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Assessing the Role of Nuclear-Nuclear Interaction in Single Ionization by Ion Impact

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Abstract

The full description of ion impact processes has been a theoretical challenge starting with the appearance of the so-called *kinematically complete experiments*. Even for high energy (nonrelativistic) ionization by ion impact, where first order theories should to work, there exist unexplained discrepancies between theory and experiment that deserve to be analyzed. In this work we consider the influence of a correct inclusion of all two-body interactions in single ionization by ion impact. The role of the nuclear-nuclear interaction is particularly assessed in events out of the scattering plane.

Keywords: Atomic physics, collisions

1 Introduction

As a result of the constant development of the experimental technique known as COLTRIMS (cold-target recoil-ion momentum spectroscopy), experiments sparked an important impulse to theory, since now it is usual to perform combined measurements involving several electrons and heavy ions (projectile and residual-target ions) [28,29]. COLTRIMS makes it possible to perform so-called *kinematically complete experiments* in the sense that it is possible to measure directly all the momenta of the particles that take part in a particular atomic process. Using single ionization of atoms by ion impact as example, the momenta of the ionized electron and the recoil ion are measured in coincidence and, using momentum conservation, the momentum transfer by the projectile is also obtained. Consequently, it is usual to record data for fully differential cross sections (FDCS) of ion-impact ionization. These measurements constitute a challenging ground for existing theoretical schemes [10]. The first measurements of FDCS, for various momentum transfers and ejected-electron energies, were reported in 2001 by Schulz *et al.* [26] for single ionization of helium by C^{6+} 100 MeV amu^{-1}. First order perturbation theories, such as the First Born Approximation (FBA), should be adequate to describe this process since the projectile charge to velocity ratio is small enough ($Z_P/v_P = 0.1$). However, unexpected contributions out of the scattering plane were observed which theories were not able to explain until now [25].

A huge amount of experiments of single ionization of helium using other projectiles and energy ranges have been performed since 2001 [24]. Picking out one example, Fischer *et al.* (2003) [9] have reported absolute experimental measurements for 2 MeV amu^{-1} C^{6+} single ionization of helium in the scattering plane, defined as the plane containing the initial and final projectile momenta, for various momentum transfers and ejected electron energies. Theoretical results reported in this work using a Continuum Distorted Wave–Eikonal Initial State (CDW-EIS) of Crothers and McCann (1983) [6] exhibit differences between experiment and theory on an absolute scale for emission in the scattering plane. Their calculations were made using the active electron approximation and hydrogenic wavefunctions for the initial and final states of the active electron [9]. Indeed, the simplest description for the helium bound initial state is to assume it has one *active* and one *passive* electron and that the *active* electron can be described as moving in the effective Coulomb field of the atomic core with an effective charge chosen (a) to reproduce the ionization energy or (b) so that the continuum wave is orthogonal to the initial state [2].

Of course, a more sophisticated way is to apply a Hartree–Fock (HF) description for both initial and final states of the active electron [14,15]. HF wave functions, however, still do not include proper angular correlations in the initial state and, for large perturbations, there might be the chance that the projectile interacts with more than one electron in a single event. An explicit two-electron description, i.e., a full–blown four–body theory might be necessary in that case.

The contribution of the internuclear potential (N–N interaction) in ionization by ion impact within the framework of distorted wave theories is still a somewhat controversial topic. There have been several models to take into account N–N interaction, but none of them has been able to reproduce the experimental data in the whole range of parameters studied. It has been shown that high energy projectiles *probe* regions very close to the target nucleus and the perturbative or Born series approach therefore might not be adequate to describe this interaction [3,12].

At a time, where only analytical work was performed and numerical computations were unusual, a semiclassical approach was developed and various schemes based in it have been in use since [18]. This scheme, with some improvements, has shown to be useful to describe several data sets for single ionization of helium by highly charged ions [3].

Nowadays, as numerical computations are quite common due to the steady increase in computational power, all the interactions between pairs of particles in a single collision process can be included, in principle, on *equal footing.* One of the latest approaches developed in this direction is the so-called 3DW-EIS by Foster *et al.* (2004) [11]. In this model, the N–N interaction is taken into account by a Coulomb wave function for the final state and an eikonal phase for the initial one. The resulting FDCS is numerically calculated using quadratures. However, even this sophisticated theory is not able to completely reproduce the available experimental data in the whole range of parameters studied [11].

Before COLTRIMS experiments, the influence of the internuclear potential in ionization by ion impact was usually overlooked since double differential cross sections (DDCS) in electron energy and angle do not depend on this interaction (to first order in $1/M_{T,P}$), as it induces only a phase to the transition amplitude [8,27].

For cross sections differential in terms of projectile scattering angle or recoil ion momentum, on the other hand, it has been shown that the N–N interaction has a relevant influence varying with the ejected electron energies and momentum transfer values [21,23,19,7].

The aim of this work is to explore the role of internuclear interaction in FDCSs of highly charged ion impact electron emission. We will incorporate this interaction in a semiclassical way and we study its influence both in the scattering plane and out of it. In the following section we briefly describe how to model the N–N interaction in this semiclassical picture within the framework of the distorted wave theories. We will use this model together with a CDW-EIS theory to perform calculations for 100 MeV amu^{-1} C^{6+} ion single ionization of helium. Analyzing the contribution of the N–N both in the scattering plane and out of it, we will be able to indicate which directions should be necessary to correctly reproduce the experimental data in the region we are applying. Atomic units are used throughout unless stated otherwise.

2 Theoretical framework

We treat helium single ionization as a single electron process assuming that in the final state the *active* target electron moves in the combined Coulomb field of the incoming projectile and the residual-ion-target with an effective charge. This charge takes into account the partial screening due to the *passive* helium electron.

Within CDW-EIS theory, electron–projectile interaction is considered by a pure Coulomb distortion in the final state and by an eikonal phase in the entrance channel [8]. The N–N interaction is usually treated as a pure Coulomb interaction between a projectile with charge Z_P and the *true* target-ion charge,

$Z_T = 1$. This approximation is fairly good for low charge projectiles and for highly charged ions in a high velocity regime. However, multicharged ions at lower velocities, may induce large polarizations in the target, modifying the screening due to passive electrons (and potentially also the active one). This effect clearly depends on the projectile impact parameter [3].

The N–N interaction is then included in the transition amplitude $\mathcal{A}_{\rm fi}(\boldsymbol{\rho})$ in the semi-classical or eikonal approximation through its multiplication by a phase factor, which in our case results in [18]

$$\mathcal{A}'_{\rm fi}(\boldsymbol{\rho}) = {\rm i}(\rho v)^{2{\rm i}\nu}\mathcal{A}_{\rm fi}(\boldsymbol{\rho}) \tag{1}$$

where $\nu = Z_P Z_T/v$ is the Sommerfeld parameter, v the projectile velocity and $\boldsymbol{\rho}$ defines the impact parameter ($\boldsymbol{\rho}\cdot\mathbf{v} = 0$). $\mathcal{A}_{\rm fi}(\boldsymbol{\rho})$ ($\mathcal{A}'_{\rm fi}(\boldsymbol{\rho})$) is the transition amplitude with (without) internuclear interaction. Using two-dimensional Fourier transforms for the transition amplitude, the CDW–EIS transition matrix can be written alternatively as a function of the momentum transfer $\mathbf{q} = \mathbf{K}_{\rm i} - \mathbf{K}_{\rm f}$, where $K_{\rm i}$ ($K_{\rm f}$) is the magnitude of the initial (final) momentum of the incident particle. $\mathbf{q}$ can also be written as a transversal $\boldsymbol{\eta}$ and a longitudinal component q_z, z being the direction of the incoming projectile velocity $\mathbf{v}$. Using energy conservation for heavy ions, it is possible to obtain $q_z = \Delta\epsilon/v$, where $\Delta\epsilon = \varepsilon_{\rm f} + \varepsilon_{\rm i}$ is the electronic energy balance. Consequently, we can write alternatively,

$$T'_{\rm fi}(\boldsymbol{\eta}') = \frac{{\rm i}v^{2{\rm i}\nu}}{(2\pi)^2}\int d\boldsymbol{\eta}\; T_{\rm fi}(\boldsymbol{\eta})\int d\boldsymbol{\rho}\;\rho^{2{\rm i}\nu}\; e^{{\rm i}(\boldsymbol{\eta}-\boldsymbol{\eta}')\cdot\boldsymbol{\rho}}\;\mathcal{A}_{\rm fi}(\boldsymbol{\rho}). \tag{2}$$

We solve the integral over the impact parameter to obtain:

$$T'_{\rm fi}(\boldsymbol{\eta}) = \nu\frac{{\rm i}v^{2{\rm i}\nu}(2\pi)^{-{\rm i}\nu}}{2^4\pi^3}\int d\boldsymbol{\eta}'\; T_{\rm fi}(\boldsymbol{\eta}')\,|\boldsymbol{\eta}-\boldsymbol{\eta}'|^{-2(1+{\rm i}\nu)} \tag{3}$$

The remaining integral in (3) is evaluated numerically. 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.

In the centre of mass (c.m.) frame, the FDCS in energy and ejection angle of the electron, and direction of the outgoing projectile is given by [16,1]

$$\frac{{\rm d}^3\sigma}{{\rm d}E_k{\rm d}\Omega_k{\rm d}\Omega_K} = N_e(2\pi)^4\mu^2 k\frac{K_{\rm f}}{K_{\rm i}}\,|T_{\rm fi}|^2\,\delta(E_{\rm f}-E_{\rm i}) \tag{4}$$

where N_e is the number of electrons in the atomic shell and μ is the reduced mass of the projectile-target subsystem. The ejected electron's energy and momentum are given by E_k and k respectively. The solid angles ${\rm d}\Omega_K$ and ${\rm d}\Omega_k$ represent the direction of scattering of the projectile and the ionized electron, respectively.

We use non-orthogonal Jacobi coordinates $(\mathbf{r}_P, \mathbf{r}_T)$ to describe the collision process (see Fig. 1) [5].

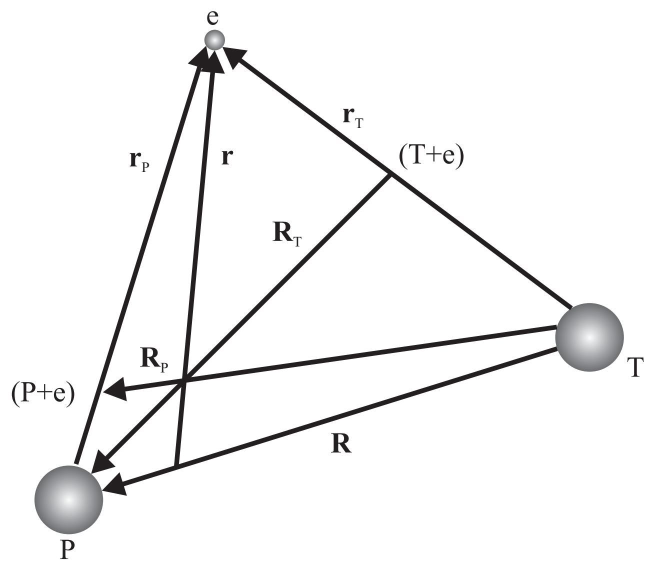

Figure 1: Jacobi coordinates for single ionization by ion impact.

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. For the full formulation, $\mathbf{R}_T$ is also needed, representing the position of the incoming projectile with respect to the c.m. of the subsystem e-T. If we neglect terms of order $1/M_T$ and $1/M_P$, where M_T is the mass of the target ion nucleus and M_P is that corresponding to the incident heavy ion, we can write $\mathbf{R}_T \approx \mathbf{r}_T - \mathbf{r}_P$. We also note that the projectile solid angle $\mathrm{d}\Omega_K = \sin\theta_K \mathrm{d}\theta_K \mathrm{d}\phi_K$ can be expressed in terms of the momentum transfer q via the relations $q \approx K_\mathrm{i} \sin\theta_K$ and $K_\mathrm{i} \approx K_\mathrm{f}$, fulfilled for heavy ion projectiles, i.e. small scattering angles.

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

$$T_{\mathrm{fi}}^{-CDW-EIS} = \left\langle \chi_f^{-CDW} \right| W_\mathrm{i} \left| \chi_i^{+EIS} \right\rangle \tag{5}$$

where the initial (final) state distorted wave χ_i^+ (χ_f^-) is an approximation to the initial (final) state which satisfies 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 Rothan–Hartree–Fock description for the initial bound-state wavefunction [4]

$$\chi_i^{+EIS} = (2\pi)^{-3/2} \exp\left(\mathrm{i}\mathbf{K}_\mathrm{i} \cdot \mathbf{R}_T\right) \psi_\mathrm{i}(\mathbf{r}_T) \mathcal{E}_v^+(\mathbf{r}_P) \tag{6}$$

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

$$\mathcal{E}_v^+(\mathbf{r}_P) = \exp\left(-\mathrm{i}\frac{Z_P}{v}\ln\left(vr_P - \mathbf{v}\cdot\mathbf{r}_P\right)\right). \quad (7)$$

The final state wavefunction is cast into the form [13]

$$\chi_f^{-CDW} = (2\pi)^{-3/2}\exp\left(\mathrm{i}\mathbf{K}_\mathrm{f}\cdot\mathbf{R}_T\right)\chi_T^-(\mathbf{r}_T)C_P^-(\mathbf{r}_P) \quad (8)$$

where C_P^- represents the Coulomb distortion of the ejected electron wave function due to the projectile:

$$C_P^-(\mathbf{r}_P) = N(\nu_P)\,{}_1F_1\left(-\mathrm{i}\nu_P, 1, -\mathrm{i}k_P r_P - \mathrm{i}\mathbf{k}_P\cdot\mathbf{r}_P\right), \quad (9)$$

with the Sommerfeld parameter $\nu_P = \frac{Z_P}{k_P}$, the relative momentum $\mathbf{k}_P$ of the e–P subsystem and the usual Coulomb factor

$$N(\nu_P) = \Gamma(1-\mathrm{i}\nu_P)\exp(\pi\nu_P/2). \quad (10)$$

$\chi_T^-(\mathbf{r}_T)$, on the other hand, is the wave function for the ejected electron in the field of the target residual ion:

$$\chi_T^-(\mathbf{r}_T) = (2\pi)^{-3/2}\exp\left(\mathrm{i}\mathbf{k}_T\cdot\mathbf{r}_T\right)N(\nu_T)\,{}_1F_1\left(-\mathrm{i}\nu_T, 1, -\mathrm{i}k_T r_T - \mathrm{i}\mathbf{k}_T\cdot\mathbf{r}_T\right) \quad (11)$$

with $\nu_T = \frac{Z_T}{k_T}$ and the relative momentum $\mathbf{k}_T$ of the e–T subsystem.

The perturbation potential W_i in (5) is defined by

$$\left(H_\mathrm{i} - E_\mathrm{i}\right)\chi_i^+ = W_\mathrm{i}\chi_i^+ \quad (12)$$

where H_i is the full electronic initial Hamiltonian (neglecting the ¸m. motion) and E_i is the total initial energy of the system in the c.m. frame. W_i is composed from two differential operators and can be written as [5]

$$W_\mathrm{i} = \frac{1}{2}\boldsymbol{\nabla}_{\mathbf{r}_P}^2 - \boldsymbol{\nabla}_{\mathbf{r}_T}\cdot\boldsymbol{\nabla}_{\mathbf{r}_P}. \quad (13)$$

We compute the FDCS, eq.(4), for single ionization of helium, using the prior CDW–EIS scheme (5) with and without taking into account the N–N interaction. We analyze the contribution of this interaction both in and out of the scattering plane. We follow the geometry used in the experiments of Schulz *et al.* (2001) (see next section) [26].

3 Results and comparisons

We first briefly describe the geometry we use to perform the theoretical calculations. We follow the experimental set up explained in Schulz *et al.* (2001)

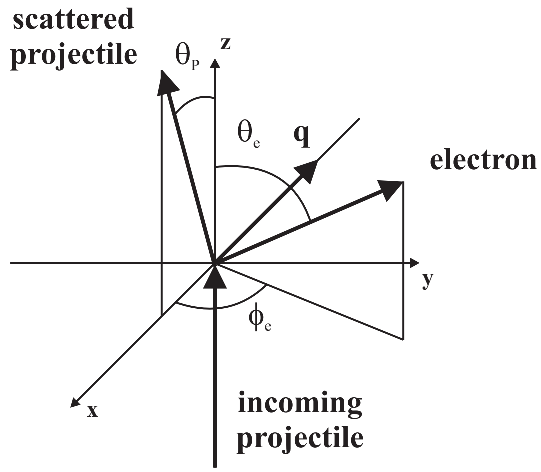

Figure 2: Spherical coordinate system used in the present work. The z axis is parallel to the direction of the incoming projectile and the $x - z$ plane is the scattering plane.

[26]. The coordinate system has the z axis parallel to the incoming projectile direction, the y axis perpendicular to the scattering plane, defined as a plane containing the initial projectile momentum $\mathbf{K}_{\mathrm{i}}$, the final projectile momentum $\mathbf{K}_{\mathrm{f}}$ and the momentum transfer $\mathbf{q}$, i.e the $x - z$ plane, and directed up. The x axis is oriented toward the left of the beam direction (see figure 2) [17].

If the projectile is scattered to the left, i.e. in the positive x direction, the binary electrons are scattered to the right in the negative x direction. The momentum transfer direction $\mathbf{q}$ is very close to 90°, which would correspond to the negative x direction in this geometry. We use standard spherical coordinates with θ_e being measured relative to the beam direction, $\phi_e = 0$ corresponds to the half-plane containing the positive x axis and $\phi_e = \pi$ corresponds to the half-plane containing the negative x axis. The binary peak appears in the $\phi_e = \pi$ half-plane and the recoil peak lies in the $\phi_e = 0$ half-plane. The FDCSs are differential in the solid angle of observation for the scattered projectile ($\mathrm{d}\Omega_K$), differential in the solid angle of observation for the ejected electron ($\mathrm{d}\Omega_k$) and differential in the energy of the ejected electron (E_e) (i.e. fully means five-fold differential in this process). Consequently, (4) can be expressed as a function of $\theta_K, \theta_e, \phi_e, E_e$ since the projectile is in the $\phi_K = 0$ plane by definition. Although the cross sections depend on the observation angles of the projectile θ_K, ϕ_K, for analytical purposes it is usually to fix the scattering angle ϕ_K and to express the projectile polar scattering angle only in terms the magnitude of the momentum transfer q.

3.1 FDCSs in Scattering plane

The present results of CDW-EIS with the N–N interaction (CDW-EIS/NN) are compared to those without this interaction (CDW-EIS) as well as to those obtained in the FBA. In figure 3 we show results for 100 MeV amu^{-1} C^{6+} single ionization of helium for different electron and projectile parameters. To plot all the results in a single graph, we define the scattering plane $x - z$ using θ'_e from 0° to 360° which corresponds first to the $\phi_e = \pi$ half-plane ($0° \leq \theta'_e \leq 180°$) followed by the $\phi_e = 0$ half-plane ($180° \leq \theta'_e \leq 360°$), the angles being measured clockwise relative to the beam direction. Following experimental requirements, the cross sections in the figures are transformed into the laboratory frame. The conversion from c.m. to laboratory frame results in a constant factor of 16 for the present FDCS.

Several important observations can be made from the results presented in figure 3. First, both experiment and theory show the same characteristic shape that is expected from scattering with electrons. There exists a larger peak at 90° (the binary peak) and a smaller peak at 270° (recoil peak). The binary peak results from a single two-particle projectile–electron collision and is located in the direction of the momentum transfer vector **q**. The recoil peak is attributed to a double scattering mechanism in which the projectile first collides with the electron and then the electron scatters at backward direction off the atomic nucleus. As apparent from figures, the recoil peak decreases rapidly with increasing momentum transfer, which is directly related to the projectile scattering angle. Both CDW-EIS/NN and CDW-EIS results are in reasonable agreement with the absolute data presented in [17] for all parameters studied. On the other hand, the FBA reproduces the shape of the FDCS, but it is about a factor of 2 smaller than the other data. For electron impact, the FBA and CDW-EIS results would be essentially identical for projectile?-electron energies above about 1 keV (velocity of about 10 a.u.). The results shown here are a bit surprising in this respect since the projectile velocity in these experiments is about 60 a.u.. Here we see noticeable differences for the lower ejected-electron energies and smaller momentum transfers resulting from the larger charge of the projectile.

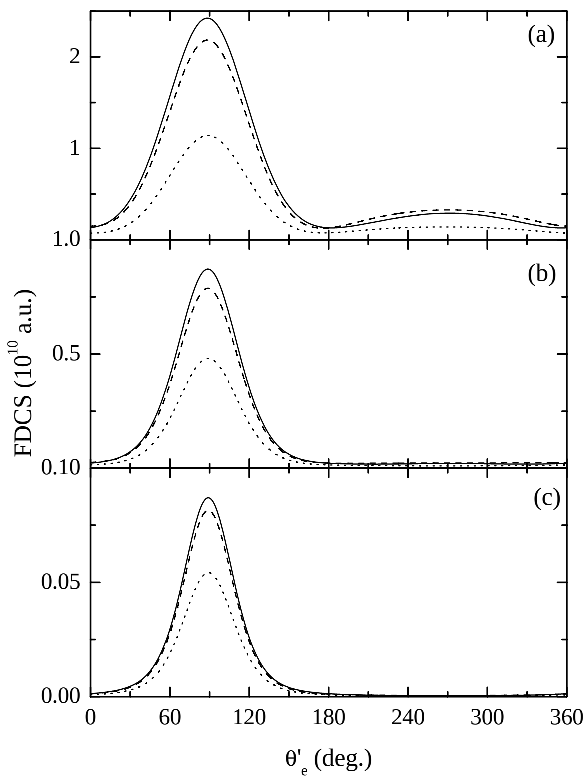

Figure 3: Comparison of in-plane FDCSs for 100 MeV amu^{-1} C^{6+} single ionization of helium. In panel (a) the energy of the ejected electron is $E_e = 6.5$ eV and the momentum transfer of the projectile is $q = 0.88$ a.u., panel (b) $E_e = 17.5$ eV, $q = 1.43$ a.u. and panel (c) $E_e = 37.5$ eV, $q = 2.65$ a.u. In all panels, solid line: CDW-EIS/NN, dashed line: CDW-EIS and dotted line: FBA.

To obtain insight in the contribution of the N–N interaction in our semiclassical picture, we plot in figure 4 the ratio between the results of CDW-EIS/NN and those without taking into account this interaction, i.e. the CDW–EIS. From these comparison we see that the N–N contributes about ±20% and hardly depends on the projectile or electron parameters. According to physical considerations, this result is contradictory, since the projectile should to be less (more) sensitive to the N–N potential at small (high) momentum transfers. This behavior of the semiclassical picture indicates room for future improvements involving this interaction.

A different source of discrepancies between theory and experiment could be experimental uncertainties, but it is seen that a convolution had only a small effect on the results [17]. Although HF wavefunctions have been used for some time now, it is still common practice to represent the final states of the active electron as hydrogenic wavefunctions for some effective charge. This last approach has the advantage to result in analytical integrals that allow us to a more detailed studies. For helium, two different effective charges are typically used: 1.3569, which yields the proper energy for ionizing the first electron, and 1.6875, which minimizes the total energy for the helium atom. Since we are interested here in studying the contribution of the internuclear interaction, we do not focus on details about the quality of initial and final electronic wavefunctions.

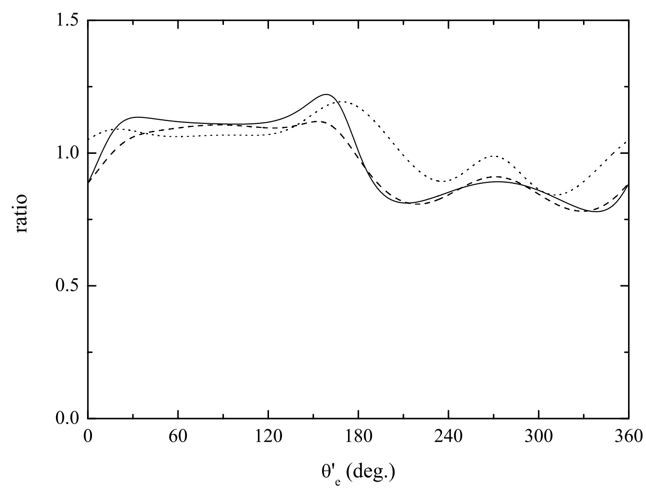

Figure 4: Ratio between CDW-EIS/NN and CDW-EIS. Solid line: $E_e = 6.5$ eV, $q = 0.88$ a.u., dashed line: $E_e = 17.5$ eV, $q = 1.43$ a.u. and dotted line: $E_e = 37.5$ eV, $q = 2.65$ a.u.

3.2 FDCSs Out-of scattering plane

According to the FBA, the cross sections are symmetric about the direction of momentum transfer. As a result, in FBA there should be no new information contained in the out-of-plane results. All the events in out-of-plane regions are a fingerprint of higher-order effects. In order to quantify the high-order information incorporated in the distorted wave theories, in figure 5 we plot FDCS of out-of-scattering plane calculations. The angular dependence of the perpendicular plane is given by the azimuthal angle ϕ_e. To make a direct comparison with the in-plane results, we define a new azimuthal angle $\beta_e = \phi_e - \pi/2$. Looking at figure 2 we can see that $\beta_e = 0$ corresponds to the y axis, $\beta_e = \pi/2$ corresponds to the momentum transfer direction $\mathbf{q}$ (negative x direction), $\beta_e = \pi$ corresponds to negative y axis and $\beta_e = 3\pi/2$ corresponds to the positive x axis.

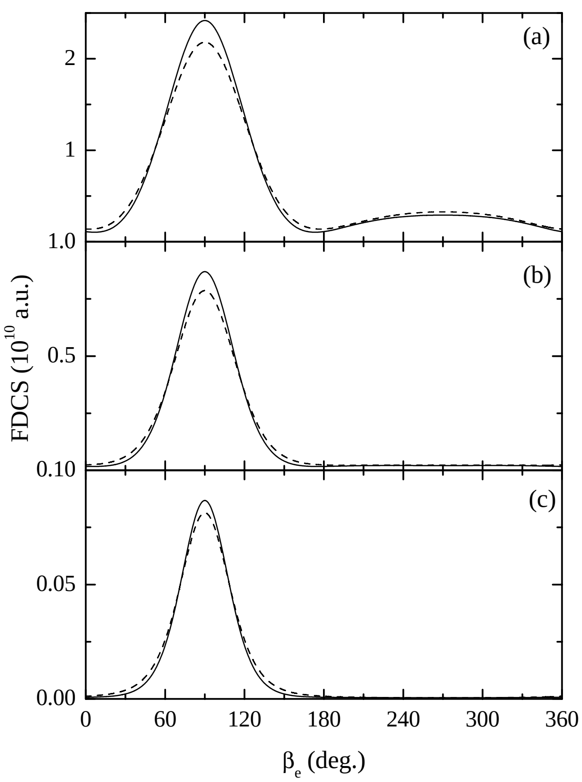

Figure 5: Comparison of out-of-scattering-plane FDCSs for 100 MeV amu^{-1} C^{6+} single ionization of helium. In panel (a) the energy of the ejected electron is $E_e = 6.5$ eV and the momentum transfer of the projectile is $q = 0.88$ a.u., panel (b) $E_e = 17.5$ eV, $q = 1.43$ a.u. and panel (c) $E_e = 37.5$ eV, $q = 2.65$ a.u. In all panels: solid line: CDW-EIS/NN, dashed line: CDW-EIS.

From the results shown in figure 5, we observe that N–N interaction contributes more to the in-plane calculations. Both calculations are in reasonable agreement with the experimental results, except in the regions $\beta_e \in [0°, 30°]$ and $\beta_e \in [135°, 160°]$, where the experimental data are a factor of 2 higher compared to our theoretical calculations [17]. As in the case of in-plane FDCS, it is illustrative to perform the ratio between the CDW-EIS/NN and the CDW-EIS results. In figure 6 we show these ratios. Supporting the first impression observed in figure 5, we see now the N–N interaction has a larger contribution in this geometry, varying between 40% and 50%, depending on the electron and projectile parameters.

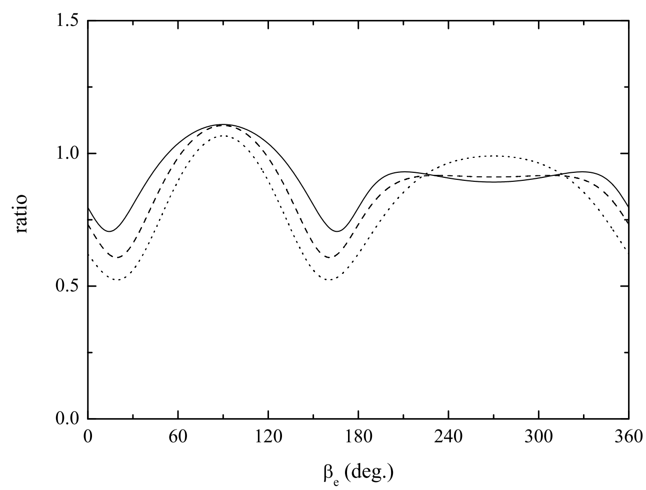

Figure 6: Same as figure 4 for the perpendicular out-of-scattering-plane geometry.

Finally, in order to compare directly our results with other theoretical approaches and to get a more global picture about the N–N contribution, we follow [17] and plot in figure 7 the ratio between the FDCSs calculated in the scattering plane and those that result from the out-of-scattering-plane events. We note that, according to the discussion above, the ratio of the cross sections for the two planes would be (essentially) unity in the FBA. As mentioned before, this means that all differences from this behavior are due to higher-order contributions. Analyzing figure 7 we observe that the trend using CDW-EIS/NN calculations is in agreement with other approaches [17], but has large discrepancies with the experiments where the shape is almost opposite. Compared to the nearly constant CDW-EIS ratios, it is obvious that the N–N interaction, at least in our semiclassical picture, contributes considerably.

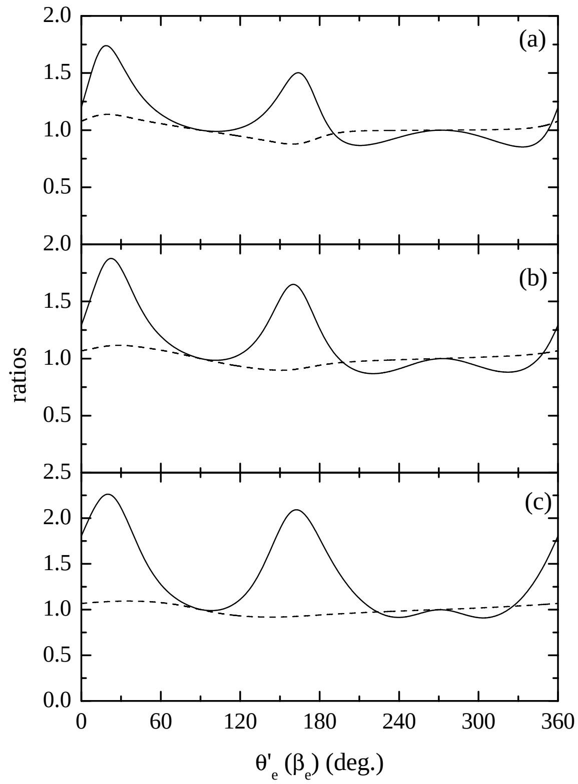

Figure 7: Ratio between results in the scattering plane and out-of-scattering plane. Panel (a) $E_e = 6.5$ eV, $q = 0.88$ a.u., panel (b): $E_e = 17.5$ eV, $q = 1.43$ a.u. and panel (c): $E_e = 37.5$ eV, $q = 2.65$ a.u. In all cases: solid line: CDW-EIS/NN; dashed line: CDW-EIS.

4 Conclusions and perspectives

We have carried out CDW-EIS calculations of FCDSs for single ionization of Helium by 100 MeV amu^{-1} C^{6+} to assess the role of the interaction between the projectile and the target ion (nuclear-nuclear interaction) using a simple semiclassical model. This semiclassical approach has the advantage to be computationally simpler and far less time consuming than more rigorous models. Analyzing the contribution of this interaction in the out-of-scattering-plane, we were able to quantify adequately its effects.

Our CDW-EIS/NN theory shows an acceptable overall agreement in the scattering plane without the need of additional 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 small contribution in the out-of-scattering plane events.

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 obtain some global conclusions about the importance of the N–N interaction.

To adequately model the ionization process and probably to solve this intriguing behavior of highly charged projectiles, 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 N–N interaction, e.g. by incorporating distorted Coulomb waves for the initial and/or final channels within a distorted wave approach. A different approach would be to attack the ionization problem using ab-initio techniques, e.g. solving numerically the Time Dependent Schrödinger Equation (TDSE), that nowadays are usual in, for example, strong laser physics (see e.g. [22] and references therein) or electron–impact ionization processes [20].

Within the physical picture provided by the usual CDW-EIS model, these improvements 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 where, on the other hand, the underlying physics is difficult to assess. So far, however, such models have shown only marginally better results when compared with simpler ones. For the time being, physically trusted models such as the CDW-EIS still are important while our understanding and modeling of these systems evolve.

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