Nonperturbative and relativistic effects in projectile-electron loss in relativistic collisions with atomic targets

A. B. Voitkiv, C. Müller, and N. Grün
Institut für Theoretische Physik der Universität Giessen, Heinrich-Buff-Ring 16, Giessen, Germany

(Received 20 June 2000; published 27 October 2000)

We calculate projectile-electron loss cross sections in ultrarelativistic collisions with neutral atomic targets. To this end we employ the first-order perturbation theory and the eikonal approximation. We show that, in general, the following main effects should be included for a proper description of the projectile-electron loss in ultrarelativistic collisions: (i) the shielding effects of electrons of the neutral target, (ii) the relativistic effects in the motion of the electron in the projectile for heavy projectiles, and (iii) the nonperturbative effects in collisions with heavy targets, especially for light projectiles.

PACS number(s): 34.10.+x, 34.50.−s, 34.50.Fa

I. INTRODUCTION

We have recently developed the plane-wave Born [1] and the first-order semiclassical [2] treatments for relativistic collisions of two composite atomic systems, which both carry active electrons. Our numerical calculations [1] for total loss cross sections from ultrarelativistic Pb^{81+} projectiles showed a reasonable agreement with available experimental data [3], [4]. In those calculations we used approximate semirelativistic wave functions for describing the electron in Pb^{81+}.

In the present paper we continue to investigate projectile-electron excitation and loss in ultrarelativistic collisions with neutral atomic targets. The goals of our paper are twofold. First, we want to make first-order perturbative calculations for electron loss from Pb^{81+} using the exact relativistic Dirac wave functions to describe the electron motion in such a heavy ion as Pb^{81+}. Second, we wish also to make some nonperturbative calculations for loss cross sections. In general these effects are not expected to be very important in ultrarelativistic collisions. However, in order to get clearer ideas about the relative importance of these effects, it is necessary to perform nonperturbative calculations. One can expect that the nonperturbative effects in ultrarelativistic collisions with neutral atoms are relatively more important compared to collisions with pointlike charges because in the former case projectile-electron excitation and loss at any possible value of the Lorentz factor γ are restricted to impact parameters $b \lesssim a_0 \sim a_B$, where a_0 is the typical dimension of the neutral atom and $a_B = 1$ a.u. is the Bohr radius.

The paper is organized as follows. In Sec. II we recall the basic formulas for cross sections and transition amplitudes obtained in the first-order perturbation theory. In this section we also give nonperturbative transition amplitudes, which are exact in the limit $\gamma \to \infty$. In Sec. III we present numerical results of our first-order calculations using semi-relativistic and exact relativistic wave functions. We also give results of our nonperturbative calculations and compare calculated results with the experimental data of Refs. [3] and [5]. Atomic units are used throughout except where otherwise stated.

II. THEORY

A. Perturbative approach

Using the first-order perturbation theory, it was shown in Ref. [1] that the cross section for a process, where the projectile electron makes a transition $0 \to n$ and a final intrinsic state of the atomic target is not observed, can be approximated by

$$\sigma_{0\to n} = \frac{4}{v^2} \sum_m \int d^2\mathbf{q}_\perp \left| \langle u_m(\boldsymbol{\tau}) | Z_A - \sum_{j=1}^{Z_A} \exp(-i\mathbf{Q}_0 \cdot \boldsymbol{\xi}_j) | u_0(\boldsymbol{\tau}) \rangle \right|^2 \times \frac{\left| \langle \psi_n(\mathbf{r}) | \left(1 - \frac{v}{c}\alpha_z\right) \exp(i\mathbf{q}_0 \cdot \mathbf{r}) | \psi_0(\mathbf{r}) \rangle \right|^2}{(q_\perp^2 + (\varepsilon_n - \varepsilon_0 + \epsilon_m - \epsilon_0)^2/v^2\gamma^2 + 2(\gamma-1)(\varepsilon_n-\varepsilon_0)(\epsilon_m-\epsilon_0)/v^2\gamma^2)^2}. \quad (1)$$

Here, $\psi_0(\mathbf{r})$ and $\psi_n(\mathbf{r})$ are the initial and final ($n \neq 0$) intrinsic states of the electron in the projectile with energies ε_0 and ε_n, respectively, where $\mathbf{r}$ is the coordinate of the electron of the projectile with respect to the projectile nucleus. The states $\psi_n(\mathbf{r})$ and the coordinate $\mathbf{r}$ are given in the rest frame of the projectile. $u_0(\boldsymbol{\tau})$ and $u_m(\boldsymbol{\tau})$ are the initial and final intrinsic states of the atom with energies ϵ_0 and ϵ_m. The set of coordinates of the atomic electrons with respect to the atomic nucleus is denoted by $\boldsymbol{\tau}=\{\boldsymbol{\xi}_1,\ldots,\boldsymbol{\xi}_{Z_A}\}$ and is given in the rest frame of the atom. Z_A is the atomic number and α_z is the Dirac matrix. Further, $\mathbf{q}_0=(\mathbf{q}_\perp,q_{min})$, $\mathbf{Q}_0=(\mathbf{q}_\perp,Q_{min})$, where $q_{min}=(\varepsilon_n-\varepsilon_0)/v+(\epsilon_m-\epsilon_0)/v\gamma$ is the minimum momentum transferred to the electron of the projectile in the rest frame of the projectile and $Q_{min}=(\epsilon_m-\epsilon_0)/v+(\varepsilon_n-\varepsilon_0)/v\gamma$ is the minimum momentum transfer to the electrons of the atom in the rest frame of the atom. In Eq. (1) the summation runs over all intrinsic atomic states, including the atomic continuum.

The cross section (1) can be split into the elastic or screening ($m=0$) contribution and the electron-electron or antiscreening (all $m\neq 0$) contribution. The elastic part reads [1]

$$\sigma^{el}_{0\to n}=\frac{4}{v^2}\int d^2\mathbf{q}_\perp\, Z^2_{A,eff}(\mathbf{Q}^s_0)\times\frac{\left|\langle\psi_n(\mathbf{r})|\left(1-\frac{v}{c}\alpha_z\right)\exp(i\mathbf{q}_0\cdot\mathbf{r})|\psi_0(\mathbf{r})\rangle\right|^2}{(q^2_\perp+(\varepsilon_n-\varepsilon_0)^2/v^2\gamma^2)^2}. \quad (2)$$

Here $\mathbf{q}_0=(\mathbf{q}_\perp,(\varepsilon_n-\varepsilon_0)/v)$ and $\mathbf{Q}^s_0=(\mathbf{q}_\perp,(\varepsilon_n-\varepsilon_0)/v\gamma)$. The effective charge of the atom in the ground state is

$$Z_{A,eff}(\mathbf{Q}^s_0)=Z_A-\langle u_0(\boldsymbol{\tau})|\sum_{j=1}^{Z_A}\exp(-i\mathbf{Q}^s_0\cdot\boldsymbol{\xi}_j)|u_0(\boldsymbol{\tau})\rangle. \quad (3)$$

The effective charge (3) can be rewritten as

$$Z_{A,eff}(\mathbf{Q}^s_0)=Z_A-\int d\boldsymbol{\xi}\,\rho_{el}(\boldsymbol{\xi})\exp(-i\mathbf{Q}^s_0\cdot\boldsymbol{\xi}), \quad (4)$$

where $\rho_{el}(\boldsymbol{\xi})$ is the charge density of the electrons in the incident atom in the rest frame of the atom. Using the Moliere parametrization of the Thomas-Fermi potential [6] or the analytical Dirac-Hartree-Fock-Slater screening functions, given by Salvat *et al.* [7] for all neutral atoms, the density $\rho_{el}(\boldsymbol{\xi})$ can be written as

$$\rho_{el}(\boldsymbol{\xi})=\frac{Z_A}{4\pi\xi}\sum_{i=1}^{3}A_i\kappa_i^2\exp(-\kappa_i\xi). \quad (5)$$

Here, A_i and κ_i are constants for a given atom [6], [7]. Using Eqs. (4) and (5), the effective charge $Z_{Aeff}(\mathbf{Q}^s_0)$ is obtained to be

$$Z_{A,eff}(\mathbf{Q}^s_0)=Z_A\left[q^2_\perp+\left(\frac{\varepsilon_n-\varepsilon_0}{v\gamma}\right)^2\right]\times\sum_{i=1}^{3}\frac{A_i}{\kappa_i^2+q^2_\perp+((\varepsilon_n-\varepsilon_0)/v\gamma)^2}. \quad (6)$$

It was shown in Ref. [1] that, using the closure approximation, the electron-electron contribution to the cross section (1) can be approximately written as

$$\sigma^{e-e}_{0\to n}=\frac{4}{v^2}\int d^2\mathbf{q}_\perp Z_{A,eff}(\mathbf{Q}^a_0)\times\frac{\left|\langle\psi_n(\mathbf{r})|\left(1-\frac{v}{c}\alpha_z\right)\exp(i\mathbf{q}_0\cdot\mathbf{r})|\psi_0(\mathbf{r})\rangle\right|^2}{(q^2_\perp+(\omega_{n0}+\Delta\epsilon)^2/v^2\gamma^2+2(\gamma-1)\omega_{n0}\Delta\epsilon/v^2\gamma^2)^2}. \quad (7)$$

In Eq. (7) $\omega_{n0}=\varepsilon_n-\varepsilon_0$, $\mathbf{Q}^a_0=(\mathbf{q}_\perp,\Delta\epsilon/v+(\varepsilon_n-\varepsilon_0)/v\gamma)$, where $\Delta\epsilon$ is the average energy for transitions of atomic electrons, and $Z_{A,eff}(\mathbf{Q}^a_0)$ is given by Eq. (6) with the replacement $\mathbf{Q}^s_0\to\mathbf{Q}^a_0$. Slightly more exact results for the electron-electron contribution can be obtained by using in Eq. (7) incoherent scattering functions rather than $Z_{A,eff}(\mathbf{Q}^a_0)$. These functions are tabulated in Refs. [8], [9] for all atomic elements.

B. Nonperturbative approach

Nonperturbative effects in projectile-electron excitation and loss in ultrarelativistic collisions should be more pronounced for collisions with heavy many-electron targets. In collisions with such targets the elastic mode is known to be dominant if the dimension of the electron orbit in the projectile is much less than the dimension of the neutral target. Therefore in this section, we will neglect the electron-electron contribution and consider only the elastic mode.

In the elastic mode the atomic target is represented by an external potential. Then the many-electron problem of two colliding atomic particles is reduced to the problem of the motion of the electron of the projectile in two fields, the field of the projectile nucleus, and the field of the target atom. In the rest frame of the projectile ion nucleus the motion of the electron of the projectile obeys the Dirac equation

$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[c\boldsymbol{\alpha}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}(\mathbf{r},t)\right)+\beta mc^2-\frac{Z_pe^2}{r}+e\Phi(\mathbf{r},t)\right]\psi(\mathbf{r},t), \quad (8)$$

where $\boldsymbol{\alpha}$ and β are the Dirac matrices, $\mathbf{r}$ is the coordinate of the electron with respect to the nucleus of the ion, and Φ and $\mathbf{A}$ are the scalar and vector potentials of the incident neutral atom. In accordance with Eq. (5), we assume that in the rest frame of the atom its scalar potential is well approximated by a short-range interaction of the type

$$\Phi'=\frac{Z_A\phi(r')}{r'} \quad (9)$$

with

$$\phi=\sum_j A_j\exp(-\kappa_jr')\quad\left(\sum_j A_j=1\right). \quad (10)$$

An interaction of the type (9)–(10) can be regarded as an interaction produced by the exchange of ‘‘massive photons’’ with masses $M_j=\kappa_j$: a photon with mass M_j is emitted by a source with a charge $Z_j=Z_A A_j$ ($\Sigma_j Z_j=Z_A$).

The scalar and vector potentials of a source Z_j of massive photons with the mass M_j, which moves with relativistic velocity v, are described by the Proca equation [10]

$$\Delta\Phi_j-\frac{1}{c^2}\frac{\partial^2\Phi_j}{\partial t^2}-M_j^2\Phi_j=-4\pi Z_j\delta[\mathbf{r}-\mathbf{R}(t)],$$

$$\mathbf{A}_j=\frac{\mathbf{v}}{c}\Phi_j. \tag{11}$$

We assume that the atom is moving in the projectile frame along a straight-line trajectory $\mathbf{R}=\mathbf{b}+\mathbf{v}t$, where $\mathbf{b}=(b_x,b_y)$ is the impact parameter and $\mathbf{v}=(0,0,v)$ is the velocity of the atom. Using the Fourier transformation in order to solve Eq. (11) the solution of Eq. (11) can be written as

$$\Phi_j(\mathbf{r},t)=\frac{Z_j}{2\pi^2}\int d^3\mathbf{k}\frac{\exp(i\mathbf{k}\cdot(\mathbf{r}-\mathbf{b})-i\mathbf{k}\cdot\mathbf{v}t)}{k^2-\frac{(\mathbf{k}\cdot\mathbf{v})^2}{c^2}+M_j^2-i0}$$

$$=\frac{Z_j}{2\pi^2}\int d^2\mathbf{k}_\perp\exp[i\mathbf{k}_\perp\cdot(\mathbf{r}_\perp-\mathbf{b})]\times\int_{-\infty}^{+\infty}dk_z\frac{\exp[ik_z(z-vt)]}{k_\perp^2+k_z^2/\gamma^2+M_j^2-i0}. \tag{12}$$

The straighforward integration of Eq. (12) results in

$$\Phi_j(\mathbf{r},t)=\frac{\gamma Z_j}{\sqrt{\gamma^2(z-vt)^2+(\mathbf{r}_\perp-\mathbf{b})^2}}\times\exp(-M_j\sqrt{\gamma^2(z-vt)^2+(\mathbf{r}_\perp-\mathbf{b})^2}). \tag{13}$$

Of course, the potential (13) can be obtained directly from Eqs. (9) and (10) using the Lorentz transformation. However, the advantage of the Fourier representation (12) is that for ultrarelativistic velocities v it allows to get straightforwardly the essential simplification for the form of the scalar and vector potentials, while the limit $v\to c$ of Eq. (13) is very delicate. For infinite γ one can drop the term k_z^2/γ^2 in the integrand of Eq. (12) and write

$$\Phi_j(\mathbf{r},t)=\frac{Z_j}{2\pi^2}\int d^2\mathbf{k}_\perp\exp[i\mathbf{k}_\perp\cdot(\mathbf{r}_\perp-\mathbf{b})]\times\int_{-\infty}^{+\infty}dk_z\frac{\exp[ik_z(z-ct)]}{k_\perp^2+M_j^2-i0}$$

$$=\frac{2Z_j}{c}\delta\left(t-\frac{z}{c}\right)K_0(M_j|\mathbf{r}_\perp-\mathbf{b}|), \tag{14}$$

where δ is the delta function and K_0 is a modified Bessel function. Then we obtain for the scalar and vector potentials created by the incident atom in the rest frame of the projectile

$$\Phi(\mathbf{r},t)=\frac{2Z_A}{c}\delta\left(t-\frac{z}{c}\right)\sum_j A_jK_0(M_j|\mathbf{r}_\perp-\mathbf{b}|),$$

$$A_z(\mathbf{r},t)=\Phi(\mathbf{r},t),\quad A_x=A_y=0. \tag{15}$$

For the potentials Φ and A_z, given by Eqs. (15), the Dirac equation (8) can be solved exactly using a method proposed in Ref. [11] to calculate electron transitions caused by collisions with a pointlike charge moving with the speed of light. In our case, where the perturbing atomic field is short ranged, the exact probability amplitude a_{0n} for the electron of the projectile to make a transition $\psi_0\to\psi_n$ between the electron states ψ_0 and ψ_n of the projectile is given by

$$a_{0n}(\mathbf{b})=\delta_{0n}+\langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right)\times\left[\exp\left(\frac{2iZ_A}{c}\sum_j A_jK_0(M_j|\mathbf{r}_\perp-\mathbf{b}|)\right)-1\right]|\psi_0\rangle$$

$$\equiv\langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right)\times\exp\left(\frac{2iZ_A}{c}\sum_j A_jK_0(M_j|\mathbf{r}_\perp-\mathbf{b}|)\right)|\psi_0\rangle. \tag{16}$$

For obtaining the second line in Eq. (16) the identity $\langle\psi_n|\alpha_z\exp(i\omega_{n0}z/v)|\psi_0\rangle\equiv v/c\langle\psi_n|\exp(i\omega_{n0}z/v)|\psi_0\rangle$ (see Ref. [12]) was used. The amplitude (16) preserves the unitarity $\Sigma_{allstates}|a_{0n}(\mathbf{b})|^2\equiv1$, as it should be for an exact solution [13]. In the limit of vanishing screening ($M_j\to0$) one can use the relation $K_0(x)\approx-\ln(x/2)-\Gamma$ for $|x|\ll1$ (see e.g., Ref. [14]), where Γ is Euler's constant. Then, neglecting an inessential coordinate-independent phase factor, the transition amplitude (16) reduces to

$$a_{0n}^{Coul}(\mathbf{b})=\langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right)\times\exp\left[\frac{-iZ_A}{c}\ln\left(\frac{\mathbf{r}_\perp-\mathbf{b}}{b}\right)^2\right]|\psi_0\rangle. \tag{17}$$

The transition amplitude (17) is identical to that derived by Baltz [11] for the electron transitions in collisions with a pointlike charge.

For finite values of γ, the transition amplitude (16) is expected to give good results if the effective duration time of the interaction $T(b)\sim b/v\gamma$ is small compared to the characteristic transition time in the system $\tau\sim1/\omega_{n0}$, i.e., for impact parameters $b\ll b_0=v\gamma/\omega_{n0}$. This region of impact parameters, where the components of the four-momentum transfer $q_\mu=(q_0,\mathbf{q}_\perp,q_z)$ to the electron are related by $q_\perp^2\gg(q_z^2-q_0^2)$, is the region of the applicability of eikonal-type approximations. For collisions with neutral atoms, we have another characteristic distance, the dimension of the neutral atom a_0. If $b_0\gg a_0$, then the amplitude (16) can be used for any impact parameter because for larger impact parameters

TABLE I. Experimental and theoretical cross sections (in kb) for ionization of 160 GeV/nucleon Pb^{81+} penetrating different solid and gas targets. The ion is initially in its ground state. The targets marked with an asterisk are atomic targets used in the experiment [5].

Target	Z_2	Experiment	[19]	[18]	Present paper				
					I	II	III	IV	V
Be	4	0.14–0.15	0.24	0.14	0.14	0.17	0.12	0.027	
C	6	0.31	0.49	0.28	0.29	0.35	0.25	0.04	
Al	13	1.3–1.4	2.0	1.1	1.2	1.42	1.1	0.08	
Ar*	18	1.75–2.11	3.7		2.2	2.56	1.86	0.11	
Cu	29	6.9–8.0	9.0	5.2	5.4	6.5	4.52	0.17	
Kr*	36	6.3–7.9	13.2		7.8	9.0	6.63	0.21	
Sn	50	15–21	25	15	15.0	17.6	12.5	0.29	12.3
Xe*	54	14.4–16.8	29.4		16.7	19.3	14.6	0.31	14.0
Au	79	42–53	60	35	35.2	40.1	29.0	0.4	27.4

$b \gtrsim b_0$, where collisions are no longer ''sudden'' for the electron, the electron-atom interaction is already negligible. Below we will refer to the transition amplitude (16) as to the eikonal amplitude.

The eikonal transition amplitude (16) is to be compared to the transition amplitude for the elastic mode that was found in Ref. [2] using the first-order perturbation theory

$$a_{0n}^{p}(\mathbf{b}) = \frac{2iZ_A}{v} \sum_j A_j \langle \psi_n | \left(1 - \frac{v}{c}\alpha_z \right) \times \exp\left(i\frac{\omega_{n0} z}{v} \right) K_0(B_j |\mathbf{r}_\perp - \mathbf{b}|) | \psi_0 \rangle, \quad (18)$$

where $B_j = \sqrt{\omega_{n0}^2/v^2\gamma^2 + M_j^2}$.

For collisions with infinite γ, the transition amplitude, given by Eq. (16), is valid for any impact parameter b. For collisions with light atoms, where $2Z_A/c \ll 1$, or at large impact parameters, where the condition $2Z_A/c\Sigma_j A_j K_0(M_j|\mathbf{r}_\perp - \mathbf{b}|) \ll 1$ holds for any atom, the transition amplitude (16) reduces to the first-order amplitude (18). Note that in the limit $\gamma \to \infty$, in contrast to collisions with pointlike charges, the eikonal transition amplitude (16) for a screened interaction does not result in infinite cross sections for dipole allowed transitions.

For collisions with high but finite values of γ, both transition amplitudes (16) and (18) are not exact. In such a case, the expressions (16) and (18), in general, are better suited to describe the transition amplitudes at small and large impact parameters, respectively. In a comparative analysis for these two amplitudes, we first consider colliding systems where $b_0 = \gamma v/\omega_{n0} \gg a_0$. In such a case one has $B_j \simeq M_j$. For large impact parameters $b \gg Z_A/Z_p c$, where the atomic field acting on the electron of the ion is weak compared to the interaction between the electron and the ion nucleus (see appendix), the exponent in Eq. (16) can be expanded in series and one sees that the transition amplitude (16) is approximately equivalent to the first-order transition amplitude for these impact parameters (if one neglects in the latter terms proportional to $1/\gamma^2$). For collisions with smaller impact parameters, where the atomic field can reach considerable magnitudes during the collisions, the first-order transition amplitude (18) is inferior to the amplitude (16). Therefore for colliding systems, which satisfy the condition $b_0 \gg a_0 \sim 1$, the eikonal transition amplitude (16) should be used for all impact parameters.

Let us now consider colliding systems where $b_0 \lesssim a_0$. In ultrarelativistic collisions the latter condition can be fulfilled for very heavy ions. If in addition $b_0 \gg a_p$, where $a_p \sim 1/Z_p$ is the typical dimension of the ground state of the electron in the ion, then a simple method can be applied to calculate cross sections (see e.g. Refs. [15], [16]). For collisions with small impact parameters $b \ll b_0$, where the atom-electron interaction can be strong, the transition probability is calculated according to the nonperturbative expression (16). For collisions with larger impact parameters $b \gg 1/Z_p \gtrsim Z_A/Z_p c$, where the perturbation is already weak (see appendix), the first order perturbation theory can be used to calculate the transition probability. This method can be employed if there exists an overlap between the regions $b \ll b_0$ and $b \gg 1/Z_p$, i.e., when $Z_p b_0 \gg 1$. Then, taking into account (16) and (18), the elastic contribution to the cross section can be written as

$$\sigma_{0\to n} = 2\pi \int_0^{b_1} db\, b\, |a_{0n}(b)|^2 + 2\pi \int_{b_1}^{\infty} db\, b\, |a_{0n}^{p}(b)|^2, \quad (19)$$

where b_1 should lie in the range of impact parameters where transition probabilities, calculated according to Eqs. (16) and (18), are approximately equal (see appendix).

RESULTS AND DISCUSSION

Table I shows a comparison between experimental data of Refs. [3], [5] and results of different calculations for the loss cross sections for Pb^{81+} penetrating various solid and gas targets at a collision energy of 160 GeV/A.

Results of the present paper for the total loss cross section $\sigma_{loss} = \sigma_{loss}^{el} + \sigma_{loss}^{e-e}$ are given in columns I, II, III, and V. Columns I and II present results of our perturbative calculations where we use the semirelativistic (Darwin) wave functions to describe the motion of the electron in the ground and continuum states of Pb^{81+}. The results of column II [17] were obtained using the nonrelativistic formula for the binding energy of the electron in the ground state, $|\varepsilon_{bind}| = Z_p^2/2$. The results of column I were calculated assuming that the binding energy is given by the relativistic formula $|\varepsilon_{bind}| = c^2(1-\sqrt{1-Z_p^2/c^2})$. The results given in column I are noticeably smaller than those in the column II. The average difference between these two sets of results is 15–20%. Surprisingly, the results of our first column are very close to those estimated in Ref. [18] where a physically appealing but rather approximate procedure was used.

Our third column contains results of the perturbative calculations where we used the relativistic (Dirac) wave functions for the ground and continuum states of the electron in Pb^{81+}. The loss cross sections were obtained by taking into account the continuum states with angular momentum κ up to ± 7 and energies up to $\varepsilon_k = 10mc^2$. The inspection of cross sections differential in energy and the inclusion of states with higher κ showed that these regions of the continuum energies and the angular momenta give practically the total contribution to the loss cross sections. The results of column III are noticeably lower than those in the first column and are considerably lower than the results in our second column. This difference shows that a proper description of the relativistic effects in the inner motion of the electron in Pb^{81+} considerably reduces the loss cross section. Our results in column III differ roughly by a factor of 2 from the results of Anholt and Becker [19].

In all these three columns the electron-electron contribution σ_{loss}^{e-e} to the total loss cross section was calculated by using Eq. (7). The application of more exact incoherent scattering functions, tabulated in Refs. [8], [9], changes the results for the total loss by no more than 5% for Be, which is the lightest target considered, where the electron-electron contribution is relatively more important. As the mean atom excitation energy $\Delta\epsilon$, we have taken the mean energy $\Delta\epsilon_{SP}$, which is used in calculations of the stopping power and is tabulated for a variety of atoms (see e.g., Ref. [20]). The accuracy of $\Delta\epsilon$ is, in fact, not crucial for our calculations [1].

In column IV we show the electron-electron contribution to the total loss cross section. This contribution was calculated using the Dirac wave functions for the ground and continuum states of the electron in Pb^{81+} and it corresponds to the total loss cross section given in column III. Analyzing the results in columns III and IV, one may conclude that the electron-electron contribution represents a small correction to the elastic contribution and that this correction is relatively more important for collisions with few-electron atoms like Be and C. For collisions with heavy targets, like Sn, Xe, and Au, the electron-electron contribution is very small ($\lesssim 2\%$).

Our calculations for the loss cross sections, using the relativistic wave functions for the ground and continuum states of the electron in Pb^{81+}, show that the total loss cross section can be rather accurately generated from the elastic contribution using the following relation $\sigma_{loss} = (1+1/Z_A)\sigma_{loss}^{el}$. The same relation also holds when we employ the semirelativistic wave functions for the ground and continuum states of the electron in Pb^{81+}. We note that this simple scaling is due to

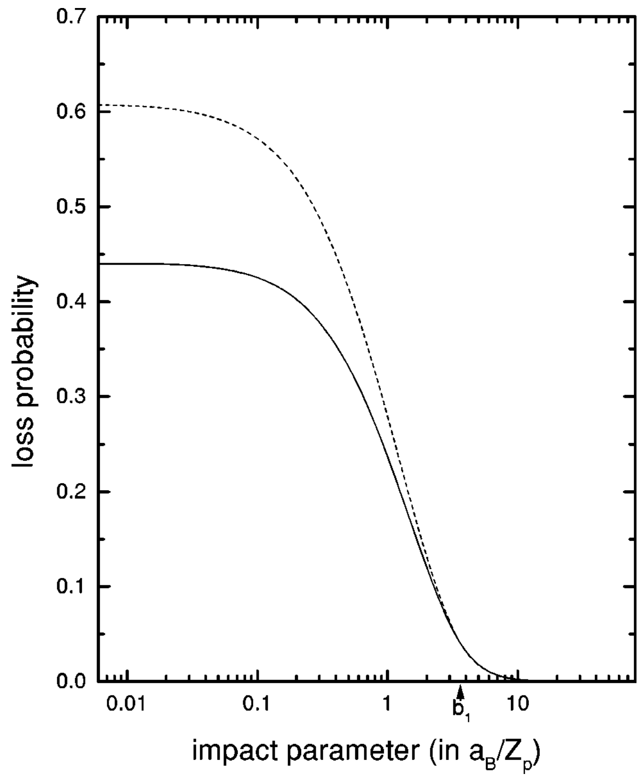

FIG. 1. The electron loss probability, as a function of the impact parameter, for the loss from 160 GeV/A Pb^{81+} in collisions with Au. Full curve: the result of the nonperturbative calculation; dashed curve: the first-order perturbative results. The impact parameter is given in units of the characteristic dimension $a_B/Z_p = 1.22\times 10^{-2}$ a.u. of the electron orbit in the ground state of Pb^{81+}.

large (on the atomic scale) momentum transfers needed to ionize the tightly bound electron in Pb^{81+}. For the electron loss from light ions this scaling may not be sufficiently accurate.

Our fifth column shows results of the nonperturbative calculations. Since we neglect the electron-electron contribution in our nonperturbative calculation, in column V we only present results for the heaviest targets, used in experiments of Refs. [3] and [5]. As it was already mentioned, for these targets the electron-electron contribution is very small. The results in column V were obtained as follows. For 160 GeV/A Pb^{81+} and taking $\omega_{eff} = 2|\varepsilon_{bind}| \approx 0.4mc^2$ as the effective transition frequency for the loss, one has $b_0 = \gamma v/\omega_{eff} \simeq 3$ a.u. This value is not much higher than $a_0 \sim 1$ a.u. Therefore the loss cross section was calculated according to Eq. (19). We set $b_1 = 3.3\times 10^{-2}$ a.u. For impact parameters in the vicinity of $b = b_1$, the eikonal and first-order loss probabilities are equal (see Fig. 1). In contrast to the first-order amplitudes (18), the eikonal transition amplitudes (16) preserve the unitarity, $\Sigma_{allstates}|a_{0n}|^2 = 1$. In addition, transitions from the ground state to the negative continuum states are negligible compared to transitions to the positive continuum. Therefore, the nonperturbative loss probability P_{loss}^{np} can be obtained not only (i) by a direct integration over the positive continuum states like in the perturbative calculation, but also as (ii) $P_{loss}^{np} = 1$

$-\Sigma_{bound}|a_{n0}|^2$, where the summation runs over all bound states. In our calculations we used the latter way. For states with the principal quantum number $n \leqslant 4$ the transition probabilities were calculated directly with Eq. (16). In order to estimate the contribution from bound states with $n > 4$ we used the approximate relation $\Sigma|a_{n0}|^2 \sim n^{-3}$, where the sum runs over all substates with the same principal quantum number n. For $b > b_1$, the loss probability was calculated in the first-order of perturbation theory. In these calculations we took into account the continuum states with angular momentum κ up to ± 7 and energies up to $\varepsilon_k = 10mc^2$.

It follows from the table that the difference between the results of our nonperturbative and perturbative calculations is very small, even for collisions with Au. Only for very small impact parameters, which do not contribute appreciably to the total loss, there is a considerable difference between the first-order and the eikonal calculations (see Fig. 1). That small difference between the ''exact'' and first-order loss cross sections can be attributed to the very high collision energy and the very tight binding of the electron in Pb^{81+}. It is known that in collisions with heavy atoms at relatively low relativistic energy, the difference between the experimental data and the first-order calculation results for the electron loss cross sections reaches 50–100 % [21]. In order to explore the influence of the binding energy on the nonperturbative effects we calculated the electron loss from a lighter projectile S^{15+}, in collisions with Au at the same collision energy per nucleon. We found $\sigma_{loss}^{pert} = 525$ kb and $\sigma_{loss} = 450$ kb using the first-order and ''exact'' [22] approaches, respectively. Thus, even at very high collision energies the nonperturbative effects can be rather important for the loss in collisions of light projectiles with heavy neutral targets. This is in contrast to the loss (ionization) in ultrarelativistic collisions with charged particles where there is a very small difference between the perturbative and nonperturbative results even for ionization of hydrogen and helium in collisions with U^{92+} [15].

Concerning the comparison of our results with the experimental data from Refs. [3] and [5], it is difficult to say which of the set of our results is, on average, in a better agreement with the data. In the more recent experiment [5] the projectile-electron loss cross sections were measured in collisions with atomic gas targets. These cross sections were found to be substantially lower than those which one could obtain by interpolating the loss cross sections measured previously in solids [3]. If we restrict the comparison of the calculated cross sections to those measured in the new experiment, then the results of the first-order calculation using the relativistic wave functions for the electron in Pb^{81+} seem to provide a better fit to the experimental data.

We have also performed first-order perturbative calculations for projectile-electron loss from 160 GeV/A Pb^{81+} in collisions with a pointlike charge Z_A. Using the Dirac wave functions for the electron in Pb^{81+} we found that $\sigma_{loss} = 8.7 \times 10^{-3} \times Z_A^2$ kb at this collision energy [23]. Neglecting the shielding effects, one would obtain for the loss cross section in collisions with neutral atoms $\sigma_{loss} = 8.7 \times 10^{-3} \times (Z_A^2 + Z_A)$ kb, where the term proportional to Z_A includes the contribution to the loss from the incoherent interaction of the projectile electron with Z_A atomic electrons. Comparing the results calculated using the above formula with the corresponding results for the neutral targets in Table I one can find that, depending on the target atom, the shielding effects reduce the unshielded loss cross section by a factor ranging from 1.4 (for Be and C) up to 1.9 (for Au).

Some additional information of interest on the process of projectile-electron excitation and loss in collisions with neutral atoms can be obtained by calculating separately the so-called longitudinal and transverse contributions [24] to cross sections. For the loss from 160 GeV/A Pb^{81+} the transverse part gives the main contribution to the total loss cross section accounting for $\gtrsim 60\%$ of the loss. Similar calculations for the loss from 160 GeV/A S^{15+} show that the transverse part contributes only 4% to the total loss. For the loss from 160 GeV/A O^{7+} we found that this part accounts for just 1% of the total loss cross section. It means that, in order to describe the electron excitation and loss from light projectiles in collisions with neutral targets at any collision velocity, one can take the interaction with the instantaneous (unretarded) scalar potential, which is relatively easy to handle, as a full interaction acting on the projectile electron. This is in sharp contrast to the loss (ionization) in relativistic collisions with charged particles where the transverse part is known to give the important contribution, which is asymptotically dominant at $\gamma \gg 1$ for the loss from both heavy and light ions.

SUMMARY

We have calculated projectile-electron loss cross sections in ultrarelativistic collisions with neutral atomic targets using the first-order perturbation theory and the ''exact'' approach. We have shown that, in general, the following main effects should be included for a proper description of the projectile-electron excitation and loss in ultrarelativistic collisions: (i) the shielding effects of electrons of a neutral target, (ii) the relativistic effects in the motion of the electron in the projectile for heavy projectiles, and (iii) the nonperturbative effects in collisions with heavy targets especially for light projectiles. We have also found that the transverse part of the neutral atom perturbation acting on the projectile electron is of minor importance for light projectiles at any collision energy. The latter point and the point (iii) are in sharp contrast to ionization in ultrarelativistic collisions with charged particles, where the nonperturbative effects are negligible for any possible pair of colliding partners and where the transverse term is asymptotically dominant. That contrast reflects the essential difference in electron transitions caused by long-range and short-range interactions.

ACKNOWLEDGMENTS

The authors are grateful to Professor R. Schuch and Dr. S. Scheidenberger for informing about the experimental results of Ref. [5] before publication. A.B.V. acknowledges with thanks the support from the Alexander von Humboldt Stiftung.

APPENDIX

Below we show that for electron loss in ultrarelativistic collisions with a pointlike charged particle one can always find a range of impact parameters where the eikonal and first-order transition amplitudes are approximately equal. We also show that a similar range of impact parameters can be found for the loss from very heavy ions in collisions with neutral atoms.

Let us first consider collisions with a pointlike charge Z_A. In this case the eikonal transition amplitude is given by Eq. (17), the first-order amplitude is given by Eq. (18), where one should set $M_j=0$. For collisions with impact parameters $b \gg 1/Z_p$, one can approximately write

$$K_0(B_0|\mathbf{r}_\perp - \mathbf{b}|) \approx K_0(B_0 b) + \frac{B_0 K_1(B_0 b)}{b}\mathbf{b}\cdot\mathbf{r}_\perp , \quad \text{(A1)}$$

where $B_0=\omega_{n0}/\gamma v$ and K_1 is a modified Bessel function. Further, we have also

$$\ln\frac{|\mathbf{b}-\mathbf{r}_\perp|}{b} \approx -\frac{\mathbf{b}\cdot\mathbf{r}_\perp}{b^2}. \quad \text{(A2)}$$

Using Eq. (A1) and keeping in mind the condition $\Sigma_j A_j = 1$, one obtains for the first-order transition amplitude (18)

$$a^p_{0n}(\mathbf{b}) \approx \frac{2iZ_A}{v}K_0(B_0 b)\langle\psi_n|\left(1-\frac{v}{c}\alpha_z\right)\exp\left(i\frac{\omega_{n0}z}{v}\right)|\psi_0\rangle + \frac{2iZ_A}{vb}B_0K_1(B_0b)\langle\psi_n|\left(1-\frac{v}{c}\alpha_z\right)\exp\left(i\frac{\omega_{n0}z}{v}\right) \times(\mathbf{r}_\perp\cdot\mathbf{b})|\psi_0\rangle. \quad \text{(A3)}$$

Using the identity

$$\langle\psi_n|\alpha_z\exp(i\omega_{n0}z/v)|\psi_0\rangle \equiv v/c\langle\psi_n|\exp(i\omega_{n0}z/v)|\psi_0\rangle$$

one sees that the first term in Eq. (A3) is proportional to $1/\gamma^2$. We will neglect this term and choose b to satisfy not only the relation $b \gg 1/Z_p$ but also $b \ll \gamma v/\omega_{n0}$. Estimating $\omega_{n0} \sim Z_p^2$ one can see that it is always possible to find the range $1/Z_p \ll b \ll \gamma v/\omega_{n0}$ for ultrarelativistic collisions when $\gamma c \gg Z_p$ for any Z_p. In this range of impact parameters, $B_0 b \ll 1$ and, correspondingly, $K_1(B_0b)\approx 1/B_0 b$ [14] and the first-order transition amplitude reads

$$a^p_{0n}(\mathbf{b}) \approx \frac{2iZ_A}{cb^2}\langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right)(\mathbf{r}_\perp\cdot\mathbf{b})|\psi_0\rangle, \quad \text{(A4)}$$

where we set $v \approx c$.

On the other hand, taking into account Eq. (A2), the eikonal transition amplitude (17) becomes

$$a^{Coul}_{0n}(\mathbf{b}) \approx \langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right)\exp\left(\frac{i2Z_A}{c}\frac{\mathbf{b}\cdot\mathbf{r}_\perp}{b^2}\right)|\psi_0\rangle. \quad \text{(A5)}$$

Since $r_\perp \sim 1/Z_p$, then, for $b \gg Z_A/Z_p c$, one can expand the exponential function in Eq. (A5) and the eikonal transition amplitude (A5) recovers the first-order transition amplitude (A4). Thus, one can conclude that for collisions with a pointlike charge (i) the first-order perturbation theory can be used for $b \gg Z_A/Z_p c$ and (ii) the eikonal and first-order transition amplitudes are approximately equal at $1/Z_p \ll b \ll \gamma v/\omega_{n0}$.

Let us now discuss briefly ultrarelativistic collisions with neutral atoms. Since for collisions with a neutral atom having atomic number Z_A, the screened atomic field for any impact parameter is not stronger than the field of a pointlike charge Z_A then the conclusion (i) is applicable for collisions with neutral atoms as well. In the eikonal amplitude

$$a_{0n}(\mathbf{b}) = \langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right) \times\exp\left(\frac{2iZ_A}{c}\sum_j A_j K_0(M_j|\mathbf{r}_\perp-\mathbf{b}|)\right)|\psi_0\rangle, \quad \text{(A6)}$$

we expand the functions $K_0(M_j|\mathbf{r}_\perp-\mathbf{b}|)$ for $b \gg 1/Z_p$ similarly to Eq. (A1). Since $b \gg \frac{1}{Z_p} > \frac{Z_A}{Z_p c}$ one can further expand the exponential function in Eq. (A6) and obtain

$$a_{0n}(\mathbf{b}) \approx \frac{2iZ_A}{cb}\sum_j A_j M_j K_1(M_j b)\langle\psi_n|(1-\alpha_z) \times\exp\left(i\frac{\omega_{n0}z}{c}\right)\mathbf{b}\cdot\mathbf{r}_\perp|\psi_0\rangle. \quad \text{(A7)}$$

For the same region of impact parameters $b \gg 1/Z_p$ the first-order transition amplitude is approximately given by

$$a^p_{0n}(\mathbf{b}) \approx \frac{2iZ_A}{cb}\sum_j A_j B_j K_1(B_j b)\langle\psi_n|(1-\alpha_z) \times\exp\left(i\frac{\omega_{n0}z}{c}\right)\mathbf{b}\cdot\mathbf{r}_\perp|\psi_0\rangle. \quad \text{(A8)}$$

As it follows from Eqs. (A7) and (A8) the eikonal and first-order amplitudes are approximately equal for $b \gg 1/Z_p$ if $B_j \simeq M_j$. If the latter condition is not fulfilled, the amplitudes (A7) and (A8) can still be approximately equal if there exists an overlap between $b \gg 1/Z_p$ and $b \ll 1/M_j$, and $b \gg 1/Z_p$ and $b \ll 1/B_j$. In the ranges $b \ll 1/M_j$ and $b \ll 1/B_j$ the amplitudes (A7) and (A8) can be further simplified using for small arguments $K_1(x)\approx 1/x$. This yields

$$a_{0n}(\mathbf{b}) \approx a^p_{0n}(\mathbf{b}) \approx \frac{2iZ_A}{cb^2}\langle\psi_n|(1-\alpha_z)\exp\left(i\frac{\omega_{n0}z}{c}\right)\mathbf{b}\cdot\mathbf{r}_\perp|\psi_0\rangle. \quad \text{(A9)}$$

The inspection of the screening constants given in Ref. [7] shows that the strict conditions $1/Z_p \ll b \ll 1/M_j$ and $1/Z_p \ll b \ll 1/B_j$ are in general not fulfilled. However, the less restrictive conditions for the overlap $1/Z_p < b < 1/M_j$ and

$1/Z_p < b < 1/B_j$ are fulfilled for very heavy projectile-ions where Z_p is considerably larger than $max\{M_j\}$.

In general the cross section (19) can be calculated according to the following simple rule. At any impact parameter the transition amplitude should be represented by the value obtained either from the eikonal or the first-order transition amplitudes, whichever gives the smallest transition probability.

[1] A.B. Voitkiv, N. Grün, and W. Scheid, Phys. Rev. A **61**, 052704 (2000).
[2] A.B. Voitkiv, M. Gail, and N. Grün, J. Phys. B **33**, 1299 (2000).
[3] H.F. Krause, C.R. Vane, S. Datz, P. Grafström, H. Knudsen, S. Scheidenberger, and R.H. Schuch, Phys. Rev. Lett. **80**, 1190 (1998).
[4] N. Claytor, A. Belkacem, T. Dinneen, B. Feinberg, and H. Gould, Phys. Rev. A **55**, R842 (1997).
[5] H.F. Krause, C.R. Vane, S. Datz, P. Grafström, H. Knudsen, U. Mikkelsen, S. Scheidenberger, R.H. Schuch, and Z. Vilakazi, Phys. Rev. A (to be published).
[6] G. Moliere, Naturforsch. **2A**, 133 (1947).
[7] F. Salvat, J.D. Martinez, R. Mayol, and J. Parellada, Phys. Rev. A **36**, 467 (1987).
[8] J.H. Hubbell, Wm.J. Veigele, E.A. Briggs, R.T. Brown, D.T. Cromer, and R.J. Howerton, J. Phys. Chem. Ref. Data **4**, 471 (1975).
[9] J.H. Hubbell and I. Øverbø, J. Phys. Chem. Ref. Data **8**, 69 (1979).
[10] J.D. Jackson, *Classical Electrodynamics* (Wiley, New York, 1975).
[11] A.J. Baltz, Phys. Rev. Lett. **78**, 1231 (1997).
[12] R. Anholt, Phys. Rev. A **19**, 1004 (1979).
[13] In fact it can be analytically proven that any transition amplitudes of the form $a_{n0} = \langle \psi_n | (1-\alpha_z) \exp(i\omega_{n0} z/c) \exp[iF(\mathbf{r}_\perp - \mathbf{b})] | \psi_0 \rangle$, where F is a real function, preserve the unitarity.
[14] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. Stegun (Dover, New York, 1965).
[15] A.B. Voitkiv and A.V. Koval, Tech. Phys. **39**, 335 (1994); J. Phys. B **31**, 499 (1998).
[16] A.J. Baltz, Phys. Rev. A **61**, 042701 (2000).
[17] This set of results was given also in Ref. [1].
[18] A.H. Sørensen, Phys. Rev. A **58**, 2895 (1998).
[19] R. Anholt and U. Becker, Phys. Rev. A **36**, 4628 (1987).
[20] U. Fano, Ann. Nucl. Sci. Eng. **13**, 1 (1963).
[21] Weick *et al.*, GSI Report No. 2000-01, 2000.
[22] For 160 GeV/A S^{15+} projectiles $b_0 = \gamma v/\omega_{eff} \approx 90$ a.u., $b_0 \gg a_0$ and the eikonal transition amplitudes (16) can be used for any impact parameter.
[23] According to this formula one obtains $\sigma^p_{loss} = 58.4$ kb for $Pb^{81+} + Pb^{82+}$ collisions. This perturbative cross section can be compared to the result $\sigma_{loss} = 55.8 - 58.2$ kb, which was calculated nonperturbatively in Ref. [16].
[24] U. Fano, Phys. Rev. **102**, 385 (1956).