Mutual ionization in atomic collisions near the electronic threshold

S F Zhang¹, X L Zhu¹, A B Voitkiv¹,², W T Feng¹, D L Guo¹, Y Gao¹, R T Zhang¹, E L Wang³ and X Ma¹

¹ Institute of Modern Physics, Chinese Academy of Sciences, 730000 Lanzhou, People’s Republic of China
² Max-Planck-Institute for Nuclear Physics, Saupfercheckweg 1, D-69117 Heidelberg, Germany
³ Department of Modern Physics, University of Science and Technology of China, Hefei, 230026, Anhui, People’s Republic of China

E-mail: x.ma@impcas.ac.cn

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Abstract

We study mutual ionization in collisions between atomic hydrogen and helium at impact velocities near the electronic threshold for this process. We show that this process is substantially influenced by the Coulomb repulsion between the emitted electrons and that the atomic nuclei are very strongly involved in the momentum balance along the collision velocity.

Keywords: mutual ionization, near the electronic threshold, electron–electron correlation, nuclei–nuclei scattering, momentum balance

Elementary collision processes are of great interest not only in atomic physics but also in plasma physics, astrophysics, etc. Two basic atomic processes can occur in a nonrelativistic collision between a bare projectile-nucleus and a target-atom. (i) The atom can be excited or ionized by the impact of the projectile. (ii) An atomic electron can be transferred into a bound or low-lying continuum state of the projectile-ion. The transfer can proceed with or without emission of radiation and is called radiative or nonradiative electron capture, respectively.

If a projectile is not fully stripped but carries initially an electron then in a collision with a target the electron can be lost. If the loss occurs simultaneously with ionization of the target the corresponding process may be termed simultaneous projectile–target ionization. This process involves at least four particles (two nuclei and two ‘active’ electrons) and represents an important case of an atomic few-body problem in which, in general, the interaction between all four particles may play a crucial role. Some aspects of this process have been already considered in the literature (see [1–5], for a broader coverage of the field and more references see also [6–9]).

The physics of mutual ionization is simpler in fast collisions in which the impact velocity $v$ is much larger than the typical orbiting velocities of the projectile and target electrons. In such a case the process proceeds mainly via a single interaction between two electrons belonging to the different colliding centers whereas the nuclei (the cores) of the projectile and target are merely spectators during the collision. This channel of mutual ionization, which we shall call the $e$–$e$ mechanism, can be described within first order perturbation theory in the projectile–target interaction.

In collisions at lower velocities another channel of mutual ionization becomes important. In this channel the process proceeds via two simultaneous interactions: the electron of the target is emitted due to the interaction with the nucleus of the projectile whereas the transition of the electron of the projectile is caused by its interaction with the nucleus of the target. This reaction channel, which can be denoted as the $n$–$e$–$n$–$e$ mechanism, appears in a theoretical description starting with the second order perturbation expansion in the projectile–target interaction. In contrast to the $e$–$e$, the nuclei are strongly involved in the $n$–$e$–$n$–$e$ process and this difference can be used for an experimental separation of these mechanisms by measuring momentum spectra of the target recoil ions [1–4].

The $e$–$e$ mechanism has an effective threshold corresponding to impact velocities at which the kinetic energy of an equivelocity free electron would be approximately equal to the sum of the binding energies of the target and projectile. When approaching this threshold the relative contribution of

4 Since the colliding electrons are initially bound, the threshold is broadened due to the Compton profiles of the corresponding bound states.
the $e-e$ mechanism strongly decreases, below the threshold it rapidly vanishes.

Due to very heavy nuclear masses the threshold for the $n-e-n-e$ mechanism is much lower. Therefore, it is widely believed (see e.g. [8, 10]) that for the mutual ionization near the $e-e$ threshold the electron–electron interaction plays merely a minor role.

However, in the present paper, where we study experimentally and theoretically mutual ionization in 70 keV $u^{-1}$ H$^0$ on He$^0$ collisions, it will be shown that the electron–electron interaction does substantially influence this process in the vicinity of the $e-e$ threshold. It will be also demonstrated that near the threshold the nuclei very actively participate in the momentum balance of the process even within the $e-e$ mechanism in which they would normally be regarded just as spectators.

An impact energy of 70 keV $u^{-1}$ corresponds to a collision velocity $v = 1.67$ au. This energy was chosen because a free electron moving with this velocity would have kinetic energy almost exactly equal to the sum of the binding energy of hydrogen and the first ionization potential of helium.

In this study we shall focus on the cross section for mutual ionization differential in the longitudinal momentum of the target recoil ions because this cross section is not only very sensitive to the major aspects of the collision dynamics (see e.g., [3], [11–13]) but also yields important information about these dynamics in a compact form [14].

Atomic units are used throughout unless otherwise stated.

The experiment was performed using the reaction microscope [15, 16] located at the beam line of the 320 kV platform for multi-discipline research with highly charged ions [17] at the Institute of Modern Physics Lanzhou, China. Proton beams extracted from the electron cyclotron resonance ion source were accelerated to an energy of 70 keV when leaving the platform. Then the proton beams were collimated and transported to the collision chamber. In front of the chamber protons were neutralized in a 20 cm-long differentially pumped gas cell in which pure N$_2$ gas was filled with a pressure of a few $10^{-4}$ mbar. The protons in the beam behind the gas cell were removed by a pair of electrostatic plates downstream of the cell. The deflection field was set to 2000 V cm$^{-1}$ so that the metastable H$^0$ produced in the neutralization processes could be quenched, and more than 99% of them are estimated to be in the ground state [18]. The remaining H$^0$ then interacted with the supersonic helium gas jet of the spectrometer. After the collisions, the projectiles were charge selected by another electrostatic deflector in front of the projectile detector. The momenta of the target fragments were obtained via the reaction microscope. Triple coincidence measurements between the electron, the recoil and the projectile detectors were employed to distinguish the interaction channels. The total cross section was not obtained since the absolute beam intensity, target density and detective efficiency of the detectors were not measured. In this experiment, only the three-dimensional momentum distribution of recoil ions was obtained. The momentum of the recoil ions was calibrated using two separate peaks in the capture channel H$^+$ + He → H$^+$ + He$^+$ (n) with final recoil He$^+$ ions in the ground (n = 1) and excited states (n $\geq$ 2). A longitudinal momentum resolution of 0.4 au (full width at half maximum) was achieved from the individual peak of recoil He$^+$ (n = 1). The peak positions can be determined with a precision of 0.02 au via a fitting procedure due to high statistics of the data in the present case.

In [2], where mutual ionization in 0.5–2 MeV He$^+$ on He collisions was studied, it was found that one more channel noticeably contributes to this process at an impact energy of 500 keV, emission of two electrons from He accompanied by capture of the electron from He$^+$. However, 70 keV H$^0$ is much less effective in producing double ionization of He than 500 keV He$^+$ and in collisions with He it is easier to ionize 70 keV H$^0$ than 500 keV He$^+$. Besides, the cross sections for electron capture from 70 keV H$^0$ and 500 keV He$^+$ by He$^{2+}$ are close. Therefore, in our case this channel is of minor importance and may be neglected.

In our theoretical treatment we regard the process of mutual ionization as an effectively four-body problem considering helium as a hydrogen-like system consisting of one (active) electron and a core with an effective charge $Z_{eff}$ determined from the first ionization potential of helium which results in $Z_{eff} = 1.345$. The process is described using the first and second order terms of the perturbative expansion in the projectile–target interaction [9].

The first order contribution to the transition amplitude reads

$$A_{fi}^{(1)}(\vec{b}) = \frac{2i}{\pi v} \int \frac{d^2q}{q^2} e^{-i\vec{q} \cdot \vec{b}} \langle \phi_f(\vec{r}) | e^{-i\vec{b} \cdot \vec{q}} | \phi_i(\vec{r}) \rangle \times \langle \psi_f(\vec{r}) | \vec{b} \cdot \vec{q} \psi_i(\vec{r}) \rangle,$$  \hfill (1)

Here, $\phi_f(\vec{r})$ and $\phi_i(\vec{r})$ are the initial and final electronic states of the projectile, where $\vec{r}$ is the coordinate of the projectile electron with respect to the projectile nucleus. $\psi_f(\vec{r})$ and $\psi_i(\vec{r})$ are the initial and final electronic states of the target, where $\vec{r}$ is the coordinate of the target electron with respect to the target nucleus. Further, $\vec{q} = (q_{\perp}, (\epsilon_f - \epsilon_i + \epsilon_f - \epsilon_i)/v)$, where $\epsilon_i$ and $\epsilon_f$ are the initial and final electronic energies of the projectile, $\epsilon_i$ and $\epsilon_f$ are the corresponding electronic energies of the target, and $\vec{b}$ is the impact parameter of the collision.

The second order contribution to the transition amplitude is given by

$$A_{fi}^{(2)}(\vec{b}) = \frac{1}{2\pi^2 v} \int \frac{d^2q_1}{q_1^2} e^{i\vec{q}_1 \cdot \vec{b}} \langle \phi_f(\vec{r}) | e^{i\vec{q}_1 \cdot \vec{r}} | \phi_i(\vec{r}) \rangle \times \int \frac{d^2q_2}{q_2^2} e^{-i\vec{q}_2 \cdot \vec{b}} \langle \psi_f(\vec{r}) | e^{i\vec{q}_2 \cdot \vec{r}} | \psi_i(\vec{r}) \rangle,$$ \hfill (2)

where $\vec{q}_1 = (q_{1\perp}, (\epsilon_f - \epsilon_i)/v)$ and $\vec{q}_2 = (q_{2\perp}, (\epsilon_f - \epsilon_i)/v)$. The first order transition amplitude is given by equation (1), and the second order transition amplitude is the sum of equations (1) and (2). Results obtained using these amplitudes are shown in figure 1 for the cross section differential in the longitudinal momentum $P_L$ of the recoil ions. In particular, it follows from the figure that the mutual ionization is dominated by the $n-e-n-e$ mechanism and that both the reaction mechanisms lead to a similar shape of the spectrum.

In figure 2 we compare the result of the above second order calculation (shown by a dashed curve) with our experimental
In order to understand possible reasons for this disagreement let us note the following. In the process of mutual ionization the initial velocities of the heavy particles—the projectile and target nuclei—are practically unchanged. However, the light particles—the electrons—do experience a substantial velocity change. The electron of the projectile, due to its interaction with the target, gets a kick opposite to the projectile motion and is, therefore, emitted from the projectile with (the longitudinal component of) a velocity noticeably smaller than that of the projectile nucleus. In turn the electron of the target in the collision gets a kick in the direction of the projectile motion and is ejected with a velocity much larger than that of the target recoil ion.

Thus, after the collision the fastest and slowest particles are the proton and the target recoil ion (which is practically at rest), respectively, and the velocities of the electrons are in between. Important to note that when the mutual ionization occurs at impact energies close to the e–e threshold the velocities of both emitted electrons are actually not very different. Moreover, since this process occurs in collisions with typical impact parameters not exceeding the size of the atoms, the electrons become close not only in the momentum but also in the position space. Therefore, one can expect that the Coulomb repulsion of the electrons in the final state may play a substantial role.

We modelled the effect of the Coulomb repulsion by introducing into the (fully differential) cross section a factor $2\pi\lambda/k_{12}/(\exp(2\pi\lambda/k_{12}) - 1)$, where $k_{12}$ is the relative momentum of the emitted electrons and $\lambda$ is a parameter. If $\lambda = 1$ we obtain the so-called Gamov factor, which is proportional to the absolute square of the Coulomb wave function describing the relative motion in a system of two electrons taken at zero relative distance (see, for instance, formula (136.2) in [19]).

From the studies of atomic ionization by electron impact it is known that if instead of the (full) Coulomb wave function only the Gamov factor is used then the repulsion effect is overestimated. Therefore, in our model we regarded $\lambda$ as a free parameter from the interval $0 \leq \lambda < 1$. Results of our calculations for the normalized cross section using three different values of $\lambda$ ($\lambda = 0, 0.3$ and $0.6$) are shown in figure 3.

According to the calculations the Coulomb repulsion between the emitted electrons shifts the longitudinal momentum distribution of the recoil ions in the positive direction and also somewhat broadens it. These effects, which appear both in the first and second order calculations, could be qualitatively understood by noting that because of the repulsion the emitted electrons try to avoid each other in the momentum space. As a result, they tend to populate in the continuum a broader energy range occupying on overall higher energy states than it would be in the absence of the repulsion. Since the longitudinal momentum transfer in the collision is proportional to the difference between the initial and final energies of the electrons, the above broadening leads to larger longitudinal momentum transfers and increases their spread. Both these points are reflected in the shape of the longitudinal momentum spectrum of the recoil ions.

The choice $\lambda = 0.6$ enables one to obtain the best agreement with the experimental data. Our calculated results

Figure 1. The cross section for mutual ionization differential in the longitudinal momentum of the target recoil ions in 70 keV H(1s) on He(1s2) collisions. Dotted and dashed curves are results of the first and second order calculations, respectively.

Figure 2. The cross section for mutual ionization differential in the longitudinal momentum of the target recoil ions in 70 keV H(1s) on He(1s2) collisions. Symbols are the experimental results. Solid (dashed) curve is the result of the calculation which takes into account (neglects) the Coulomb repulsion between the emitted electrons.

data. Note that since the experimental cross sections are not measured on an absolute scale, both measured and calculated cross sections are normalized by setting their maxima to 1 in this figure. Besides, the calculated results were convoluted with an experimental resolution of $\Delta P_\parallel = 0.4$ au. It is seen, in the figure, that the agreement between the theory and experiment is not very good: the theory overestimates the experiment at $P_\parallel < 0$ but substantially underestimates it at $P_\parallel > 1$. Besides, the positions of the maxima in the experimental and calculated spectra differ by $\approx 0.25$ au, which is much larger than the uncertainty of 0.02 au in the peak position determination.
with $\lambda = 0.6$, convoluted with the experimental resolution of $\Delta P_{lg} = 0.4$, are shown in figure 2 by a solid curve. It is seen that the account of the Coulomb repulsion brings the calculated spectrum in much better agreement with the experiment.

The closeness of the electrons in the position and momentum space, which makes the Coulomb repulsion quite effective, can also impact the process of mutual ionization via the electron exchange effect. Therefore, we estimated the influence of the latter on the longitudinal momentum spectrum within the first order of perturbation theory. However, according to the estimate, the shape of the spectrum and the position of its maximum turned out to be very weakly influenced by the exchange effect.

It is well known (see e.g. [2]) that at high impact velocities, where the $e-e$ mechanism dominates, the longitudinal spectrum of the recoil ions is almost symmetric with respect to the point $P_{lg} = 0$ where the maximum of the spectrum is located. At lower velocities (but still far above the $e-e$ threshold) the $n-e-n-e$ channel becomes important which makes the spectrum asymmetric with the interval $P_{lg} > 0$ be more populated compared to $P_{lg} < 0$.

An interesting peculiarity of the mutual ionization at impact velocities near the $e-e$ threshold is that the longitudinal spectrum of the recoil ions is more asymmetric, is stronger shifted to the positive $P_{lg}$ than at high impact velocities and that this holds not only for the $n-e-n-e$ but also for the $e-e$ reaction channel (see figure 1).

The reason for this is that at impact velocities near the threshold the electrons, in order to be emitted via the $e-e$ mechanism, have to ‘borrow’ momentum-energy from the coupling to their parenteral nuclei that affects the momentum spectra of the nuclei. As the collision velocity approaches the $e-e$ threshold, the internal motion of the electrons in their initial bound states starts to have a pronounced effect on the ionization process.

Indeed, near the threshold the most favourable condition for the mutual ionization to occur is when the electron of the projectile in its initial bound state possesses a positive projection of the orbiting velocity on the direction of the projectile motion whereas the electron of the target has initially a negative component of the orbiting velocity along this motion: such a velocity configuration provides the largest relative momentum and energy for the colliding electrons.

Since the momenta of the electron and the nucleus in a bound atomic state compensate each other (in the atomic centre-of-mass frame) the above configuration of the electron momenta leads to a mirrored configuration of the momenta of the nuclei in which the nucleus of the projectile (target) has a negative (positive) projection of its orbiting momentum on the collision velocity in the initial bound state. Being preferential for the mutual ionization this configuration of the initial nuclear momenta is ‘selected’ in the collisions that results, in particular, in a shift of the longitudinal momentum distribution of the target recoil ions towards positive $P_{lg}$.

The peculiarities in this distribution near the $e-e$ threshold can be analysed using the conservation of energy and longitudinal momentum in the collision that leads to the following general constraint on the possible values of the longitudinal momentum of the target recoil ion in the final state (no matter what the reaction channel is)

$$P_{lg} \geq \frac{k_i^2}{2v} - \epsilon_i + \frac{\epsilon_f - \epsilon_i}{v} - \frac{v}{2} \quad (3)$$

Here, $\epsilon_i$ and $\epsilon_f$ are the initial energies of the electrons bound in the target and projectile, respectively, $\epsilon_f$ is the energy of the electron emitted from the projectile (as it is viewed in the rest frame of the projectile) and $k_i$ is the absolute value of the transverse momentum component of the electron emitted from the target given in the target frame.

At high impact velocities the constraint (3) does not really set limitations but it becomes quite restrictive when the velocity approaches the $e-e$ threshold. For instance, for the mutual ionization in 70 keV H on He collisions we obtain $P_{lg} \geq 0.001$ au \footnote{Because of a finite resolution the experimental data (as well as the theory results after the convolution with experimental resolution) partly spread to $P_{lg} < 0$.} and, thus, the spectrum of the recoil ions simply cannot have a maximum at $P_{lg} = 0$ and be symmetric with respect to this point as it would be at high impact velocities.

In conclusion, we have considered the process of mutual ionization in collisions of 70 keV hydrogen with helium by exploring the cross section differential in the longitudinal momentum of the target recoil ions. Our results show that, although at impact velocities in the vicinity of the $e-e$ threshold the electron–electron interaction is not the main mechanism inducing mutual ionization, it nevertheless substantially influences this process via the Coulomb repulsion between the emitted electrons. Besides, we have also demonstrated that near the threshold the nuclei of the colliding particles are much stronger involved in the momentum balance of the reaction than it would be at high impact energies.

Figure 3. The cross section for mutual ionization differential in the longitudinal momentum of the target recoil ions in 70 keV H(1s) on He(1s) collisions. Dashed, dotted and solid curves are calculated results obtained setting $\lambda = 0, 0.3$ and 0.6, respectively.
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