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Time-dependent density functional theory calculations for collisions of bare ions with helium

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Abstract

We present net capture and ionisation cross sections for the collision systems p-He and He^{2+}–He with emphasis on microscopic response effects during the collision. The calculations rely on the basis generator method (BGM). In both collision systems the response of the effective electronic interaction to the time-dependent density leads to a significant change of the net cross sections.

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1. Introduction

Time-dependent density functional theory (TDDFT) provides a sound basis for the description of interacting many-particle systems in terms of single-particle equations [1]. It has been used very recently to calculate charge transfer in Ar^{8+}–Ar collisions [2] and ionisation in $\bar{p}$-He collisions [3,4]. We have calculated charge transfer and ionisation in the collision systems p-He and He^{2+}–He using TDDFT within the so-called exchange-only approximation, i.e. time-dependent screening and exchange effects are treated on a microscopic level, while electron correlations are neglected. The comparison with experimental data and with calculations in which time-dependent changes in the effective potential are also neglected sheds light on the role of different

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aspects of the electron-electron interaction. Atomic units ($\hbar = m_e = e = 1$) are used throughout.

2. Theory

Within the framework of TDDFT the single-particle equations for an N-electron ion–atom collision system are

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

with the Hamiltonian

$$\hat{h}(t) = -\frac{1}{2}\Delta - \frac{Z_\mathrm{T}}{r} - \frac{Z_\mathrm{P}}{|\mathbf{r}-\mathbf{R}(t)|} + v_{ee}([n(t)],\mathbf{r},t) \tag{2}$$

and the one-particle density

$$n(\mathbf{r},t) = \sum_{j=1}^{N} |\psi_j(\mathbf{r},t)|^2. \tag{3}$$

We assume that the projectile is moving on a straight line trajectory $\mathbf{R}(t) = (b,0,Vt)$ with impact parameter b and constant velocity V.

For collisions of bare ions with a helium target in the groundstate, i.e. a two-electron spin singlet system, the effective electronic potential within the exchange-only approximation reads

$$v_{ee}(\mathbf{r},t) = \frac{1}{2}\int \frac{n(\mathbf{r}',t)}{|\mathbf{r}-\mathbf{r}'|}\,\mathrm{d}^3r' \tag{4}$$

and the density is given by $n(\mathbf{r},t) = 2|\psi(\mathbf{r},t)|^2$. As one can see, v_{ee} fulfils the Poisson equation

$$\Delta v_{ee}(\mathbf{r},t) = -\frac{1}{2}4\pi n(\mathbf{r},t). \tag{5}$$

To solve the time-dependent single-particle equation (1) we use a basis representation obtained from the basis generator method (BGM) [5]

$$\psi(\mathbf{r},t) = \sum_{K=0}^{L}\sum_{J=0}^{M}\sum_{k=1}^{N'} c_k^{KJ}(t)\chi_k^{KJ}(\mathbf{r},t), \tag{6}$$

$$\chi_k^{KJ}(\mathbf{r},t) = W_\mathrm{T}(r,\epsilon_\mathrm{T})^K W_\mathrm{P}(\mathbf{r},t,\epsilon_\mathrm{P})^J \chi_k^{00}(\mathbf{r}), \tag{7}$$

$$W_\mathrm{T}(r,\epsilon_\mathrm{T}) = \frac{1-\exp(-\epsilon_\mathrm{T} r)}{r}, \tag{8}$$

$$W_\mathrm{P}(\mathbf{r},t,\epsilon_\mathrm{P}) = \frac{1-\exp(-\epsilon_\mathrm{P}|\mathbf{r}-\mathbf{R}(t)|)}{|\mathbf{r}-\mathbf{R}(t)|}, \tag{9}$$

with $W_\mathrm{P/T}$ denoting the regularised Coulomb interactions with respect to the projectile and target centers, respectively. The set of bound eigenfunctions of the undisturbed helium atom $\chi_k^{00}(\mathbf{r})$ accounts for the elastic and target excitation channels, while the set of pseudostates $\chi_k^{KJ}(\mathbf{r},t)$ describes ionisation and capture. To simplify the construction and to reduce the amount of BGM states, only states generated with W_P ($L = 0$) are used for the results presented here. This scheme has proven to yield reasonable convergence in a number of applications [6].

In order to solve the Poisson equation we represent v_{ee} according to [4]

$$v_{ee}(\mathbf{r},t) = \sum_{\lambda=1}^{\Lambda}\sum_{l=0}^{D}\sum_{m=0}^{l} d_{lm}^{\lambda}(t) W_\mathrm{T}(r,\epsilon_\mathrm{T})^{\lambda} Y_{lm}^{T}(\Omega_\mathrm{T}) + \sum_{\lambda'=1}^{\Lambda'}\sum_{l'=0}^{D'}\sum_{m'=0}^{l'} b_{l'm'}^{\lambda'}(t) W_\mathrm{P}(\mathbf{r},t,\epsilon_\mathrm{P})^{\lambda'} Y_{l'm'}^{P}(\Omega_\mathrm{P}). \tag{10}$$

The radial parts are described by the $W_\mathrm{T/P}$-hierarchy (8), (9), the angular parts by spherical harmonics. The coefficients $d_{lm}^{\lambda}(t)$ and $b_{l'm'}^{\lambda'}(t)$ are determined at each timestep of the collision. Within the *no-response* approximation that we apply for the sake of comparison the electron-electron potential is frozen to the initial ground state configuration ($v_{ee}(\mathbf{r},t) = v_{ee}^0(r)$).

We calculate single-particle transition probabilities with respect to the eigenfunctions of the time-dependent Hamiltonian (2) at large internuclear separations. As these functions fulfil the boundary conditions of the collision system only approximately, the transition probabilities do not necessarily become perfectly stable with respect to time (for a detailed discussion of this topic see [4]). From the single-particle probabilities for attachment to the projectile (P_P) and the continuum contribution (P_C) we calculate net probabilities for capture and ionisation by

$$P_{\mathrm{net}}^{x} = 2P_x \quad x\text{: } P, C. \tag{11}$$

As net probabilities, that correspond to average electron numbers, can be explicitly expressed as