experimental data extracted from [7]. All calculations and experimental data correspond to 75 keV p single ionization of helium, for electrons ejected in the scattering plane with  $E_e = 5.4$  eV, and different transverse momentum transfer values  $q_t$ . Recent studies of fully differential single ionization cross sections indicate that systematically the interaction between the projectile and the residual target core (PI interaction) poses the biggest problem to theory. In the following, we will therefore focus the discussion on the role of that interaction in our model. To this end we will analyse both the magnitude and the angular dependence of the cross sections.

We see in figure 1 that, for small values of  $q_t$ , the experimental data show a broad peak in the forward direction, but with a slight relative minimum at  $\theta_e = 0^\circ$ . As the momentum transfer is increased, this structure evolves into a pronounced narrow peak, at an angle which roughly coincides with the direction of  $\mathbf{q}$ , and a much smaller peak at negative angles. The former structure corresponds to the well-known binary peak.



**Figure 1.** Fully differential cross sections for electrons with an energy 5.4 eV ejected into the scattering plane in 75 keV p+He collisions.  $\theta_e$  corresponds to the electron emission angle (see the text for details). The transverse momentum transfer  $q_t$  are (from bottom to top) 0.13 au, 0.41 au, 0.73 au and 1.38 au. Solid lines: CDW-EISPI (see the text); dashed lines: CDW-EIS (see the text); dotted lines: SE (see the text); points: experimental data [7].

Although both calculations do show the main features of the experimental data, it is clear that the low  $q_t$  data are not well described by the CDW-EISPI calculation. On the other hand, in the absolute magnitude much better agreement is achieved with the CDW-EIS calculation. We have already observed the same behaviour in high-energy  $C^{6+} + He$  collisions [23]. This suggests that the PI interaction is overestimated by the CDW-EISPI calculation at small  $q_t$ . This can be understood as follows: low-energy electron emission at small momentum transfer favours large impact parameter collisions. In this situation it is possible that both the passive and the active electron could partially screen the target nucleus, leading to a weaker PI interaction than what is taken into account in the theory. As we look at larger  $q_t$ , smaller impact parameters become increasingly important, the active electron screening is reduced and the PI interaction is better described by our theory. Indeed, much better agreement in magnitude is obtained with the CDW-EISPI calculation at large  $q_t$ . Although this explanation is based on semiclassical arguments, it still indicates the need for a refined theory that includes the variations in the PI interaction strength when small  $q_t$  are considered.

In the experiment, the binary peak does not move very much as  $q_t$  increases (from  $25^\circ$  at smallest value to  $45^\circ$  at the largest value of  $q_t$  while the direction of  $\mathbf{q}$  itself moves from  $11^\circ$  to  $65^\circ$ ). At small  $q_t$  the binary peak is shifted in the backward direction relative to

$\mathbf{q}$  and at large  $q_t$  it is shifted in the forward direction. The experimentalists presented a simple classical double collision model to explain this observation. In this model, the PI interaction would lead to a backward shift if the projectile passed the target atom outside the electron cloud, but to a forward shift if it penetrated the target atom [10]. Although neither of our calculations reproduce the shift of the binary peak observed in the experiment, there is nevertheless an element of qualitative agreement. In the calculation without the PI interaction there is an increasing forward shift with increasing  $q_t$ . This suggests that the post-collision interaction (PCI) between the outgoing projectile and the ejected electron becomes stronger with increasing  $q_t$ , contrary to previous belief. On the other hand, in the calculation including the PI interaction the forward shift of the binary peak is significantly reduced, especially at large  $q_t$ . This demonstrates that indeed the PI interaction can lead to a backward shift. However, in our calculation this backward shift occurs for all  $q_t$ , which may indicate that even at large  $q_t$  the projectile is not likely to penetrate the target atom. The forward shift at large  $q_t$  is probably due to a dominance of PCI over the PI interaction. The fact that in the CDW-EISPI calculation the binary peak remains practically at  $\mathbf{q}$  results from a coincidental cancellation of the forward shift due to the PCI by the backward shift due to the PI interaction. A comparison with the experimental peak position then suggests that not only the PI interaction, but PCI too may be overestimated in our calculations at small  $q_t$ . In any case, the insensitivity of the binary peak position to  $q_t$  observed in the experiment is consistent with a strong role taken by the PI interaction.

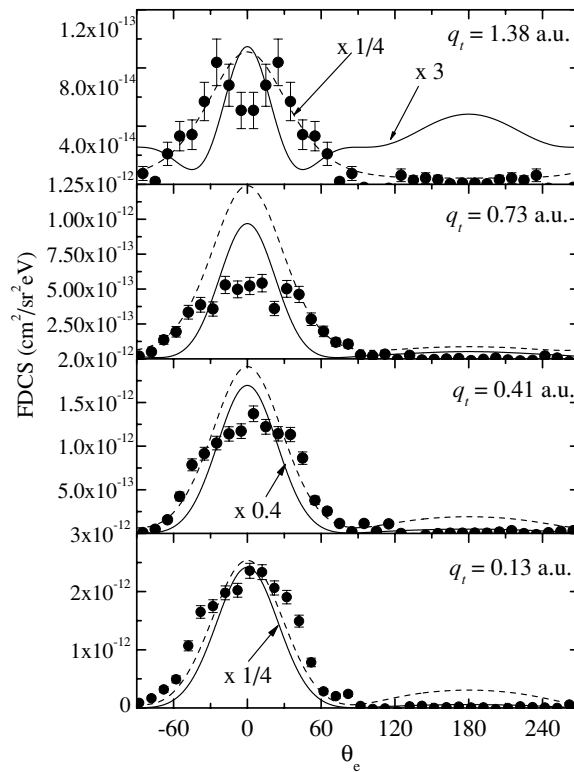
In order to complete the picture about PCI effects, we have performed calculations using the symmetric eikonal (SE) model (see [34] for details). This model minimizes the PCI, i.e. the electron–projectile interaction in the final channel, within the distorted wave formalism. We can see in all cases studied the strong importance of the PCI, since the SE values have to be renormalized adequately to be compared both with the experimental data and with the other theoretical CDW-EIS-based models.

Finally, we note that in the experiment the binary peak at large  $q_t$  is much narrower than in the distorted wave calculations. Similarly, narrow structures have already been reported at lower projectile impact energies [35], and explained in terms of a quasimolecular model. A strong PI interaction is consistent with a quasimolecular picture: this interaction is an essential ingredient for the formation of a quasimolecule, and indeed the calculation with the PI interaction yields a significantly narrower binary peak than the one without it. However, even in the CDW-EISPI calculation the peak is not as narrow as in the experimental data.

The structure at negative angles has also been interpreted in terms of the PI interaction. If the projectile passes the target atom outside the electron cloud, it ejects the electron and the residual-target-ion in opposite directions. If the momentum transfer goes predominantly to the ion, then the final recoil momentum is likely to point near the momentum transfer direction and the electrons occur at negative angles [10, 36]. This structure is reproduced by theory at least at large  $q_t$ . At small  $q_t$  the experimental data do not show a structure fully resolved from the binary peak. At the same time the CDW-EISPI calculation significantly overestimates the magnitude and possibly the width of the binary peak (as it clearly does at large  $q_t$ ). It is therefore difficult to evaluate to what extent this structure is reproduced by our calculations at small  $q_t$ .

A particularly sensitive test of the description of higher-order contributions in the theory is provided by the dependence of the FDCS in the perpendicular plane. As mentioned above, signatures of the PI interaction are observed in the scattering plane. Such effects should be even more pronounced in the perpendicular plane. Because of momentum conservation, a first-order ionization process can only eject the electron out of the scattering plane if the electron had, at the instant of the primary interaction with the projectile, a momentum component outside the





**Figure 2.** Fully differential cross sections for electrons with an energy 5.4 eV ejected into the perpendicular plane in 75 keV p+He collisions. The transverse momentum transfer  $q_t$  are the same as figure 1. Solid lines: CDW-EISPI (see the text), dashed lines: CDW-EIS (see the text), points: experimental data [7].

scattering plane already in the initial bound state of the target atom. Therefore, the relative importance of higher-order contributions tends to increase with increasing departure from the scattering plane. The measured FDCS and a comparison to our theoretical calculation for the perpendicular plane are plotted as a function of  $\theta_e$  in figure 2 for the same  $q_t$  as the FDCS for the scattering plane of figure 1. Except for  $q_t = 1.38$  au, the experimental FDCS exhibit a strong peak at  $\theta_e = 0^\circ$ . As  $q_t$  increases this maximum becomes increasingly broader and eventually separates into two peaks at about  $\theta_e \approx 30^\circ$  for the largest  $q_t$  leaving a minimum at  $\theta_e = 0^\circ$ . Again, like for the scattering plane, the CDW-EIS calculation reasonably reproduces the magnitude of the measured cross sections at small  $q_t$ . At large  $q_t = 1.38$  au, in contrast, both the CDW-EIS and the CDW-EISPI calculations are in poor agreement with the data. Nevertheless, qualitative improvement by the inclusion of the PI interaction is achieved in one aspect: a peak structure not located along the projectile beam axis is found, although the peak positions ( $\pm 80^\circ$ ) strongly deviate from the experimentally observed maxima ( $\pm 30^\circ$ ). The same behaviour was obtained with the 3DW calculations (which also contains the PI interaction) shown in [10]. These peak structures break the cylindrical symmetry about  $\mathbf{q}$  strictly required by a first-order ionization process and thus are a clear signature of higher-order processes. The description of such higher-order contributions in our calculations is evidently rather incomplete. Again, a better description of the PI interaction appears to be particularly urgent.



#### 4. Conclusions and perspectives

We have carried out CDW-EIS calculations of FDCS for single ionization of helium by 75 keV proton impact. We have assessed the post-collisional interaction using a simple distorted wavefunction to take into account both the interaction between the residual–target–ion with the ionized electron and with the outgoing projectile (PI). For the former, we have used the usual CDW-EIS model with a Coulomb with an effective charge to take into account, at least partially, the screening of the passive electron. Additionally, the interaction between the projectile and the target ion was accounted for in a semiclassical picture. Both approaches have the advantage of being computationally simpler and far less time consuming than fully numerical models.

Our theory shows an acceptable overall agreement in the scattering plane without the need of normalization factors and a marginal accordance when we applied it to the perpendicular plane. We found that the CDW-EIS calculations without internuclear interaction yield better results for small momentum transfer. The lack of internuclear interaction can be explained if both active and the passive electron screening takes place, which is perfectly compatible with collisions with small momentum transfer and low emission energy.

The ionization events out of scattering plane are dominated by higher-order processes that are not accurately described by our theory. However, we were able to elucidate some global conclusions about the importance of post-collisional interactions. SE calculations are in agreement with the conclusions stated above, i.e. PCI are important enough so that they should not be neglected.

To adequately model the ionization process at intermediate projectile energies, it might be necessary to include (at the FDCSs level) well-known improvements to the CDW-EIS model, namely (i) to incorporate non-Coulombian effects for the ejected electron and the residual–target–ion interaction, e.g. by using model potentials; (ii) to go beyond the semiclassical or eikonal approach for the PI interaction, e.g. incorporating distorted Coulomb waves for the initial and/or final channels within a distorted wave approach and (iii) to assess the importance of the target excitation, since for this energy such process is known to have considerable contribution.

These improvements, however, within the physical picture provided by the usual CDW-EIS model, might be insufficient to provide substantial changes in the description of ionization events, at the FDCS level. There are more elaborated pathways to refine the CDW-EIS-based theories, all of them implying a large amount of computational calculations, and whose underlying physics is difficult to assess. These include going beyond the single active electron approximation (four-body theories) [37], taking into account the heavy ions' movement quantum mechanically [3, 24] and the use of correlated distorted wave models [38], among others. However, and so far, such elaborated models have shown marginally better results when compared with simpler ones, at the expense of more difficult analysis. For the time being, trusted models as the CDW-EIS still have a role to play while our understanding and our modelling of these systems evolve.

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## References

- [1] Moshhammer R *et al* 1994 *Phys. Rev. Lett.* **73** 3371
- [2] Schulz M, Moshhammer R, Fischer D, Kollmus H, Madison D H, Jones S and Ullrich J 2003 *Nature* **422** 48
- [3] Foster M, Madison D H, Peacher J L, Schulz M, Jones S, Fischer D, Moshhammer R and Ullrich J 2004 *J. Phys. B: At. Mol. Opt. Phys.* **37** 1565
- [4] Schulz M *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** L305
- [5] Schulz M and Madison 2006 *Int. J. Mod. Phys. A* **21** 3649
- [6] Fischer D, Moshhammer R, Schulz M, Voitkiv A and Ullrich J 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** 3555
- [7] Maydanyuk N V, Hasan A, Foster M, Tooke B, Nanni E, Madison D H and Schulz M 2005 *Phys. Rev. Lett.* **94** 243201
- [8] Schulz M, Moshhammer R, Perumal A N and Ullrich J 2002 *J. Phys. B: At. Mol. Opt. Phys.* **35** L161
- [9] Ehrhardt H, Jung K, Knoth G and Schlemmer P 1986 *Z. Phys. D* **1** 3 and references therein
- [10] Schulz M, Hasan A, Maydanyuk N V, Foster M, Tooke B and Madison D H 2006 *Phys. Rev. A* **73** 062704
- [11] Cheshire I M 1964 *Proc. Phys. Soc.* **84** 89
- [12] Belkič D 1978 *J. Phys. B: At. Mol. Phys.* **11** 3529
- [13] Crothers D S F 1982 *J. Phys. B: At. Mol. Phys.* **15** 2061
- [14] Crothers D S F and McCann J F 1983 *J. Phys. B: At. Mol. Phys.* **16** 3229
- [15] Stolterfoht N, DuBois R D and Rivarola R D 1997 *Electron Emission in Heavy Ion–Atom Collisions* (Berlin: Springer)
- [16] Vajnai T, Gaus A D, Brand J A, Htwe W, Madison D H, Olson R E, Peacher J L and Schulz M 1995 *Phys. Rev. Lett.* **74** 3588
- [17] Schulz M, Vajnai T, Gaus A D, Htwe W, Madison D H and Olson R E 1996 *Phys. Rev. A* **54** 2951
- [18] Moshhammer R, Perumal A, Schulz M, Rodríguez V D, Kollmus H, Hagmann S and Ullrich J 2001 *Phys. Rev. Lett.* **87** 223201
- [19] Sánchez M D, Cravero W R and Garibotti C R 2000 *Phys. Rev. A* **61** 062709
- [20] Rodríguez V D and Barrachina R O 1998 *Phys. Rev. A* **57** 215
- [21] Fainstein P D and Gulyás L 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** 317
- [22] Jones S and Madison D H 2002 *Phys. Rev. A* **65** 052727
- [23] Ciappina M F and Cravero W R 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** 2183
- [24] Foster M, Madison D H, Peacher J L and Ullrich J 2004a *J. Phys. B: At. Mol. Opt. Phys.* **37** 3797
- [25] McCarroll R and Salin A 1968 *J. Phys. B: At. Mol. Phys.* **1** 163
- [26] McCarroll R and Salin A 1978 *J. Phys. B: At. Mol. Phys.* **11** L693
- [27] Bethe H 1930 *Ann. Phys. Lpz.* **5** 325
- [28] Inokuti M 1971 *Rev. Mod. Phys.* **43** 297
- [29] Berakdar J, Briggs J S and Klar H 1993 *J. Phys. B: At. Mol. Opt. Phys.* **26** 285
- [30] Clemente E and Roetti C 1974 *At. Data Nucl. Data Tables* **14** 177
- [31] Garibotti C R and Miraglia J E 1980 *Phys. Rev. A* **21** 572
- [32] Crothers D S F and Dubé L J 1992 *Adv. At. Mol. Opt. Phys.* **30** 287–337
- [33] Ciappina M F and Cravero W R 2006 *J. Phys. B: At. Mol. Opt. Phys.* **39** 1091
- [34] Fainstein P D, Ponce V H and Rivarola R D 1991 *J. Phys. B: At. Mol. Opt. Phys.* **24** 3091
- [35] Dörner R, Khemliche H, Prior M H, Cocke C L, Gary J A, Olson R E, Mergel V, Ullrich J and Schmidt-Böcking H 1996 *Phys. Rev. Lett.* **77** 4520
- [36] Olson R E and Fiol J 2003 *J. Phys. B: At. Mol. Opt. Phys.* **36** L365
- [37] Pedlow R T, O'Rourke S F C and Crothers D S F 2005 *Phys. Rev. A* **72** 062719
- [38] Gasaneo G, Colavecchia F D, Garibotti C R, Macri P and Miraglia J E 1997 *Phys. Rev. A* **55** 2809