

## Plane-wave Born treatment of projectile-electron excitation and loss in relativistic collisions with atomic targets

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Electron excitation and loss of relativistic ion projectiles colliding with atomic targets are studied within the framework of the first order of the plane-wave Born approximation. General expressions are derived for the elastic and electron-electron contributions to the electron excitation and loss cross sections. In the limit of nonrelativistic collision velocities these expressions go over into known nonrelativistic formulas. In ultrarelativistic collisions shielding effects are shown to be very important for the excitation and loss cross sections even for collisions of highly charged projectiles with light atomic targets. Results of our calculations for the electron loss cross sections are in reasonable agreement with available experimental data on projectile-electron loss in relativistic collisions.

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### I. INTRODUCTION

Processes of excitation and loss of the projectile electron in collisions with atomic targets at nonrelativistic collision velocities have been extensively studied during the last few decades (see [1–3] and references therein). The result of these studies is a rather good understanding of these processes, especially those which can be considered within first-order perturbation theory. Some nonperturbative approaches are also available at present to treat the projectile-electron excitation and loss in nonrelativistic collisions (see, e.g., [4] and references therein).

The process of the projectile-electron loss in relativistic collisions with atomic targets was considered in several papers of Anholt and collaborators (see [5–7] and references therein). In these papers electron loss cross sections were calculated. The method used by these authors is based on the first-order perturbative treatment of ionization in relativistic collisions with structureless pointlike charges [8,9]. In order to take into account the fundamental difference between a pointlike charge and a neutral atom, they employed results for the projectile-electron loss in nonrelativistic collisions with neutral atoms and introduced some intuitive assumptions to adapt the nonrelativistic results to relativistic collisions. The most complete set of results for the loss process in relativistic collisions, obtained in this way, was presented in a paper of Anholt and Becker [7]. In that paper the electron loss cross sections were given for a variety of projectile-target pairs for collisions up to relativistic projectiles with  $\gamma \leq 1000$ , where  $\gamma$  is the Lorentz factor.

In a recent experiment [10] electron capture and loss with Pb ions as projectiles were investigated for several targets (from Be to Au) at a collision energy  $E = 160$  GeV/nucleon and a considerable difference between the theory [7] and the experimental data was found for the projectile electron loss cross sections.

The reason for this disagreement, revealed by Sørensen [11], is that the loss cross section, obtained in [7], does not correctly describe shielding effects in ultrarelativistic collisions. In the paper of Sørensen [11], within the framework of first-order perturbation theory, a simple and physically attractive semiquantitative investigation was given for the so-called elastic (for the target), or screening, contribution to the electron loss process. Within this approach the elastic contribution to the loss cross section is separated into a close and a distant collision contribution. The close-collision contribution was evaluated within the binary-encounter approximation for the collisions between the projectile electron and the nucleus of the neutral atom. The distant-collision contribution was estimated by using the method of equivalent photons. The so-called electron-electron, or antiscreening, contribution to the loss cross section, which cannot be treated within such an approach, was estimated by applying a relation between the electron-electron and elastic contributions which follows from the free collision model of Bohr (see, e.g., [1,2]). The results, calculated in [11], are in reasonable agreement with the experimental data [10].

In a recent paper [12] another approach was applied to treat the elastic contribution to the projectile electron loss cross section. In the rest frame of the projectile-ion the incident atom was described as a beam consisting of the nucleus and the electrons moving with a constant relativistic velocity along straight-line classical trajectories. The scalar and vector potentials, created by this beam, were calculated. The quantum nature of the atomic electrons was taken into account by averaging these potentials over the density distribution of the electrons “frozen” in the ground state of the incident atom. The time-dependent Dirac equation for the electron of the ion, making transitions in the field of the incident relativistic atom, was treated in the first-order of the perturbation theory in the electron-atom interaction and the screening cross section was calculated. Since the approach used in [12] can hardly be generalized to incorporate the electron-electron contribution, this contribution to the loss cross section was estimated in a similar manner as done in [11]. The results obtained in [12] agree well with the experiment [10].

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The present paper is an attempt to give a more general treatment of projectile-electron excitation and loss in relativistic collisions with atomic targets within the first order of the plane-wave Born approximation (PWBA). Our consideration is mainly restricted to projectiles carrying a single electron. In this case the transitions of the projectile electron can be described in the first order perturbation theory for the electron-target interaction if (i)  $Z_A < Z_I$ , where  $Z_A$  is the charge of the target nucleus and  $Z_I$  is the charge of the nucleus of the projectile-ion, or (ii)  $Z_A < v$ , where  $v$  is the collision velocity. In relativistic collisions the latter condition  $Z_A < v$  is fulfilled for any atomic number  $Z_A$ .

The present study is mainly focused in deriving general expressions for cross sections of the projectile-electron excitation and loss. In addition, some calculations for the loss cross sections are also presented.

The paper is organized as follows. In Sec. II we present the PWBA theory for the projectile-electron excitation and loss in relativistic collisions. In Sec. III we introduce the approximation of a ‘‘nonrelativistic atom’’ and evaluate the elastic and electron-electron contributions to the cross sections within this approximation. In Sec. IV we give a comparison of results of our numerical calculations with experimental data of [10] and [13] and with other theoretical results [7,11,12].

Atomic units are used throughout except where otherwise stated.

## II. GENERAL CONSIDERATION

In order to describe electronic transitions in composite atomic systems which are subject to the electromagnetic interaction in the collision, we start with the transition  $S$ -matrix element (see, e.g., [14])

$$S_{fi} = \left( -\frac{i}{c} \int d^4x J_\mu^I(x) A_A^\mu(x) \right)_{fi}, \quad (1)$$

where  $J_\mu^I(x)$  is the electromagnetic four-current of the projectile ion at a space-time point  $x$ ,  $A_A^\mu(x)$  is the four-potential of the electromagnetic field created by the target atom at the same point  $x$ , and  $c$  is the speed of light. Here and below the indices  $I$  and  $A$  stand for the ion and atom, respectively.

The potential obeys the Maxwell equation

$$\square A_A^\mu(x) = -\frac{4\pi}{c} J_A^\mu(x), \quad (2)$$

where  $J_A^\mu(x)$  is the four-current of the target atom and

$$\square = \Delta - \frac{\partial^2}{c^2 \partial t^2}$$

is the D'Alembert operator. Below the transition  $S$ -matrix element (1) will be evaluated within first-order perturbation theory in the projectile-target interaction.

Before we proceed further, let us make two rather obvious but important remarks, which allow us to simplify considerably the treatment of the problem in question. First, since the

nuclear and atomic energy scales are very different, Coulomb collisions between the ion and the atom, resulting in excitation of nuclear degrees of freedom, are of negligible importance for cross sections of electron transitions. Therefore the atomic and ionic nuclei can be treated as pointlike structureless charges. Second, in a reference frame, where the atom or the ion is initially at rest, its typical recoil velocity after the collision is not only nonrelativistic but also much less than the Bohr velocity  $v_0 = 1$  a.u. (see the Appendix).

Taking into account the remarks mentioned above, a convenient way to calculate the transition matrix element (1) is the following. First, we evaluate the ion current  $J_\mu^I(x)$  in the reference frame  $K_I$ , where the ion is initially at rest. Second, we calculate the atom current  $J_A^\mu(x_A)$  in the reference frame  $K_A$ , where the atom is initially at rest, and obtain the potential  $A_A^\mu(x_A)$  in this frame. Then we transform the potential to the frame  $K_I$  and calculate the transition matrix elements and corresponding cross sections in this frame.

Assuming that the ion carries only one electron the transition four-current  $J_\mu^I$  of the ion in the frame  $K_I$  reads

$$\begin{aligned} J_0^I(x) &= c \int d^3\mathbf{R}_I \int d^3\mathbf{r} \Psi_f^\dagger(\mathbf{R}_I, \mathbf{r}, t) \\ &\quad \times [Z_I \delta^3(\mathbf{x} - \mathbf{R}_I) - \delta^3(\mathbf{x} - \mathbf{R}_I - \mathbf{r})] \Psi_i(\mathbf{R}_I, \mathbf{r}, t), \\ J_i^I(x) &= -c \int d^3\mathbf{R}_I \int d^3\mathbf{r} \Psi_f^\dagger(\mathbf{R}_I, \mathbf{r}, t) \\ &\quad \times \alpha_i \delta^3(\mathbf{x} - \mathbf{R}_I - \mathbf{r}) \Psi_i(\mathbf{R}_I, \mathbf{r}, t). \end{aligned} \quad (3)$$

In Eqs. (3),  $Z_I$  is the atomic number of the ion,  $\mathbf{R}_I$  is the coordinate of the ion nucleus,  $\mathbf{r}$  is the coordinate of the electron of the ion with respect to the ion nucleus,  $\alpha_i$  are the Dirac matrixes for the electron of the ion, and  $\delta^{(3)}$  is the three-dimensional delta-function. Since in the frame  $K_I$  the three-velocity of the ion nucleus is negligible when compared with that of the ion electron, we have neglected in the second line in Eqs. (3) the contribution to the ion three-current due to the motion of the nucleus.

Further, in Eqs. (3) the wave functions of the initial and final states read

$$\Psi_j(\mathbf{R}_I, \mathbf{r}, t) = \frac{1}{\sqrt{V_I}} \exp(i\mathbf{P}_j^I \cdot \mathbf{R}_I - iE_j^I t) \psi_{0,n}(\mathbf{r}). \quad (4)$$

Here the symbol  $j$  stands for both  $i$  and  $f$ , which refer to the initial and final states of the ion, respectively,  $\mathbf{P}_i^I$  and  $\mathbf{P}_f^I$  are the total three-momenta ( $\mathbf{P}_i^I = 0$ ),  $E_i^I$  and  $E_f^I$  the total energies (including the rest energies) of the ion,  $\psi_0$  and  $\psi_n$  are the relativistic Dirac bispinors for the initial and final intrinsic states of the ion, and  $V_I$  is a normalization volume for the plane wave describing a free motion of the ion before and after the collision. Below we will be interested only in collisions where the intrinsic state of the ion is changed:  $n \neq 0$ . For the process of electron excitation the final state  $\psi_n$  is a

discrete state of the ion. Otherwise the state  $\psi_n$  is a continuum state of the ion, properly normalized, and describes the electron loss process.

The ansatz (4) represents a common form (see, e.g., [17]) of a wave function for a free atomic system moving with a nonrelativistic velocity [18], where we have neglected the spin of the nucleus and the difference between the coordinate of the nucleus of the ion and the coordinate of the center of mass of the ion. The justification of both approximations lies in the extremely large difference between the masses of nuclei and of electrons (see, e.g., the discussion in [16] devoted to the justification of the neglect of the spin of a heavy particle in the equivalent photon method).

Inserting Eq. (4) into Eq. (3) and integrating over  $\mathbf{R}_l$  we obtain for  $n \neq 0$

$$J_\mu^l(x) = c \frac{F_\mu^l(n0; \mathbf{P}_f^l - \mathbf{P}_i^l)}{V_l} \exp[i(\mathbf{P}_f^l - \mathbf{P}_i^l)\mathbf{x} - i(E_f^l - E_i^l)t]. \quad (5)$$

We denote the four-component quantity  $F_\mu^l(n0; \mathbf{P}_f^l - \mathbf{P}_i^l)$  with components

$$F_0^l(n0; \mathbf{P}_f^l - \mathbf{P}_i^l) = - \int d^3\mathbf{r} \psi_n^\dagger(\mathbf{r}) \exp[i(\mathbf{P}_f^l - \mathbf{P}_i^l)\mathbf{r}] \psi_0(\mathbf{r}),$$

$$F_i^l(n0; \mathbf{P}_f^l - \mathbf{P}_i^l) = - \int d^3\mathbf{r} \psi_n^\dagger(\mathbf{r}) \exp[i(\mathbf{P}_f^l - \mathbf{P}_i^l)\mathbf{r}] \alpha_i \psi_0(\mathbf{r}), \quad (6)$$

as the inelastic form factor of the ion. It can be seen from Eqs. (6) that the quantity  $F_\mu^l/V_l$  forms a four-vector.

Now we proceed to the calculation of the potential created by the atom. First we calculate the current  $J_A'^\mu(x_A)$  of the atom in the reference frame  $K_A$  where the atom is initially at rest and obtain the potential  $A_A'^\mu(x_A)$  in this frame. Here,  $x_A = (ct_A, \mathbf{x}_A)$  is the space-time four-vector in  $K_A$ . In a way similar to that used to get the ion current (5), we obtain for the four-current of the atom

$$J_A'^\mu(x_A) = c \frac{F_A'^\mu(m0; \mathbf{P}_f^A - \mathbf{P}_i^A)}{V_A'} \times \exp[i(\mathbf{P}_f^A - \mathbf{P}_i^A)\mathbf{x}_A - i(E_f^A - E_i^A)t_A]. \quad (7)$$

In Eq. (7),  $\mathbf{P}_{i,f}^A$  ( $\mathbf{P}_i^A = 0$ ) are the three-momenta and  $E_{i,f}^A$  the total energies (including rest energies) of the atom in the initial and final states, respectively, and  $V_A'$  is a normalization volume for the atom in the frame  $K_A$ . The components of the form factor of the atom  $F_A'^\mu$  are determined as follows:

$$F_0^A(m0; \mathbf{Q}) = Z_A \delta_{m0} - \int \prod_{i=1}^{N_A} d^3\xi_i u_m^\dagger(\boldsymbol{\tau}_{N_A}) \times \sum_{j=1}^{N_A} \exp(i\mathbf{Q} \cdot \boldsymbol{\xi}_j) u_0(\boldsymbol{\tau}_{N_A}),$$

$$F_i^A(m0; \mathbf{Q}) = - \int \prod_{i=1}^{N_A} d^3\xi_i u_m^\dagger(\boldsymbol{\tau}_{N_A}) \times \sum_{j=1}^{N_A} \alpha_{l(j)} \exp(i\mathbf{Q} \cdot \boldsymbol{\xi}_j) u_0(\boldsymbol{\tau}_{N_A}). \quad (8)$$

Here  $\mathbf{Q} = \mathbf{P}_f^A - \mathbf{P}_i^A$ ,  $Z_A$  is the atomic number,  $N_A$  is the number of the electrons of the atom,  $\alpha_{l(i)}$  are the Dirac matrices for the  $i$ th electron,  $u_{0,m}$  are the wave functions describing initial and final intrinsic states of the atom, and  $\boldsymbol{\tau}_{N_A} = \{\boldsymbol{\xi}_1, \boldsymbol{\xi}_2, \dots, \boldsymbol{\xi}_{N_A}\}$  represents the coordinates of the  $N_A$  atomic electrons with respect to the atomic nucleus. Since the intrinsic motion of the (inner) electrons in heavy atomic systems is relativistic, then, in general, the wave functions  $u_{0,m}$  are relativistic electronic wave functions. Exact solutions for the Dirac equation with two and more electrons are not known; however, approximate wave functions for such systems can be constructed from individual electron wave functions.

Equations (7) and (8) were obtained using approximations, similar to those used to get Eqs. (5) and (6). The only essential difference between the two form factors (6) and (8) is that we consider for the atom also the possibility to make no transitions between its intrinsic states in the collision. The zeroth components of the ion (6) and atom (8) form factors have the familiar form of the atomic form factor appearing in the nonrelativistic theory of projectile excitation and loss (see, e.g., [1]). The three other components of these form factors have no counterpart in the nonrelativistic theory. Note also that the quantity  $F_A'^\mu/V_A'$  forms a four-vector.

In order to solve Eq. (2) it is convenient to use a four-dimensional Fourier transformation

$$A_A'^\mu(x_A) = \frac{1}{(2\pi)^2} \int d^4k B_A'^\mu(k) \exp(ikx_A),$$

$$J_A'^\mu(x_A) = \frac{c}{V_A'} \int d^4k \exp(ikx_A) \times \delta^{(4)}(k + P_f^A - P_i^A) F_A'^\mu(m0; -\mathbf{k}). \quad (9)$$

In Eq. (9),  $kx_A$  denotes a scalar product of the two four-dimensional vectors  $k$  and  $x_A$ ,  $P_{i,f}^A$  are the four-momenta of the atom in the frame  $K_A$ , and  $\mathbf{k}$  is the ‘‘spatial’’ part of  $k$ . Inserting Eq. (9) into  $\square' A_A'^\mu(x_A) = (-4\pi/c) J_A'^\mu(x_A)$  we find the Fourier transform  $B_A'^\mu(k)$  to be

$$B_A'^\mu(k) = 4\pi \frac{(2\pi)^2 \delta^{(4)}(k + P_f^A - P_i^A)}{k^2 - i0} \frac{F_A'^\mu(m0; -\mathbf{k})}{V_A'} \quad (10)$$

and obtain the four-potential

$$A_A'^\mu(x_A) = 4\pi \frac{\exp[i(P_f^A - P_i^A)x_A]}{(P_f^A - P_i^A)^2 - i0} \frac{F_A'^\mu(m0; \mathbf{Q})}{V_A'}. \quad (11)$$

In Eq. (11), the term  $-i0$  gives a prescription (see, e.g., [14]) to handle the singularity. This singularity would appear if  $(P_i^A - P_f^A)^2 = (\mathbf{P}_i^A - \mathbf{P}_f^A)^2 - (E_i^A - E_f^A)^2/c^2 = 0$ . The latter condition holds only if the electromagnetic interaction between the colliding systems is due to an exchange of a photon with  $k^2 = 0$ .

Let  $a_{\mu\nu}$  be the Lorentz transformation matrix from the frame  $K_A$  to the frame  $K_I$ . Then for the potential in the frame  $K_I$  we have

$$A_A^\mu(x) = a_{\nu}^\mu A_A^\nu(a^{-1}x) \\ = 4\pi \frac{\exp[i(P_i^A - P_f^A)x]}{(P_i^A - P_f^A)^2 - i0} a_{\nu}^\mu \frac{F_A^\nu(m0; \mathbf{Q})}{\gamma V_A}. \quad (12)$$

In Eq. (12),  $P_{i(f)}^A$  is the initial (final) four-momentum of the atom in the frame  $K_I$ ,  $V_A = V_A'/\gamma$  is the normalization volume for the atom in  $K_I$ ,  $\gamma = 1/\sqrt{1-v^2/c^2}$  is the Lorentz factor, and  $\mathbf{v}$  is the velocity of the incident atom in  $K_I$  and is identical to the collision velocity.

Using the Lorentz transformation the three-momentum transfer to the atom  $\mathbf{Q} = \mathbf{P}_f^A - \mathbf{P}_i^A$ , given in the frame  $K_A$ , which enters Eq. (12), can be rewritten as

$$\mathbf{Q} = \left( \mathbf{P}_{f\perp}^A - \mathbf{P}_{i\perp}^A, \frac{1}{\gamma}(P_{f\parallel}^A - P_{i\parallel}^A) + \frac{v}{c^2}(E_i^A - E_f^A) \right) \\ \approx \left( \mathbf{P}_{f\perp}^A - \mathbf{P}_{i\perp}^A, \frac{1}{\gamma}(P_{f\parallel}^A - P_{i\parallel}^A) - \frac{v}{c^2}(\epsilon_m - \epsilon_0) \right), \quad (13)$$

where  $\mathbf{P}_\perp^A$  and  $P_\parallel^A$  are the transverse and longitudinal parts of the three-momentum  $\mathbf{P}^A$  of the atom in the frame  $K_I$ . In Eq. (13) and below we use the letters  $\epsilon$  and  $\varepsilon$  to denote the

electron energy of the atom (in the frame  $K_A$ ) and the ion (in the frame  $K_I$ ), respectively. In Eq. (13),  $\epsilon_0$  and  $\epsilon_m$  are the electron energies of the atom in the initial (0) and final ( $m$ ) states, respectively. In the second line of Eq. (13) we have neglected the recoil energy of the atom in the frame  $K_A$ . The components  $\mathbf{P}_\perp^A$  and  $P_\parallel^A$  are perpendicular and parallel to the collision velocity  $\mathbf{v}$ , respectively. Note that the transverse and longitudinal components of the momentum transfer  $\mathbf{P}_f^A - \mathbf{P}_i^A$  to the atom in the frame  $K_I$  enter the atomic form factor in Eq. (12) differently, which results in important peculiarities in the shielding of the atomic nucleus by atomic electrons in ultrarelativistic collisions.

Inserting the right hand sides of Eqs. (5) and (12) into Eq. (1) and integrating over  $d^4x$  in Eq. (1) we obtain

$$S_{fi} = -i \frac{4\pi}{V_I V_A} (2\pi)^4 \delta^{(4)}(P_i^I + P_i^A - P_f^I - P_f^A) G_{fi}, \quad (14)$$

where

$$G_{fi} = \frac{F_\mu^I(n0; \mathbf{q}) \gamma^{-1} a_{\nu}^\mu F_A^\nu(m0; \mathbf{Q})}{(P_i^A - P_f^A)^2 - i0} \quad (15)$$

and  $\mathbf{q} = \mathbf{P}_f^I - \mathbf{P}_i^I = \mathbf{P}_i^A - \mathbf{P}_f^A$  is the three-dimensional momentum transfer to the ion (given in the frame  $K_I$ ). We recall that the form factors  $F_\mu^I$  and  $F_A^\nu$ , given by Eqs. (6) and (8), are determined in the reference frames  $K_I$  and  $K_A$ , respectively.

Using the standard technique in order to get cross sections from known transition  $S$ -matrix elements (see, e.g., [14]) and taking into account Eqs. (13) and (15), we obtain for the cross section of a process where the electron of the ion makes the transition  $\psi_0 \rightarrow \psi_n$  and those of the atom the transition  $u_0 \rightarrow u_m$

$$\sigma_{0 \rightarrow n}^{0 \rightarrow m} = \frac{4}{v^2} \frac{E_f^A}{E_i^A} \sum_{s_I} \sum_{s_A} \int d^2\mathbf{q}_\perp |G_{fi}|^2 \\ = \frac{4}{v^2} \frac{E_i^A + E_i^I - E_f^I}{E_i^A} \sum_{s_I} \sum_{s_A} \int d^2\mathbf{q}_\perp \frac{|F_\mu^I(n0; \mathbf{q}_\perp, q_{\min}) \gamma^{-1} a_{\nu}^\mu F_A^\nu(m0; -\mathbf{q}_\perp, -q_{\min}/\gamma - (v/c^2)(\epsilon_m - \epsilon_0))|^2}{[q_\perp^2 + q_{\min}^2 - (E_f^I - E_i^I)^2/c^2]^2}, \quad (16)$$

where  $E_i^A$  and  $E_f^A = E_i^A + E_i^I - E_f^I$  are the initial and final total energies of the atom given in the rest frame of the ion. The summation indicated in Eq. (16) runs over the spin degrees of freedom of the electron of the ion and over those of the atom. This summation implies proper spin averaging, i.e., an average over initial and sum over final spin states of the electrons participating in the process. In the above equation the integration over the absolute value of the transverse part  $\mathbf{q}_\perp$  of the momentum transfer  $\mathbf{q}$  runs from 0 to some maximal value  $q_\perp^{\max}$  which for our case can be set equal to infinity. With the same accuracy the factor  $E_f^A/E_i^A$  in Eq. (16) can be set to unity. We have omitted in Eq. (16) the term  $-i0$

because of reasons which will be discussed below. The minimum momentum transfer  $q_{\min} = |\mathbf{P}_i^I| - |\mathbf{P}_f^I|$ , entering Eq. (16), is to be determined from the energy conservation in the collision:

$$E_i^I + \sqrt{c^2 \mathbf{P}_i^A{}^2 + M_{Ai}^2 c^4} = E_f^I + \sqrt{c^2 \mathbf{P}_f^A{}^2 + M_{Af}^2 c^4}, \quad (17)$$

where  $M_{Ai}$  and  $M_{Af}$  are the rest masses of the atom being in the initial and final states,  $u_0$  and  $u_m$ , respectively. Due to a very large difference between masses of the ion and that of the electron, the recoil energy of the ion in the frame  $K_I$  can be neglected. Then in this frame the difference in total ener-

gies of the ion before and after the collision can be approximated as  $E_f^I - E_i^I \approx \varepsilon_n - \varepsilon_0$ , where  $\varepsilon_0$  and  $\varepsilon_n$  are the energies of the electron of the ion in the initial and final intrinsic states  $\psi_0$  and  $\psi_n$ , respectively. Taking into account that (i) the change of the three-momentum of the incident atom is small compared to its initial value,  $|\mathbf{P}_f^A| + |\mathbf{P}_i^A| \approx 2|\mathbf{P}_i^A|$ , (ii) the difference in the rest masses of the atom is small compared to its initial value,  $M_{Ai} + M_{Af} \approx 2M_{Ai}$ , and (iii) the total energy of the relativistic incoming atom in the frame  $K_I$  is much larger than the difference between the final and initial energies of the ion in that frame,  $E_i^A \gg |E_f^I - E_i^I| \approx |\varepsilon_n - \varepsilon_0|$ , Eq. (17) is approximately solved to yield

$$q_{\min} = \frac{\varepsilon_n - \varepsilon_0}{v} + \frac{(M_{Af} - M_{Ai})c^2}{v\gamma} = \frac{\varepsilon_n - \varepsilon_0}{v} + \frac{\epsilon_m - \epsilon_0}{v\gamma}. \quad (18)$$

Here, neglecting the recoil energy of the atom in the frame  $K_A$ , we set  $(M_{Af} - M_{Ai})c^2$  to be equal to the difference between the final,  $\epsilon_m$ , and initial,  $\epsilon_0$ , energies of the electrons of the atom in that frame.

It is convenient also to introduce the quantity

$$Q_{\min} = \frac{q_{\min}}{\gamma} + \frac{v}{c^2}(\epsilon_m - \epsilon_0) = \frac{\epsilon_m - \epsilon_0}{v} + \frac{\varepsilon_n - \varepsilon_0}{v\gamma}, \quad (19)$$

which plays the same role for the atom as the quantity  $q_{\min}$  for the ion.

Taking into account Eqs. (18) and (19) the cross section (16) can be rewritten in the form which clearly shows the symmetry of the quantities of the atom and of the ion in the cross section:

$$\sigma_{0 \rightarrow m}^{0 \rightarrow m} = \frac{4}{v^2} \sum_{s_I} \sum_{s_A} \int d^2 \mathbf{q}_{\perp} \frac{\left| F_{\mu}^I \left( n0; \mathbf{q}_{\perp}, \frac{\varepsilon_n - \varepsilon_0}{v} + \frac{\epsilon_m - \epsilon_0}{v\gamma} \right) \gamma^{-1} a_{\nu}^{\mu} F_A^{\nu} \left( m0; -\mathbf{q}_{\perp}, -\frac{\epsilon_m - \epsilon_0}{v} - \frac{\varepsilon_n - \varepsilon_0}{v\gamma} \right) \right|^2}{\left( q_{\perp}^2 + \frac{(\varepsilon_n - \varepsilon_0 + \epsilon_m - \epsilon_0)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{(\varepsilon_n - \varepsilon_0)(\epsilon_m - \epsilon_0)}{v^2 \gamma^2} \right)^2}. \quad (20)$$

Here we have consistently neglected the recoil energy of the ion also in the denominator of the integrand in Eq. (16),  $E_f^I - E_i^I \approx \varepsilon_n - \varepsilon_0$ . Equations (16) and (20) are the first main result of the present paper.

If the atom and the ion are initially in their ground states, it follows from Eq. (20) that the singularity in the integrand in Eqs. (16) and (20) does not appear. From the physical point of view it means that for collisions of composite atomic systems, which are initially in the ground states, the restrictions imposed by the momentum-energy conservation in the collision do not permit an electromagnetic interaction between the systems to occur via an exchange of a real photon with the energy-momentum relation  $k^2 = 0$ . We consider below only such collisions and omit the term  $-i0$  in Eqs. (16) and (20).

Before we proceed further, however, it is worthwhile to say a few words about the situation when one of the two collision partners is initially in the ground state while the other one is in an excited state and when the collision leads to the excitation of the first particle and the deexcitation of the second one. The analysis of the denominator in Eq. (20) shows that the electromagnetic interaction between the colliding composite systems can occur via an exchange of a photon with the energy-momentum relation  $k^2 = 0$  which is inherent to a real photon [19]. In this case the corresponding cross section calculated within the present formalism is infinite, which reflects the breakdown of the first-order treatment in such a case even for finite  $\gamma$  [20]. In order to get a deeper insight into the reason which undermines the validity of the first-order treatment in this case, let us consider the denomi-

nator in the integrands in Eqs. (16) and (20) in more detail. This denominator can be equal to zero if

$$q_{\min}^2 - \frac{(\varepsilon_n - \varepsilon_0)^2}{c^2} \leq 0. \quad (21)$$

To be definite, let us assume that the ion gets excited ( $\varepsilon_n - \varepsilon_0 > 0$ ) and the atom is deexcited ( $\epsilon_m - \epsilon_0 < 0$ ) in the collision. Then, taking into account Eq. (18), we obtain that the inequality (21) holds if

$$|\epsilon_m - \epsilon_0| \sqrt{\frac{c-v}{c+v}} \leq \varepsilon_n - \varepsilon_0 \leq |\epsilon_m - \epsilon_0| \sqrt{\frac{c+v}{c-v}}. \quad (22)$$

Because of the relativistic Doppler effect, the emission of photons in the atomic frame  $K_A$  (in all directions) with a fixed frequency  $\omega_0$  results in a photon spectrum in the ion frame  $K_I$  with the frequencies  $\omega$ :

$$\omega_0 \sqrt{\frac{c-v}{c+v}} \leq \omega \leq \omega_0 \sqrt{\frac{c+v}{c-v}}. \quad (23)$$

Comparing Eqs. (22) and (23) we see that the interaction between the atom and the ion in the collision process occurs via the emission of a photon with the energy  $\omega_0 = |\epsilon_m - \epsilon_0|$  by the atom in the frame  $K_A$  and the absorption of the same photon, but with the energy  $\omega = \varepsilon_n - \varepsilon_0$ , by the ion in the frame  $K_I$ . Thus, the collision process in this case is a resonant process which cannot be treated within the first order.

Now we return to the consideration of relativistic collisions between atomic systems which are initially in the

ground states. Using the explicit form of the Lorentz transformation matrix  $a_\nu^\mu$  (see, e.g., [2]) the relativistic coupling of the form factors in Eqs. (16)–(20) can be written in the following symmetrical form:

$$F_\mu^l \gamma^{-1} a_\nu^\mu F_A^\nu = \left( F_0^l - \frac{v}{c} F_3^l \right) \left( F_A^0 - \frac{v}{c} F_A^3 \right) + \frac{F_3^l F_A^3}{\gamma^2} + \frac{F_1^l F_A^1 + F_2^l F_A^2}{\gamma}. \quad (24)$$

Compared to the known form of the nonrelativistic cross section (see, e.g., [1,3] and references therein) Eqs. (16), (20), and (24) contain two types of relativistic effects. The first type is connected with the collision velocity  $v$  and disappears when  $v/c \ll 1$ . This type includes the retardation effect, described by the term  $(E_f^l - E_i^l)^2/c^2 \approx (\epsilon_n - \epsilon_0)^2/c^2$  in the denominator in Eq. (16), and the different dependences of the form factors of the atom and ion on the transition energies  $(\epsilon_n - \epsilon_0)$  and  $(\epsilon_m - \epsilon_0)$  and also the coupling between the zeroth and third components of the form factors in Eq. (24). The second type is due to relativistic effects in the inner motion of the electron of the ion and the electrons of the atom, and it does not disappear when  $v/c \ll 1$ . It includes

the coupling between the space components of the corresponding form factors in Eq. (24). In the limit  $c \rightarrow \infty$  both types of relativistic effects vanish and Eq. (20) recovers the form of the corresponding nonrelativistic cross section.

If a final intrinsic state of the atom is not observed, one has to sum over all possible states of the atom. Equation (16) then gives

$$\sigma_{0 \rightarrow n} = \frac{4}{v^2} \sum_{s_I} \sum_m \int d^2 \mathbf{q}_\perp \times \frac{|F_\mu^l(n0; \mathbf{q}_\perp, q_{\min}) \gamma^{-1} a_\nu^\mu F_A^\nu(m0; -\mathbf{q}_\perp, -Q_{\min})|^2}{[q_\perp^2 + q_{\min}^2 - (\epsilon_n - \epsilon_0)^2/c^2]^2}. \quad (25)$$

The summation over the atomic states in Eq. (25) includes also the summation over all spin degrees of freedom of the atomic electrons. The cross section (25) can be split into the elastic ( $m=0$ ) and electron-electron (all  $m \neq 0$ ) contributions to the total cross section for the transition  $0 \rightarrow n$  of the electron of the ion. Taking Eq. (18) into account we obtain for the elastic part

$$\sigma_{0 \rightarrow n}^{eI} = \frac{4}{v^2} \sum_{s_I} \int d^2 \mathbf{q}_\perp \frac{|F_\mu^l(n0; \mathbf{q}_\perp, q_{\min}) \gamma^{-1} a_\nu^\mu F_A^\nu(00; -\mathbf{q}_\perp, -q_{\min}/\gamma)|^2}{\left( q_\perp^2 + \frac{(\epsilon_n - \epsilon_0)^2}{v^2 \gamma^2} \right)^2}. \quad (26)$$

Correspondingly for the electron-electron contribution we have

$$\sigma_{0 \rightarrow n}^{e-e} = \frac{4}{v^2} \sum_{s_I} \sum_{m \neq 0} \int d^2 \mathbf{q}_\perp \frac{|F_\mu^l(n0; \mathbf{q}_\perp, q_{\min}) \gamma^{-1} a_\nu^\mu F_A^\nu(m0; -\mathbf{q}_\perp, -Q_{\min})|^2}{\left( q_\perp^2 + \frac{(\epsilon_n - \epsilon_0 + \epsilon_m - \epsilon_0)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{(\epsilon_n - \epsilon_0)(\epsilon_m - \epsilon_0)}{v^2 \gamma^2} \right)^2}. \quad (27)$$

### III. APPROXIMATION OF A “NONRELATIVISTIC” ATOM

The coupling (24) between the form factors of the ion and atom is rather complicated. In order to get more tractable equations for the electron loss cross sections we introduce the following approximation: we neglect the space components of the atomic form factor. Below some semiquantitative arguments are given in its favor.

Let us consider the atomic form factor (8) in more detail. The component  $F_A^0(m0; \mathbf{Q})$  of the atomic form factor is connected with the charge distribution inside the atom. The components  $F_A^l(m0; \mathbf{Q})$  are connected with the current, created by the motion of the electrons inside the atom in the rest frame of the atom. One can estimate roughly the magnitude of  $F_A^l(m0; \mathbf{Q})$  as  $F_A^l(m0; \mathbf{Q}) \sim (v_e/c) F_A^0(m0; \mathbf{Q})$  where  $v_e$  is a characteristic velocity of the atomic electrons. For light and

not too heavy atoms one has  $v_e \ll c$  for all atomic electrons and one can neglect all three components  $F_A^l(m0; \mathbf{Q})$  in Eq. (8) compared to  $F_A^0(m0; \mathbf{Q})$ . In heavy atoms the very inner electrons can have relativistic velocities. However, because the number of these electrons is relatively small compared to the total number of atomic electrons, they are not expected to increase considerably the absolute value of  $F_A^l(m0; \mathbf{Q})$ . Therefore, the neglect of  $F_A^l(m0; \mathbf{Q})$  is approximately justified also for heavy atoms.

We will refer to this approximation as to the nonrelativistic atom (NRA) approximation. The NRA approximation breaks the symmetry in which the form factors of the ion and of the atom enter Eqs. (16) and (20)–(27). Therefore, in general, one can expect that this approximation fits better to the screening mode. In this mode the electron of the ion makes a transition while those of the atom do not, and the symmetry between the ion and atom is already broken to some extent. Indeed the analysis of the elastic atomic form factor shows

that for the screening mode the NRA approximation can be used for all possible collision energies and colliding partners.

The situation becomes more complicated when we use the NRA approximation for the antiscreeing mode. In the argumentation given above we considered typical electron velocities in the atom ground state. In collisions with heavy projectile ions the minimum momentum transfer  $Q_{\min} = (\varepsilon_n - \varepsilon_0)/v\gamma + (\varepsilon_m - \varepsilon_0)/v$  can be large compared to the typical electron momenta in the atom. In the antiscreeing mode of such collisions the atomic electrons can acquire velocities which are considerably higher than the typical electron velocities in the ground state of the atom. Since we have assumed that the atomic electrons are nonrelativistic in the collisions, it means that the condition  $Q_{\min} \ll m_e c$ , where  $m_e = 1$  is the electron rest mass, should be fulfilled. If we approximate  $\varepsilon_n - \varepsilon_0$  by  $Z_I^2$ , then we obtain the limitation  $\gamma \gg Z_I^2/vc$  for the use of the NRA approximation in relativistic collisions. The latter condition is certainly met for collisions with, say,  $\gamma > 4$  for any heavy ion.

There is another important limitation for the use of the NRA approximation for the antiscreeing mode. Our analysis of the properties of the inelastic atomic form factor in the limit of small momentum transfers shows that the condition  $(\varepsilon_n - \varepsilon_0)/\gamma \gg (\varepsilon_m - \varepsilon_0)$  should also be met for all transitions of the atomic electrons contributing considerably to the antiscreeing part of the loss cross section. This condition imposes an upper limit on the collision energies which can be considered within the NRA approximation. However, since we are interested mainly in the description of electron loss from very heavy ions, this condition does not seem to be very restrictive for collisions with light atoms when the antiscreeing mode is relatively important. On the other hand, for collisions with heavy atoms, where the NRA approximation may not be well justified for ultrarelativistic collisions,

the antiscreeing mode is not expected to give a noticeable contribution to the total electron excitation or loss.

We also note that in order to provide a reasonable asymptotical limit for the electron-electron contribution to the cross section, which for  $\gamma \rightarrow \infty$  should be  $\gamma$  independent, it is sufficient to take the first term  $[F_0^I - (v/c)F_3^I][F_A^0 - (v/c)F_A^3]$  of the full coupling of the form factors in Eq. (24).

Keeping in mind that the arguments given above are qualitative rather than quantitative we use below the NRA approximation for our calculations.

Neglecting  $F_A^I(m_0; \mathbf{Q})$  we obtain for the elastic cross section (26)

$$\sigma_{0 \rightarrow n}^{eI} = \frac{4}{v^2} \sum_{s_I} \int d^2 \mathbf{q}_\perp Z_{A,eff}^2(\mathbf{Q}_0^s) \times \frac{\left| \left\langle \psi_n(\mathbf{r}) \left| \left( 1 - \frac{v}{c} \alpha_z \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}) \right| \psi_0(\mathbf{r}) \right\rangle \right|^2}{\left( q_\perp^2 + \frac{(\varepsilon_n - \varepsilon_0)^2}{v^2 \gamma^2} \right)^2}. \quad (28)$$

Here  $\mathbf{q}_0 = (\mathbf{q}_\perp, q_{\min})$ ,  $\mathbf{Q}_0^s = (\mathbf{q}_\perp, q_{\min}/\gamma)$ , and we use Dirac's notation for the vectors of electronic states. The effective charge of the incident atom in the ground state is [see Eq. (8)]

$$Z_{A,eff}(\mathbf{Q}_0^s) = Z_A - \left\langle u_0(\tau_{N_A}) \left| \sum_{j=1}^{N_A} \exp(-i \mathbf{Q}_0^s \cdot \boldsymbol{\xi}_j) \right| u_0(\tau_{N_A}) \right\rangle. \quad (29)$$

In the same way the electron-electron contribution (27) can be written as

$$\sigma_{0 \rightarrow n}^{e-e} = \frac{4}{v^2} \sum_{s_I} \sum_{m \neq 0} \int d^2 \mathbf{q}_\perp \left| \left\langle u_m(\tau_{N_A}) \left| \sum_{j=1}^{N_A} \exp(-i \mathbf{Q}_0^a \cdot \boldsymbol{\xi}_j) \right| u_0(\tau_{N_A}) \right\rangle \right|^2 \times \frac{\left| \left\langle \psi_n(\mathbf{r}) \left| \left( 1 - \frac{v}{c} \alpha_z \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}) \right| \psi_0(\mathbf{r}) \right\rangle \right|^2}{\left( q_\perp^2 + \frac{(\varepsilon_n - \varepsilon_0 + \varepsilon_m - \varepsilon_0)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{(\varepsilon_n - \varepsilon_0)(\varepsilon_m - \varepsilon_0)}{v^2 \gamma^2} \right)^2}, \quad (30)$$

where  $\mathbf{Q}_0^a = (\mathbf{q}_\perp, Q_{\min})$ .

According to Eq. (11) the approximation  $F_A^I(m_0; \mathbf{Q}) \approx 0$ , used to obtain Eqs. (28) and (30), in fact means that we have neglected the vector potential, created by the atom in the frame  $K_A$ , compared to its scalar potential in this frame. Then the scalar potential  $A^0$  and the vector potential  $\mathbf{A}$  of the atom in the frame  $K_I$  are connected by the simple relation  $\mathbf{A} = (\mathbf{v}/c)A^0$ , and Eqs. (25) and (27) are reduced to Eqs. (28) and (30). The latter equations are the second main result of the present paper.

For ions carrying  $N_I$  electrons ( $N_I > 1$ ) the cross sections (28) and (30) can be generalized to yield

$$\sigma_{0 \rightarrow n}^{eI} = \frac{4}{v^2} \sum_{s_I} \int d^2 \mathbf{q}_\perp Z_{A,eff}^2(\mathbf{Q}_0^s) \frac{\left| \left\langle \psi_n(\boldsymbol{\rho}_{N_I}) \left| \sum_{i=1}^{N_I} \left( 1 - \frac{v}{c} \alpha_{z(i)} \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}_i) \right| \psi_0(\boldsymbol{\rho}_{N_I}) \right\rangle \right|^2}{\left( q_\perp^2 + \frac{(\varepsilon_n - \varepsilon_0)^2}{v^2 \gamma^2} \right)^2} \quad (31)$$

and

$$\begin{aligned} \sigma_{0 \rightarrow n}^{e-e} = & \frac{4}{v^2} \sum_{s_I} \sum_{m \neq 0} \int d^2 \mathbf{q}_\perp \left| \left\langle u_m(\boldsymbol{\tau}_{N_A}) \left| \sum_{j=1}^{N_A} \exp(-i \mathbf{Q}_0^a \cdot \boldsymbol{\xi}_j) \right| u_0(\boldsymbol{\tau}_{N_A}) \right\rangle \right|^2 \left| \left\langle \psi_n(\boldsymbol{\rho}_{N_I}) \left| \sum_{i=1}^{N_I} \left( 1 - \frac{v}{c} \alpha_{z(i)} \right) \right. \right. \\ & \left. \left. \times \exp(i \mathbf{q}_0 \cdot \mathbf{r}_i) \right| \psi_0(\boldsymbol{\rho}_{N_I}) \right\rangle \right|^2 \left( q_\perp^2 + \frac{(\varepsilon_n - \varepsilon_0 + \varepsilon_m - \varepsilon_0)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{(\varepsilon_n - \varepsilon_0)(\varepsilon_m - \varepsilon_0)}{v^2 \gamma^2} \right)^{-2}. \end{aligned} \quad (32)$$

In Eqs. (31) and (32),  $\boldsymbol{\rho}_{N_I} = \{\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_{N_I}\}$  are the coordinates of the  $N_I$  electrons of the ion with respect to the ion nucleus, and  $\alpha_{z(i)}$  is the Dirac matrix for the  $i$ th electron.

Below we restrict our consideration to ions carrying only one (active) electron.

### A. Elastic contribution (screening)

In this subsection we consider the elastic contribution (28) to the total cross section in more detail.

The effective charge (29) can be rewritten as

$$Z_{A,eff}(\mathbf{Q}_0^s) = Z_A - \int d\xi \rho_{el}(\boldsymbol{\xi}) \exp(-i \mathbf{Q}_0^s \cdot \boldsymbol{\xi}), \quad (33)$$

where  $\rho_{el}(\boldsymbol{\xi})$  is the charge density of the electrons in the incident atom in rest frame of the atom. In a paper of Salvat *et al.* [22] analytical Dirac-Hartree-Fock-Slater screening functions are given for neutral atoms with atomic numbers  $Z_2 = 1-92$ . The density is written as

$$\rho_{el}(\boldsymbol{\xi}) = \frac{Z_A}{4\pi\xi^2} \sum_{i=1}^3 A_i \kappa_i^2 \exp(-\kappa_i \xi). \quad (34)$$

Here,  $A_i$  and  $\kappa_i$  are constants for a given atom which are tabulated for all atomic elements in [22]. Using Eqs. (33) and (34) the effective charge  $Z_{A,eff}(\mathbf{Q}_0^s)$  is obtained to be

$$\begin{aligned} Z_{A,eff}(\mathbf{Q}_0^s) = & Z_A \left( 1 - \sum_{i=1}^3 \frac{A_i \kappa_i^2}{\kappa_i^2 + q_\perp^2 + q_{\min}^2 / \gamma^2} \right) \\ = & Z_A (q_\perp^2 + q_{\min}^2 / \gamma^2) \sum_{i=1}^3 \frac{A_i}{\kappa_i^2 + q_\perp^2 + q_{\min}^2 / \gamma^2}. \end{aligned} \quad (35)$$

For obtaining the second line on the right hand side of Eq. (35) the condition  $\sum_i A_i = 1$  (see [22]) was used.

Inserting Eq. (35) into Eq. (28) we get

$$\begin{aligned} \sigma_{0 \rightarrow n}^{eI} = & \frac{4Z_A^2}{v^2} \sum_{s_I} \sum_{i,j} A_i A_j \int d^2 \mathbf{q}_\perp \\ & \times \frac{\left| \left\langle \psi_n(\mathbf{r}) \left| \left( 1 - \frac{v}{c} \alpha_z \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}) \right| \psi_0(\mathbf{r}) \right\rangle \right|^2}{\left( \mathbf{q}_\perp^2 + \frac{\omega_{n0}^2}{v^2 \gamma^2} + \kappa_i^2 \right) \left( \mathbf{q}_\perp^2 + \frac{\omega_{n0}^2}{v^2 \gamma^2} + \kappa_j^2 \right)}. \end{aligned} \quad (36)$$

Here  $\omega_{n0} = \varepsilon_n - \varepsilon_0$ . The above equation is exactly the same as that obtained in [12].

For an atom without any electrons, i.e., a bare nucleus, we set in Eq. (36) all  $\kappa_i$  equal to zero and recover the well-known form for cross sections for collisions with bare nuclei (see, e.g., [2]). In collisions with bare nuclei the main contribution to the cross section stems from the range of small values of  $q_\perp$ ,  $0 \leq q_\perp \leq \omega_{n0}/v\gamma$ , resulting in a logarithmic growth of the cross section with  $\gamma$ :  $\sigma_{0n} \sim \ln \gamma$  (see, e.g., [2]).

For collisions with neutral atoms Eq. (36) shows an important general feature of the shielding in relativistic collisions which is not present in nonrelativistic ones. If the ion is a highly charged ion ( $Z_I \gg 1$ ) and the atom is a light atom with all screening constants  $\kappa_i$  of the order of unity, the shielding is not important in nonrelativistic collisions because the term  $\omega_{n0}^2/v^2 \sim Z_I^4/v^2$  dominates over all  $\kappa_i^2$  in the denominator of the integrand on the right hand side of Eq. (36). However, the situation changes drastically for ultrarelativistic collisions, where  $\gamma \gg 1$ . In this case the terms  $\kappa_i^2$  can be larger than the term  $\omega_{n0}^2/v^2 \gamma^2 \sim Z_I^4/v^2 \gamma^2$ . This results in a reduction of the cross section. Our numerical calculations (see below) confirm that, in contrast to nonrelativistic collisions, in ultrarelativistic collisions the shielding is important even for collision partners consisting of a heavy ion and a light atom. It is worthwhile to emphasize that this important feature follows directly from Eq. (13) and, hence, it is independent of the particular model (34), taken to describe the shielding.

In conclusion of this subsection we note that the analysis of Eq. (36) shows that, in collisions with neutral atoms, the cross section  $\sigma_{0 \rightarrow n}^{eI}$  is independent of  $\gamma$  in the limit of very high values of  $\gamma$ .

### B. Electron-electron contribution (antiscreeing)

Equation (30) can be considerably simplified by making use of the closure method (see [3] and references therein). In its simplest form the same average energy  $\Delta \varepsilon$  is assigned to all possible transitions of the atomic electrons. This approximation is known to give good results in nonrelativistic collisions at velocities well above the energy threshold for the ionization of the ion by a beam of free electrons. This approximation is used below in order to get a simpler and more tractable form for the part of the cross section due to the electron-electron contribution (30). Using the analogy with nonrelativistic collisions, one can expect that the closure approximation gives reasonable results also for collisions at  $v \approx c$  when the kinetic energy  $T$  of an equivelocity free elec-

tron is much larger than the binding energy of the electron of the ion:  $T = m_e c^2 (\gamma - 1) \gg |\epsilon_0|$ . This condition is well fulfilled for any heavy ion starting with, say,  $\gamma \geq 3-4$  which is quite close to the lower limit imposed by the use of the NRA approximation.

Under this approximation one can apply the closure relation for the electronic states of the atom,

$$\sum_m |u_m\rangle \langle u_m| = \mathbf{I}, \quad (37)$$

in order to perform the summation in Eq. (30) over the final states of the atom. It yields

$$\begin{aligned} \sigma_{0 \rightarrow n}^{e-e} = & \frac{4}{v^2} \sum_{s_1} \int d^2 \mathbf{q}_\perp \\ & \times \frac{\left| \left\langle \psi_n(\mathbf{r}) \left| \left( 1 - \frac{v}{c} \alpha_z \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}) \right| \psi_0(\mathbf{r}) \right\rangle \right|^2}{\left( q_\perp^2 + \frac{(\omega_{n0} + \Delta \epsilon)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{\omega_{n0} \Delta \epsilon}{v^2 \gamma^2} \right)^2} \\ & \times \left( \left\langle u_0 \left| \sum_{i,j} \exp[-i \mathbf{Q}_0^a(\xi_j - \xi_i)] \right| u_0 \right\rangle \right. \\ & \left. - \left| \left\langle u_0 \left| \sum_j \exp(-i \mathbf{Q}_0^a \xi_j) \right| u_0 \right\rangle \right|^2 \right), \quad (38) \end{aligned}$$

where we redefined  $\mathbf{Q}_0^a$  as  $\mathbf{Q}_0^a = (\mathbf{q}_\perp, \Delta \epsilon / v + (\epsilon_n - \epsilon_0) / v \gamma)$ . If a range of large (on the atomic scale) momentum transfers  $\mathbf{Q}_0^a$  contributes most to the integral on the right hand side of Eq. (38), only the diagonal terms  $i = j$  in the double sum in Eq. (38) give nonvanishing contributions. The double sum and the last sum in Eq. (38) are reduced simply to the number of the atomic electrons and the cross section  $\sigma_{0 \rightarrow n}^{e-e}$  describes transitions of the electron of the ion due to an incoherent electromagnetic interaction with  $Z_A$  free electrons.

In general, Eq. (38) can be further simplified if the antisymmetrization of the ground state of the atom is ignored and the wave function of the ground state is expressed as

$$u_0 = \prod_\lambda \phi_\lambda(\xi_\lambda), \quad (39)$$

where  $\phi_\lambda(\xi)$  are the single electron orbitals. It was shown in [5] (see also [23]) that under these conditions one has

$$\begin{aligned} & \left\langle u_0 \left| \sum_{i,j} \exp[-i \mathbf{Q}_0^a(\xi_j - \xi_i)] \right| u_0 \right\rangle \\ & - \left| \left\langle u_0 \left| \sum_j \exp(-i \mathbf{Q}_0^a \xi_j) \right| u_0 \right\rangle \right|^2 \\ & = Z_A - \sum_\lambda |\langle \phi_\lambda | \exp(-i \mathbf{Q}_0^a \cdot \xi) | \phi_\lambda \rangle|^2. \quad (40) \end{aligned}$$

Inserting the right hand side of Eq. (40) into Eq. (38) we obtain

$$\begin{aligned} \sigma_{0 \rightarrow n}^{e-e} = & \frac{4}{v^2} \sum_{s_1} \int d^2 \mathbf{q}_\perp \\ & \times \frac{\left| \left\langle \psi_n(\mathbf{r}) \left| \left( 1 - \frac{v}{c} \alpha_z \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}) \right| \psi_0(\mathbf{r}) \right\rangle \right|^2}{\left( q_\perp^2 + \frac{(\omega_{n0} + \Delta \epsilon)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{\omega_{n0} \Delta \epsilon}{v^2 \gamma^2} \right)^2} \\ & \times \left( Z_A - \sum_\lambda \left| \langle \phi_\lambda | \exp(-i \mathbf{Q}_0^a \cdot \xi) | \phi_\lambda \rangle \right|^2 \right). \quad (41) \end{aligned}$$

Anholt [5] has pointed out that

$$\begin{aligned} & \sum_\lambda \langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle \\ & \leq \sum_\lambda |\langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle|^2 \\ & \leq \frac{1}{Z_A} \left| \sum_\lambda \langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle \right|^2. \quad (42) \end{aligned}$$

He made calculations [7] using both replacements

$$\sum_\lambda |\langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle|^2 \rightarrow \sum_\lambda \langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle$$

and

$$\begin{aligned} & \sum_\lambda |\langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle|^2 \\ & \rightarrow \frac{1}{Z_A} \left| \sum_\lambda \langle \phi_\lambda | \exp(-i \mathbf{Q} \cdot \xi) | \phi_\lambda \rangle \right|^2 \end{aligned}$$

and has found that the difference between the results of these calculations is very small. Therefore, we simply set

$$\begin{aligned} & Z_A - \sum_\lambda |\langle \phi_\lambda | \exp(-i \mathbf{Q}_0^a \cdot \xi) | \phi_\lambda \rangle|^2 \\ & \rightarrow Z_A - \sum_\lambda \langle \phi_\lambda | \exp(-i \mathbf{Q}_0^a \cdot \xi) | \phi_\lambda \rangle \\ & = Z_{A,eff}(\mathbf{Q}_0^a), \quad (43) \end{aligned}$$

where  $Z_{A,eff}(\mathbf{Q}_0^a)$  is determined by Eq. (33) with an evident replacement  $\mathbf{Q}_0^s \rightarrow \mathbf{Q}_0^a$ . Then for the electron-electron contribution we finally have

TABLE I. Experimental and theoretical cross sections (in kb) for the ionization of 10.8 GeV/nucleon Au<sup>78+</sup> penetrating various solid targets. The ion is initially in its ground state.

Atom	$Z_A$	Experiment	Anholt and Becker	Sørensen	Present work
C	6	0.31	0.31	0.27	0.31
Al	13	1.18	1.28	1.15	1.24
Cu	29	5.26	5.8	5.37	5.65
Ag	47	16.2	14.4	13.7	14.7
Au	79	38.2	38.8	38	38.5

$$\sigma_{0 \rightarrow n}^{e-e} = \frac{4}{v^2} \sum_{s_l} \int d^2 \mathbf{q}_\perp Z_{A,eff}(\mathbf{Q}_0^a) \times \frac{\left| \left\langle \psi_n(\mathbf{r}) \left| \left( 1 - \frac{v}{c} \alpha_z \right) \exp(i \mathbf{q}_0 \cdot \mathbf{r}) \right| \psi_0(\mathbf{r}) \right\rangle \right|^2}{\left( q_\perp^2 + \frac{(\omega_{n0} + \Delta \epsilon)^2}{v^2 \gamma^2} + 2(\gamma - 1) \frac{\omega_{n0} \Delta \epsilon}{v^2 \gamma^2} \right)^2}. \quad (44)$$

It is important to note that the relativistic peculiarities in the antiscreening mode are not affected by all the approximations used to obtain Eq. (44).

#### IV. RESULTS AND DISCUSSION

Table I shows a comparison between the experimental data of Claytor *et al.* [13] and theoretical results of Anholt and Becker [7], of Sørensen [11], and our calculations. In the experiment [13] the loss cross sections for Au<sup>78+</sup> ions penetrating different solid targets were measured at a collision energy of 10.8 GeV/nucleon corresponding to  $\gamma = 12.6$ . Our numerical calculations are based on Eqs. (36) and (44) where the final states of the electron of the ion are now the continuum states of the ion and where the integration over the continuum states is carried out. In order to describe the electronic states we took the same approximations for the wave functions for the bound and continuum states as those which were taken in [24], [9], and [12]. These approximations were proved to give good results even for *K*-shell ionization of heavy elements like gold and lead (see, e.g., [8,9,24]). Both

electron transitions with and without spin flip were taken into account. In order to calculate the cross section (44) we need to know a value of the averaged excitation energy of the atom  $\Delta \epsilon$ . To our knowledge, there is no strict and simple prescription to choose this parameter for multielectron atoms [1,3]. In our calculations we have set  $\Delta \epsilon = \Delta \epsilon_{SP}$ , where  $\Delta \epsilon_{SP}$  is the mean excitation energy, which is used in calculations of the stopping power. Values of  $\Delta \epsilon_{SP}$  are tabulated for a variety of atoms (see, e.g., [25], p.25). Note that in fact the accuracy of  $\Delta \epsilon$  is not crucial for the present calculations. For the electron loss from the highly charged ions, like Au<sup>78+</sup> and Pb<sup>81+</sup>, in collisions with light targets like Be, C, and Al considered here, the terms with  $\Delta \epsilon$  in Eq. (44) are of negligible importance for both ultrarelativistic cases studied experimentally in [13,10]. The latter collision is considered below (Table II). For collisions of Au<sup>78+</sup> and Pb<sup>81+</sup> with heavier targets (Cu, etc.; see Tables I and II) the electron-electron contribution to the total loss cross section is already only a very small correction, less than 3–4 %, to the elastic contribution [26]. Therefore there is no need in the present calculations to use more exact values for the parameter  $\Delta \epsilon$ .

It follows from Table I that there is no significant difference between the experimental data and all the calculations as well as between different calculations at an incident energy of 10.8 GeV/nucleon.

The situation is changed noticeably for the higher-energy case studied experimentally in [10]. In this experiment the loss cross sections for Pb<sup>81+</sup> ions were measured at a collision energy of 160 GeV/nucleon. In this case  $\gamma = 168$  is already very high and the shielding becomes important. Table II gives a comparison between the experimental data of Krause *et al.* [10] and different theoretical results. We have added a few more columns than in Table I. Calculations of Sørensen [11] are now given in two columns showing his results for the loss cross sections in collisions with a bare atomic nucleus and a neutral atom, respectively. Our calculations are also given in two columns. The first of the two columns presents the results for the electron loss cross sections in collisions with a bare atomic nucleus, when there is no screening effect and no electron-electron contribution and when the cross section is proportional to  $Z_A^2$ . The second column is for collisions with a neutral atom calculated with Eqs. (36) and (44) where both the screening effect of the atomic electrons in the elastic contribution, which reduce the loss cross section, and the electron-electron contribution, in-

TABLE II. Experimental and theoretical cross sections (in kb) for ionization of 160 GeV/nucleon Pb<sup>81+</sup> penetrating different solid targets. The ion is initially in its ground state.

Atom	$Z_A$	Experiment	Anholt and Becker		Sørensen		Present work	
			Atom	Bare nucleus	Atom	Bare nucleus	Atom	
Be	4	0.14–0.15	0.24	0.15	0.14	0.2	0.17	
C	6	0.31	0.49	0.33	0.28	0.45	0.35	
Al	13	1.3–1.4	2.0	1.6	1.1	2.14	1.42	
Cu	29	6.9–8.0	9.0	7.8	5.2	10.6	6.5	
Sn	50	15–21	25	23	15	31.5	17.6	
Au	79	42–53	60	58	35	78.7	40.1	

creasing the loss, are included.

Our results for the cross sections in collisions with atoms are considerably less than those of [7] and are in a fairly good agreement with the experimental data. Compared to calculations of [11] our results are somewhat larger, especially for collisions with a bare atomic nucleus where the difference reaches about 30%. Our results practically coincide with those obtained in [12].

A rather small difference between our results for the electron loss in collisions with neutral Be and  $\text{Be}^{4+}$  is due to the electron-electron contribution to the total cross section. For collisions with few-electron targets the antiscreening mode gives a relatively large contribution. This contribution reaches about 20% of the total electron loss in collisions with Be. Our calculations show that for 160 GeV/nucleon collisions the shielding effects in the elastic and electron-electron [27] contributions to the cross sections reduce the total electron loss cross section by a factor of 1.4 for  $\text{Pb}^{81+}$ -Be collisions and by a factor of 2 for  $\text{Pb}^{81+}$ -Au collisions.

In conclusion of this section we note that the general good agreement with the experiment at quite different values of  $\gamma$ , obtained in our calculations, gives some additional indirect justification for the use of the NRA approximation in relativistic collisions.

## V. SUMMARY

In this paper we have considered projectile electron excitation and loss in relativistic collisions with atomic targets. Our treatment of the processes is based on the first-order relativistic perturbation theory for the electromagnetic interaction of the four-current of the projectile with the four-current of the target. General expressions have been derived for the cross sections for the excitation and loss. In the limit  $c \rightarrow \infty$  these expressions go over into known nonrelativistic formulas for the corresponding cross sections. In ultrarelativistic collisions these expressions describe an important peculiarity in the shielding of the atomic nucleus by the atomic electrons. Results of our numerical calculations are in reasonable agreement with available experimental data.

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## APPENDIX

In this section we prove that in a reference frame, where the atom or the ion is initially at rest, its typical recoil velocity after the collision is not only nonrelativistic but also much less than the Bohr velocity  $v_0 = 1$  a.u. Let us consider a Coulomb collision between two bare nuclei with charges  $Z_1$  and  $Z_2$ , respectively. The nucleus with charge  $Z_1$  and mass  $M_1$  is initially at rest and the second nucleus moves with relativistic velocity  $v$  along a classical straight-line trajectory. The energy, transferred to the first nucleus in the collision, can be estimated as (see, e.g., [15])

$$\Delta E_1 = \frac{2Z_1^2 Z_2^2}{b^2 v^2 M_1}, \quad (\text{A1})$$

where  $b$  is the impact parameter of the collision. Correspondingly the recoil velocity of the first nucleus after the collision is

$$v_{rec} = \sqrt{\frac{2\Delta E_1}{M_1}} = \frac{2Z_1 Z_2}{bv M_1}. \quad (\text{A2})$$

It follows from Eq. (A2) that for fixed  $b$  and  $v$  the recoil velocity  $v_{rec}$  reaches the highest value in the collision, where the second nucleus has the largest possible charge and the first nucleus has the highest possible ratio  $Z_1/M_1$ . Choosing an uranium nucleus as the projectile and a proton as the target, for  $b_{\min} = a_1 + a_2$  ( $a_1 \sim 1$  fm  $= 2 \times 10^{-5}$  a.u. is the dimension of the proton and  $a_2 \approx 1.5 \times 10^{-4}$  a.u. is that for the uranium nucleus) and putting  $v \approx c = 137$  we have  $v_{rec, \max} \approx 4v_0$ . Impact parameters, contributing most to cross sections for transitions of the projectile electron in relativistic collisions, can be estimated as  $b \sim q_{\perp}^{-1} \sim \min(v\gamma/\omega_{n0}; 1/\kappa_i)$  (see Sec. II A), where  $\omega_{n0}$  is the electron transition frequency,  $\kappa_i$  are the atomic screening constants. Since such impact parameters are at least two orders of magnitude larger than  $\sim 10^{-4}$  a.u., one can conclude that the recoil velocity of the ion or the atom in a reference frame, where the ion or the atom is initially at rest, is negligible compared to the Bohr velocity  $v_0$ .

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