Four-body quantum dynamics of two-center electronic transitions in relativistic ion-atom collisions and target recoil momentum spectroscopy

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Abstract

We consider relativistic collisions of heavy hydrogen-like ions with hydrogen and helium atoms in which the ion-atom interaction causes both colliding particles to undergo transitions between their internal states. Using an approach enabling one, for the first time, to give a detailed description of this important case of the relativistic quantum few-body problem we concentrate on the study of the longitudinal momentum spectrum of the atomic recoil ions. We discuss the role of relativistic and higher order effects, predict a surprisingly strong influence of the projectile’s electron on the momentum transfer, draw the general picture of the recoil ion formation and show that the important information about the doubly inelastic collisions could be obtained in experiment merely by measuring the recoil momentum spectrum.

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The interaction between two point-like charged particles, whose relative velocity is much less than the speed of light $c = 137$ a.u., is approximated with an excellent accuracy by the famous Coulomb law. As a result, this law underlies a vast amount of phenomena studied by atomic physics. Note, however, that even with such simplest form of the pair-wise interaction, one encounters large difficulties in attempts to get a detailed understanding of the dynamics of atomic collisions involving three and more ‘active’ particles.

When the relative velocity approaches the speed of light, the form of the pair-wise electromagnetic interaction becomes much more complicated. Consequently, a detailed description of relativistic atomic collisions involving three and more active particles, an important case of the fundamental quantum few-body problem (in its relativistic dynamic version), represents a particularly strong challenge for theory and many phenomena occurring in such collisions are much less understood compared to their non-relativistic counterparts.

Highly charged projectiles produced at accelerators of heavy ions often carry one or more very tightly bound electrons. When such a projectile-ion impinges on a target-atom the interaction between them can cause both the ion and atom to undergo transitions between their internal electronic states. Such ion-atom collisions are termed ‘doubly inelastic’.

Doubly inelastic collisions of light ions with atoms at nonrelativistic impact energies have been extensively studied experimentally and theoretically (see e.g. [1] and references therein). However, for the relativistic domain of impact energies, especially for collisions involving very highly charged ions, not only no results of coincidence measurements for doubly inelastic processes have been reported so far but also the existing theoretical approaches actually did not enable one to address them.

From the theoretical point of view the main difficulties are connected with the complicated form of the pair-wise relativistic interaction and also with the fact that, at any values of the relative ion-atom velocity, doubly inelastic processes in collisions with very highly charged ions cannot be correctly described within first order approaches in the projectile-target interaction.

The main obstacle for detailed experimental studies of the doubly inelastic processes is that cross sections for excitation and loss of an electron, tightly bound in a highly charged projectile, are by orders of magnitude smaller than those for ionization of a neutral atom. Therefore, it might seem to be extremely difficult to extract a small amount of doubly inelastic events out of a very large background produced by singly inelastic collisions in which only the atom undergoes electronic transitions.

In this letter we consider doubly inelastic processes in collisions between a very heavy hydrogen-like ion, whose nucleus has a charge $Z_I \gg 1$ a.u. and moves with a velocity approaching the speed of light, and hydrogen and helium atoms. In particular, it will be shown that, due to the surprisingly ‘prominent’ role of the projectile electron in the momentum transfer, the important information about these processes could be obtained in an experiment just by measuring the longitudinal momentum spectrum of the target recoil ions.

In high-energy atomic collisions the changes in the velocities of the atomic and ionic nuclei are negligible. Therefore, in order to describe these collisions it is convenient to introduce the following two reference frames. In one of them, denoted by $K_A$, the nucleus of the atom having a charge $Z_A$ is at rest and taken as the origin of $K_A$. In the other frame, $K_I$, the nucleus of the ion rests and its position is taken to be the origin of $K_I$.

Let $\varphi_0$ and $\varphi_n$ ($n \neq 0$) represent the initial and final internal states of the atom in the frame $K_A$ whose energies in this frame are $\varepsilon_0$ and $\varepsilon_n$, respectively. Let $\chi_0$ and $\chi_m$ ($m \neq 0$) be the initial and final internal states of the ion in the frame $K_I$ and $\varepsilon_0$ and $\varepsilon_m$ be their energies in $K_I$. In the frame $K_A$ the incident projectile has a velocity $\boldsymbol{v} = (0, 0, v)$, and $\gamma = 1/\sqrt{1 - v^2/c^2}$ is the corresponding collisional Lorentz factor.

At $Z_I/v \ll 1$ (atomic units are used) the physics of doubly inelastic ion-atom collisions is mainly governed...
by the so called two-center dielectronic interaction, which couples two electrons orbiting the different colliding centers and occurs predominantly via a single photon exchange [3], and can be well described within the first order approaches [4]. However, since \( v < c \), the condition \( Z_I/v \ll 1 \) is never fulfilled in collisions with very highly charged projectiles for which a much more sophisticated treatment is needed.

By using a refined version (to be discussed in detail elsewhere) of the relativistic eikonal model, developed recently in [5], one can show that the transition amplitude for the doubly inelastic collisions between a hydrogen-like ion and a two-electron atom is given by

\[
S_{fi}(Q) = -\frac{2i}{v} \int d^2p_1 \int d^2p_2 \int d^2\kappa \frac{f(p_1, \nu) f(p_2, \nu) f(\kappa, -\eta)}{(\kappa^4 + \kappa - p_1 - p_2)^2 - (\epsilon_0 - \epsilon_f)^2} \times \Phi^0_\mu(n; 0; \kappa^4 + \kappa - p_1 - p_2; p_1; p_2) 
\gamma^{-1} \Lambda^\alpha_\mu F^\alpha_I(m_0; \kappa^4 - \kappa + p_1 + p_2)) ,
\]

where \( Q \) is the transverse part, \( Q \cdot v = 0 \), of the total momentum \( q^4 \) transferred to the atomic target in the collision. In (1) the integration runs over the two-dimensional transverse vectors \( p_1, p_2 \) and \( \kappa \) (0 \( \leq p_j < \infty, p_j \cdot v = 0; \) \( 0 \leq \kappa < \infty, \kappa \cdot v = 0, \nu = Z_I/v, \eta = Z_I Z_A/v \) and

\[
f(a, \tau) = \frac{\Gamma(1-i\tau)\Gamma(1/2 + i\tau)}{2\pi \Gamma(1/2) \Gamma(2\tau)} d^{\delta - 2 + 2i\tau},
\]

where \( \delta \to +0 \) and \( \Gamma(x) \) is the gamma-function. Further, \( F^\alpha_I \) and \( F^\alpha_\mu \) (\( \alpha, \mu = 0, 1, 2, 3 \)) are the inelastic form-factors of the ion and atom, respectively, \( \Lambda^\alpha_\mu \) is the Lorentz transformation matrix and the summation over the repeated Greek indices is implied in Eq. (1). The explicit form of the coupling of the form-factors in Eq. (1) is somewhat cumbersome

\[
\Phi^\alpha_\mu \gamma^{-1} \Lambda^\alpha_\mu F^\alpha_I = \left( \Phi^\alpha_0 + \frac{v}{c} \Phi^\alpha_3 \right) \left( F^0_I + \frac{v}{c} F^3_I \right) + \frac{\Phi^\alpha_4 F^3_I}{\gamma^2} + \frac{\Phi^\alpha_4 F^2_I}{\gamma} + \frac{\Phi^\alpha_1 F^1_I + \Phi^\alpha_2 F^2_I}{\gamma} ,
\]

reflecting rather complicated nature of the interaction between two relativistic transition four-currents.

The components of the atomic two-electron form-factors are given by

\[
\Phi^\alpha_0(n; 0; k; p_1; p_2) = \langle \varphi_n | Z_A \exp(ik \cdot r_1 + ip_2 \cdot r_2) - \exp(ip_1 \cdot r_1 + ip_2 \cdot r_2) \times (\exp(ik \cdot r_1) + \exp(ik \cdot r_2)) | \varphi_0 \rangle,
\]

\[
\Phi^\alpha_l(n; 0; k; p_1; p_2) = \langle \varphi_n | \exp(ip_1 \cdot r_1 + ip_2 \cdot r_2) \times (\alpha_{l,1} \exp(ik \cdot r_1) + \alpha_{l,2} \exp(ik \cdot r_2)) | \varphi_0 \rangle ,
\]

where the indices 1 and 2 refer to the first and second atomic electron, \( r_j \) (\( j = 1, 2 \)) are the coordinates of the \( j \)-th atomic electron in the frame \( K_A \) and \( \alpha_{l,(j)} \) are the Dirac matrices for this electron.

The components of the inelastic form-factor of the ion \( F^I_\alpha(m; 0; k) \) are given by

\[
F^I_\alpha(m; 0; k) = -\langle \chi_m | \exp(ik \cdot \xi) | \chi_0 \rangle,
\]

\[
F^I_\beta(m; 0; k) = \langle \chi_m | \alpha_l \exp(ik \cdot \xi) | \chi_0 \rangle ,
\]

where \( \xi \) are the coordinates of the electron of the ion in the frame \( K_I \).

In the frame \( K_A \) the momentum \( q^4 \) transferred to the atom is given by

\[
q^4_A = \frac{(Q, q^4_{\text{min}})}{v} + \frac{\epsilon_n - \epsilon_0}{\gamma v},
\]

\[
q^4_{\text{min}} = \frac{\epsilon_n - \epsilon_0}{\gamma v} + \frac{\epsilon_m - \epsilon_0}{\gamma v} ,
\]

where \( q^4_{\text{min}} \) is the component of this momentum along the velocity \( v \) and represents the minimum momentum transfer to the atom in the frame \( K_A \). The momentum transfer \( q^4 \) to the ion, viewed in the frame \( K_I \), reads

\[
q^4_I = (-Q, -q^4_{\text{min}}) \]

\[
q^4_{\text{min}} = \frac{\epsilon_n - \epsilon_0}{\gamma v} + \frac{\epsilon_m - \epsilon_0}{\gamma v} .
\]

Below we shall consider only collisions in which the target gets ionized.

In collisions at \( Z_I \sim v \sim c \) the spectra of electrons emitted from the target and projectile show strong effects caused by both the relativity and the multiple exchanges of virtual photons between the colliding ion and atom. We, however, shall discuss these spectra elsewhere and here concentrate on the spectrum of the target recoil ions given as a function of the longitudinal component \( p_{R,||} \) of the recoil momentum \( (p_{R,||} \parallel v) \).

In order to go over into the first order transition amplitude [3] but very substantially differs from the latter when \( \nu \) approach 1. In contrast to the first order amplitude, the amplitude \( \Phi^\alpha_\mu \) takes into account all six pair-wise interactions between the constituents of the projectile and the target [4].

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FIG. 1: The longitudinal momentum spectrum of the target
recoil ions produced in 100 MeV/u Nd\(^{59+}\)(1s)\+H(1s) collisions.
Dash, dot and dash-dot curves at large \( p_{R,\parallel} \) correspond to the
Nd\(^{59+}\)(n=2), Nd\(^{59+}\)(n=3) and Nd\(^{60+}\) + e\(^-\) states of the projectile,
respectively. Besides, solid curve displays the total contributions
of the above channels to the recoil spectrum at small \( p_{R,\parallel} \).

FIG. 2: The projectile excitation into states with the principal
quantum number \( n = 2 \) accompanied by target single ionization in
collisions of 100 MeV/u Nd\(^{59+}\)(1s) (a) and 325 MeV/u U\(^{91+}\)(1s)
(b) with He(1s\(^2\)). Dash and solid curves display results of the
purely nonrelativistic (\( c = \infty \)) and fully relativistic calculations,
respectively. Dot curves were obtained by assuming \( c = \infty \) only
in the description of the internal electron states. Dash-dot curves
were calculated by setting \( c = \infty \) only in the treatment of the
relative ion-atom motion.

The relativistic effects influencing the form of the recoil
spectrum can be subdivided into those depending on the
collision velocity \( v \) and those related to the inner motions
of electrons within the colliding centers. As is seen in
figure 2 in the momentum spectrum these two groups of
the effects counteract.

In figure 2 we display results for the projectile excitation
into states with \( n = 2 \) accompanied by the single ionization of helium target. We see that the relativistic and
nonrelativistic calculations predict rather different
positions and shape of the target recoil peak.

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of electrons within the colliding centers. As is seen in
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The relativistic effects in the inner motion of the electron
in the ion lead to the energy splitting of the levels
having the total angular momentum \( j = 1/2 \) and \( j = 3/2 \)
and increase the energy differences between them and
the ground state. Because of the splitting the peak in the
recoil momentum spectrum becomes broader and the
splitting is also partly responsible for the decrease in the
height of the peak. As a result of the increase in the
energy differences the peak position is shifted to larger
values of \( p_{R,\parallel} \). However, the relativistic effects due to the
relative ion-atom motion soften the recoil of the residual
atomic core which shifts the peak position to lower values
of \( p_{R,\parallel} \). In the examples shown in figure 2 the value of
the collision velocity is very close to the value of the typical
orbiting velocity of the electron in the ground state of the ion
but the shift of the recoil peak due to the relativistic effects in the relative ion-atom motion turns out
to be larger by about a factor of 2.

The processes considered above are of course not the
only ones which produce target recoil ions. Therefore,
the important question is whether the signatures of the
projectile-electron excitation and loss in the momentum spectrum of the target recoil ions will not be masked by
other processes (especially if the final state of the projectile is not detected). To answer this question we have
performed a more extensive study of the target recoil
momentum spectrum produced in collisions in which the
initial internal state of the projectile may change or may
remain the same. Some results of this study are shown in
figure 3 which actually illuminates the very general features
in the formation of the longitudinal recoil spectrum in
collisions with very heavy hydrogen-like ions at moderate
values of \( \gamma \). According to this figure one can separate
four different regions of \( p_{R,\parallel} \) in which the formation is
dominated by qualitatively different mechanisms.

(a) At small values of \( p_{R,\parallel} \) the recoil spectrum is generated
via the indirect coupling between the projectile,
whose internal state is unchanged, and the target core:
the projectile induces a transition of the target electron
and the electron exchanges its momentum with the target
core. In relativistic collisions this channel is characterized
by very large impact parameters \(( \gg 1 \) a.u.) and is very
efficient in transferring small values of the momentum to
the target recoil. At larger \( p_{R,\parallel} \), however, it rapidly loses
its effectiveness which leads to the very strong decrease
in the longitudinal spectrum when \( p_{R,\parallel} \) grows.

(b) Eventually with increasing \( p_{R,\parallel} \) the direct coupling between the nuclei of the ion and atom (the Rutherford scattering) may start to dominate the formation of the spectrum. This channel ‘works’ in collisions with very small impact parameters \((\sim Z_1 Z_A/v \sqrt{M_A p_{R,\parallel}})\), where \( M_A \) is the mass of the atomic nucleus and, provided \( Z_1 \sim v \), the nuclear scattering is accompanied by target ionization with the probability close to 1 but the inner state of the projectile remains unchanged [8].

(c) With the further increase in \( p_{R,\parallel} \) \((3Z_1^2/8v \lesssim p_{R,\parallel} \lesssim Z_1^2/v)\) the channel involving the excitation and loss of the tightly bound electron of the projectile comes into the play. Compared to the nucleus-nucleus collisions this channel is characterized by much larger values of the typical impact parameters, which at \( Z_1 \sim v \) are of the order of the size of the projectile ground state, and is much more effective. Since the absolute charge of the electron is negligibly small compared to the mass of the nuclei, such an effectiveness is quite surprising and may have interesting consequences.

Consider, for instance, two very heavy projectiles whose atomic numbers differ just by 1 and whose masses are very close \((\text{e.g. } ^{239}_{89}\text{Bi} \ (A = 208.98) \text{ and } ^{209}_{82}\text{Po} \ (A = 208.98), A \text{ is the atomic mass}). Let one of them be represented by a bare nucleus with a charge \( Z_1^{(1)} \) and the second be a hydrogen-like ion with a net charge \( Z_1^{(2)} - 1 = Z_1 \). Thus, the projectiles possess practically equal charge-to-mass ratios and seem to behave almost identically in external electric fields. However, if these projectiles collide with atoms, the atoms can easily ‘recognize’ whether the projectile is a bare nucleus or an hydrogen-like ion since in the latter case the spectrum of the target recoil ions possesses a prominent resonance-like structure, reflecting the excitation and loss of the projectile’s electron (superimposed on the smooth background from collisions elastic for the projectile).

(d) At even higher \( p_{R,\parallel} \) the recoil spectrum is formed almost solely by the nucleus-nucleus scattering [9].

In very asymmetric collisions \((M_I \gg M_A)\), where \( M_I \) is the mass of the ion nucleus the contributions to the cross section \( d\sigma/dp_{R,\parallel} \) due to the nuclear Rutherford scattering and due to the excitation of the electron of the ion scale as \( Z_2^2/M_A \) and \( Z_2^2 \), respectively. Therefore, the relative strength of the latter channel in the spectrum formation is weakest for collisions with atomic hydrogen.

In summary, we have considered the doubly inelastic collisions of relativistic heavy hydrogen-like ions with the lightest atoms and shown that the physics of such collisions is strongly influenced by the higher order effects in the ion-atom interaction. We have discussed the manifestations of the relativistic effects caused by both the relative ion-atom motion and the electron motion in the internal states of the ion. Our results have enabled one to draw the general picture of the formation of the longitudinal momentum spectrum of the target recoil ions produced in high-energy collisions with very heavy hydrogen-like ions. These results also show a surprisingly strong effect of the projectile electron on the momentum transfer to the atomic recoil ion.

In collisions of very highly charged ions with atoms the doubly inelastic cross sections are by several orders of magnitude smaller than the cross section for the pure atomic ionization. However, since at moderate \( \gamma \) the regions of \( p_{R,\parallel} \) relevant to the singly and doubly inelastic processes are well separated and because of the unexpectedly ‘prominent’ behavior of the projectile electron in the transfer of large \( p_{R,\parallel} \), a great deal of information about the doubly inelastic collisions with relativistic heavy ions could be obtained in an experiment just by measuring the longitudinal momentum spectrum of the target recoil ions.

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[4] A.B.Voitkiv, Phys.Rep. 392 191 (2004)
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[6] The doubly inelastic transition amplitude for collisions with atomic hydrogen can be obtained from Eq. 4 if the integration over, say, \( p_2 \) is removed and the function \( f(p_2, \nu) \) is set to 1. Besides, in the rest of the integrand of 4, \( p_2 \) should be set to 0 and the obvious changes have to be made in the atomic form-factors.
[7] In collisions with highly charged ions the two-center di-electronic interaction is modulated by multiple interactions between the ionic nucleus and the electron of the target which, under the conditions of figure 1, decreases the height of the peak at \( p_{R,\parallel} \approx 0 \) by about 25% compared to the prediction of the first order theory.
[8] To describe this channel of momentum transfer Eqs. 3 have to be corrected by adding a term \( {Q_1}^2/(2M_A v) \) into the equation for \( g_{\text{min}} \) (a similar change has to be made also in 2). Note that this correction becomes important only at very small impact parameters whose contribution to the doubly inelastic cross sections is negligible and, therefore, can safely be neglected when the latter are calculated.
[9] So far we have not mentioned the capture of a target electron by the projectile. This process occurs via the radiative and coulomb capture channels. At the impact energies under consideration the last channel is quite weak and is characterized by very small recoil peaks located at large negative \( p_{R,\parallel} \) \((p_{R,\parallel} = -(I_f - I_i)/v - m_e c^2(1 - 1/\gamma)/v, \) where \( I_i \) and \( I_f \) are the initial and final binding energies of the electron). The relatively strong radiative capture
channel results only in quite low values of the target re-
coil momenta where its effect is fully masked by the direct
target ionization.