# Excitation of heavy hydrogenlike ions by light atoms in relativistic collisions with large momentum transfers

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We present a theory for excitation of heavy hydrogenlike projectile ions by light target atoms in collisions where the momentum transfers to the atom are very large on the atomic scale. It is shown that in this process the electrons and the nucleus of the atom behave as (quasi-) free particles with respect to each other and that their motion is governed by the field of the nucleus of the ion. The effect of this field on the atomic particles can be crucial for the contribution to the excitation of the ion caused by the electrons of the atom but, because of large nuclear mass, may be neglected in the contribution to the excitation due to the nucleus of the atom. The theory is applied to calculate excitation of  $Bi^{82+}(1s)$  ions in collisions with hydrogen.

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### I. INTRODUCTION

Projectile-electron excitation and loss occurring in collisions of projectile ions with atomic targets in the nonrelativistic domain of impact energies and projectile charges have been extensively studied during the past few decades (for a review, see [1,2]). Starting with pioneering articles of Bates and Griffing [3], most of the theoretical studies of these processes have been based on the first-order perturbation theory in the projectile-target interaction [4].

In contrast to nonrelativistic collisions, in the relativistic domain of collision parameters the first consistent theoretical approaches for treating projectile-electron excitation and loss was formulated relatively recently [5]. Like in the nonrelativistic domain, the simplest description of these processes is given by the first-order theory in the interaction between the projectile and the target. This theory is strictly valid provided the following conditions are fulfilled simultaneously: (i)  $Z_I \ll v$  and (ii)  $Z_A \ll v$ , where  $Z_I$  and  $Z_A$  are the atomic numbers of the projectile ion and target atom, respectively, and v is the collision velocity (atomic units are used throughout except where otherwise stated).

In the present paper we shall discuss excitation of heavy hydrogenlike projectiles in collisions with very light atoms when the condition  $Z_A \ll v$  is very well fulfilled but the atomic number of the projectile ion is so high that one has  $Z_I \simeq v$ even for collision velocities from the relativistic domain  $v \sim c$ , where *c* is the speed of light. In such a case the field of the target *per se* represents just a weak perturbation for the electron of the projectile. Nevertheless, large higher-order contributions to the projectile-electron excitation may arise "indirectly"since the strong field of the nucleus of the projectile can substantially distort the motion of the target electrons, which in turn changes the cross section for excitation.

Note that some aspects of projectile-electron excitation and loss in asymmetric collisions ( $Z_I \gg Z_A$ ) have been already considered in [6] and [7] where eikonal-like theories of these processes were formulated for the nonrelativistic [6] and relativistic [7] domains. Those theories, however, were based on the assumption that both in the initial and final channels the motion of the electrons of the atomic target is mainly driven by the field of the atomic nucleus while the field of the projectile ion just distorts somewhat this motion. In the present paper, the work on which was triggered by a recent experiment performed at GSI (Darmstadt, Germany) [8], we consider a situation in which the above assumption is no longer true. It is realized in collisions characterized by momentum transfers which are very large on the scale of the target atom. It turns out that under such a condition it is the field of the nucleus of the projectile-ion which is the main driving force in the collision, not only for the electron of the projectile but also for those of the atomic target.

The paper is organized as follows. In the next section, based on the first-order theory in the projectile-target interaction, we show that in collisions with large momentum transfers the electrons and the nucleus of the target atom act in the excitation process incoherently behaving like quasifree particles with respect to each other. In this section we also show that in such collisions the motion of the particles constituting the atom is driven primarily by the field of the nucleus of the ion and that this field may strongly affect the motion of the atomic electrons. As a result, a better (compared to the first order) treatment of the excitation can be obtained by describing the electrons of the atom in their initial and final states as moving in the field of the nucleus of the ion.

Since the electrons and the nucleus of the atom excite the ion independently and the excitation by the nucleus is very simply related to the excitation by a proton, in Secs. III and IV we present treatments for the excitation by proton and electron impacts, respectively. In Sec. V the theory is illustrated by calculating cross sections for excitation of  $Bi^{82}(1s)$  ions in relativistic collisions with hydrogen.

## II. SOME PECULIARITIES OF EXCITATION OF A HEAVY ION IN COLLISIONS WITH LIGHT ATOMS

Let us consider excitation of a heavy hydrogenlike ion in collisions with a light atom. For the moment we shall assume, for the sake of simplicity, that the atom consists of a nucleus with a charge  $Z_A$  and just one electron.

It can be shown (see, e.g., [9]) that within the first-order approximation in the ion-atom interaction the cross section for

the ion-atom collision reads

$$\frac{d^{2}\sigma_{0\to n}^{0\to m}}{d^{2}\mathbf{q}_{\perp}} = \frac{4}{v^{2}} \frac{\left| \left(F_{0}^{I} + \frac{v}{c}F_{3}^{I}\right) \left(F_{A}^{0} + \frac{v}{c}F_{A}^{3}\right) + \frac{F_{3}^{I}F_{A}^{3}}{\gamma^{2}} + \frac{F_{1}^{I}F_{A}^{1} + F_{2}^{I}F_{A}^{2}}{\gamma} \right|^{2}}{\left(\mathbf{q}_{i}^{2} - \frac{(\varepsilon_{n} - \varepsilon_{0})^{2}}{c^{2}}\right)^{2}}.$$
(1)

Here,  $\varepsilon_0$  and  $\varepsilon_n$  are initial and final internal energies of the ion, respectively, and  $\mathbf{q}_i$  is the three-momentum transferred to the ion; all the quantities are given in the rest frame of the ion. We also introduce quantities  $\epsilon_0$ ,  $\epsilon_m$ , and  $\mathbf{q}_a$  which have similar meanings but are for the atom and given in the rest frame of the atom. The momentum transfers are defined by  $\mathbf{q}_i = (\mathbf{q}_{\perp}, q_{\min}^i)$  and  $\mathbf{q}_a = (-\mathbf{q}_{\perp}, -q_{\min}^a)$ , where  $\mathbf{q}_{\perp}$  is the two-dimensional part of the momentum transferred to the atom, which is perpendicular to the collision velocity  $\mathbf{v}$ , and the components of the momentum transfers along the collision velocity read

$$q_{\min}^{i} = \frac{\varepsilon_{n} - \varepsilon_{0}}{v} + \frac{\epsilon_{m} - \epsilon_{0}}{v\gamma},$$

$$q_{\min}^{a} = \frac{\epsilon_{m} - \epsilon_{0}}{v} + \frac{\varepsilon_{n} - \varepsilon_{0}}{v\gamma},$$
(2)

where  $\gamma = 1/\sqrt{1 - v^2/c^2}$  is the collisional Lorentz factor. The inelastic four-component form factor of the ion (in the ion frame) and the four-component form factor of the atom (in the atom frame) are given by

$$F_0^I \equiv F_0^I(\mathbf{q}_i) = -\langle \varphi_n | \exp(i\mathbf{q}_i \cdot \mathbf{r}) | \varphi_0 \rangle,$$
  

$$F_l^I \equiv F_l^I(\mathbf{q}_i) = \langle \varphi_n | \exp(i\mathbf{q}_i \cdot \mathbf{r}) \alpha_l | \varphi_0 \rangle,$$
(3)

$$F_A^0 \equiv F_A^0(\mathbf{q}_a) = Z_A \delta_{m0} - \langle u_m | \exp(i\mathbf{q}_a \cdot \boldsymbol{\xi}) | u_0 \rangle,$$
  

$$F_A^l \equiv F_A^l(\mathbf{q}_a) = -\langle u_m | \alpha_l \exp(i\mathbf{q}_a \cdot \boldsymbol{\xi}) | u_0 \rangle,$$
(4)

respectively (l = 1, 2, 3). In Eq. (3)  $\varphi_0 = \varphi_0(\mathbf{r})$  and  $\varphi_n = \varphi_n(\mathbf{r})$  are the initial and final internal states of the ion,  $\mathbf{r}$  the coordinates of the ion electron with respect to the ion nucleus, and  $\alpha_l$  the Dirac matrices for the electron of the ion. In Eq. (4)  $u_0 = u_0(\boldsymbol{\xi})$  and  $u_m = u_m(\boldsymbol{\xi})$  are the initial and final internal states of the atom, and  $\boldsymbol{\xi}$  are the coordinates of the atomic electron with respect to the atomic nucleus.

If one is interested only in the electron transitions in the ion, without knowing what happens to the atom in the collision, then one has to consider the cross section

$$\frac{d^2\sigma_{0\to n}}{d^2\mathbf{q}_{\perp}} = \sum_{m} \frac{d^2\sigma_{0\to m}^{0\to m}}{d^2\mathbf{q}_{\perp}},\tag{5}$$

where the sum runs over all possible internal states of the atom including its initial state and the atomic continuum. The cross section (5) can be conveniently written as the sum of the contributions from the elastic (m = 0) and inelastic ( $m \neq 0$ ) atomic collision modes

$$\frac{d^2\sigma_{0\to n}}{d^2\mathbf{q}_{\perp}} = \frac{d^2\sigma_{0\to n}^{0\to 0}}{d^2\mathbf{q}_{\perp}} + \sum_{m\neq 0} \frac{d^2\sigma_{0\to n}^{0\to m}}{d^2\mathbf{q}_{\perp}},\tag{6}$$

where the sum over  $m \neq 0$ , which represents the contribution from the inelastic atomic mode, includes also the sum over the continuum states of the atom.

In collisions resulting in excitation of heavy hydrogenlike ions the momentum transfer to the atom  $q_a$  can, under certain conditions, be much larger than the typical momentum  $(\simeq Z_A)$  of the electron bound in the atom. From the second equation in (2) one may see that this will be the case when  $(\varepsilon_n - \varepsilon_0)/(v\gamma) \gg Z_A$ . Taking into account that  $\varepsilon_n - \varepsilon_0 \sim Z_I^2$ we obtain that provided the condition

$$\frac{Z_I^2}{Z_A} \gg v\gamma \tag{7}$$

is fulfilled, the collision will always be characterized by momentum transfers to the atom which are very large on its scale. This enables one to greatly simplify and, as we shall see below, also to improve the description of the excitation of the ion. In what follows we shall assume that the condition (7) is fulfilled.

Let us first consider the elastic atomic mode. In this mode, because of the rapidly oscillating exponent  $\exp(i\mathbf{q}_a \cdot \boldsymbol{\xi})$ , the elastic form factors of the atom can be approximated by  $F_A^0 = Z_A - \langle u_0 | \exp(i\mathbf{q}_a \cdot \boldsymbol{\xi}) | u_0 \rangle \approx Z_A$  and  $F_A^l = -\langle u_0 | \alpha_l \exp(i\mathbf{q}_a \cdot \boldsymbol{\xi}) | u_0 \rangle \approx 0$ , respectively. Then, taking into account (1), we obtain

$$\frac{d^2 \sigma_{0 \to n}^{0 \to 0}}{d^2 \mathbf{q}_{\perp}} = \frac{4Z_A^2}{v^2} \frac{\left| \left\langle \varphi_f \left| \exp(i\mathbf{q}_0 \cdot \mathbf{r}) \left( 1 - \frac{v}{c} \alpha_3 \right) \right| \varphi_i \right\rangle \right|^2}{[\mathbf{q}_{\perp}^2 + (\varepsilon_n - \varepsilon_0)^2 / (v^2 \gamma^2)]^2}, \quad (8)$$

where  $\mathbf{q}_0 = (\mathbf{q}_{\perp}, (\varepsilon_n - \varepsilon_0)/v)$ .

Let us now turn to the inelastic atomic mode. The rapidly oscillating term  $\exp(i\mathbf{q}_a \cdot \boldsymbol{\xi})$  in the inelastic form factors (4) of the atom tends to make their magnitude very small unless its oscillations are compensated by similar oscillations in the final atomic state. For this the latter has to be a continuum state, in which the momentum  $\mathbf{k}_a$  of the electron emitted from the atom is approximately equal to  $\mathbf{q}_a$ . Since in order to balance large  $\mathbf{q}_a$  the absolute value of the momentum of the emitted electron has to be as large (and thus  $k_a \gg Z_A$ ) the state of this electron can be to a good approximation described by replacing the Coulomb atomic wave by the corresponding plane wave.

The simultaneous realization of the conditions  $\mathbf{k}_a \approx \mathbf{q}_a$  and  $k_a \gg Z_A$  physically means that the electron of the atom in the collision process can be treated as quasifree with respect to the nucleus of the atom. The fact that initially the electron was bound is reflected merely by the Compton profile of the state  $u_0$ . Note that this profile appears in the consideration in a natural way once the final atomic state has been approximated by a plane wave.

Based on the above considerations of the elastic and inelastic atomic modes we arrive at a rather simple picture of the collision process. In this picture, due to very large momentum transfers involved, the excitation of the ion is produced by the independent (incoherent) actions of the two quasifree particles—the nucleus and the electron—constituting initially the atom.

One has, however, to keep in mind the following. Large momentum transfers are associated with a very large difference between the initial and final energies of the electron of the ion. This difference is in turn the consequence of a very high charge of the nucleus of the ion. Because of the latter the field produced by the nucleus of the ion in the collision can be so strong that it may determine the character of the motion of the electron of the atom.

In order to see this let us make some simple estimates. This is convenient to do in the rest frame of the ion. The range of impact parameters  $b_e$  of the incident atomic electron with respect to the nucleus of the ion, which are typical for the excitation process, can be roughly estimated by comparing the collision time  $T \sim b_e / \gamma_e v_e$  ( $v_e \approx v$  is the velocity of the atomic electron with respect to the nucleus of the ion and  $\gamma_e \approx$  $\gamma$  the corresponding Lorentz factor) with the transition time  $\tau \sim Z_I^{-2}$  of the electron of the ion. Since for the excitation to proceed effectively one needs  $T \lesssim \tau$ , we obtain  $b_e \lesssim \gamma_e v_e / Z_I^2$ . On the other hand, by comparing the force, which acts between the atomic electron and the nucleus of the atom, with the force exerted on this electron by the nucleus of the ion, we see that the latter will be the dominant one when the atomic electron enters the sphere, which is centered on the nucleus of the ion and has the radius  $R_I = R_A \sqrt{Z_I/Z_A}$  (where  $R_A \simeq 1/Z_A$  is the size of the atom). Therefore, provided the inequality  $b_e \ll R_I$ , which can be written in the form

$$\sqrt{\frac{Z_I}{Z_A}} \frac{Z_I^2}{Z_A} \gg \gamma v, \tag{9}$$

is fulfilled the motion of the atomic electron in the projectileelectron excitation process will be predominantly governed by the field of the nucleus of the ion. Comparing (9) and (7) and taking into account that  $\sqrt{Z_I/Z_A} > 1$  (or  $\gg 1$ ), we see that in collisions with momentum transfers, which are very large on the scale of the atom, the condition (9) is indeed always fulfilled.

Provided the condition (7) is fulfilled, the main interaction acting on the nucleus of the atom in the collision process is of course also due to the field of the nucleus of the ion.

A simple estimate for the magnitude of the effect of the field of the ionic nucleus on the motion of the electrons and the nucleus of the atom in the process of excitation can be obtained in the following way. Assume that there is a particle with a charge z and mass m which is incident with a velocity v on the nucleus  $Z_I$ . The change in the momentum of this particle caused by the field of  $Z_I$  is roughly given by  $q \sim Z_I z/(bv)$ , where b is the impact parameter. For the problem of excitation the typical impact parameters are of the order of  $1/Z_I$  or larger. One can estimate the effect of the field by using the ratio  $\varsigma = |q|/p_i$ , where  $p_i = m\gamma v$  is the initial momentum of the incident particle and, thus,

$$\varsigma = \frac{|z|}{m\gamma} \frac{Z_I^2}{v^2}.$$
 (10)

From this estimate it is obvious that for the impact energies of interest the field of the nucleus of the ion does not really affect the motion of the nucleus of the atom  $(|z|/m_N\gamma < 10^{-3})$  but may very strongly change the motion of the atomic electrons  $(|z|/m_e\gamma < 1)$ .

The first-order cross section (1), with which we have started our current discussion, of course does not take into account the effect of the nucleus of the ion on the motion of the electrons of the atom. Besides, this cross section also does not account for the exchange effect of the atomic and ionic electrons. We, however, have already seen that in very asymmetric collisions the general two-center problem of excitation can be reduced to a single-center one in which only one center of force—the nucleus of the ion—is effectively present. Therefore, one can improve the description of the excitation process in collisions with large momentum transfers if, instead of regarding the atomic electrons as (quasi-) free, we would treat these electrons, both in their initial and final states, as moving in the field of the nucleus of the ion and, besides, would take into account the exchange effect.

In such an approach the cross section  $\sigma_A$  for the excitation of a heavy highly charged ion in collisions with an atom is given by the incoherent addition of the cross sections for excitation by the impacts of the atomic nucleus and electrons:

$$\sigma_A = Z_A^2 \sigma_p + Z_A \sigma_e, \tag{11}$$

where  $\sigma_p$  and  $\sigma_e$  are the cross sections for excitation by proton and electron, respectively. This means that, if one would be able to compute the cross sections for the excitation by protons and electrons, one could use them for evaluating excitation cross sections in collisions with atoms [10]. Therefore, in the next two sections we shall discuss excitation of heavy hydrogenlike ions in collisions with protons and electrons.

### **III. EXCITATION IN COLLISIONS WITH PROTONS**

Let us first consider the excitation of a heavy hydrogen-like ion by protons. The charge of the proton is much smaller than that of the highly charged nucleus of the ion. This means that the interaction between the proton and the electron of the ion in the process of excitation is much weaker than the interaction between the electron and the ionic nucleus and, hence, can be treated as a weak perturbation. Further, the proton mass is much heavier than that of the electron and, as was already mentioned, for collision energies of interest for the present study the influence of the field of the ionic nucleus on the proton motion can be ignored. Therefore, regarding the proton as a Dirac particle, one can approximate the initial and final states of the proton by (Dirac) plane waves.

In our consideration the nucleus of the ion will be taken as infinitely heavy representing, thus, just an external field. We shall work in the rest frame of this nucleus and choose its position as the origin.

Taking all the above into account the transition amplitude for the excitation of the ion by proton impact can be written according to

$$S_{\rm fi}^{\rm pr} = -\frac{i}{c^2} \int d^4x \int d^4y \, j_\mu(x) \, D^{\mu\nu}(x-y) J_\nu(y). \tag{12}$$

Here,  $j_{\mu}(x)$  and  $J_{\nu}(y)$   $(\mu, \nu = 0, 1, 2, 3)$  are the electromagnetic transition four-currents generated by the electron of the ion at a space-time point x and by the proton at a space-time point y, respectively, and  $D^{\mu\nu}(x - y)$  is the propagator of the electromagnetic field which transmits the interaction between these particles. The contravariant  $a^{\mu}$  and covariant  $a_{\mu}$  fourvectors are given by  $a^{\mu} = (a^0, \mathbf{a})$  and  $a_{\mu} = (a^0, -\mathbf{a})$ . The metric tensor  $g_{\mu\nu}$  of the four-dimensional space is defined by  $g_{00} = -g_{11} = -g_{22} = -g_{33} = 1$  and  $g_{\mu\nu} = 0$  for  $\mu \neq \nu$ . In (12) the summation over the repeated Greek indices is implied.

The transition currents of the electron and proton are given by

$$j_{\mu}(x) = -c\overline{\psi}_{f}(\mathbf{r},t)\gamma_{\mu}\psi_{i}(\mathbf{r},t)$$
(13)

and

$$J_{\mu}(y) = c\overline{\Psi}_{f}(\mathbf{R}, T)\gamma_{\mu}\Psi_{i}(\mathbf{R}, T), \qquad (14)$$

respectively, where  $\gamma_{\mu}$  are the gamma matrices. In Eq. (14) the vector  $\mathbf{r}_e$  denotes the electron coordinates, and  $\psi_i(\mathbf{r}_e,t) = \varphi_i(\mathbf{r}_e) \exp(-i\varepsilon_i t)$  and  $\psi_f(\mathbf{r}_e,t) = \varphi_f(\mathbf{r}_e) \exp(-i\varepsilon_f t)$  are the initial and final states of the electron with total energies  $\varepsilon_i$  and  $\varepsilon_f$ , respectively. These states describe the motion of the electron in the field of the nucleus of the ion.

Further, **R** are the coordinates of the proton,  $\Psi_i(\mathbf{R}, T) = \phi_i(\mathbf{R}) \exp(-iE_iT)$  and  $\Psi_f(\mathbf{R}, T) = \phi_f(\mathbf{R}) \exp(-iE_fT)$  are the initial and final states of the proton with corresponding total energies  $E_i$  and  $E_f$ . These states describe a free proton with a given value of spin projection.

By applying the Fourier transformation to the currents and the photon propagator in the integrand of (12) the transition amplitude can be rewritten in a more convenient form,

$$S_{\rm fi}^{\rm pr} = -\frac{4\pi i}{c^3} \int d^4q \, \tilde{j}_{\mu}(q) \frac{1}{q^2 + i0} \tilde{J}^{\mu}(-q), \tag{15}$$

where

$$\widetilde{j}_{\mu}(q) = \frac{1}{4\pi^2} \int d^4x \ j_{\mu}(x) \exp(-iqx)$$

$$= \frac{1}{2\pi} \delta(q_0 + (\varepsilon_i - \varepsilon_f)/c) \int d^3 \mathbf{r} \ \overline{\varphi}_f(\mathbf{r}) \gamma_{\mu}$$

$$\times \exp(i\mathbf{q} \cdot \mathbf{r}) \varphi_i(\mathbf{r}),$$

$$\widetilde{J}_{\mu}(-q) = \frac{1}{4\pi^2} \int d^4y \ J_{\mu}(y) \exp(iqy)$$

$$= \frac{1}{2\pi} \delta(q_0 - (E_i - E_f)/c) \int d^3 \mathbf{R} \ \overline{\phi}_f(\mathbf{R}) \gamma_{\mu}$$

$$\times \exp(-i\mathbf{q} \cdot \mathbf{R}) \phi_i(\mathbf{R}). \tag{16}$$

Due to the relatively large mass of the proton the change in its initial momentum caused by the collision is much smaller than the initial momentum itself. As a result, the proton not only moves in the collision practically along a straight line but also, as one can easily show, the change in the direction of its spin is very unlikely. Taking this into account, assuming for definiteness that initially the proton moves along the *z* axis and using the explicit form of the Dirac plane-wave states for the proton the expression for the four-current  $\tilde{J}_{\mu}(-q)$  in (16) can be greatly simplified:

$$\widetilde{J}_{0}(-q) = \frac{1}{2\pi} \delta(q_{0} - (E_{i} - E_{f})/c) \delta^{(3)}(\mathbf{P}_{i} - \mathbf{q} - \mathbf{P}_{f}), 
\widetilde{J}_{3}(-q) = \frac{v}{2\pi c} \delta(q_{0} - (E_{i} - E_{f})/c) \delta^{(3)}(\mathbf{P}_{i} - \mathbf{q} - \mathbf{P}_{f}), 
\widetilde{J}_{1}(-q) = 0, \quad \widetilde{J}_{2}(-q) = 0.$$
(17)

In the above equations  $\mathbf{P}_i = (0, 0, P_i)$  and  $\mathbf{P}_f$  are the initial and final momenta of the proton, respectively,  $(|\mathbf{P}_i - \mathbf{P}_f| \ll |\mathbf{P}_i|)$  and v is the proton velocity with respect to the nucleus, which to excellent accuracy remains a constant in the collision.

Using Eqs. (15) and (17) and the expression for the electron transition current from Eq. (16) the transition amplitude is

obtained to be

$$S_{\rm fi}^{\rm pr} = \frac{i}{\pi} \frac{\delta(\varepsilon_i + E_i - \varepsilon_f - E_f)}{\mathbf{q}^2 - (\varepsilon_f - \varepsilon_i)^2/c^2} \\ \times \int d^3 \mathbf{r} \, \varphi_f^{\dagger}(\mathbf{r}) \exp(i\mathbf{q} \cdot \mathbf{r}) \left(1 - \frac{v}{c}\alpha_3\right) \varphi_i(\mathbf{r}) \\ = \frac{i}{\pi} \delta(\varepsilon_i + E_i - \varepsilon_f - E_f) \frac{\langle \varphi_f | \exp(i\mathbf{q} \cdot \mathbf{r}) (1 - \frac{v}{c}\alpha_3) | \varphi_i \rangle}{\mathbf{q}^2 - (\varepsilon_f - \varepsilon_i)^2/c^2},$$
(18)

where  $\mathbf{q} = \mathbf{P}_i - \mathbf{P}_f$  is the momentum transfer to the ion,  $\alpha_3$  is the Dirac matrix, and the delta function expresses the energy conservation in the collision.

Using the well-known procedure in order to obtain the cross section from the transition amplitude for the excitation cross section differential in the momentum transfer we get

$$\frac{d^{3}\sigma_{\rm fi}}{d\mathbf{q}^{3}} = \frac{4}{v} \frac{\left|\left\langle\varphi_{f}\left|\exp(i\mathbf{q}\cdot\mathbf{r})\left(1-\frac{v}{c}\alpha_{3}\right)\right|\varphi_{i}\right\rangle\right|^{2}}{[\mathbf{q}^{2}-(\varepsilon_{f}-\varepsilon_{i})^{2}/c^{2}]^{2}} \times \delta(\varepsilon_{i}+E_{i}-\varepsilon_{f}-E_{f}).$$
(19)

In the above consideration we have already used the fact that the change in the momentum of the proton caused by the collision is very small compared to its initial value. Using this fact again one can show that, to an excellent accuracy, the change in the proton energy is very simply related to the z component,  $q_z$ , of the momentum transfer vector  $\mathbf{q}$ :  $E_i - E_f = vq_z$ . This enables us to integrate the cross section (19) over  $q_z$ and obtain

$$\frac{d^2\sigma_{\rm fi}}{d\mathbf{q}_{\perp}^2} = \frac{4}{v^2} \frac{\left|\left\langle\varphi_f \left|\exp(i\mathbf{q}_0\cdot\mathbf{r})\left(1-\frac{v}{c}\alpha_3\right)\right|\varphi_i\right\rangle\right|^2}{\left[\mathbf{q}_0^2 - (\varepsilon_f - \varepsilon_i)^2/c^2\right]^2},\qquad(20)$$

where

$$\mathbf{q}_0 = (\mathbf{q}_\perp, q_{\min}), \qquad (21)$$

with  $\mathbf{q}_{\perp}$  being the transverse part of the momentum transfer  $(\mathbf{q}_{\perp}\cdot\mathbf{v}=0)$  and

$$q_{\min} = \frac{\varepsilon_f - \varepsilon_i}{v} \tag{22}$$

is the minimum momentum transfer in the collision. It is not difficult to see that the only difference between the cross section (8), obtained in the previous section, and the cross section (20) and is that the latter was derived by assuming  $Z_A = 1$ .

The initial and final bound states of the electron in (20) are given by

$$\varphi_{i}(\mathbf{r}_{e}) = \begin{pmatrix} g_{n_{i}\kappa_{i}}(r_{e}) & \chi_{\kappa_{i}}^{\mu_{i}}(\hat{\mathbf{r}}_{e}) \\ if_{n_{i}\kappa_{i}}(r_{e}) & \chi_{-\kappa_{i}}^{\mu_{i}}(\hat{\mathbf{r}}_{e}) \end{pmatrix}$$
(23)

and

$$\varphi_f(\mathbf{r}_{\mathbf{e}}) = \begin{pmatrix} g_{n_f \kappa_f}(r_e) & \chi_{\kappa_f}^{\mu_f}(\hat{\mathbf{r}}_{\mathbf{e}}) \\ i f_{n_f \kappa_f}(r_e) & \chi_{-\kappa_f}^{\mu_f}(\hat{\mathbf{r}}_{\mathbf{e}}) \end{pmatrix},$$
(24)

respectively. In Eqs. (23) and (24)  $g_{n\kappa}$  ( $f_{n\kappa}$ ) are the large (small) components of the radial Dirac-Coulomb states of the electron in the field of the nucleus with a charge  $Z_1$ .

If we denote  $\zeta = Z_I \alpha$ , where  $\alpha = e^2/\hbar c = 1/137.04$  is the fine structure constant, and  $\Lambda = \sqrt{\kappa^2 - \zeta^2}$ , then the energies

and the radial wave functions of the bound states are given, respectively, by (see, e.g., [11])

$$\varepsilon = mc^2 \left[ 1 + \left(\frac{\zeta}{n' + \Lambda}\right)^2 \right]^{-\frac{1}{2}}$$
(25)

and

$$\begin{cases} g_{n\kappa} \\ f_{n\kappa} \end{cases} = \pm (1 \pm \varepsilon/mc^2)^{\frac{1}{2}} \frac{\sqrt{2}k^{\frac{5}{2}}\lambda_e}{\Gamma(2\Lambda+1)} \\ \times \left(\frac{\Gamma(2\Lambda+n'+1)}{n'!\zeta(\zeta-\kappa k\lambda_e)}\right)^{1/2} (2kr)^{\Lambda-1}e^{-kr} \\ \times \left[ \mp n'_1F_1(-n'+1,2\Lambda+1;2kr) \\ - \left(\kappa - \frac{\zeta}{k\lambda_e}\right)_1F_1(-n',2\Lambda+1;2kr) \right].$$
(26)

Here,  $\Gamma(x)$  and  ${}_{1}F_{1}(a,b;z)$  are the gamma function and confluent hypergeometric function [12], respectively,  $\lambda_{e} = \hbar/mc$  is the electron Compton wavelength,  $k = \frac{\zeta}{\lambda_{e}}[\zeta^{2} + (n' + \Lambda)^{2}]^{-\frac{1}{2}}$ ,  $n = n' + |\kappa|$  is the principal quantum number, and the quantity  $\kappa$  is related to the orbital momentum l and the total angular momentum j by

$$l = \begin{cases} \kappa, & \text{if } \kappa > 0\\ -\kappa - 1 & \text{if } \kappa < 0 \end{cases} \text{ and } j = |\kappa| - \frac{1}{2}. \quad (27)$$

Further,  $\chi_{\kappa}^{\mu}$  are the normalized spin-angular functions (see, e.g., [11]) which read

$$\chi^{\mu}_{\kappa}(\hat{\mathbf{r}}_{\mathbf{e}}) = \sum_{m_l} \begin{pmatrix} l & \frac{1}{2} \\ m_l & \mu - m_l \end{pmatrix} Y^*_{lm_l}(\hat{\mathbf{r}}_{\mathbf{e}}) \chi^{\mu - m_l}_{\frac{1}{2}}, \quad (28)$$

where

$$\chi_{\frac{1}{2}}^{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{\frac{1}{2}}^{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$
 (29)

are the Pauli spinors and  $Y_{lm_l}$  are the spherical harmonics.

# IV. EXCITATION IN COLLISIONS WITH ELECTRONS

Let us now turn to the excitation of a heavy hydrogenlike ion by electron impact. As in the previous section we assume that the nucleus of the ion is infinitely heavy and taken as the origin.

Like in the case of collisions with protons, the interaction between the incident electron and the electron of the ion is comparatively very weak. Therefore, this interaction can be treated as arising due to just single-photon exchange between the electrons.

However, as was already mentioned, there are two important differences between the excitation of a highly charged ion by proton and electron impacts. First, the mass of an electron is much lighter than that of a proton. As a result, in contrast to the proton case, the motion of the incident (and scattered) electron can be very substantially distorted by its interaction with the nucleus of the ion. Second, since the electrons are indistinguishable, the exchange effect has to be taken into account. The first point can be addressed by describing not only the bound but also the continuum electron as moving in the Coulomb field of the nucleus of the ion. The second point leads to the necessity to include an additional first order diagram (the so-called exchange diagram) into the theoretical treatment of electron-impact excitation.

Taking all the above into account the transition amplitude for electron-impact excitation is given by

$$S_{\rm fi}^{\rm tot} = S_{\rm fi}^{\rm dir} + S_{\rm fi}^{\rm exc},\tag{30}$$

where  $S_{\rm fi}^{\rm dir}$  and  $S_{\rm fi}^{\rm exc}$  are the direct and exchange contributions, respectively, to the total transition amplitude.

Similarly to the case of proton impact for the direct contribution one can obtain

$$S_{\rm fi}^{\rm dir} = -\frac{4\pi i}{c^3} \int d^4q \, \tilde{j}_{\mu}^{\rm dir}(q) \frac{1}{q^2 + i0} \tilde{J}_{\rm dir}^{\mu}(-q), \qquad (31)$$

where

$$\widetilde{j}_{\mu}^{\text{dir}}(q) = \frac{1}{2\pi} \delta(q_0 + (\varepsilon_i - \varepsilon_f)/c) \\ \times \int d^3 \mathbf{r} \, \overline{\varphi}_f(\mathbf{r}) \gamma_\mu \exp(i\mathbf{q} \cdot \mathbf{r}) \varphi_i(\mathbf{r})$$
(32)

describes the current generated by the electron in its boundbound transition in the ion and

$$\widetilde{J}_{\mu}^{\text{dir}}(-q) = \frac{1}{2\pi} \delta(q_0 - (E_i - E_f)/c) \\ \times \int d^3 \mathbf{r} \,\overline{\varphi}_{\mathbf{p}_f}(\mathbf{r}) \gamma_{\mu} \exp(-i\mathbf{q} \cdot \mathbf{r}) \varphi_{\mathbf{p}_i}(\mathbf{r}) \quad (33)$$

represent the current generated by the incident and scattered electron with asymptotic momenta  $\mathbf{p}_i$  and  $\mathbf{p}_f$ , respectively (continuum-continuum transition).

The exchange part of the transition amplitude reads

$$S_{\rm fi}^{\rm exc} = +\frac{4\pi i}{c^3} \int d^4 q \, \tilde{j}_{\mu}^{\rm exc}(q) \frac{1}{q^2 + i0} \, \tilde{J}_{\rm exc}^{\mu}(-q). \tag{34}$$

In this expression

$$\widetilde{j}_{\mu}^{\text{exc}}(q) = \frac{1}{2\pi} \delta(q_0 + (\varepsilon_i - E_f)/c) \\ \times \int d^3 \mathbf{r} \,\overline{\varphi}_{\mathbf{p}_f}(\mathbf{r}) \gamma_\mu \exp(i\mathbf{q} \cdot \mathbf{r}) \varphi_i(\mathbf{r}) \quad (35)$$

describes the current generated by the electron, which was initially bound in the ion and emitted during the collision having asymptotically a momentum  $\mathbf{p}_f$  (bound-continuum transition). Further,

$$\widetilde{J}_{\mu}^{\text{exc}}(-q) = \frac{1}{2\pi} \delta(q_0 - (E_i - \varepsilon_f)/c) \\ \times \int d^3 \mathbf{r} \,\overline{\varphi}_f(\mathbf{r}) \gamma_\mu \exp(-i\mathbf{q} \cdot \mathbf{r}) \varphi_{\mathbf{p}_i}(\mathbf{r})$$
(36)

represent the current generated by the electron, which was initially incident on the ion with an asymptotic momentum  $\mathbf{p}_i$  and become bound in the collision (continuum-bound transition).

In the above expressions the form of the bound states is given, as before, by Eqs. (23)–(27). The continuum states [the incident and scattered electron(s)] are described using

the corresponding Dirac wave function in the Coulomb field of the nucleus of the ion.

Namely, for the incident electron which propagates initially in the positive *z*-axis direction  $[\mathbf{p}_i = (0,0,p_i)]$  and has spin projection  $m_s$  one has

$$\psi_i^{(m_s)}(\mathbf{r},t) = e^{-iE_it} \sqrt{\frac{\pi c^2}{2p_i E_i}} \sum_{\kappa_i} i^l \sqrt{4\pi (2l+1)} \begin{pmatrix} l & \frac{1}{2} & j_i \\ 0 & m_s & m_s \end{pmatrix}$$
$$\times e^{i\Delta_{\kappa_i}} \begin{pmatrix} g_{E_i\kappa_i}(r) & \chi_{\kappa_i}^{m_s}(\hat{\mathbf{r}}) \\ if_{E_i\kappa_i}(r) & \chi_{-\kappa_i}^{m_s}(\hat{\mathbf{r}}) \end{pmatrix}.$$
(37)

The state of the scattered electron, which asymptotically has a momentum  $\mathbf{p}_f$  and spin projection  $m_s$ , reads

$$\psi_{f}^{(m_{s})}(\mathbf{r},t) = e^{-iE_{f}t} 4\pi \sqrt{\frac{\pi c^{2}}{2p_{f}E_{f}}} \sum_{\kappa_{f}\mu_{f}} i^{l} \begin{pmatrix} l & \frac{1}{2} & j_{f} \\ m_{l} & m_{s} & \mu_{f} \end{pmatrix}$$
$$\times e^{-i\Delta_{\kappa_{f}}} Y_{lm_{l}}^{*}(\hat{\mathbf{p}}_{f}) \begin{pmatrix} g_{E_{f}\kappa_{f}}(r) & \chi_{\kappa_{f}}^{\mu_{f}}(\hat{\mathbf{r}}) \\ if_{E_{f}\kappa_{f}}(r) & \chi_{-\kappa_{f}}^{\mu_{f}}(\hat{\mathbf{r}}) \end{pmatrix}. \quad (38)$$

The radial wave functions  $g_{E\kappa}(r)$  and  $f_{E\kappa}(r)$  are given by

$$\begin{cases} g_{E\kappa} \\ f_{E\kappa} \end{cases} = \pm (E \pm mc^2)^{\frac{1}{2}} \frac{2p^{\frac{1}{2}}}{c\pi^{\frac{1}{2}}} (2pr)^{\Lambda-1} e^{\pi\eta/2} \frac{|\Gamma(\Lambda + i\eta)|}{\Gamma(2\Lambda + 1)} \\ \times \begin{cases} \operatorname{Re} \\ \operatorname{Im} \end{cases} e^{-ipr} e^{i\delta_{\kappa}} (\Lambda + i\eta)_1 F_1 \\ \times (\Lambda + 1 + i\eta; 2\Lambda + 1, 2ipr), \end{cases}$$
(39)

where  $\eta = \frac{Z_I E}{pc^2}$  is the Sommerfeld parameter, the Coulomb phase shift  $\delta_{\kappa}$  is defined by the relation

$$e^{2i\delta_{\kappa}} = \frac{-\kappa + ic^2\eta/E}{\Lambda + i\eta}$$

and  $\Delta_{\kappa} = \delta_{\kappa} - \arg\Gamma(\Lambda + i\eta) - \frac{\pi}{2}\Lambda$  (see [11]). In expression (39) the notations Re and Im mean that one has to take the real or the imaginary part, respectively, of its second line.

#### V. SOME NUMERICAL RESULTS AND DISCUSSION

In this section we shall briefly consider excitation of  $Bi^{82+}(1s)$  projectiles into the *L*-shell occurring in collisions with atomic hydrogen:  $Bi^{82+}(1s) + H(1s) \rightarrow Bi^{82+}(n = 2, j) + p^+ + e^-$ , where j (j = 1/2 and j = 3/2) is the total angular momentum of the electron in the final state of the Bi ion. This consideration is based on two theoretical approaches. One of them (approach I) is the first-order perturbation theory in the ion-atom interaction [see Eqs. (1)–(6)]. The other is the approach presented in this paper (approach II). It relates the cross sections in collisions with an atom to the cross sections in collisions with protons and electrons constituting the atom [see formula (11)], and fully takes into account the interaction between these electrons and the nucleus of the highly charged ion and also the electron exchange effect.

Figure 1 shows the contribution of the inelastic target mode to the excitation cross sections. The figure contains two sets of theoretical results. One of them, depicted by dash curves, was obtained by using approach I. The other one, displayed by solid curves, was calculated by employing approach II. Let



FIG. 1. Cross sections for excitation of  $Bi^{82+}(1s)$  projectiles into the *L*-shell in collisions with hydrogen in the inelastic target mode. Dash and solid curves show the results obtained using approach I and approach II, respectively. For more explanation, see the text.

us remind the reader that within the latter the inelastic target mode is simply equal to collisions with electrons.

As it follows from Fig. 1, there is a large difference between these two sets of the results with approach II yielding substantially higher cross sections. This is especially obvious in the case of the excitation of the  $1s_{1/2}-2s_{1/2}$  transition where even at an impact energy as high as  $\simeq 700$  MeV/u the difference is still of a factor of 2.

The origin of this difference may lie in the strong attraction between the electron of the atom and the nucleus of the ion which increases the probability for the atomic electron to come closer to the electron of the ion. Such a "focusing" could be especially effective namely in the excitation of the  $1s_{1/2}-2s_{1/2}$ transition since the latter needs small impact parameters in order to proceed.

In Fig. 2 we compare the cross sections for excitation of Bi<sup>82+</sup>(1s) ions by the impact of the proton and electron which have (initially) equal velocities with respect to the ion. Note that according to approach II these cross sections also correspond to the contributions to the excitation by the elastic (proton) and inelastic (electron) target modes in collisions with atomic hydrogen. It is seen that in the interval of collision velocities considered in the figure the results for excitation by electrons and protons are rather different. In particular, despite the incident protons possess kinetic energy, which is by three orders of magnitude larger than that of the equivelocity electrons, it turns out that the latter ones can be more effective in exciting the  $1s_{1/2}-2s_{1/2}$  and  $1s_{1/2}-2p_{1/2}$  transitions.

The larger efficiency of the electrons in the excitation process is most substantial for the  $1s_{1/2}-2s_{1/2}$  transition for which the electron is more efficient by a factor of 2.5 at the lower boundary of the velocity interval. The origin of this difference most likely lies in a very strong distortion of the motion of the incident electron by the field of the nucleus of the ion. While the heavy proton moves in the collision practically undeflected the strong attraction of the light incident electron by the field of the sector.



FIG. 2. Cross sections for excitation of  $Bi^{82+}(1s)$  ions into the *L*-shell by the impact of equivelocity electrons (solid curves) and protons (dash curves).

to come closer to the location of the bound electron. Since the  $1s_{1/2}$ -  $2s_{1/2}$  transition, as a nondipole one, occurs at small impact parameters, the focusing of the incident electron by the field of the nucleus may increase the chances for the excitation.

### VI. CONCLUSIONS

We have considered excitation of highly charged hydrogenlike ions in relativistic collisions with light atoms in which the momentum transfer to the atom is very large on the typical atomic scale. In the process of excitation in such collisions the nucleus and the electrons of the atom behave as quasifree particles with respect to each other and it is the field of the nucleus of the ion which is the main force acting on them. Therefore, excitation of the ion essentially proceeds via two distinct reaction pathways, which involve the collision of the electron of the ion either with the atomic nucleus or with the atomic electrons, whose contributions add up incoherently in the cross section.

Since the nucleus of the atom is much heavier than the electron, its motion remains practically not distorted by the interaction with the field of the nucleus of the ion. Because of that and also due to the condition  $Z_I \gg Z_A$  the contribution to the excitation of the ion, caused by the interaction with the nucleus of the atom, can be evaluated already within the first-order perturbation theory in the interaction between the nucleus of the atom and the projectile ion.

Contrary to this, the field of the nucleus of the projectile in collisions with large momentum transfer has a crucial impact on the motion of the electrons of the atom. Therefore, for a proper description of the excitation by atomic electrons one needs to take into account the distortion of their states both in the initial and final reaction channels. Besides, since there is in general a noticeable overlap between the phase spaces of the electron of the ion and those of the atom, the exchange effect has to be taken into account.

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- E. C. Montenegro, W. E. Meyerhof, and J. H. McGuire, Adv. At. Mol. Opt. Phys. 34, 249 (1994).
- [2] N. Stolterfoht, R. D. DuBois, and R. D. Rivarola, *Electron Emission in Heavy Ion-Atom Collisions* (Springer, Berlin, 1997).
- [3] D. R. Bates and G. Griffing, Proc. Phys. Soc. London, Sect. A 66, 961 (1953); 67, 663 (1954); 68, 90 (1955).
- [4] J. H. McGuire, Electron Correlation Dynamics in Atomic Collisions (Cambridge University Press, Cambridge, UK, 1997).
- [5] A. B. Voitkiv, N. Grün, and W. Scheid, Phys. Rev. A 61, 052704 (2000);
   A. B. Voitkiv, M. Gail, and N. Grün, J. Phys. B 33, 1299 (2000).
- [6] A. B. Voitkiv and B. Najjari, J. Phys. B 38, 3587 (2005).

- [7] A. B. Voitkiv, Phys. Rev. A 72, 062705 (2005).
- [8] A. Gumberidze and Th. Stöhlker (private communication).
- [9] A. B. Voitkiv and J. Ullrich, *Relativistic Collisions of Structured Atomic Particles* (Springer-Verlag, Berlin, 2008); A. B. Voitkiv, Phys. Rep. **392**, 191 (2004).
- [10] In general, the cross section for excitation by electron impact should be averaged over the Compton profile of the atomic electrons.
- [11] M. E. Rose, *Relativistic Electron Theory* (John Wiley and Sons, New York, 1961).
- [12] Handbook of Mathematical Functions, edited by M. Abramovitz and I. Stegun (Dover Publications, New York, 1964).