Non-perturbative relativistic calculations of the K-shell-vacancy production in Xe–Xe^{54+} collisions

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Abstract. Non-perturbative calculations of the relativistic quantum dynamics of electrons in the Xe-Xe^{54+} collisions at 30 AMeV are performed. The calculations are based on an independent-electron model and use the coupled-channel approach with atomic-like Dirac-Fock-Sturm orbitals. Special attention is paid to the inner-shell processes. The role of the relativistic and many-particle effects is studied.

1. Introduction

Heavy-ion collisions play a very important role in investigations of the relativistic quantum dynamics of electrons in presence of strong electromagnetic fields [1]. Moreover, if the total charge of the colliding nuclei is larger than the critical one, $Z_1 + Z_2 > 173$, such collisions can provide a unique tool for tests of quantum electrodynamics at the supercritical regime [2]. The CRYRING [5] at the present GSI SIS18/ESR facility and, especially, the realization of the FAIR [3, 4] project will provide unique opportunities for studying new physics with low-energy heavy-ion-atom collisions. These studies require corresponding theoretical calculations which have to describe in details the relativistic quantum dynamics of electrons.

In the present paper, we perform the relativistic non-perturbative quantum-mechanical calculations of the Xe-Xe^{54+} collision at 30 AMeV within an independent electron model using the coupled-channel approach with atomic-like Dirac-Fock-Sturm orbitals [6, 7]. We evaluate the K-shell-vacancy production in this collision and investigate the role of the many-electron and relativistic effects.

Atomic units ($\hbar = e = m_e = 1$) are used throughout the paper.

2. Method

In the following, we briefly present the formalism used, for a complete description see Refs. [6, 8, 9]. Using the semiclassical approximation, where the atomic nuclei move along the classical trajectories and are considered as sources of a time-dependent external potential, we have to solve the time-dependent many-particle Dirac equation for electrons involved in the process. The method we employ is based on an independent particle model, where the many-electronic Hamiltonian $\hat{H}$ is approximated by a sum of effective single-electron Hamiltonians, $\hat{H}^{\text{eff}} = \sum \hat{h}^{\text{eff}}$, reducing the electronic many-particle problem to a set of single-particle Dirac equations for all electrons of the colliding system:

$$i\frac{\partial \psi_i(t)}{\partial t} = \hat{h}_i^{\text{eff}}(t)\,\psi_i(t) \quad \text{with} \quad i = 1, \ldots, N, \tag{1}$$

where the wave functions $\psi_i(t)$ have to satisfy the initial conditions for the N electrons:

$$\lim_{t \to -\infty} (\psi_i(t) - \psi_i^0(t)) = 0 \quad \text{with} \quad i = 1, \ldots, N. \tag{2}$$

As the effective single-electron Hamiltonian $\hat{h}^{\text{eff}}$ we use the two-center Dirac-Kohn-Sham Hamiltonian:

$$\hat{h}^{\text{eff}} = c(\vec{\alpha} \cdot \vec{p}) + \beta\, c^2 + V_{\text{nucl}}^A(\vec{r}_A) + V_{\text{nucl}}^B(\vec{r}_B) + V_C[\rho] + V_{xc}[\rho]\,, \tag{3}$$

where c is the speed of light and $\vec{\alpha}$, β are the Dirac matrices. Here $V_{\text{nucl}}^{\alpha}(\vec{r}_\alpha)$ and $V_C[\rho] = \int d^3\vec{r'}\, \frac{\rho(\vec{r'})}{|\vec{r} - \vec{r'}|}$ are the electron-nucleus interaction and the electron-electron Coulomb potentials, respectively, and $\rho(\vec{r})$ is the electron density of the system. The exchange-correlation potential $V_{xc}[\rho]$ is taken in the Perdew-Zunger parametrization [10].

Solving the effective single-particle equations (1) is based on the coupled-channel approach with atomic-like Dirac-Sturm-Fock orbitals, localized at the ions (atoms) [9]. The many-particle probabilities are calculated in terms of the single-particle amplitudes employing the formalism of inclusive probabilities [11, 12], which allows one to describe the many-electron collision dynamics.

3. Results and discussion

In the present paper, we applied the methods described in Sec. 2 to calculate the inner-shell processes in low-energy collisions of neutral atoms with bare ions. The calculations were performed for the Xe-Xe^{54+} collision, which experimental investigation was recently carried out at GSI (Darmstadt) [13]. Since we were mainly interested in the dynamics of electrons in presence of the strongest electric field, we focused on the study of the K-shell electron population probabilities of the colliding ions.

Figure 1 shows the probabilities of the q-vacancy creation in the K shell of the target atom (neutral xenon) as functions of the impact parameter. In order to investigate the role of many-electron effects we performed the calculations using both the many-electron approach and the active-electron approximation. The results are indicated in Fig. 1 by bold and thin lines, correspondingly. In the active-electron approximation only the K-shell electrons of the target are considered as the active electrons and participate in excitation and charge-transfer processes, while the others provide a screening potential. In both cases the probabilities have a rather similar oscillatory behaviour, but the magnitudes of the peaks and bottoms are changed while their positions are preserved.

In order to investigate the role of the relativistic effects we performed the corresponding calculations in the nonrelativistic limit by multiplying the standard value of the speed of light by the factor 1000 (in atomic units). The comparison of the obtained relativistic and nonrelativistic results is presented in Fig. 2. As one can see from this figure, the relativistic (bold lines) and nonrelativistic (thin lines) curves have the same oscillatory behavior but the nonrelativistic curves are shifted toward larger impact parameters.

To summarize, the many-particle and relativistic effects on the probabilities of the q-K-shell vacancy production in the Xe-Xe^{54+} collision at 30 AMeV have been investigated. The contributions of these effects are of the same order of magnitude but of different type. The many-electron effects decrease the magnitudes of the oscillatory behavior, while the relativistic ones shift the oscillatory curves toward smaller impact parameters. These corrections are rather substantial and have to be taken into account.

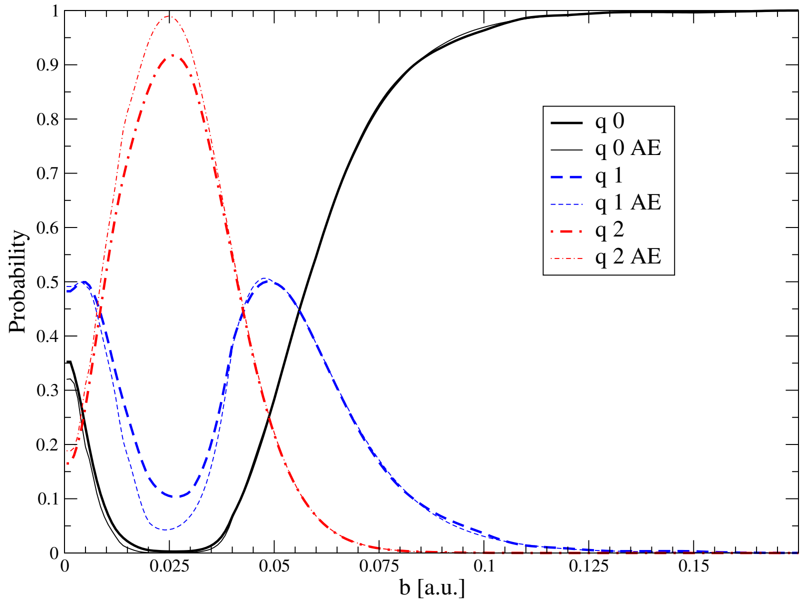

Figure 1. The probabilities of the target Xe q-K-shell-vacancy production as functions of the impact parameter b for the Xe-Xe^{54+} collision at the projectile (Xe^{54+}) energy of 30 MeV/u. The bold and thin lines indicate the results of the calculation using the many-electron approach and the active-electron (AE) approximation, correspondingly.

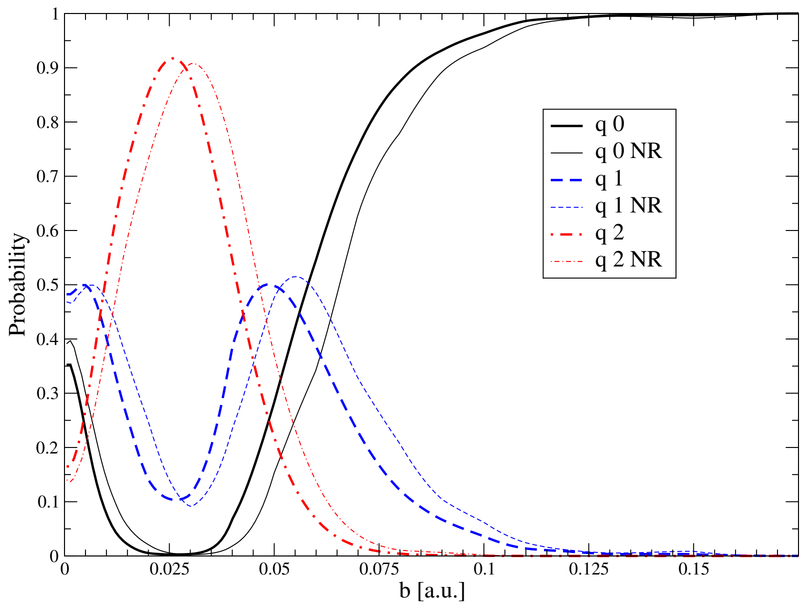

Figure 2. The probabilities of the target Xe q-K-shell-vacancy production as functions of the impact parameter b for the Xe-Xe^{54+} collision at the projectile (Xe^{54+}) energy of 30 MeV/u. The bold and thin lines indicate the relativistic and non-relativistic (NR) results of the calculation, correspondingly.

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