LETTER TO THE EDITOR

Dynamical electron-electron Correlation in C^{2+} + He Simultaneous Target-Projectile Ionization

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Abstract. Simultaneous target and projectile single ionization in 3.6 MeV/u C^{2+} + He collisions is considered within a 6-body Classical Trajectory Monte Carlo model. Analysis of the relative azimuthal angle between the two emitted electrons allows one to discriminate the ionization contribution produced by the two-center dynamical electron-electron interaction from that due to nuclear-electron interactions. The present calculations agree well with cross sections measurements recently performed in kinematically complete experiments.

PACS numbers: 34.50.Fa, 34.80.Kw

Submitted to: *J. Phys. B: At. Mol. Opt. Phys.*

1. Introduction

Collisions resulting in the ionization of both target and projectile provide a basis to study the effect of electron-electron (e-e) and nuclear-electron (N-e) interactions. Interest on such collisions arises mainly because they are the simplest processes where dynamical electron correlation can be studied in competition with the nuclear-electron forces. Unlike ionization of multiple-electron targets by bare ions, where static initial state correlation plays the primary role, dynamical correlation between electrons on different centers significantly contributes to simultaneous ionization in collisions between "dressed" particles (Montenegro *et al* 1992, 1994).

A clear separation of the contribution due to interactions between electrons belonging to different centers (e-e interactions) from that of nucleus-electron (N-e) interactions is of particular practical interest. Experimental conditions that allow one to isolate the effect of two center e-e interactions in ion-atom collisions may lead to a practical technique to measure electron-ion scattering processes, which are important in plasma physics.

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Numerous efforts have been made to identify and separate the contribution of e-e and N-e interactions to the simultaneous ionization (Hülsköter *et al* 1989, Montenegro *et al* 1992, Dörner *et al* 1994, Wu *et al* 1994). Theoretical and experimental data have been interpreted in terms of screening and antiscreening interactions (Anholt *et al* 1986). The screening interaction is defined as the potential between the electron in one center and the (screened) nuclear charge in the opposite center. This contribution includes both the pure Coulomb electron-nuclear interaction and the screening due to the static average potential of the electrons in the initial state. On the other hand, the antiscreening contribution is ascribed to the dynamical electron-electron interaction between nuclear centers (Montenegro *et al* 1994 and references therein).

The simultaneous single ionization of the target and the projectile in $C^{2+} + He$ collisions at 3.6 MeV/u ($v = 12$a.u.)

$$C^{2+} + He \rightarrow C^{3+} + He^{+} + 2\,e \tag{1}$$

is investigated within the Classical Trajectory Monte Carlo (CTMC) theory. The 6-body calculations include the two helium K-shell electrons and the two L-shell electrons of the C^{2+} ion. In this model, each electron interacts with the two nuclei and with each of the two electrons initially bound to the other center. The present calculations are similar to those presented in a previous paper for the $He^{+} + Ne$ system (Fiol *et al* 2001).

Correlation between electrons belonging to different centers may be studied by considering magnitudes that must be conserved in two-body processes. In particular, the cross section differential in the relative azimuthal angle between the two ionized electrons φ_{eP-eT} has recently been proposed with this purpose (Fiol *et al* 2001). In a purely binary electron-electron collision both particles are emitted on the same plane ($\varphi_{eP-eT} = 180°$). On the other hand, for ionization by the simultaneous interaction of each emitted electron with the nucleus in the opposite center, the angular distribution does not present any preferential direction. This simple property has been used to determine the contribution from dynamical e-e interaction in simultaneous ionization in $He^{+} + Ne$ collisions. For this system the calculations showed that the electron-electron interaction produces approximately 35% of the target-projectile simultaneous ionization cross section at incident energies between 1 and 16 MeV/u. However, the theoretical predictions for the angular distributions were not experimentally confirmed, since there are no available data for this system.

Recently, new data of simultaneous ionization cross sections in 3.6 MeV/u $C^{2+} + He$ collisions have been reported (Kollmus *et al* 2002). The experiment, performed at the GSI (UNILAC) accelerator, detected the emerging C^{3+} projectile in coincidence with the measurement of the two emitted electrons and target ion nucleus He^{+} momenta. The new kinematically-complete data suggests the feasibility of using this technique to study electron-ion scattering processes. The aim of the present work is to analyze the separation of the nuclear-electron and electron-electron interactions in C^{2+} and He simultaneous ionization and compare the theoretical CTMC results to the newly available experimental data.

2. Results

As mentioned in the introduction, the relative azimuthal angle between the two emitted electrons has been shown to be a suitable quantity to study e-e correlation (Fiol *et al* 2001, Kollmus *et al* 2002). Figure 1 shows the cross section for reaction (1) differential in the relative azimuthal angle φ_{eP-eT} and momentum transfer $\boldsymbol{Q} = \boldsymbol{P} - \boldsymbol{K}$, where $\boldsymbol{P} = M_P\boldsymbol{v}$ and $\boldsymbol{K}$ are the initial and final momenta of the carbon ion projectile of mass M_P. Observe that the momentum associated to the incident velocity $m_e v$ has been subtracted to the momentum transfer in the horizontal axis. This shift accounts for the momentum loss due to the emission of the electron from the projectile. The distribution on the left panel of figure 1 shows favorable emission at $\varphi_{eP-eT} = 180°$ for small values of the momentum transfer $Q^* = Q - m_e v$. For larger values of Q^* the emission is isotropic indicating that simultaneous ionization is mainly produced by the interaction of each emitted electron with the nucleus in the opposite center.

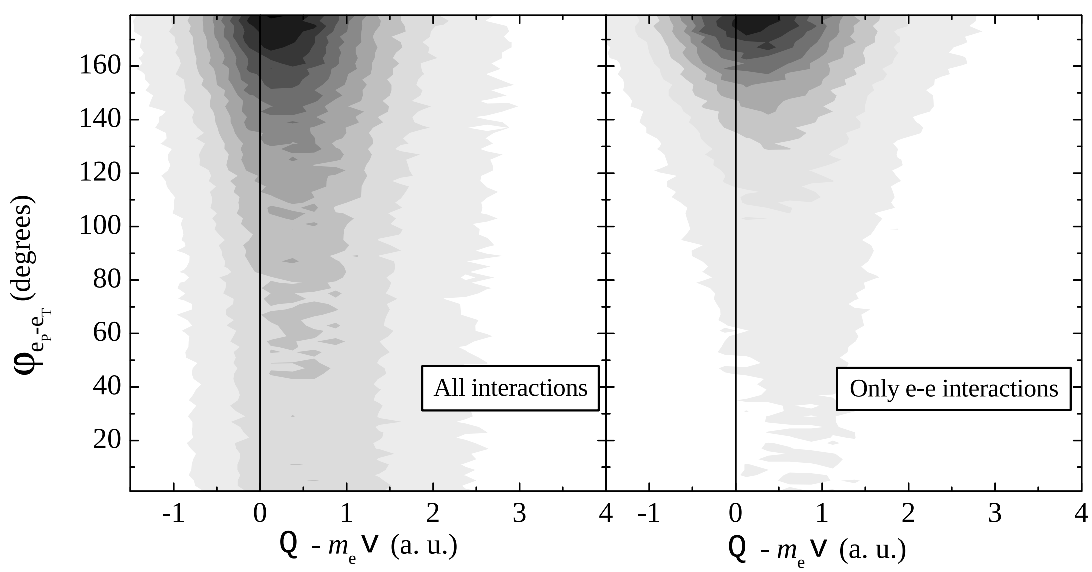

Figure 1. CTMC differential cross sections as a function of the (shifted) momentum transfer $Q^* = Q - m_e v$ and the relative azimuthal angle φ_{eP-eT} between both ionized electrons. Left: all interactions between particles belonging to different centers are active. Right: CTMC results within the simplified model where each electron only interacts with its parent nucleus and the two electrons in the other center.

Two simplified models are considered in addition to the “full” 6-body CTMC calculations before described. The first model neglects the potential interaction between electrons initially belonging to different nucleus. Each electron only interacts with the two bare nuclei. The second model is complementary to the first one. Each electron does not interact with the nucleus in the opposite center. In this later model the ionization only takes place by electron-electron collisions. We remark that in all calculations, interactions between electrons of the same center have been neglected, since they are known to produce unstableness in the classical description of bound states. The right plot in figure 1 shows results for the simplified model where only e-e interactions are active.

The calculated distributions for the C^{2+} + He are qualitatively similar to those observed previously in the He^{+} + Ne case for the same projectile energy (Fiol *et al* 2001). On the left, the calculations including all the interactions show a maximum for small values of the translated momentum $Q^{*} = Q - m_e v$. The correlation between the two emitted electrons is reflected in a maximum at 180° in the relative azimuthal angle. For higher values of the momentum transfer, simultaneous ionization is mainly produced by the interaction of each emitted electron with the screened nucleus in the opposite center, producing a isotropic distribution of azimuthal angles φ_{eP-eT}. Accordingly, the plot on the right, obtained including only e-e interactions, shows that the distribution is strongly favored in the electron-electron scattering plane $\varphi_{eP-eT} = 180°$.

Figure 2 shows CTMC single differential cross section in the relative azimuthal angle $\mathrm{d}\sigma/\mathrm{d}\varphi_{eP-eT}$ for simultaneous ionization of the target and projectile in C^{2+} + He. Together with the 6-body CTMC calculations are shown the results for the two simplified models that include only either e-e or N-e interactions, respectively. As discussed previously, the antiscreening (e-e) contribution gives rise to angular distributions in the relative azimuthal angle with preferential emission in a plane. Our calculations exhibit a pronounced maximum at azimuthal angle $\varphi_{eP-eT} = 180°$ with a tail, due to the overlapping Compton profiles of the electrons that produces counts at smaller angles. On the other hand, the contribution of the two combined N-e interactions shows an isotropic distribution in the relative azimuthal angle. Note that in figure 2 the CTMC results are absolute simultaneous ionization cross section for each model.

The computed single differential cross sections are compared in figure 3 with recent measured data. The experimental distribution, obtained in a kinematically complete experiment performed at the UNILAC of GSI (Kollmus *et al* 2002), has been shifted by an angle $\varphi_{eP-eT} = 10°$. Observe that this shift of the experimental data ensures proper symmetry of the spectrum around $\varphi_{eP-eT} = 180°$. The separation performed in figure 3 assumes that the contributions from screening and antiscreening modes simply add to the observed cross section. However, this is not necessarily true for collisions out of a perturbative regime. In fact, for He^{+} + Ne collisions the two mechanisms cannot be considered as independent even at incident energies as high as 4 MeV/u (Fiol *et al* 2001). In the present case, with only two active electrons in each center, a perturbative approach describes correctly the process and a simple additive separation may be expected.

The change in the momentum of the participating particles is a measure of how hard was the collision they experienced. Ionization due to binary e-e collisions is expected to transfer larger momentum to the electrons than to the nuclei (Kollmus *et al* 2002). On the other hand, simultaneous ionization due to N-e interactions would lead to higher momentum transferred to the nuclei than to their electrons. Following this line of

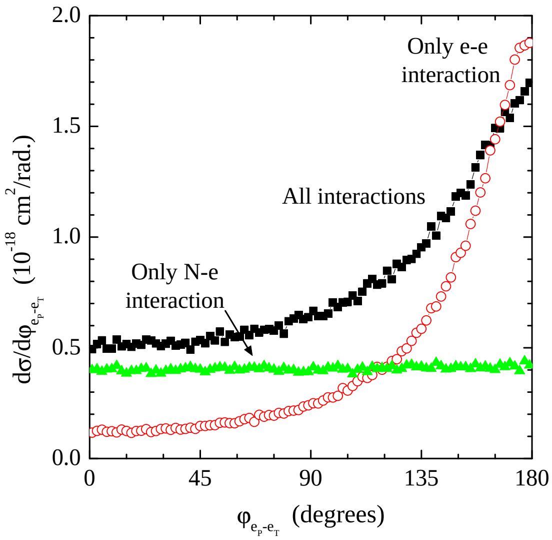

Figure 2. Single differential 6-body CTMC cross sections in the azimuthal angle between the two emitted electrons for the three models considered. The calculations including only e-e interactions show a pronounced maximum at $\varphi_{eP-eT} = 180°$ while those including only nuclear-electron interactions present a flat behavior.

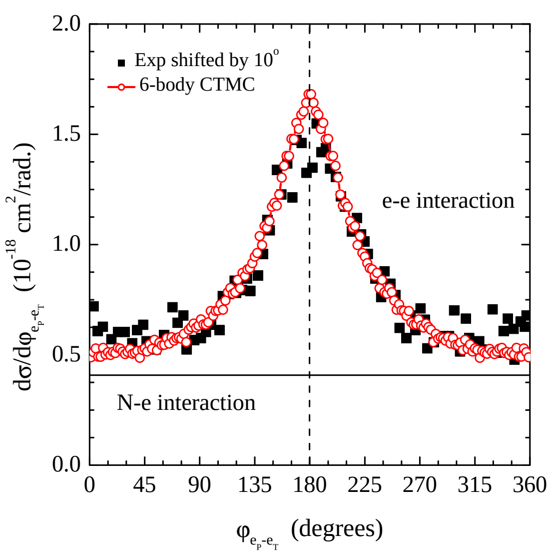

Figure 3. Single differential 6-body CTMC (open circles) and experimental (full squares) cross sections in the relative azimuthal angle between the two ionized electrons are compared. The experimental data has been shifted by 10° in order to obtain a distribution that is symmetric around $\varphi_{eP-eT} = 180°$ and for a better comparison with the theory.

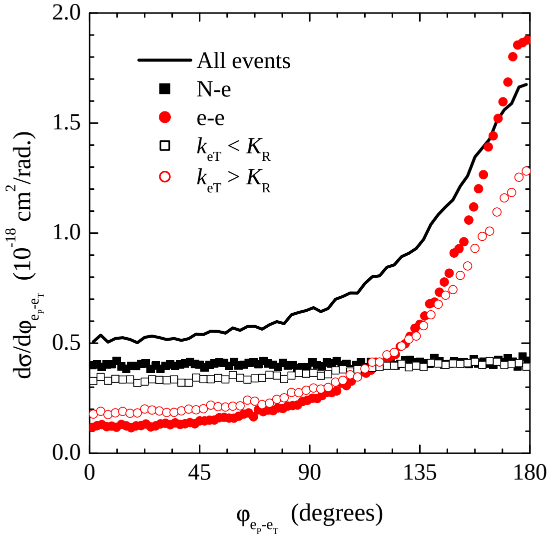

Figure 4. The e-e and N-e contributions (lines) are compared to calculations considering all interactions but where only events verifying either that the electron momentum k_e is larger or smaller than the recoil momentum K_R are recorded (symbols).

reasoning, the distributions obtained by selecting events with momentum of the target electron either larger or smaller than the momentum of the residual ion are related to the two simplified models considered in this work. In figure 4, 6-body CTMC cross sections obtained selecting only those events verifying the condition $k_e > K_R$ ($K_R > k_e$) are compared with the results obtained when only e-e (N-e) interactions are active. The angular distribution for those events with $k_e < K_R$ is nearly uniform, confirming that those ionization events are mainly produced by nucleus-electron interactions. The distribution for the case with only e-e active interactions presents a more pronounced maximum than the obtained for all the interactions but $k_e > K_R$.

There is an obvious equivalence between projectile and target centers. Ionization via N-e interactions result in final states where the change in the projectile momentum must account for the energy deposited in order to ionize the target electron. A small change in projectile momentum is expected from processes dominated by e-e collisions. Figure 5 displays CTMC simultaneous ionization cross sections obtained selecting only those events when either the change in the nucleus projectile momentum is more or less important than the momentum acquired by its electron ($k_P < Q$ and $k_P > Q$ respectively). Observe that this selection must be performed in a reference system attached to the initial velocity of the projectile, such that the relative electron-projectile momentum $k_P = k_{eP} - m_e v$ must be considered rather than the electron momentum k_{eP}.

This separation of e-e and N-e contributions results in cross sections whose shape is remarkably similar to those observed for equivalent selections on the target, with the

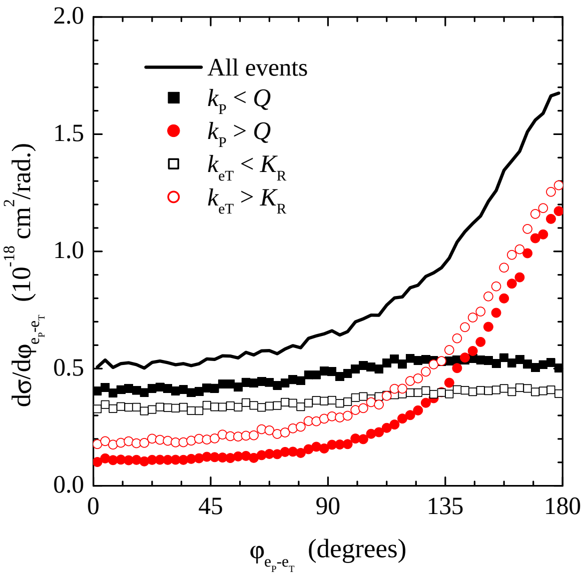

Figure 5. CTMC computed cross sections considering all interactions but where only events verifying either that the relative projectile's electron momentum k_P is larger or smaller than the momentum transfer Q are recorded (symbols). These selections are compared with equivalent selections where only $k_e < K_R$ or $k_e > K_R$ are considered (see figure 4).

conditions $k_{eT} > K_R$ and $k_{eT} < K_R$ respectively. However, surprising discrepancies are observed in the magnitudes of the screening and antiscreening ionization cross sections obtained by these two methods. The contribution from N-e collisions obtained with the the selection on the targets fragment's momenta are 15% smaller than when projectile fragments momenta are used. The origin of these differences can be found in the asymmetries in the initial state of the two centers. The binding energy of the helium atom (24.6 eV) is much smaller than the energy needed to ionize the C^{2+} ion (48 eV). Thus, electron-electron collisions resulting in helium ionization do not necessarily will produce the ionization of the carbon ion. On the other hand, in close collisions where the energy transferred between the electrons is enough to ionize the C^{2+} ion the electron bound to the helium atom will likely be ionized.

3. Conclusions

The present work shows that the analysis in terms of the azimuthal relative angle proposed in previous works offers a sensible method for the discrimination of so-called screening and antiscreening contributions. It does not only give a qualitative description of the relative importance of electron-electron and nuclear-electron collisions, but also a fair estimation of each contribution. For the present case, the screened N-e interactions were found to be responsible of about 70% of the observed simultaneous ionization events.

Different methods for identify the e-e and N-e contributions were investigated. The comparison between relative contributions obtained by studying target's and projectile's particles showed the consistency of the proposed selection criteria. Quantitative discrepancies between the results obtained with the different methods were found to be related to the asymmetry between projectile and target initial states. Present n-body Classical Trajectory Monte Carlo computations show remarkable agreement with new kinematically-complete experimental data.

Acknowledgments

The authors acknowledge support from the Office of Fusion Energy Sciences - DOE.

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