Relativistic calculations of the K-K charge transfer and K-vacancy production probabilities in low-energy ion-atom collisions

I. I. Tupitsyn,[1] Y. S. Kozhedub,[1] V. M. Shabaev,[1] A. I. Bondarev,[1] G. B. Deyneka,[2] I. A. Maltsev,[1]
S. Hagmann,[3] G. Plunien,[4] and Th. Stöhlker[3,5,6]

[1]*Department of Physics, St. Petersburg State University, Oulianovskaya 1, Petrodvorets, 198504 St. Petersburg, Russia*
[2]*St. Petersburg State University of Information Technologies, Mechanics and Optics, Kronverk av. 49, 197101 St. Petersburg, Russia*
[3]*Gesellschaft für Schwerionenforschung, Planckstrasse 1, D-64291 Darmstadt, Germany*
[4]*Institut für Theoretische Physik, Technische Universität Dresden, Mommsenstrasse 13, D-01062 Dresden, Germany*
[5]*Physikalisches Institut, Universität Heidelberg, Philosophenweg 12, D-69120 Heidelberg, Germany*
[6]*Helmholtz-Institut Jena, D-07743 Jena, Germany*

(Received 14 December 2011; published 28 March 2012)

The previously developed technique for evaluation of charge transfer and electron-excitation processes in low-energy heavy-ion collisions [Tupitsyn *et al.*, Phys. Rev. A **82**, 042701 (2010)] is extended to collisions of ions with neutral atoms. The method employs the active-electron approximation, in which only the active-electron participates in the charge transfer and excitation processes while the passive electrons provide the screening density-functional theory (DFT) potential. The time-dependent Dirac wave function of the active electron is represented as a linear combination of atomic-like Dirac-Fock-Sturm orbitals, localized at the ions (atoms). The screening DFT potential is calculated using the overlapping densities of each ion (atom), derived from the atomic orbitals of the passive electrons. The atomic orbitals are generated by solving numerically the one-center Dirac-Fock and Dirac-Fock-Sturm equations by means of a finite-difference approach with the potential taken as the sum of the exact reference ion (atom) Dirac-Fock potential and of the Coulomb potential from the other ion within the monopole approximation. The method developed is used to calculate the K-K charge transfer and K-vacancy production probabilties for the Ne($1s^2 2s^2 2p^6$)-F^{8+}($1s$) collisions at the F^{8+}($1s$) projectile energies 130 and 230 keV/u. The obtained results are compared with experimental data and other theoretical calculations. The K-K charge transfer and K-vacancy production probabilities are also calculated for the Xe-Xe^{53+}($1s$) collision.

DOI: 10.1103/PhysRevA.85.032712 PACS number(s): 34.10.+x, 34.50.−s, 34.70.+e

I. INTRODUCTION

Collisions of highly charged ions provide a unique tool for tests of relativistic and quantum electrodynamics (QED) effects in the scattering theory [1–3]. Investigations of such processes can also give access to QED in supercritical fields, provided the total charge of the colliding nuclei is larger than the critical one, $Z_c = 173$ (see, e.g., Ref. [4] and references therein). One of the most attractive ways for indirect observation of the supercritical field created in the collision is to investigate the dynamics of inner-shell electrons, which can be rather sensitive to the collision parameters. The most favorable conditions for studying the electron dynamics in the supercritical field regime correspond to the projectile energy of about the Coulomb barrier [5]. In the case of U-U collisions this requires energy of about 6 MeV/u, which means a low-energy collision. One of the key processes in such collisions is the charge transfer of electrons (see, e.g., Ref. [6] and references therein). A systematic approach to relativistic calculations of the charge transfer probabilities and electron-excitation probabilities in low-energy heavy-ion collisions was developed in our previous paper [7], where the consideration was restricted to collisions of H-like ions with bare nuclei. Since the experimental study of such collisions for high-Z systems is presently rather problematic, an extention of the method to collisions of highly charged ions with neutral atoms, which can be studied in experiments with the current GSI facility and future GSI Facility for Antiproton and Ion Research (FAIR) [8,9], is needed. In this paper we present the desired extention and perform calculations for low-energy ion-atom collisions. To examine the approach we calculate the K-K charge transfer and K-vacancy production probabilities for low-energy collision of H-like F (F^{8+}) and neutral Ne, the process of which has been investigated both experimentally [10] and theoretically [11–13]. The calculations are performed at the F^{8+} projectile energies 130 and 230 keV/u. We also evaluate the probabilities of the K-K charge transfer and K-vacancy production in the Xe-Xe^{53+}($1s$) collision at the projectile energy 3.6 MeV/u. The latter processes are planned to be studied in the near future in experiments at GSI [8,9].

The paper is organized as follows. In Sec. II A we describe the time-dependent one-electron equation in the so-called active-electron approximation [14] and the method for constructing the local Kohn-Sham potential induced by the passive electrons. The wave function of the active electron is expanded in terms of the Dirac-Fock and Dirac-Fock-Sturm basis functions, which are central-field four-component Dirac bispinors centered at the ions. The two-center relativistic Kohn-Sham equation in the finite basis set is briefly discussed in Sec. II B. The basis functions are obtained by solving numerically the atomic Dirac-Fock and Dirac-Fock-Sturm equations in an external field with a special choice of the weight function, as was proposed in Refs. [15,16]. The external potential is a spherically symmetric Coulomb-Hartree potential of the other ion (atom) taken in the monopole approximation. The basis set constructed in this way and the related calculation procedures are described in Sec. II C. Basic formulas for the K-vacancy production probability are

given in Sec. II D. In Sec. III we present the results of the relativistic calculations of the Ne K-shell-vacancy production and K-K charge transfer probabilities in the Ne-F^{8+} collisions as a function of the impact parameter b at the projectile energies 130 and 230 keV/u. In this section we also present the results of the neutral Xe K-shell-vacancy production and K-K charge transfer probabilities in the Xe-$Xe^{53+}(1s)$ collision.

II. THEORY

A. Dirac-Kohn-Sham equation in the active-electron approximation

In this paper we use so-called active-electron approximation [14] to describe the ion-atom collision. In this approximation, we consider only the active electron which participates in the charge transfer and excitation processes, while the other passive electrons provide a screening potential. In our calculations the screening potential is defined by the density-functional theory (DFT) in the local-density approximation (LDA). In this approach the time-dependent wave function $\psi(\boldsymbol{r},t)$ of the active electron is the solution of the relativistic time-dependent Kohn-Sham equation. In atomic units ($\hbar = m = e = 1$), this equation is given by

$$i\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} = h_{\rm D}\psi(\boldsymbol{r},t). \tag{1}$$

Here $h_{\rm D}$ is the two-center Dirac-Kohn-Sham Hamiltonian defined by

$$\begin{aligned} \hat{h}_{\rm D} &= c(\boldsymbol{\alpha}\cdot\boldsymbol{p}) + \beta c^2 + V_{AB}(\boldsymbol{r}), \\ V_{AB}(\boldsymbol{r}) &= V_H[\rho] + V_{\rm xc}[\rho], \end{aligned} \tag{2}$$

where c is the speed of light and $\boldsymbol{\alpha}$ and β are the Dirac matrices. $V_H[\rho]$ and $V_{\rm xc}[\rho]$ are the Hartree and exchange-correlation potentials, respectively. Both of them are the functionals of the electron density $\rho(\boldsymbol{r})$. The Hartree potential $V_H[\rho]$ includes the electron-nucleus interaction and the electron-electron Coulomb repulsion $V_{\rm C}[\rho]$:

$$\begin{aligned} V_H[\rho] &= V^A_{\rm nucl}(\boldsymbol{r}_A) + V^B_{\rm nucl}(\boldsymbol{r}_B) + V_{\rm C}[\rho], \\ \boldsymbol{r}_A &= \boldsymbol{r} - \boldsymbol{R}_A, \quad \boldsymbol{r}_B = \boldsymbol{r} - \boldsymbol{R}_B, \end{aligned} \tag{3}$$

where

$$V_{\rm nucl}(\boldsymbol{r}) = \int d^3\boldsymbol{r}'\frac{\rho_{\rm nucl}(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}, \quad V_{\rm C}[\rho] = \int d^3\boldsymbol{r}'\frac{\rho(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}, \tag{4}$$

$\rho_{\rm nucl}(\boldsymbol{r})$ and $\rho(\boldsymbol{r})$ are the nuclear and electron densities, respectively. The exchange-correlation potential $V_{\rm xc}[\rho]$ was taken in the Perdew-Zunger parametrization [17] including the self-interaction correction (SIC).

The electron density $\rho(\boldsymbol{r})$, obtained with the many-electron wave function which is represented by a Slater determinant, is invariant with respect to the rotations in the occupied orbitals' space. For this reason, to obtain the electron density we can use atomiclike orbitals, localized on both centers (A and B). In this case the electron density, constructed from the orthogonal localized orbitals, can be represented as a sum of densities $\rho_A(\boldsymbol{r})$ and $\rho_B(\boldsymbol{r})$ which are localized on the centers A and B. This is not the case, however, if the orbitals localized on the different centers overlap and are nonorthogonal. The electron density, derived from nonorthogonal orbitals, is given by

$$\rho(\boldsymbol{r}) = \sum_{i,j}\psi^{(p)*}_i(\boldsymbol{r})(S^{-1})_{ij}\psi^{(p)}_j(\boldsymbol{r}), \tag{5}$$

where $\psi^{(p)}_i(\boldsymbol{r})$ are the atomiclike wave functions of the passive electrons and matrix S is the overlapping matrix. Note that the electron density is normalized on the number of passive electrons,

$$\int d^3\boldsymbol{r}\rho(\boldsymbol{r}) = N - 1, \tag{6}$$

where N is the total number of electrons. The electron density $\rho(\boldsymbol{r})$ can be divided into three parts,

$$\rho(\boldsymbol{r}) = \rho_A(\boldsymbol{r}) + \rho_B(\boldsymbol{r}) + \rho^{\rm (ovlp)}_{AB}(\boldsymbol{r}), \tag{7}$$

if we split the summation over indices i,j into the sum over $i,j \in A$, the sum over $i,j \in B$, and the remaining overlapping part. We can also split the overlapping density into two parts dividing the space into two regions, A and B,

$$\rho^{\rm (ovlp)}_{AB}(\boldsymbol{r}) = \rho^{\rm (ovlp)}_{A}(\boldsymbol{r}) + \rho^{\rm (ovlp)}_{B}(\boldsymbol{r}). \tag{8}$$

This can be done by the plane passing through the middle of the internuclear distance (see Ref. [7] for details).

For simplicity, let us consider spherically average values of the electron densities in each region,

$$\begin{aligned} \overline{\rho}_A(r_A) &= \int d\Omega_A\left[\rho_A(\boldsymbol{r}) + \rho^{\rm (ovlp)}_A(\boldsymbol{r})\right], \\ \overline{\rho}_B(r_B) &= \int d\Omega_B\left[\rho_B(\boldsymbol{r}) + \rho^{\rm (ovlp)}_B(\boldsymbol{r})\right]. \end{aligned} \tag{9}$$

This procedure does not change the normalization of the total electron density,

$$\int d^3\boldsymbol{r}\overline{\rho}(\boldsymbol{r}) = \int d^3\boldsymbol{r}[\overline{\rho}_A(r_A) + \overline{\rho}_B(r_B)] = N - 1. \tag{10}$$

As a result, the potential $V_{AB}(\boldsymbol{r})$ can be approximated by the sum of the spherically symmetric potentials of the two different centers,

$$V_{AB}(\boldsymbol{r}) \simeq V_A[\overline{\rho}_A](r_A) + V_B[\overline{\rho}_B](r_B). \tag{11}$$

The overlapping densities must be taken into account especially for the short internuclear distances. Otherwise, the Pauli principle is violated and, as a result, the number of electrons on the $1s$ shell of the united system can exceed 2.

It should also be noted that the time-dependent wave function $\psi(\boldsymbol{r},t)$ of the active electron is orthogonalized to the wave functions $\psi^{(p)}_i(\boldsymbol{r})$ of the passive electrons. This means that the transitions of the active electron to the states occupied by the passive electrons are forbidden in accordance with the Pauli principle.

B. Two-center Dirac-Kohn-Sham equation

The two-center expansion of the time-dependent wave function $\psi(\boldsymbol{r},t)$ can be written in the form

$$\psi(\boldsymbol{r},t) = \sum_{\alpha=A,B}\sum_a C_{\alpha a}(t)\varphi_{\alpha,a}(\boldsymbol{r} - \boldsymbol{R}_\alpha(t)), \tag{12}$$

where index $\alpha = A,B$ labels the centers, index a enumerates basis functions at the given center, and $\varphi_{\alpha,a}(\boldsymbol{r} - \boldsymbol{R}_\alpha)$ is the central-field bispinor centered at point α. In what follows, the shorthand notations $|j\rangle \equiv |\varphi_j\rangle \equiv |\varphi_{\alpha,a}\rangle$ for states $j \equiv \alpha,a$ are used. The expansion coefficients $C_{a\alpha}(t)$ of the time-dependent wave function $\psi(\boldsymbol{r},t)$ can be obtained by solving the linear system of first-order differential equations:

$$i \sum_k S_{jk} \frac{dC_k(t)}{dt} = \sum_k (H_{jk} - T_{jk}) C_k(t), \tag{13}$$

where indices j and k enumerate the basis functions of both centers, and the matrix elements of H and S are

$$H_{jk} = \langle j|\hat{h}_{\rm D}|k\rangle, \quad S_{jk} = \langle j|k\rangle. \tag{14}$$

The matrix elements of T are given by

$$T_{jk} = i\langle j|\frac{\partial}{\partial t}|k\rangle = T^*_{kj} + i\frac{\partial}{\partial t} S_{jk}. \tag{15}$$

Obviously the matrix T is non-Hermitian, if the overlapping matrix S depends on time.

The functions $\varphi_{\alpha,a}$ depend on time due to two reasons. First, the basis functions centered at the target and projectile nuclei move together with the nuclei. Second, the basis functions depend parametrically on the distance between the nuclei, since their radial parts are obtained from the radial equations, where for each center the potential of the other ion (atom) is included in the so-called monopole approximation (see Sec. II C).

C. Basis functions

In our approach the basis set contains Dirac-Fock and Dirac-Fock-Sturm orbitals. The Dirac-Fock-Sturm orbitals can be considered as pseudostates, which should be included in the basis to take into account the contribution of the positive- and negative-energy Dirac continuum. Both types of basis functions $\varphi_{\alpha a}$ are central-field Dirac bispinors centered at the position $\boldsymbol{R}_\alpha$ ($\alpha = A,B$) of the corresponding ion,

$$\varphi_{n\kappa m}(\boldsymbol{r}) = \begin{pmatrix} \frac{P_{n\kappa}(r)}{r}\chi_{\kappa m}(\Omega) \\ i\,\frac{Q_{n\kappa}(r)}{r}\chi_{-\kappa m}(\Omega) \end{pmatrix}, \tag{16}$$

where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are the large and small radial components, respectively, and $\kappa = (-1)^{l+j+1/2}(j+1/2)$ is the relativistic angular quantum number. The large and small radial components are obtained by solving numerically the Dirac-Fock and Dirac-Fock-Sturm equations in the central-field approximation. The radial Dirac-Fock equation is

$$\begin{gathered} \left[h^{\rm DF}_\alpha + V_{\rm ext}(r)\right] F_{\alpha n\kappa}(r) = \varepsilon_{\alpha n\kappa} F_{\alpha n\kappa}(r), \\ F_{\alpha n\kappa}(r) = \begin{pmatrix} P_{\alpha n\kappa}(r) \\ Q_{\alpha n\kappa}(r) \end{pmatrix}, \end{gathered} \tag{17}$$

where $h^{\rm DF}_\alpha$ is the radial Dirac-Fock Hamiltonian of ion α ($\alpha = A,B$), $F_{\alpha n\kappa}(r)$ is the two-component radial wave function, and $V_{\rm ext}(r)$ is a local external potential. The explicit form of the radial Dirac-Fock equation and the description of the corresponding computer code are presented in Ref. [18]. For the details of the method see also Ref. [19]. The radial components of the Dirac-Fock-Sturm orbitals $\overline{\varphi}_{n\kappa m}$, which we denote by $\overline{F}_{n\kappa}(r)$, are the solutions of the generalized Dirac-Fock-Sturm eigenvalue problem,

$$\left[h^{\rm DF}_\alpha + V_{\rm ext}(r) - \varepsilon_{\alpha n_0\kappa}\right] \overline{F}_{\alpha n\kappa}(r) = \lambda_{\alpha n\kappa}\, W_\kappa(r)\, \overline{F}_{\alpha n\kappa}(r). \tag{18}$$

Here $\lambda_{\alpha n\kappa}$ can be considered as the eigenvalue of the Dirac-Fock-Sturm operator and $W_\kappa(r)$ is a constant sign weight function. The energy $\varepsilon_{\alpha n_0\kappa}$ is fixed in the Dirac-Fock-Sturm equation. If the weight function $W(r) \to 0$ at $r \to \infty$, all Sturmian functions have the same asymptotic behavior at $r \to \infty$. It is clear that for $\lambda_{\alpha n\kappa} = 0$ the Sturmian function $\overline{\varphi}_{n\kappa m}$ coincides with the reference Dirac-Fock orbital $\varphi_{n_0\kappa m}$. In our calculations we use the following weight function

$$W_\kappa(r) = -\frac{1 - \exp[-(\alpha_\kappa r)^2]}{(\alpha_\kappa r)^2}. \tag{19}$$

In contrast to $1/r$, this weight function is regular at the origin. It is well-known that the Sturmian operator is Hermitian. It does not contain continuum spectra, in contrast to the Dirac operator. Therefore, the set of the Sturmian eigenfunctions forms a discrete and complete basis set of one-electron wave functions.

The external central-field potential $V_{\rm ext}(r)$ in Eqs. (17) and (18) is arbitrary, and, therefore, it can be chosen to provide most appropriate Dirac-Fock and Dirac-Fock-Sturm basis orbitals. At small internuclear distances the wave function of the atomic electron experiences also the strong Coulomb field of the other ion (atom). To the leading order this effect can be taken into account by including the Coulomb-Hartree potential of the second ion (atom) as the external potential $V_{\rm ext}(r)$ within the monopole approximation. For instance, the external central-field potential $V^A_{\rm ext}(r)$ is given by

$$V^A_{\rm ext}(r) = V^B_{\rm mon}(r) = \frac{1}{4\pi}\int d\Omega_A V^B_H(\boldsymbol{r} - \boldsymbol{R}_{AB}), \tag{20}$$

where $V^B_{\rm mon}(r)$ is the spherically symmetric part of the reexpansion of the Coulomb-Hartree potential $V^B_H(\boldsymbol{r} - \boldsymbol{R}_{AB})$ of the ion B with respect to the center A and $\boldsymbol{R}_{AB}$ is the internuclear distance vector.

The matrix elements H_{jk}, S_{jk}, and T_{jk} [Eqs. (14) and (15)] are expressed in terms of the one- and two-center integrals which are evaluated by the method described in detail in our previous paper [7]. The time-dependent Dirac-Kohn-Sham equation for the active electron is solved using the two-center basis set expansion. The expansion coefficients are determined employing the direct evolution (exponential) operator method [7], which is more stable compared to the others, such as, e.g., the Crank-Nicholsen propagation scheme [20] and the split-operator method [21]. To obtain the matrix representation of the exponential operator in the finite basis set one has to diagonalize the generalized complex Hamiltonian matrix at each time step. Since our basis set is not too large, the diagonalization procedure is not too time-consuming.

D. Charge transfer and vacancy production probabilities

The amplitudes of the charge transfer and excitations to different bound states of the projectile and target ions are calculated by projecting the time-dependent wave function of the active electron onto the atomic Dirac-Fock orbitals of the projectile and target. The corresponding calculations for collisions of H-like ions with bare nuclei were described in detail in our work [7]. That is why here we restrict our

consideration only to the new features of the calculation procedure that occur for atom-ion collisions within the one active electron approximation.

Consider the collision of a neutral atom A (target) with a H-like ion B (projectile). We assume that before the collision the active electron occupies the $1s$ state of the target with spin up (in the relativistic case, with the total angular moment projection $\mu = 1/2$) and the passive electron of the H-like ion occupies the $1s$ state with spin down. In what follows, we are interested in two processes: the K-K charge transfer and the K-shell-vacancy production.

Let $P_A(1s)$ denote the probability to find the active electron in the $1s$ state of the target after the collision and $P_B(1s)$ denote the probability to find one active electron in the $1s$ state of the projectile or, in other words, the probability $P_{K\text{-}K}$ of the K-K shell charge transfer of one electron. To obtain the probabilty $P_{\rm vac}$ of the K-shell-vacancy production, we introduce the probabilities $P(E_1)$ and $P(E_2)$ of the events E_1 and E_2, when a hole is created in the $1s$ state of the target with spin up and spin down, respectively. The probabilities of these events are defined by

$$\begin{aligned} P(E_1) &= 1 - P_A(1s), \\ P(E_2) &= 1 - P_A(1s) - P_B(1s). \end{aligned} \tag{21}$$

Assuming the events E_1 and E_2 are independent, the probability of production of at least one hole in the $1s$ state of the target is given by

$$\begin{aligned} P_{\rm vac} &= P(E_1) + P(E_2) - P(E_1)P(E_2) \\ &= 1 - P_A(1s)[P_A(1s) + P_B(1s)]. \end{aligned} \tag{22}$$

We note that, since the sum of the probabilities $P_A(1s)$ and $P_B(1s)$ is less than 1, the vacancy production probability satisfies the condition $0 \leqslant P_{\rm vac} \leqslant 1$. It should also be noted that the K-shell-vacancy production defined by Eq. (22) includes the production of two holes in the target K shell.

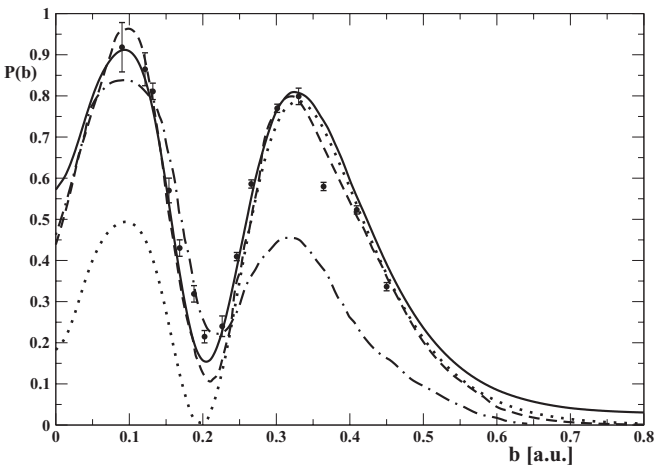

FIG. 1. The results of the present calculations for the probabilities $P(b)$ of the Ne K-shell-vacancy production (solid line) and of the K-K-shell charge transfer (dotted line) as functions of the impact parameter b for the Ne-$F^{8+}(1s)$ collision at the projectile energy 230 keV/u. The circles indicate experimental results by Hagmann *et al.* [10]. The dashed and dash-dotted lines present theoretical results by Fritsch and Lin [11] and by Thies *et al.* [13], respectively.

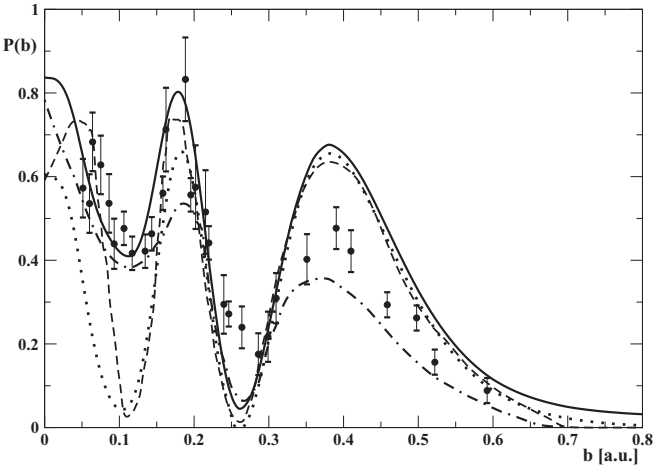

FIG. 2. The results of the present calculations for the probabilities $P(b)$ of the Ne K-shell-vacancy production (solid line) and of the K-K-shell charge transfer (dotted line) as functions of the impact parameter b for the Ne-$F^{8+}(1s)$ collision at the projectile energy 130 keV/u. The circles indicate experimental results by Hagmann *et al.* [10]. The dashed and dash-dotted lines present theoretical results by Lin *et al.* (taken from Ref. [10]) and by Thies *et al.* [13], respectively.

III. RESULTS OF THE CALCULATIONS AND DISCUSSION

To test the approach we have studied the Ne-$F^{8+}(1s)$ collision for low energies where experimental and nonrelativistic theoretical results are available [10–13]. In this case the nuclear charge numbers are rather small and, therefore, relativistic effects are negligible. We stress, however, that our approach can be directly applied to heavier systems where the relativistic effects become stronger or even dominant.

In our calculations the projectile (F^{8+}) moves on a straight line with constant velocity and the target (Ne) is fixed. In Fig. 1 we present the results of our calculations for the probabilities $P(b)$ of the Ne K-shell-vacancy production (solid line) and of the K-K-shell charge transfer (dotted line) as functions

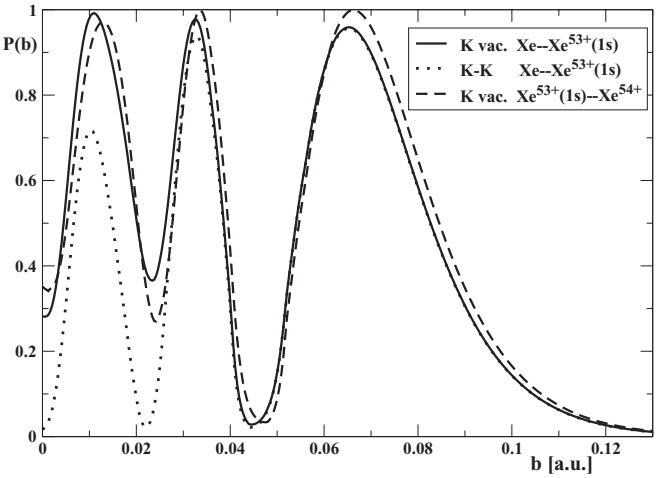

FIG. 3. The probabilities $P(b)$ of the Xe K-shell-vacancy production (solid line) and of the K-K-shell charge transfer (dotted line) in the Xe-$Xe^{53+}(1s)$ collision as functions of the impact parameter b. The dashed line indicates the K-shell-vacancy production for the $Xe^{53+}(1s)$-Xe^{54+} collision.

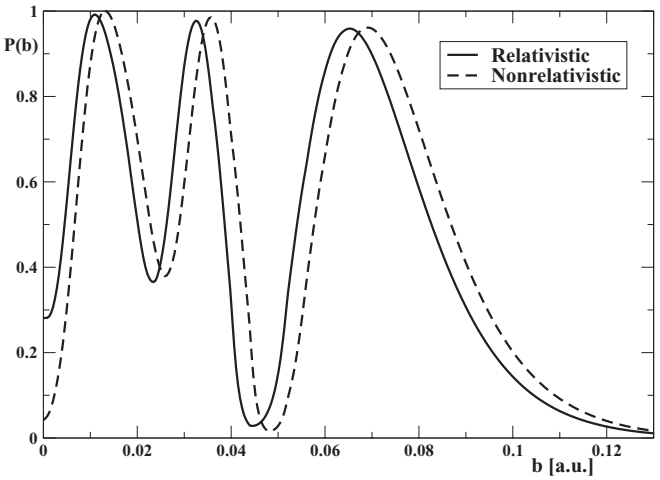

FIG. 4. The probability $P(b)$ of the Xe K-shell-vacancy production in the Xe-Xe$^{53+}(1s)$ collision as a function of the impact parameter b. The solid and dashed lines present relativistic and nonrelativistic results, respectively.

of the impact parameter b for the Ne-F$^{8+}(1s)$ collision at the projectile energy 230 keV/u. The results for the Ne K-vacancy production are compared with experimental values (circles) [10] and with theoretical results obtained by Fritsch and Lin (dashed line) [11] and by Thies *et al.* (dash-dotted line) [13]. It can be seen that our results are in perfect agreement with the experimental ones.

The related results for the Ne-F$^{8+}(1s)$ collision at the projectile energy 130 keV/u are presented in Fig. 2, where the same notations as in Fig. 1 are used. We note that our theoretical results are in good agreement with the experimental ones at small impact parameters. However, in contrast to Fig. 1, the agreement is not so good for medium and large impact parameters, although the theoretical predictions for the maximum and minimum positions agree rather well with the experimental ones.

As one can see from Figs. 1 and 2, for both energies at large impact parameters the K-vacancy production is mainly determined by the K-K-shell charge transfer, which is indicated by the dotted line. The difference between the K-vacancy production and the K-K-shell transfer probabilities at small impact parameters is due to the contribution from the charge transfer excitation into the $2s$, $2p$, and higher vacant states of the projectile. This is in accordance with the experimental results of Ref. [22], where the K-vacancy production in the Ne-F$^{6+}[(1s)^2 2s]$ collision was studied. The calculation of the latter process is currently under way and will be published elsewhere.

In this work we also performed the related calculations for the Xe-Xe$^{53+}(1s)$ collision at the projectile energy 3.6 MeV/u. The experimental study of this process is planned at GSI (Darmstadt) [8,9]. The probabilities $P(b)$ of the Xe K-shell-vacancy production and of the K-K-shell charge transfer as functions of the impact parameter b are plotted in Fig. 3. The solid and dotted lines represent the vacancy production and the charge transfer, respectively. For comparison, in the same figure we display the K-shell-vacancy production for the Xe$^{53+}(1s)$-Xe^{54+} collision that is indicated by the dashed line. We note again that at large impact parameters the K-vacancy production is almost completely determined by the K-K-shell charge transfer. It can be also seen that in the case under consideration the screening effect is rather small.

To investigate the role of the relativistic effects we performed the same calculations for the Xe-Xe$^{53+}(1s)$ collision in the nonrelativistic limit by multiplying the standard value of the speed of light by the factor 1000. The obtained relativistic and nonrelativistic results are presented in Fig. 4. As one can see from the figure, the oscillatory behavior of both curves is the same but the nonrelativistic curve is shifted toward larger impact parameters.

IV. CONCLUSION

In this paper the method that was previously developed for evaluation of the electron-excitation and charge transfer processes in collisions of H-like ions with bare nuclei has been extended to collisions of ions with neutral atoms. The extention is based on the active-electron approximation, in which the interaction of the active electron with the passive electrons is accounted for by the screening DFT potential.

The method developed has been applied to evaluate the K-vacancy production and the K-K charge transfer in the low-energy Ne-F^{8+} collision. The results of the calculation are compared with available experimental data and with theoretical calculations by other authors. The influence of the relativistic effects on the K-vacancy production probability is investigated for the Xe-Xe^{53+} collision. It is demonstrated that the relativistic and nonrelativistic probabilities as functions of the impact parameter exhibit the same oscillatory behavior at low energies but the relativistic curves are shifted toward lower impact parameters compared to the nonrelativistic ones.

In our further investigation we plan to continue calculations of low-energy heavy-ion collisions that are of interest for current and near future experiments at GSI and FAIR in Darmstadt. Special attention will be paid to the critical regime, when the ground-state level of the united quasimolecule can become so deeply bound to allow for spontaneous filling by electron-positron pair creation. In the Dirac single-particle picture this corresponds to the diving of the ground-state level into the negative-energy Dirac continuum.

As is known (see, e.g., Refs. [4,23]), for a proper account of the negative-energy continuum one should use the second quantization formalism. Such a formulation, which is especially important in the near critical regime, and the corresponding calculations will be presented in a forthcoming paper.

ACKNOWLEDGMENTS

This work was supported by DFG (Grants No. PL 254/7-1 and No. VO 1707/1-1), by RFBR (Grants No. 10-02-00450 and No. 11-02-00943-a), by GSI, by DAAD, by the Ministry of Education and Science of the Russian Federation (Grant No. P1334), and by the grant of the President of the Russian Federation (Grant No. MK- 2106.2012.2). The work of A.I.B. and I.A.M. was also supported by the Dynasty Foundation. Y.S.K. and A.I.B. acknowledge financial support from the FAIR–Russia Research Center.

[1] J. Eichler and W. E. Meyerhof, *Relativistic Atomic Collisions* (Academic Press, New York, 1995).
[2] V. M. Shabaev, Phys. Rep. **356**, 119 (2002).
[3] J. Eichler and T. Stöhlker, Phys. Rep. **439**, 1 (2007).
[4] W. Greiner, B. Müller, and J. Rafelski, *Quantum Electrodynamics of Strong Fields* (Springer-Verlag, Berlin, 1985).
[5] B. Müller and W. Greiner, Z. Naturforsch. **31a**, 1 (1976).
[6] B. H. Bransden and M. R. C. McDowell, *Charge Exchange and the Theory of Ion-Atom Collisions* (Oxford University Press, New York, 1992).
[7] I. I. Tupitsyn, Y. S. Kozhedub, V. M. Shabaev, G. B. Deyneka, S. Hagmann, C. Kozhuharov, G. Plunien, and Th. Stöhlker, Phys. Rev. A **82**, 042701 (2010).
[8] S. Hagmann *et al.*, "Electron Emission following 1*s* Adiabatic Ionization and Quasi-resonant 1*s*-1*s* Charge Transfer in Symmetric Ion-Atom Collisions," GSI proposal (unpublished).
[9] S. Hagmann *et al.*, AIP Conf. Proc. **1336**, 115 (2011); P. D. Fainstein, J. Phys. B **37**, 817 (2004).
[10] S. Hagmann, S. Kelbch, H. Schmidt-Böcking, C. L. Cocke, P. Richard, R. Schuch, A. Skutlartz, J. Ullrich, B. Johnson, M. Meron, K. Jones, D. Trautmann, and F. Rösel, Phys. Rev. A **36**, 2603 (1987).
[11] W. Fritsch and C. D. Lin, Phys. Rev. A **31**, 1164 (1985).
[12] A. Toepfer, A. Henne, H. J. Lüdde, M. Horbatsch, and R. M. Dreizler, Phys. Lett. A **126**, 11 (1987).
[13] B. Thies, W. D. Sepp, and B. Fricke, Phys. Lett. A **139**, 161 (1989).
[14] C. D. Lin and P. Richard, *Inner Shell Vacancy Production in Ion-Atom Collisions*, Advances in Atomic and Molecular Physics, edited by D. Bates and B. Bederson (Academic, New York, 1981), Vol. 17, p. 275.
[15] I. I. Tupitsyn, V. M. Shabaev, J. R. Crespo López-Urrutia, I. Draganić, R. S. Orts, and J. Ullrich, Phys. Rev. A **68**, 022511 (2003).
[16] I. I. Tupitsyn, A. V. Volotka, D. A. Glazov, V. M. Shabaev, G. Plunien, J. R. Crespo López-Urrutia, A. Lapierre, and J. Ullrich, Phys. Rev. A **72**, 062503 (2005).
[17] J. P. Perdew and A. Zunger, Phys. Rev. B **23**, 5048 (1981).
[18] V. F. Bratsev, G. B. Deyneka, and I. I. Tupitsyn, Bull. Acad. Sci. USSR, Phys. Ser. **41**, 173 (1977).
[19] I. P. Grant, Adv. Phys. **19**, 747 (1970).
[20] J. Crank and P. Nicholson, Proc. Cambridge Philos. Soc. **43**, 50 (1947).
[21] M. D. Feit, J. A. Fleck Jr., and A. Steiger, J. Comput. Phys. **47**, 412 (1982).
[22] S. Hagmann, C. L. Cocke, J. R. Macdonald, P. Richard, H. Schmidt-Böcking, and R. Schuch, Phys. Rev. A **25**, 1918 (1982).
[23] E. S. Fradkin, D. M. Gitman, and S. M. Shvartsman, *Quantum Electrodynamics with Unstable Vacuum* (Springer-Verlag, Berlin, 1991).