A four-body fully distorted wave - eikonal initial state model for ionization of He targets by ion impact

J. M. Monti†, O. A. Fojón†, J. Hanssen‡ and R. D. Rivarola†
† Instituto de Física Rosario (CONICET-UNR) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Pellegrini 250, 2000 Rosario, Argentina.
‡ Institut de Physique, Laboratoire de Physique Moléculaire et des Collisions, Université Paul Verlaine - Metz, 1 Bv. Arago, 57078 Metz Cedex 3, France.
E-mail: jmonti@ifir.edu.ar

Abstract. A four body-distorted wave model is introduced to study collisions between swift bare ions and dielectronic atomic targets. Both electrons are considered as active, being one of them ionized while the other one remains bound to the residual target. The relevance of electron correlation on the resulting emission electron spectra is investigated for the case of protons impacting on He atoms.

1. Introduction
The reaction of single electron ionization of atomic and simple molecular targets by impact of swift heavy ions has been a matter of active research in the last forty years. An increasing interest on this subject was produced following the development of a new experimental technique known as cold target recoil ion momentum spectroscopy (COLTRIMS) [1]. Employing this technique a complete mapping of the momentum of all particles resulting from the reaction can be obtained. From the theoretical point of view, one-active electron models were commonly used to describe this multiple particle process. The reduction of this single ionization problem to a one electron treatment was formally given by Fainstein et al. [2] assuming that the time evolution of the active electron is produced independently of the other ones (passive electrons), which are supposed to remain as frozen during the collision. This implies the concept of independent electrons: the active one and the core of passive electrons of the residual target. So, the multiple body reaction (projectile, active and passive electrons, and target nucleus) is described using a three-body model (projectile, active electron and residual target). A certain success was obtained in representing single ionization experimental data for numerous collision systems [3-6]. Moreover, in the case of a multiple-electron process where all electrons are considered as active ones, when the independent electron model (IEM) is used, each one of the electrons is considered to evolve in time independently of the dynamical evolution of the other ones. So, in such representation electrons are assumed to be statically and dynamically decorrelated. By static electron correlation we understand the interaction among the active electrons in the asymptotic initial state and by dynamical correlation the fact that all electrons evolve simultaneously at the 'same' time.

Focussing our interest in the case of a bare swift ion impacting on a two-electron atomic target, a four-body theoretical representation appears as necessary to include static and dynamic
correlations. We propose thus the treatment of the four-body reaction as a real four-body problem, avoiding the limitations of a three-body representation. It implies to deal with harder computational difficulties, than the ones corresponding to the simpler IEM. Studies using four-body models for ionization of two-electron atomic targets are scarce in the existing literature (for a review on these type of models applied to different electronic reactions, see Ref. [7]). The continuum distorted wave - eikonal initial state approximation was used in a four-body formalism (4B-CDW-EIS) to analyse single electron detachment of negative atomic hydrogen H\(^-\) by proton impact [8], showing the important role played by the static electron correlation on ionization total cross sections. Correct boundary conditions were preserved in both the entry and exit channels and the electron remaining in the residual H atom was supposed to occupy its fundamental state. However, the distortion of the two-electron initial and final wavefunctions provoked by the projectile potential was considered to affect only the ionized electron, in an unequal treatment of both target electrons.

In the present work, the influence of the projectile potential on the initial wavefunction is considered on equal footing for both electrons, so that two associated distortion continuum eikonal phases are included describing the interaction of the impinging bare ion with each one of these electrons. In the exit channel the non-ionized electron is distorted by a projectile continuum eikonal phase according to the symmetric eikonal (SE) model employed with success to study electron excitation [9]. In the final wavefunction, a product of the continuum target wavefunction and a projectile continuum factor is proposed to represent the ionized electron moving in the combined fields of the residual target and projectile, according to the CDW-EIS approximation for ionization [11]. We call the present model, the four-body fully distorted wave - eikonal initial state approximation (4B-FDW-EIS).

Atomic units will be used in the text, except otherwise stated.

2. Theory

Let us consider the following reaction produced by the impact of a bare ion of nuclear charge \(Z_P\) on a He atom of nuclear charge \(Z_T\):

\[
Z_P + (Z_T, 2e^-) \rightarrow Z_P + (Z_T, e^-)^+ + e^-
\]

where one of the electrons is ionized and the other one remains bound to the target nucleus.

An initial distorted wave function is chosen as

\[
\chi^+_\alpha = \varphi_\alpha(x_1, x_2) \exp(-i\varepsilon_\alpha t)L^+_\alpha(s_1, s_2) \exp[i\frac{Z_PZ_T}{v} \ln(vR + vR)]
\]

In (2), \(\varphi_\alpha\) is the initial two-electron bound state, \(v\) is the collision velocity, \(R\) is the position of the projectile with respect to the target nucleus and \(\varepsilon_\alpha\) the initial atomic energy. Also, \(x_j\) (with \(j = 1, 2\)) and \(s_j\) (with \(j = 1, 2\)) give the positions of the \(j\)th-electron seen from a reference frame fixed on the target nucleus and on the projectile, respectively. The term \(L^+_\alpha\) is the distortion function given by

\[
L^+_\alpha(s_1, s_2) = \exp[-i\frac{Z_P}{v} \ln(vs_1 + v.s_1)] \exp[-i\frac{Z_P}{v} \ln(vs_2 + v.s_2)]
\]

Eq. (3) indicates that the eikonal forms of the continua of both electrons in the projectile field are included into the initial channel. The last multiplicative factor in (2) represents the elastic scattering between the nuclei.

The final distorted wavefunction is chosen as

\[
\chi^-_\beta = \varphi_\beta(x_1, x_2) \exp(i\varepsilon_\beta)N^*(\frac{Z_P}{p})F_1(-i\frac{Z_P}{v}, 1, -i(ps_1 + p.s_1)) \exp[i\frac{Z_PZ_T}{v} \ln(vs_2 - v.s_2)] \exp[-i\frac{Z_PZ_T}{v} \ln(v - v.R)]
\]
where \( \varphi_\beta \) represent a final target state with one of the electrons bound and the other one traveling in the continuum of this three-body subsystem, and \( \varepsilon_\beta = -i k^2 t - i \varepsilon t \) the corresponding energy, with \( k \) the momentum of the ejected electron with respect to the target nucleus and \( \varepsilon \) the orbital energy corresponding to the bound electron. Also, \( F_1 \) is a Kummer’s confluent hypergeometric function representing the continuum factor of an electron moving with momentum \( p \) in the projectile field, as seen from a reference frame fixed on this nucleus. \( N(\frac{\varepsilon}{p}) \) is the normalization constant of the Kummer’s function. Thus, according to expression (4), the ejected electron moves in the combined field of the residual target and the projectile, while the other electron is considered to be bound to the target nucleus but at same time moving in a projectile continuum (given by its eikonal approximation). The last multiplicative factor in (4) describes the relative internuclear movement.

3. Results and conclusions

In this first work, the case of proton impact is analyzed considering that a large amount of experimental double differential cross sections (DDCS) exist. For multiply charged projectiles the influence of dynamical correlation could be expected to be even more relevant than for the proton case, because the collision time at equal projectile velocities will be larger, allowing thus dynamical correlation to play a role during the collision. Different initial \( \varphi_\alpha(x_1, x_2) \) and final \( \varphi_\beta(x_1, x_2) \) wavefunctions are chosen. For the initial channel we take a product of 1s1s configuration of single Z-functions (with \( Z = 1.6875 \)) or a two-electron Hylleraas-Eckart wavefunction [11, 12] with two variational Z-charges (1s1s’ configuration) with \( Z_1 = 2.15 \) and \( Z_2 = 1.19 \). These wavefunctions take into account approximately 80% and 90% of the radial static correlation, respectively. In the exit channel we consider \( \varphi_\beta = \phi_{1s}(x_2)\phi_\alpha(x_1) \), where \( \phi_{1s}(x_2) \) is the wavefunction corresponding to the dominant residual He\(^+\)(1s) state and \( \phi_\alpha(x_1) \) is taken as a Coulomb continuum wavefunction in the residual target field. An effective charge is considered in this continuum state: \( \zeta = \sqrt{-2\varepsilon_1} \), with \( \varepsilon_1 = -0.91795 \) the initial orbital energy of the ionized electron as given by a Roothaan-Hartree-Fock calculation [13]. We have verified that the use of an asymptotic \( \zeta = 1 \) does not produce noticeable changes in DDCS for all cases treated in this work. So, in the following only DDCS computed employing the effective charge are presented.

In Fig. 1, DDCS are shown as a function of the emitted electron energy at fixed ejection angles of \( 0^\circ \), \( 30^\circ \), \( 50^\circ \) and \( 90^\circ \) for impact of 1 MeV protons. 4B-FDW-EIS results obtained employing both initial configurations indicated above are compared with 3B-CDW-EIS calculations [2] and with existing experiments for \( 30^\circ \), \( 50^\circ \) and \( 90^\circ \). Present calculations using the simplest 1s1s configuration are in close agreement with 3B-CDW-EIS predictions, except in the binary encounter region, where the last ones coincides with 4B-FDW-EIS results corresponding to the 1s1s’ configuration. In general, DDCS obtained for the initial 1s1s’ configuration overestimate, at high enough emitted electron energies, the other calculations shown in figure, which seem to fit better the experimental data. The largest difference between 4B-FDW-EIS corresponding to 1s1s’ and 1s1s configurations appears for the \( 0^\circ \) case, where unhappily no experiments are available. In order to study this behavior, we present in Fig. 2 DDCS at \( 0^\circ \)-emission angle but for energies of 50 keV, 100 keV and 1.5 MeV, for which experimental data exist. At emission energies lower than the ones corresponding to the capture to continuum peak, experiments place under the 4B-FDW-EIS predictions for a 1s1s’ configuration and above the other theoretical results. In the binary encounter region, for the lower impact energies considered, experiments are in better agreement with 3B-CDW-EIS and 4B-FDW-EIS (1s1s configuration) calculations. On the contrary, for 1.5 MeV impact energy, 3B-CDW-EIS and 4B-FDW-EIS (1s1s’ configuration) are in better accordance.

In conclusion, a four body treatment of the single ionization reaction for impact of bare ions on dielectronic targets is presented. It has been applied to the case of the H\(^+\)+He(1s\(^2\))
Figure 1. DDCS for electron emission in collisions of 1 MeV H\(^+\) with He as a function of electron energy at fixed ejection angles. Theory: ——, 4B-FDW-EIS 1s1s' configuration; - - - -, 4B-FDW-EIS 1s1s configuration; · · · · · ·, 3B-CDW-EIS [2]. Experimental data: ◦, [14]

Figure 2. DDCS at 0\(^°\) electron emission angle in collisions of 50 keV, 100 keV and 1.5 MeV H\(^+\) with He. ——, 4B-FDW-EIS 1s1s' configuration; - - - -, 4B-FDW-EIS 1s1s configuration. 50 keV and 100 keV: · · · · · ·, 3B-CDW-EIS calculations [15]; ◦, experimental data [16]. 1.5 MeV: · · · · · ·, 3B-CDW-EIS [17]; ◦, experimental data [18].

collision. Comparisons are given with existing DDCS experimental data and with three body calculations. The role played by electron correlation is analyzed. The use of more elaborated initial wavefunctions including radial and angular correlations is being the matter of our present research. Preliminary 4B-FDW-EIS results obtained in this way show a promissory close agreement with experiments at all ejection energies. We are now focusing our interest on the application of this four-body theory to multiply charged projectile impact on He atoms.

4. References
[1] Moshammer R et al. 1994 Phys. Rev. Lett. 73 3371.
[2] Fainstein P D, Ponce V H and Rivarola R D 1988 J. Phys. B: At. Mol. Phys. 21 2989.
[3] Stolterfoht N, DuBois R D and Rivarola R D 1997 Electron Emission in Heavy Ion – Atom Collisions (Berlin: Springer).
[4] Rivarola R D and Fainstein P D 2003 Nucl. Instr. Meth. B 205 448.
[5] Foster M et al. 2004 J. Phys. B: At. Mol. Opt. Phys. 37 3797 and references therein.
[6] Ciappina M F and Cravero W R 2006 J. Phys. B: At. Mol. Opt. Phys. 39 2183 and references therein.
[7] Belkic Dz, Mancev I and Hanssen J 2008 Rev. Mod. Phys. 80 249.
[8] Belkic Dz 1997 Nucl. Instr. Meth. B 124 365.
[9] Deco G R, Fainstein P D 1986 J. Phys. B: At. Mol. Phys. 19 213.
[10] Crothers D S F and McCann J F 1983 J. Phys. B: At. Mol. Phys. 16 3229.
[11] Hylleraas E A 1929 Z. Physik 54 347.
[12] Eckart C 1930 Phys. Rev. 36 878.
[13] Clementi E and Roetti C 1974 Atomic Data and Nuclear Data Tables 14 177.
[14] Rudd M E, Toburen L H and Stolterfoht N 1976 At. Data Nucl. Data Tables 18 413
[15] M F Ciapina, W R Cravero and C R Garibotti 2004 Phys. Rev. A 70 062713
[16] G C Bernardi et al. 1989 Phys. Rev. A 40 6863
[17] P D Fainstein, V H Ponce and R D Rivarola 1991 J. Phys. B: At. Mol. Phys. 24 3091
[18] D H Lee et al. 1990 Phys. Rev. A 41 4816