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LETTER TO THE EDITOR

Simultaneous projectile and target ionization in He^+ + Ne collisions

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Abstract

Cross sections for single and multiple ionization of the target atom with simultaneous ionization of the projectile have been measured for 1–4 MeV collisions of He^+ with Ne. The observations are interpreted using the n-body classical trajectory Monte Carlo method. The 11-body calculations include the L-shell electrons of the Ne and the K-shell electron on the He^+. In this model, each electron interacts with both nuclei and with all the electrons belonging to the other centre. For single ionization from both centres, it is found that the dynamical electron–electron (e–e) interaction produces a clear signature in the relative azimuthal angle distribution between the ionized electrons. For low values of momentum transfer q, this interaction is reflected in a pronounced enhancement near 180° in the azimuthal angle between electrons. Integral values of the azimuthal angle events, summed over all q values, indicate that it is possible to determine the relative importance of the e–e versus the nuclear–electron (N–e) interactions.

Simultaneous ionization of both the projectile and target atom provides a unique opportunity to study the interplay between the dynamical electron–electron (e–e) and screened nuclear–electron (N–e) interactions in atomic collisions. In order to determine the relative importance of the two-centre e–e versus the N–e interactions, original work concentrated on measuring the total cross sections as a function of energy, and compared these results with Born calculations for the two separate interactions (Hülskötter *et al* 1989, Montenegro *et al* 1992a). The advent of recoil ion momentum spectroscopy provided a more direct determination of the N–e and e–e interactions with the observation of two separate maxima in the transverse momentum of the recoil ion as a function of longitudinal momentum (Dörner *et al* 1994, Wu *et al* 1994). However, distinct maxima only occur for select systems and energies, and are clouded by the fact that the recoil longitudinal momentum moves towards zero as the collision velocity increases. It is the purpose of this letter to illustrate that the signature of the e–e and N–e

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interactions is clearly profiled in the relative azimuthal angle between the ionized electrons, irrespective of the behaviour of the recoil ion.

In this letter we concentrate on the 1–4 MeV collision processes

$$He^{+} + Ne \rightarrow He^{2+} + Ne^{i+} + (i + 1)e. \tag{1}$$

Multiple-ionization cross sections have been measured for Ne^{i+} for final charge states $i = 0$–3 using the apparatus described in Santos *et al* (2001). These data are used to benchmark 11-body classical trajectory Monte Carlo (*n*CTMC) computations that explicitly include the interaction of each electron with both nuclei, the N–e interactions, and the e–e interactions between all pairs of electrons each belonging to a different nuclear centre. This version of the *n*CTMC method was originally developed to investigate the competition between electron loss and electron capture to the continuum processes for collisions involving partially stripped ions (Schultz *et al* 1990). Because the *n*CTMC method provides a kinematically complete description of the scattering, it has been very successful in developing an understanding of the collision dynamics in multiple-ionization reactions (Cocke and Olson 1991, Ullrich *et al* 1997). The method has previously been used in the interpretation of the relative importance of the e–e and N–e interactions for He^{+} + He recoil ion momenta measurements (Dörner *et al* 1994), and for the kinematically complete measurements for 3.6 MeV u^{-1} C^{2+} + He simultaneous ionization (Moshammer 2000).

Experimental data for the He^{+} + Ne *total* electron loss cross sections have been interpreted in terms of antiscreening (e–e interaction) and screening (N–e interaction) contributions introduced by McGuire *et al* (1981) and Anholt (1986); see also Montenegro *et al* (1994). These two collision mechanisms have different collision dynamics. In general, the screening (N–e) interaction dominates in hard, small impact parameter collisions, while the antiscreening (e–e) interaction dominates in large impact parameter collisions. This can give rise to different signatures on the recoil ion momenta and, as we will show, in coincidence measurements of the ionized electron distributions. Reaction (1) is especially interesting since calculations, which for light targets such as He and H_2 tend to the high-energy Born limit, indicate that the screening and antiscreening interactions share almost equal weight when $i = 1$ (Voitkiv *et al* 1999).

Important to our discussion is a clear definition of the terms screening (N–e) and antiscreening (e–e) interactions. What we term e–e interactions are those that directly contribute to the ionization cross sections via dynamical interactions of the electrons between nuclear centres. The screening (N–e) events are interactions between the ionized electron and the *screened* nuclear charge on the other centre. It is important to note that the e–e interaction potential in the Hamiltonian thus has two contributions, one of screening the nuclear charge and the other of dynamically inducing ionization events via binary collisions between the electrons on the two nuclear centres. Here, we attempt to isolate the dynamical e–e contribution from its static nuclear screening function.

From a theoretical point of view, the complexity of the problem arises mainly due to the large number of interactions involved, which increases quadratically as $(n^2 - n)/2$ where n is the number of particles. In the *n*CTMC calculations performed here we have neglected the e–e interactions between target electrons and have incorporated this correlation by using a static screened interaction between the nuclei and each of their electrons. With this simplification the number of interactions decreases significantly. It is worth noting, however, that the relevant ionizing interactions, i.e. those between particles on the two centres, are considered in an exact way. Thus, the Hamiltonian for the *n*CTMC method is written as

$$H = (H_0 + V_{\mathrm{NP-eP}} + V_{\mathrm{NT-eT}}) + V_{\mathrm{NP-NT}} + V_{\mathrm{NT-eP}} + V_{\mathrm{NP-eT}} + V_{\mathrm{eP-eT}} \tag{2}$$

where H_0 is the kinetic energy and all the interactions are as schematized in figure 1. The terms

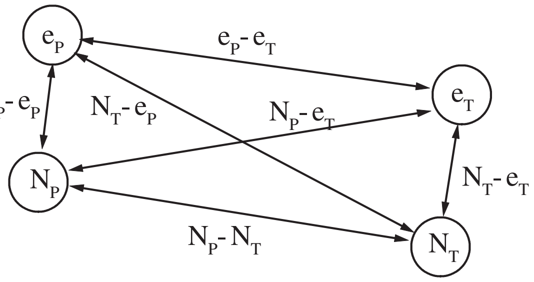

Figure 1. Diagram of the interactions considered in the *n*CTMC calculations.

in parentheses in equation (2) describe the separate centres that cannot produce transitions. Also, it is well known that the internuclear interaction does not contribute significantly to the total cross sections since the nuclei do not exchange a large amount of energy. The simultaneous ionization of both centres is produced by the combined and competing N–e and e–e interactions.

The contributions from the e–e interaction to the collision dynamics can be illuminated if equation (2) is rewritten as

$$H = (H_0 + V_{\mathrm{NP-eP}} + V_{\mathrm{NT-eT}}) + V_{\mathrm{NP-NT}} + \{V_{\mathrm{NT-eP}} + \langle V_{\mathrm{eP-eT}}\rangle_{\mathrm{T}}\} \\ +\{V_{\mathrm{NP-eT}} + \langle V_{\mathrm{eP-eT}}\rangle_{\mathrm{P}}\} + \{V_{\mathrm{eP-eT}} - \langle V_{\mathrm{eP-eT}}\rangle_{\mathrm{T}} - \langle V_{\mathrm{eP-eT}}\rangle_{\mathrm{P}}\}. \tag{3}$$

Here $\langle V_{\mathrm{eP-eT}}\rangle_{\mathrm{T}}$ is the 'mean' potential interaction between the projectile electron and the target electrons. In a quantum mechanical model it can be described as the e–e interaction averaged over the target ground state wavefunction. Thus, the first term between braces is the screened nuclear contribution from the target to the projectile ionization. A similar role is played by $\langle V_{\mathrm{eP-eT}}\rangle_{\mathrm{P}}$ and the term in the second set of braces in the target ionization. The last term between braces is the dynamical contribution from the e–e interaction, which contributes to the excitation of both collision partners (antiscreening). For the calculations we have assumed that the K-shell electrons on the Ne do not significantly contribute to the cross sections. Thus, we include the two nuclei, the He^+ electron, and the eight 2s and 2p electrons in the L-shell of Ne for an 11-body calculation.

The experiment consists of measuring the charge-state analysed projectile both non-coincident and coincident with the Ne recoil ions. The experimental arrangement has been described previously (Montenegro *et al* 1992b, Sant'Anna *et al* 1998). The modifications and the calibration procedures for coincidence measurements with heavy recoil ions are described in detail by Santos *et al* (2001). Beams of He^+ with 1–4 MeV energy delivered by the van de Graaff accelerator at Pontificia Universidade Católica do Rio de Janeiro impinge on a Ne gas target. The emergent beams (He^+ and He^{2+}) are charge-analysed by a magnetic field and recorded by two surface barrier detectors. The recoil ions are recorded by a microchannel plate at the end of a time-of-flight spectrometer. The absolute detection efficiency of the spectrometer was obtained through the measurement of recoil ions in coincidence with single electron capture for C^{3+} on Ne. These latter data were then compared to single (non-coincidence) measurements for this channel under the same experimental conditions. Standard fast electronics are used to select recoil ions in coincidence with the He^+ and He^{2+} emergent beams.

The experimental results are compared with the calculations using the Hamiltonian given by equation (2). Figure 2 shows the experimental and *n*CTMC total cross sections of He^+ ionization occurring in coincidence with different final charge states of the target (Ne^{i+}, $i = 0, 1, 2, 3$). We observe that the total electron loss cross section for He^+ mainly consists

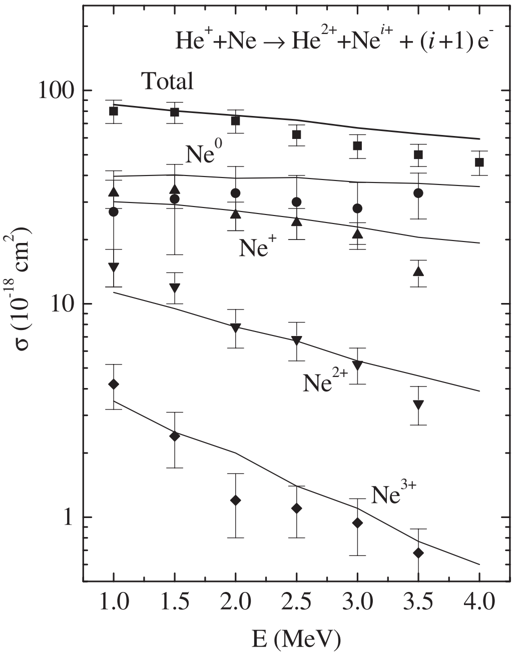

Figure 2. For He^+ + Ne collisions, the total cross section for simultaneous projectile and target ionization is displayed for final target charge states 1–4 as a function of the projectile energy. The experimental results (symbols) are compared with the nCTMC calculations (curves).

of contributions from the Ne target 'elastic' ($i = 0$) and single ionization ($i = 1$) reactions. However, at the lower energies (below 2 MeV), double ionization of Ne adds more than 10% to the total cross section. The cross sections for higher stages of target ionization are reasonably portrayed by the nCTMC calculations. This is because unitarity is preserved in the calculations and experimental binding energies are employed to describe multiple ionization. For the latter, the energy deposition required for multiple ionization is not underestimated, which would result in an overestimation of the cross sections, as is the case for independent electron model calculations (Cocke and Olson 1991).

The reasonable accord between experimental and theoretical cross sections lends credibility to the predictions that follow. Since the calculations are kinematically complete, we attempted to find signatures of the e–e and N–e interactions for reaction (1) with $i = 1$ that can be tested experimentally. At each energy investigated, 1, 4 and 16 MeV, full calculations were made using the Hamiltonian given by equation (2). Then, to illustrate only the dynamical e–e interactions, the Hamiltonian was modified by removing the nuclear–nuclear and the nuclear–electron interactions between centres. By so doing, all interactions between centres were used in one calculation, and then compared in a consistent manner to those using only the e–e interaction. After investigating various coincidence events between recoil ion and the two ionized electrons, we found that the relative azimuthal angle between ionized electrons provides a clear signature of dynamical e–e interactions. Of course, such a correlation presumes that the collision energy is sufficiently high so that the dynamical e–e interaction can produce simultaneous ionization from both centres. Also, the collision velocity should be such that the projectile and target ionized electrons are spatially separated from one another so that post-collision e–e interactions do not distort the interpretation.

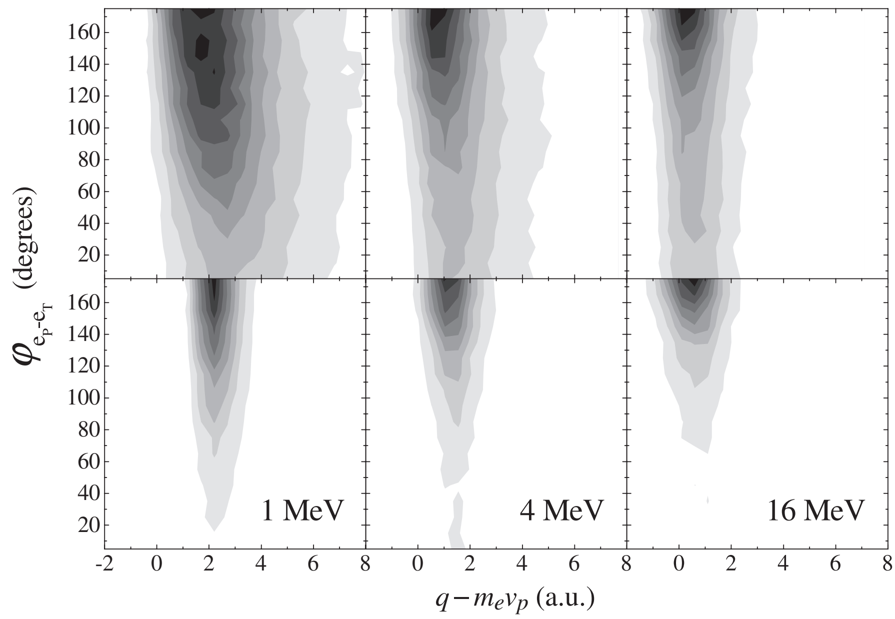

Figure 3. Differential cross sections are presented for the $He^{+} + Ne \rightarrow He^{2+} + Ne^{+} + 2e$ reaction. The ordinate is the relative azimuthal angle between the ionized electrons $\phi_{eP-eT} = \phi_{eP} - \phi_{eT}$. The abscissa is the magnitude of the momentum transfer q minus the mass loss momentum of the ionized projectile electron. The plots in the upper row are nCTMC calculations including all interactions as given by equation (2). For comparison, in the lower row are nCTMC calculations with only the e–e interactions between electrons on different centres. A linear scale is used for the intensity.

In figure 3 the relative azimuthal angle between the two emitted electrons in the simultaneous projectile and target single-ionization process is shown as a function of the magnitude of the momentum transfer vector. The momentum transfer vector is defined by

$$\boldsymbol{q} = \boldsymbol{P}_0 - \boldsymbol{P}_{\mathrm{f}}, \tag{4}$$

where $\boldsymbol{P}_0$ is the initial momentum of the He^{+} projectile, and $\boldsymbol{P}_{\mathrm{f}}$ is the final momentum of the scattered He^{2+}. We note that the emitted electron from the projectile takes away a momentum equal to $m_{\mathrm{e}} v_{\mathrm{P}}$. In order to aid comparisons, on the abscissa in figure 3 we have accounted for the change in mass of the projectile by subtracting the momentum loss due to the ionization of its electron. After this procedure, we observe that the main contribution to the simultaneous ionization comes from values $q – m_{\mathrm{e}} v_{\mathrm{P}} \approx \Delta E_{\mathrm{e}}/v_{\mathrm{P}}$, where ΔE_{e} is the change in the energy of the electrons relative to their parent nuclei. At high collision velocities the electrons have low energy relative to their nuclear centre so that ΔE_{e} is approximately the sum of their binding energies. Hence, the maxima in figure 3 tend toward zero with increasing collision velocity. Note that the scale is linear with the events weighted by their contribution to the total cross section.

In figure 3 the top row is the full calculation, while the bottom row is the calculation with only the e–e interactions between centres. In the full calculation, note that for large momentum transfer where the screened N–e interaction dominates, the structure is isotropic. One would expect isotropic behaviour for the screened N–e interaction, as long as the collision velocity is high enough so that the ionized electrons are not influenced by their post collision e–e interaction. The lower row of figure 3 illustrates the calculations made where only the interactions V_{eP-eT} between electrons of different centres are active.

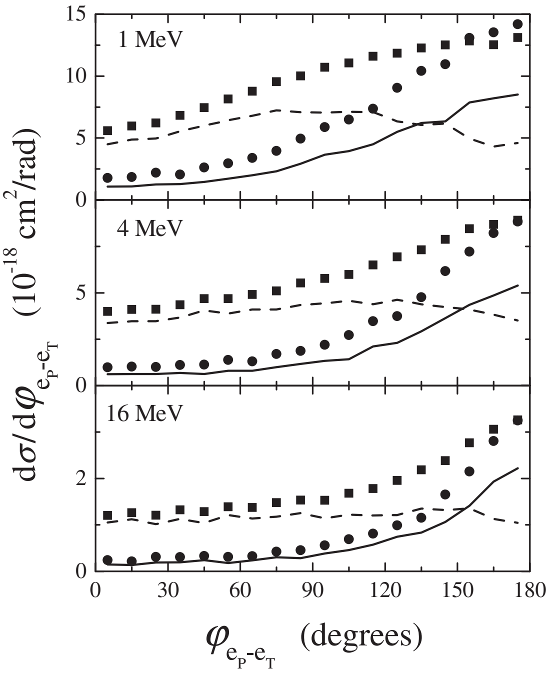

Figure 4. Cross sections for simultaneous single ionization in the *n*CTMC model are given as a function of the relative azimuthal angle between ionized electrons. Comparison is made between the calculations including all interactions (squares) with those made with only the e–e interactions between centres (circles). The solid curves are the e–e results normalized as explained in the text, and the dashed curves are our estimates of the contribution from the screened N–e interactions.

The experimental testing of the plot given in figure 3 requires kinematically complete experiments that are presently only possible in a few laboratories. However, at lower order, it is possible to integrate over momentum transfer in order to obtain the relative contributions of the dynamical e–e and screened N–e interactions to the cross section. The only thing lost is an indication of the impact parameter dependencies. In figure 4 the integral values corresponding to figure 3 are given. The squares are the full calculation, while the circles are for the dynamical e–e simulation.

First note that it is possible for the present e–e calculations to exceed those of the full calculation near 180°. This is because both calculations preserve unitarity. The ionization reaction investigated is far removed from the perturbation regime with non-coincidence ionization probabilities for both the He^+ and Ne exceeding 50% at small impact parameters. Further evidence of the strength of these collisions is given by the large multiple-ionization cross sections observed for this reaction, figure 2. Thus, in the full calculation, both the e–e and N–e interactions compete for flux. In contrast, the dynamical e–e calculation is unhindered by the screened N–e interaction.

To determine the relative contributions of the dynamical e–e and the screened N–e interactions, the e–e calculations were renormalized to reflect unitarity of flux. The assumption is made that the N–e interaction produces an isotropic distribution and is not distorted appreciably by the post-collision e–e correlation. This approximation is supported by calculations made with the e–e interaction of equation (2) removed. At all energies, the e–e azimuthal angle correlation was then found to be isotropic.

The dashed curves reflect our fits to the data for the screened N–e interaction. This was accomplished by multiplying the e–e calculation by a constant, then subtracting the renormalized e–e values (solid curve) from the calculations using the full Hamiltonian. At the three energies studied, we find that the screened N–e interaction contributes approximately 65%, and the dynamical e–e interaction 35% to the overall cross section for reaction (1) and $i = 1$. This is in contrast to the results for light targets like He where it is found that the dynamical e–e interaction dominates the simultaneous ionization channel at these energies (Montenegro 1992a, Dörner *et al* 1994). However, for the He system the collision strength is not as strong as for Ne, which has six active 2p electrons and a 10+ core. Our conclusions regarding the predominant contribution of the N–e interaction to the *total loss* agree with those of Voitkiv *et al* (2000). However, in the present calculations the two-centre e–e was not dropped, unlike in the work of Voitkiv *et al*.

Thus, in summary, we have presented a method by which the relative contributions of the dynamical e–e and screened N–e interactions can be determined experimentally through the measurements of only the electron momenta. We predict that the observation of the relative azimuthal angle correlation between ionized projectile and target electron will provide a useful tool to probe two-centre e–e correlation dynamics.

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