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Bare- and Dressed-Ion Impact Collisions from Neon Atoms Studied Within a Nonperturbative Mean-Field Approach

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Abstract

We study electron removal processes in collisions of bare and dressed doubly charged ions with neon atoms in the 20 keV/u to 1 MeV/u impact energy regime. The many-electron problem is represented by a single mean field, which in the case of dressed-ion impact includes the projectile electrons. Moreover, the same basis is used to propagate all active orbitals thereby ensuring orthogonality at all times and allowing for a final-state analysis in terms of standard Slater determinantal wave functions. The same approach was used in a recent work for B^{2+}-Ne collisions [Phys. Rev. A 88 012712], in which we examined the role of the projectile electrons for target-recoil-charge-state production. The present study expands on that work by considering additional collision channels and comparing results of equicharged dressed and bare ions in order to shed more light on the role of the projectile electrons.

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1. Introduction

Recently, results from collision experiments of dressed B^{2+} projectiles with atomic neon targets were reported [1, 2]. Collision systems like this are a challenge for theoretical descriptions, since one has to deal with electrons not only on the target, but also on the projectile. One approach to describe such collisions is to only consider the active target electrons while the initial projectile electrons are solely taken into account in terms of a screening potential. Such calculations have been performed in the independent particle model (IPM), for example with the continuum distorted wave with eikonal initial state (CDW-EIS) method [2, 3]. In a recent work we discussed the advantages of considering active electrons on the dressed-ion projectile as well as on the target in the description of projectile charge state coincident multiple ionization of neon [4]. In the present work we compare results of such calculations for dressed-ion impact with those of equicharged bare ion impact, specifically the collisions of B^{2+} and He^{2+} with Ne. Atomic units are used throughout this work, unless stated otherwise.

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2. Method

The collisions are described in an IPM in which the nuclear potentials are screened by mean-field potentials of their electrons. The collisions discussed here are fast enough to describe the nuclear motion by straight line trajectories. The many-electron system is separated into independent problems for N initial conditions, which correspond to the N orbitals that are occupied on the projectile and the target at an asymptotic time before the collision. All initial states are propagated with the same Hamiltonian

$$\hat{h}(t) = -\frac{1}{2}\Delta - \frac{Z_\mathrm{t}}{r_\mathrm{t}} + v_\mathrm{ee}^\mathrm{t}(r_\mathrm{t}) - \frac{Z_\mathrm{p}}{r_\mathrm{p}} + v_\mathrm{Ha}^\mathrm{p}(r_\mathrm{p}) \tag{1}$$

where $-Z_\mathrm{t}/r_\mathrm{t}$ and $-Z_\mathrm{p}/r_\mathrm{p}$ are the nuclear target and projectile potentials, respectively. The projectile is screened by the Hartree potential $v_\mathrm{Ha}^\mathrm{p}(r_\mathrm{p})$. At asymptotic distances the effective projectile potential $-Z_p/r_p + v_\mathrm{Ha}^\mathrm{p}(r_\mathrm{p})$ approaches $-q_\mathrm{p}^i/r_\mathrm{p}$ with the initial projectile charge state q_p^i. The potential $v_\mathrm{ee}^\mathrm{t}(r_\mathrm{t})$ includes Hartree and exchange terms, i.e. it compensates self interaction [5], and is therefore asymptotic to $-1/r_\mathrm{t}$. We are using the no-response approximation in which the effective potentials do not change their forms, but reflect the electron configuration at the initial time throughout the collision. The potentials used in our calculations are obtained from the optimized potential method [5].

Using the same Hamiltonian, i.e. a common mean field, preserves orthogonality of the propagated states. The downside of using the Hamiltonian (1) for all initially occupied orbitals is that it is not possible to ensure the correct asymptotic behaviour for both collision centres at the same time. In this work we choose to have the asymptotically correct potential for the target, as our focus is on removal and capture of target electrons. The single-particle equations

$$\mathrm{i}\partial_t \psi_\nu(\mathbf{r},t) = \hat{h}(t)\psi_\nu(\mathbf{r},t), \quad \nu = 1,\ldots,N \tag{2}$$

are solved with the two-centre basis generator method (TC-BGM) [6, 7] which is a basis expansion method. The basis is formed by atomic eigenstates of the target, ionic eigenstates of the projectile, and pseudo states to represent the continuum. For the present calculations our basis consists of the 19 neon eigenstates $2s\ldots4f$ and 20 projectile eigenstates $1s\ldots4f$ of the hydrogen-like bare helium or the dressed boron ion. In addition 79 pseudostates generated from target orbitals are included.

For each initial condition (index ν) and for all final states (bound target or projectile states), labelled by μ, we obtain transition amplitudes $c_{\nu\mu}$ and single-particle probablities $p_{\nu\mu} = |c_{\nu\mu}|^2$. The latter can be used for a direct comparison with experiments that provide net recoil ion production cross sections:

$$\sigma_+ = 2\pi \int_0^\infty b P_\mathrm{net}^\mathrm{rec}(b)\,\mathrm{d}b. \tag{3}$$

The impact parameter b dependent net recoil ion production $P_\mathrm{net}^\mathrm{rec}(b)$ is found by summing up the single-particle probabilities $p_{\nu\mu}$ corresponding to bound target states:

$$P_\mathrm{net}^\mathrm{rec}(b) = N_\mathrm{t} - \sum_\nu \sum_{\mu\in T} n_\nu p_{\nu\mu}(b). \tag{4}$$

N_t is the number of electrons initially at the target. For the collisions of Ne with the bare He^{2+} projectile the inital conditions are the neon $2s$ to $2p_1$ orbitals, each occupied by $n_\nu = 2$ electrons. For the dressed B^{2+} projectile the boron $1s$ and $2s$ states are propagated in addition. In both calculations the neon $1s$ orbital is neither propagated nor included in the basis. These K-shell electrons are considered passive and only contribute to the screening potential v_ee^t.