Nonperturbative Treatment of Excitation and Ionization in $U^{92+} + U^{91+}$ Collisions at 1 GeV/amu

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Inner-shell excitation and ionization processes in relativistic collisions of very heavy ions are treated by a nonperturbative method for the first time. The time-dependent Dirac equation is solved by a finite-difference method for the scattering of U^{92+} on U^{91+} at a value of E_{lab} corresponding to 1 GeV/amu and zero impact parameter. The K-shell-ionization probabilities are compared with those resulting from first-order perturbation theory.

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Our theoretical investigations were motivated by the current measurements[1-3] of electron excitation processes in relativistic collisions of the heaviest ions accessible to experimental observations. For example, the measurements of Anholt *et al.*[3] of the total K-shell-ionization cross sections in relativistic heavy-ion collisions can be reproduced by atomic reaction theories in which the interaction is treated in first-order perturbation theory. Calculations of the cross sections have been carried out by Anholt *et al.*[3] using the plane-wave Born approximation and by Becker, Grün, and Scheid[4] using first-order perturbation theory within the semiclassical approximation (SCA). The latter calculations have demonstrated[4,5] that the K-shell-ionization probabilities exceed the unitary limit for very heavy ions and small impact parameters if they are calculated in first-order perturbation theory. Therefore, nonperturbative methods are needed for the evaluation of the inner-shell excitation and ionization probabilities at small impact parameters, which certainly will be measured in the near future.

Nonperturbative methods in heavy-ion collisions are usually based on the SCA which treats the relative motion of the ions classically and the electronic motion by quantum mechanics. Following this method one can describe the dynamical fate of a single electron initially bound to a very heavy nucleus by the time-dependent Dirac equation

$$i\hbar\,\partial\psi(\mathbf{r},t)/\partial t = \{c\boldsymbol{\alpha}\cdot[\mathbf{p}+(e/c)\mathbf{A}(\mathbf{r},t)]+\beta mc^2 - eV(\mathbf{r},t)\}\psi(\mathbf{r},t), \tag{1}$$

where $\psi(\mathbf{r},t)$ denotes the four-component spinor. In the nonrelativistic regime of the internuclear motion the Dirac equation was successfully solved by use of a quasimolecular expansion of the electronic state for symmetrical collision systems[6] or a one-center atomic expansion for asymmetrical ones.[7] Furthermore, Bottcher and Strayer[8] employed a time-dependent finite-element method to investigate electron-positron pair creation.

In this paper we present a nonperturbative solution of the time-dependent Dirac equation for relativistic collisions of U^{92+} on U^{91+} by application of a finite-difference algorithm and discuss the results in comparison with those obtained by first-order perturbation theory.

Nonperturbative solution of Dirac equation.—The finite-difference method chosen for solving Eq. (1) is described in a previous publication.[9] Other numerical techniques are presented in the review of Bottcher[10] and in the references therein. In order to keep the numerical procedure manageable, we restrict the calculations to rotationally symmetrical electromagnetic fields about the internuclear axis. Furthermore, we assume that the projectile nucleus moves with constant velocity v along the z axis and the target is fixed at $z=0$. The potentials are given for extended charges with charge numbers Z_P and Z_T and radii R_P and R_T:

$$\begin{aligned} V &= eZ_T f_T(r) + eZ_P\gamma f_P(r'),\\ \mathbf{A} &= eZ_P(v/c)\gamma f_P(r')\mathbf{e}_z, \end{aligned} \tag{2}$$

where

$$\begin{aligned} \gamma &= 1/(1-v^2/c^2)^{1/2},\\ r' &= [x^2+y^2+\gamma^2(z-z_0-vt)^2]^{1/2},\\ f_I(r) &= \begin{cases} 1/r, & r \geqslant R_I,\\ (3-r^2/R_I^2)/2R_I, & r\leqslant R_I, \end{cases} \end{aligned} \tag{3}$$

with $I=P,T$. For the solution of Eq. (1) we employed cylindrical coordinates z and $\rho=(x^2+y^2)^{1/2}$. The chosen grid in the finite-difference method consists of 264×800 meshes of size $\Delta z=\Delta\rho=26.5$ fm. A variation of the grid size did not affect the excitation proba-

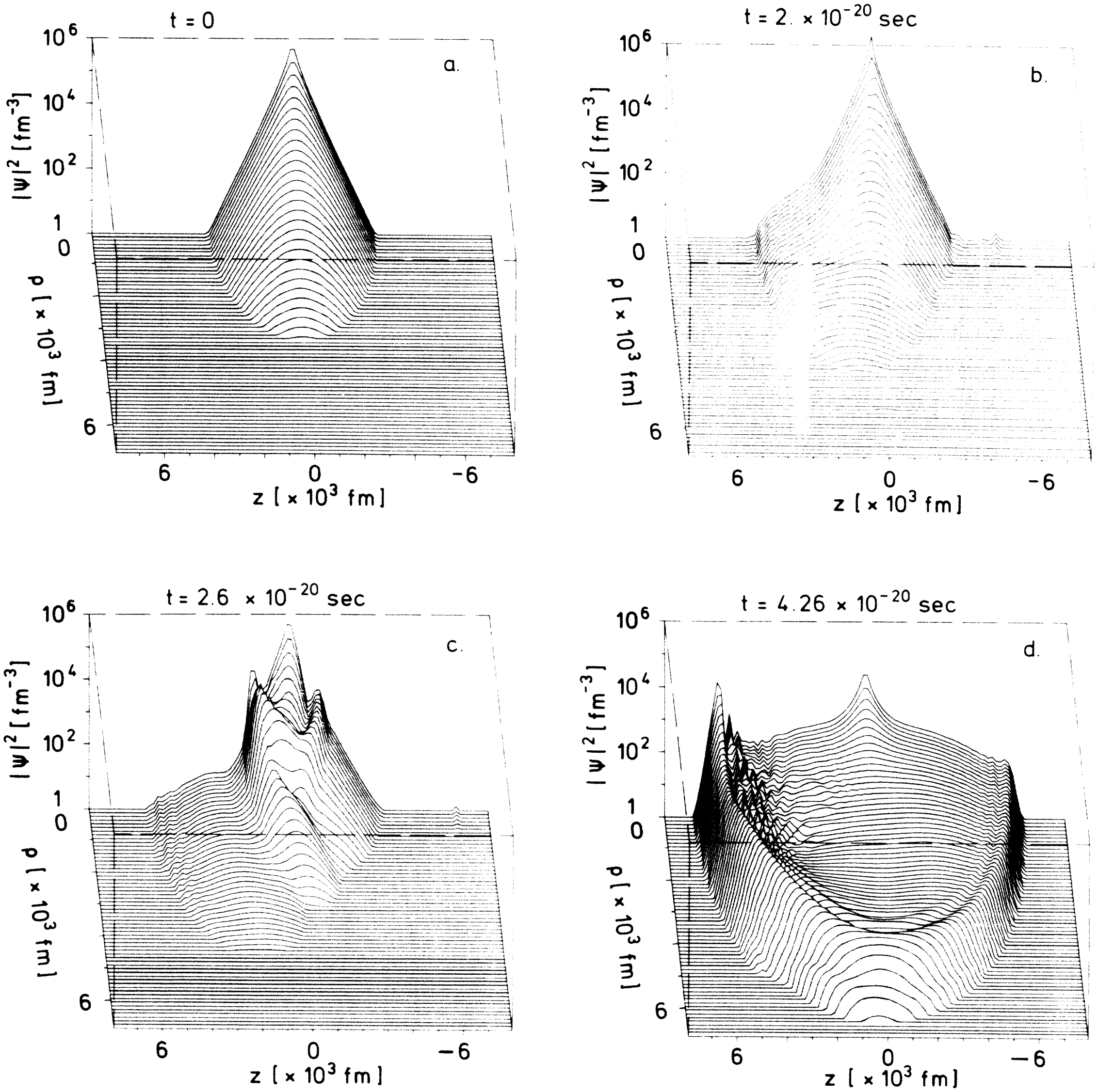

FIG. 1. Time development of the electron density distribution in the z-ρ plane for a collision of U^{92+} on U^{91+} at $E_{\text{lab}}=1$ GeV/amu. The position of the target nucleus is fixed at $z=0$ and $\rho=0$. The projectile nucleus moves along the z axis from the negative to the positive z direction with the position at $z_P(t)$. (a) $t=0$, $z_P=-5300$ fm, (b) $t=2\times10^{-20}$ sec, $z_P=-44$ fm, (c) $t=2.6\times10^{-20}$ sec, $z_P=1533$ fm, (d) $t=4.26\times10^{-20}$ sec, $z_P=5896$ fm.

bilities of the electron. The time steps are taken as 10^{-22} sec. Initially the electron occupies the $1s_{1/2}$ state in the U^{91+} ion. The Coulomb potentials of the projectile and target nuclei are calculated by assuming an artificial radius of $R_P=R_T=2\Delta z=53$ fm. As demonstrated in Ref. 9 these radii represent an optimal choice to guarantee the stability of the unperturbed initial $1s_{1/2}$ state. The problem of fermion doubling[11] is avoided by using a filter which removes the rapidly oscillating solutions on the grid (for details see Ref. 9).

Figure 1 shows the time development of the probability density of the electron in a collision of U^{92+} on U^{91+} at a value of E_{lab} corresponding to 1 GeV/amu and zero impact parameter. At the initial time $t=0$ the density of the electron is determined by the $1s_{1/2}$ state of hydrogenlike uranium, whereas the projectile nucleus is assumed to be at $z_P=-5300$ fm. During the approach of the projectile the wave function of the electron does not change much which can be deduced by the comparison of the density for $t=0$ and 2×10^{-20} sec. In contrast to nonrelativistic collisions a strong localization of the electron wave function is not observed. After the projectile has passed the point of closest approach, the main excitation and ionization processes take place. In the densities at $t=2.6\times10^{-20}$

sec and 4.26×10^{-20} sec we observe an ionization component which leads to an emission of the electron with approximately the velocity of the projectile. At the last depicted time ($t=4.26\times10^{-20}$ sec) we projected the numerically evaluated wave function on the set of eigenstates of the Hamiltonian of the pointlike uranium nucleus. After the collision the initial $1s_{1/2}$ state is only occupied by 13% and the excited bound states by about 10%.

Figure 2 shows the differential ionization probabilities (solid curves) as a function of the total energy E_f of the ionized electron. The small undulations, seen on the solid curves, are caused by the finiteness of the grid and the projection on nonlocalized continuum wave functions and, therefore, have no physical meaning. For the discussion we depict also approximate ionization probabilities obtained by the first-order perturbation theory in SCA (dashed curves in Fig. 2). By comparing the differential ionization probabilities belonging to s states ($\kappa_f=-1$), we find the results of the first-order approximation to be a factor of 2.5 larger than the nonperturbative ones. Nevertheless, the slopes of the solid and dashed curves agree roughly for all values of κ_f.

Perturbation theory gives a total ionization probability of about 0.83 if integrated over the positive-energy continuum for energies from 0.511 to 1.5 MeV. This large number reflects the nonunitarity of the approximate method. In contrast the finite-difference method conserves the norm of the wave function and yields only the value 0.56 for the corresponding ionization probability.

Figure 3 shows the K-shell-ionization probability for a collision of a projectile of charge Z_P with a uranium target at $E_{\text{lab}}=1$ GeV/amu as a function of the impact parameter. This probability, calculated by the first-order perturbation theory within the SCA, has a logarithmic falloff given by $\exp(-b/d_K)$, where $d_K=565$ fm. Compared with $d_K=20$ fm for the nonrelativistic U+U collision at $E_{\text{lab}}=5.9$ MeV/amu,[12] this large value of d_K demonstrates the increasing importance of larger impact parameters for ionization at relativistic velocities. The perturbation theory predicts a total ionization cross section of 5.4×10^4 b at 1 GeV/amu. Corresponding experimental data are not yet available. For the lower bombarding energy of 422 MeV/amu the theoretical result[3,4] ($\sigma_K=5.5\times10^4$ b) is in fair agreement with the experimental value[3] [$\sigma_K=(6.7\pm1)\times10^4$ b]. The projection of the wave function on eigenstates of the negative-energy continuum yields differential probabilities for electron-positron pair production of the order of 10^{-3}/MeV in agreement with the perturbation theory.

After the collision the density distribution in Fig. 1(d) shows a first component of ionization isotropically distributed around the target nucleus and a second

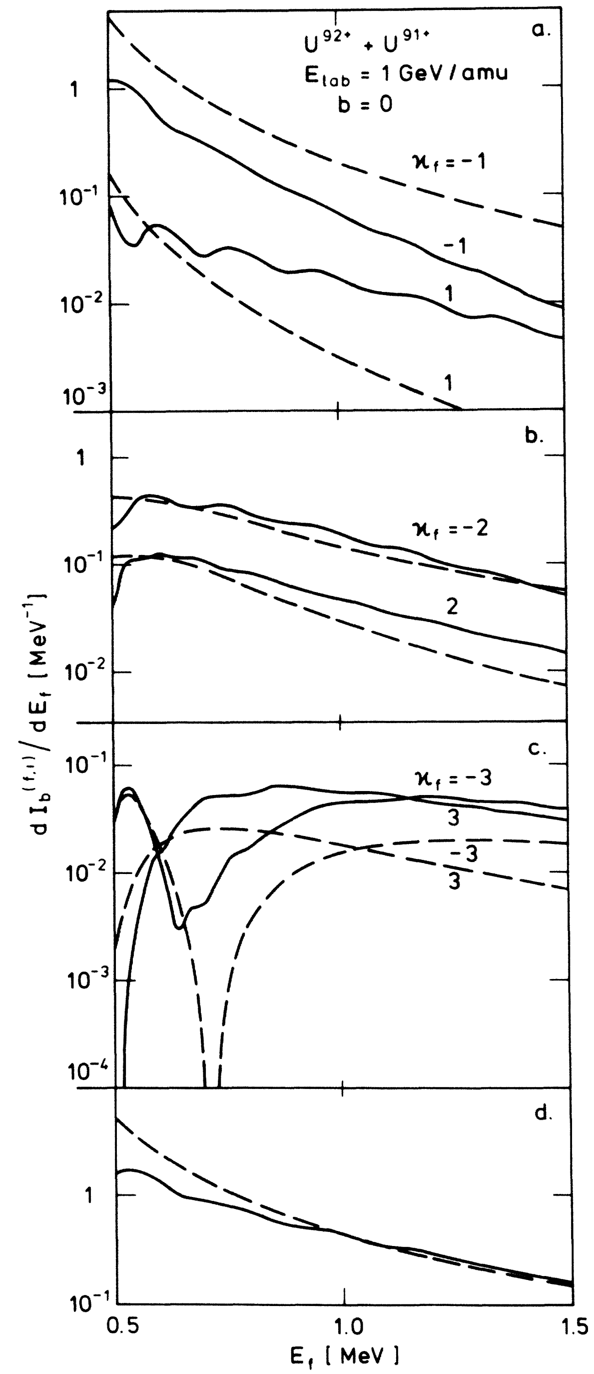

FIG. 2. The differential ionization probabilities for the transition of the $1s_{1/2}$ electron into the positive-energy continuum as a function of the final electron energy E_f for a collision of U^{92+} on U^{91+} at $E_{\text{lab}}=1$ GeV/amu and zero impact parameter. The final states are (a) the $s_{1/2}(\kappa_f=-1)$ and $p_{1/2}(\kappa_f=1)$ states, (b) the $p_{3/2}(\kappa_f=-2)$ and $d_{3/2}(\kappa_f=2)$ states, (c) the $d_{5/2}(\kappa_f=-3)$ and $f_{5/2}(\kappa_f=3)$ states, and (d) the sum over the states of the positive-energy continuum. The solid curves are obtained by projecting on the wave function of the electron calculated by the finite-difference method at $t=4.26\times10^{-20}$ sec. The dashed curves are calculated by employing first-order perturbation theory within the SCA.

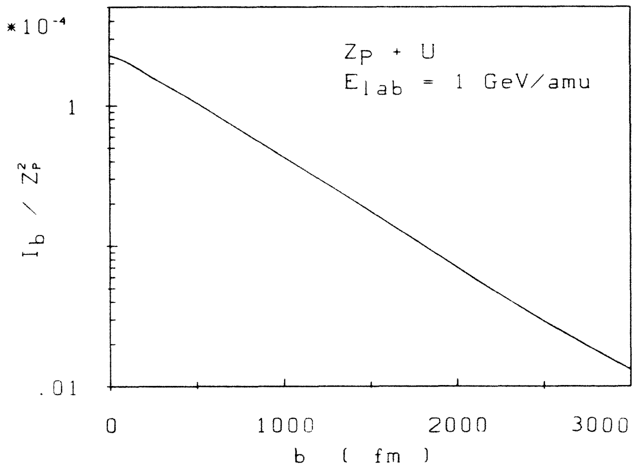

FIG. 3. K-shell-ionization probability calculated by first-order perturbation theory as a function of the impact parameter for a collision of a projectile of charge Z_P on U at $E_{\rm lab} = 1$ GeV/amu.

one strongly peaked in the direction of the projectile. The latter component becomes important with increasing relative velocities.[3,5] This is indicated by the values of the ionization probabilities integrated over the emitted electron energy as a function of the quantum number κ. In our example (1 GeV/amu), the finite-difference method yields probabilities of 0.20 and 0.22 for the ionization into the $s_{1/2}$ and $p_{3/2}$ continua, respectively. For higher relative energies, higher values of κ become more essential than lower ones which reflects an increase of the ionization in the direction of the projectile. Only a small part of the forward component leads to charge exchange into bound states of the projectile.

A more mathematical point of view of our calculations is provided by the fact that the complex collision of U^{92+} on U^{91+} is treated without major approximations and, therefore, the results can be utilized for correcting approximate theories. For example, first-order perturbation theory needs a proper treatment of the unitarity for small impact parameters.

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