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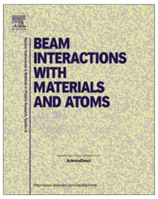

A critical study on electronic processes involving electron capture and ionization of He targets by interaction with multiply charged ion beams

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ABSTRACT

The interest of the present work is focused on theoretical calculations of single electron ionization, single electron capture and transfer-ionization reactions of He targets interacting with bare ion beams. In order to investigate all these processes, the corresponding transition probabilities are determined in the framework of the prior-version of the three-body Continuum Distorted Wave-Eikonal Initial State model (3B-CDW-EIS). A theoretical description using a trinomial probability analysis based on 3B-CDW-EIS is also presented to analyze its limitations for the studied reactions. The cases of He^{2+} and Li^{3+} projectiles are considered at intermediate and high collision energies. A unitarization procedure is employed to avoid transition probabilities larger than one at intermediate velocities.

1. Introduction

Dynamical interaction of bare ion projectiles impacting on He atoms is the simplest multi-electronic system to investigate electron transitions. The study of these collisional systems is crucial to fully understand the mechanisms underlying these basic reactions. Moreover, they are of interest in several fields such as astrophysics [1], thermonuclear fusion [2] and hot plasmas [3], among other areas.

In the early days, experimental data for electronic reactions were provided mainly measuring projectile or target ion charges in the exit channel, combining them in some cases with the resulting radiation emission. Moreover, the corresponding cross sections were usually normalized to other theoretical and experimental predictions. Nowadays, using cold target recoil ion momentum spectroscopy (COLTRIMS) techniques, kinematically complete experiments are feasible [4], allowing to investigate separately different electronic reactions, such as single ionization, single capture and transfer-ionization. Thus, these new facilities open the possibility to test new theoretical descriptions in the same way as experiments were done, for a more appropriate comparison between them and for a better understanding of the different electron transition processes studied.

The aim of this work is to present single electron ionization (SI), single electron capture (SC) and two-electron-transfer-ionization (TI) cross sections of He targets impacted by He^{2+} and Li^{3+} projectiles at intermediate and high collision energies. They are computed through the determination of transition probabilities as a function of the impact parameter in the framework of the 3B-CDW-EIS model. A unitarization procedure appears as necessary to avoid overestimations of 3B-CDW-EIS impact parameter probabilities. Two different models are employed, 3B-CDW-EIS developed by Rivarola and co-workers for single-electron capture [5] as well as for single electron ionization [6], and another one, where a trinomial probability analysis (TPA) based on 3B-CDW-EIS ones are used [7,8]. Both approximations are calculated in order to discern their adequacy to describe the different electronic reactions. It must be mentioned that an approximation employing binomial probabilities has been previously applied with some success to describe multiple electron ionization of atomic and molecular targets at high impact energies [9–11].

Unless otherwise stated, atomic units ($m_e = \hbar = e = 1$) will be used.

2. Theory

The 3B-CDW-EIS model is employed to calculate the transition probabilities for both single electron ionization [12] and single electron capture [13,14]. Originally, Crothers and McCann developed this model [15] for SI of hydrogenic targets and later on it

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was extended [6] with great success for multielectronic targets, assuming that except for the active electron all the residual ones remain as frozen in their initial orbitals. This is a key point in our analysis. Within the straight-line version of the impact parameter approximation ($\mathbf{R} = \boldsymbol{\rho} + \mathbf{v}t$, with $\mathbf{R}$ being the internuclear vector, $\boldsymbol{\rho}$ the impact parameter, $\mathbf{v}$ the collision velocity and t the evolution time) this formulation was based on a deduction previously obtained for SC [5] and which has a general character, independently of the theoretical model employed. Thus, for SI or SC the problem was reduced to find scattering solutions of a one-active electron Hamiltonian

$$H = -\nabla^2/2 - Z_T/x - Z_P/s + V_{ap}(\mathbf{x}) + V_S(\mathbf{R}), \tag{1}$$

where Z_T and Z_P are the target and projectile nucleus charges, $\mathbf{x}$ and $\mathbf{s}$ represent the position vectors of the active electron with respect to the target and projectile, respectively, and,

$$V_{ap}(\mathbf{x}) = \left\langle \varphi_p(\{\mathbf{x}_{p\,i}\}) \middle| \sum_{i=1}^{N_p} \frac{1}{|\mathbf{x} - \mathbf{x}_{p\,i}|} \middle| \varphi_p(\{\mathbf{x}_{p\,i}\}) \right\rangle \tag{2}$$

is a potential that takes into account the interaction of the active electron with the passive ones, being $\varphi_p(\{\mathbf{x}_{p\,i}\})$ the wavefunction corresponding to the N_p passive electrons and $\mathbf{x}_{p\,i}$ is the ensemble of position vectors of the i th passive electrons with respect to the target nucleus. Also in Eq. (2), $V_S(\mathbf{R})$ is the static potential

$$V_s(\mathbf{R}) = \frac{Z_P Z_T}{R} + \left\langle \varphi_p(\{\mathbf{x}_{p\,i}\}) \middle| - \sum_{i=1}^{N_p} \frac{Z_P}{|\mathbf{R} - \mathbf{x}_{p\,i}|} \middle| \varphi_p(\{\mathbf{x}_{p\,i}\}) \right\rangle, \tag{3}$$

which considers the interaction between the residual target and the projectile. In order to facilitate the calculations, the potentials $(-Z_T/x + V_{ap}(\mathbf{x}))$ are replaced by a coulombic one $(-Z_T^*/x)$, where an effective charge Z_T^* is chosen as $Z_T^* = \sqrt{-2n_i^2\varepsilon_i}$ [16], where n_i is the principal quantum number of the target electron orbital and ε_i is the corresponding active electron binding energy.

The initial wave function in a reference frame located on the target nucleus, both for ionization and capture, is chosen as

$$\begin{aligned}\chi_i^{ion,\ cap} &= \varphi_i(\mathbf{x}) \exp(-i\varepsilon_i t) \exp[-i\tfrac{Z_P}{v} \ln(vs + \mathbf{vs})] \\ &\quad \times \exp\{-i \textstyle\int_{-\infty}^{t} V_S(\mathbf{R})dt'\} = \\ &= \Phi_i^{ion,\ cap}(\mathbf{x}, t) \exp\{-i \textstyle\int_{-\infty}^{t} V_S(\mathbf{R})dt'\},\end{aligned} \tag{4}$$

where $\varphi_i(\mathbf{x})$ is the initial active electron bound state described within the Roothan-Hartree-Fock approximation [17].

The final wavefunction for ionization is chosen as

$$\begin{aligned}\chi_f^{ion} &= (2\pi)^{-3/2} \exp(-i\varepsilon_f^{ion} t + i\mathbf{kx}) N^*(\xi)_1 \times F_1(-i\xi; 1; -ikx - i\mathbf{kx}) \\ &\quad \cdot N^*(\zeta)_1 F_1(-i\zeta; 1; -ips - i\mathbf{ps}) \times \exp\{i \textstyle\int_t^{+\infty} V_S(\mathbf{R})dt'\} \\ &= \Phi_f^{ion}(\mathbf{x}, t) \exp\{i \textstyle\int_t^{+\infty} V_S(\mathbf{R})dt'\},\end{aligned} \tag{5}$$

where $\mathbf{k}\,(\mathbf{p} = \mathbf{k} - \mathbf{v})$ is the linear momentum of the ejected electron with respect to the target (projectile) nucleus, $\varepsilon_f^{ion} = k^2/2$ is the final electron energy, $N(a) = \exp(\pi a/2)\Gamma(1 + ia)$ with Γ the Gamma function, $\xi = Z_T^*/k$, $\zeta = Z_P/p$ and ${}_1F_1(a; 1; b)$ is the Coulomb continuum factor.

The final wavefunction for electron capture is taken as

$$\begin{aligned}\chi_f^{cap} &= \varphi_f(\mathbf{s}) \exp(-i\varepsilon_f^{cap} t + i\mathbf{vx} - i\tfrac{v^2}{2}t) \cdot N^*(\beta)_1 F_1(-i\beta; 1; -ivx - i\mathbf{vx}) \\ &\quad \times \exp\{i \textstyle\int_t^{+\infty} V_S(\mathbf{R})dt'\} = \Phi_f^{cap}(\mathbf{s}, t) \exp\{i \textstyle\int_t^{+\infty} V_S(\mathbf{R})dt'\},\end{aligned} \tag{6}$$

with $\varphi_f(\mathbf{s})$ the final active electron bound state, ε_f^{cap} the corresponding orbital energy and $\beta = Z_T^*/v$. It has been demonstrated that with these choices of wavefunctions, radial electron correlation is included in the entry channel and the interaction between the passive and active electrons (dynamical screening) is considered in the exit one [18,19]. Hereby, the so-called two-center effect is taken into account in the 3B-CDW-EIS approximation.

Transition amplitudes

$$\begin{aligned}A_{if}^{ion,\ cap}(\boldsymbol{\rho}, \mathbf{k}) &= -i \int_{-\infty}^{+\infty} dt \left\langle \chi_f^{ion,\ cap} \middle| H - i\frac{\partial}{\partial t} \middle| \chi_i^{ion,\ cap} \right\rangle \\ &= -i \exp\{-i \int_{-\infty}^{+\infty} V_S(\mathbf{R})dt\} \cdot \int_{-\infty}^{+\infty} dt \Big\langle \Phi_f^{ion,\ cap} \Big| H_e \\ &\quad - i\frac{\partial}{\partial t} \Big| \Phi_i^{ion,\ cap} \Big\rangle = a_{if}^{ion,\ cap} \exp\{-i \int_{-\infty}^{+\infty} V_S(\mathbf{R})dt\}\end{aligned} \tag{7}$$

with

$$H_e = H - V_S(\mathbf{R}) \tag{8}$$

as a function of the impact parameter, both for ionization and capture, are analyzed.

We define the one-active electron ionization probability as,

$$\frac{d^3 P_{ion}(\rho, \mathbf{k})}{dE_k d\Omega_k} = \frac{k}{2\pi} \int_0^{2\pi} d\varphi_\rho |a_{if}^{ion}(\boldsymbol{\rho}, \mathbf{k})|^2, \tag{9}$$

where E_k is the emitted electron energy and Ω_k is the ejection angle.

Proceeding in a similar way, the impact-parameter-dependent single-particle probability for electron capture is given by,

$$P_{cap}(\rho) = \frac{1}{2\pi} \int_0^{2\pi} d\varphi_\rho |a_{if}^{cap}(\boldsymbol{\rho})|^2, \tag{10}$$

where φ_ρ is the azimuthal angle of the impact parameter vector. It is clear that the interaction between the projectile and the residual target does not affect the ionization and capture probabilities defined by Eqs. (9) and (10). This behavior is supported by employment of the straight line version of the impact parameter approximation, which has been extensively used with success for both, ionization [12] and electron capture reactions [20]. Total cross sections (TCS) for SI and SC can be computed by means of,

$$\sigma_{SI,SC} = 2\pi \int \rho P_{tot}^{ion,cap}(\rho) d\rho, \tag{11}$$

where P_{tot}^{ion} is obtained after integration of Eq. (9) on E_k and Ω_k. Total probabilities can be calculated using two different theoretical descriptions, 3B-CDW-EIS derived by Rivarola and co-workers, where SI and SC total probabilities are given by,

$$P_{tot}^{ion,cap}(\rho) = 2P_{ion,cap}(\rho), \tag{12}$$

and a second one, where a trinomial probability analysis is employed [21]. The TPA approximation was introduced to investigate the reaction of capture of m electrons and the ionization of l ones, so that the corresponding total probability is written as,

$$P_{m,l}(\rho) = \frac{N!}{m!l!(N-m-l)!} (P_{cap}(\rho))^m (P_{ion}(\rho))^l (1 - P_{ion}(\rho) - P_{cap}(\rho))^{N-m-l}, \tag{13}$$

where N is the total number of target electrons. For SI and SC Eq. (13) is reduced to

$$P_{TPA}^{ion,cap}(\rho) = 2P_{ion,cap}(\rho) \cdot (1 - P_{ion,cap}(\rho) - P_{cap,ion}(\rho)). \tag{14}$$

Considering that for transfer-ionization involving He atoms, $N - m - l = 0$, both models give the same TCS, so that one obtains,

$$P_{TI}(\rho) = 2P_{ion}(\rho) \cdot P_{cap}(\rho). \tag{15}$$

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