Experimental and theoretical results on electron emission in collisions between He targets and dressed \( \text{Li}^{q+} (q = 1, 2) \) projectiles

D Fregenal\(^1\), J M Monti\(^2\), J Fiol\(^1\), P D Fainstein\(^1\), R D Rivarola\(^2\), G Bernardi\(^1\) and S Suárez\(^1\)

\(^1\)Centro Atómico Bariloche, Comisión Nacional de Energía Atómica, 8400 San Carlos de Bariloche (Río Negro) and Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina

\(^2\)Laboratorio de Colisiones Atómicas, Instituto de Física Rosario (CONICET-UNR) and Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Avenida Pellegrini 250, 2000 Rosario, Argentina

E-mail: fregenal@cab.cnea.gov.ar

Received 14 March 2014, revised 22 May 2014
Accepted for publication 16 June 2014
Published 28 July 2014

Abstract

We investigate experimentally and theoretically the electron emission in collisions between He atoms and \( \text{Li}^{q+} (q = 1, 2) \) projectiles at intermediate to high incident energies. We report on measured absolute values of double-differential cross-sections, as a function of the emitted electron energy and angle, at a collision energy of 440 keV u\(^-1\). The different contributions from target ionization, projectile ionization, and simultaneous target–projectile ionization are calculated with the quantum-mechanical continuum distorted wave and continuum distorted wave–eikonal initial state models, and with classical trajectory Monte Carlo simulations. There is an overall good agreement of the calculations with the experimental data for electron emission cross-sections.

Keywords: ionisation, ion-atom collision, cross-section

(Some figures may appear in colour only in the online journal)

1. Introduction

The study of electronic reactions in collisions between partially dressed projectiles and atomic and molecular targets has received increasing interest in the past two decades. These systems provide a suitable framework in which to investigate the relative importance of the electron–electron interactions versus the electron–nucleus interactions. In particular, electron emission has received a great part of the attention, because it is the main mechanism leading to energy loss of swift ions in matter. Therefore, detailed knowledge of the mechanisms of electron emission in collisions between fast partially dressed ions with atomic and molecular targets is relevant in many scientific areas, such as astrophysics and plasma physics, and it also plays a predominant role in applied areas, like in the design of fusion reactors, in radiation damage and in hadron therapy. A large amount of experimental data for double-differential cross-sections (DDCS) are available (see for example appendix C of [1]) involving bare and partially dressed ions impinging on atomic or molecular targets at intermediate and high collision energies. However, to the best of our knowledge, besides the results presented by Monti et al [2], where the ionization of He atoms by \( \text{Li}^{3+} \) impact was investigated, there are no reports of DDCS for electron emission considering Li ions as projectiles or as targets.

In this work we compare the experimental data against well-known theories, that have been tested for many different systems: a four-body classical trajectory Monte Carlo (CTMC) model, and two quantum-mechanical modified distorted wave models, reported previously by Monti et al [3, 4].

CTMC has been shown to be a very versatile technique to use in studying collisions involving many bodies. During the past few decades, several variants of the CTMC method have been developed and employed to investigate ionization collisions between many-electron systems. The main
difficulties with this approach arise from the well-known instabilities of a classical description of bound states with three or more bodies, that lead to spontaneous break-up. In the present case, of many-electron ions and atoms, the Coulomb interactions produce a fast auto-ionization of at least one electron. Among the proposed approximations, the simplest approach consists in omitting completely the interactions between electrons in the target atom, in the independent electron model. More elaborate models, that include dynamical screening, energy- or momentum-dependent potentials that incorporate the quantum-mechanical uncertainty relations, and semiclassical time propagations have also been investigated [5–12]. In particular $n$-CTMC, where interactions between electrons belonging to the same centre are neglected but interactions between electrons of different atoms are fully included, provides a simple framework in which to investigate the relative importance of nucleus–electron and electron–electron interactions in collisions between dressed ions and atoms [10, 13].

The quantum distorted wave models presented in [3, 4] are extensions of the well-known continuum distorted wave (CDW) [14, 15] and continuum distorted wave–eikonal initial state (CDW–EIS) [16] models to the case of dressed projectiles. Such extensions were obtained by approximating the interaction of the projectile with the active target electron by an analytic two-parameter Green–Sellin–Zachor (GSZ) model potential [17–19]. In these models it was also assumed that the projectile electrons are bound deeply enough to be considered as passive electrons (not changing their state during the collision). These models were successfully applied to study several systems, among which are the ionization of He [3, 16], U21+ and 600 keV u−1 Au11+ impact (see [21] and [4], respectively). In all the collision systems reported in [3, 4] the projectile internal structure was considered ‘frozen’ and projectile ionization was neglected.

In the present case the projectile electrons have binding energies similar to the binding energies in the helium target. Therefore target, projectile and even simultaneous ionization may give a substantial contribution to the electron emission process.

We present in this work a new set of experimental absolute DDCS for electron emission in collisions of 440 keV/u Li+ (q = 1, 2) ions impinging on atomic He targets, as a function of the electron energy, for a wide range of fixed emission angles. We compare the experimental data against the above mentioned four-body CTMC, CDW and CDW–EIS theoretical models. Target, projectile and simultaneous ionization are theoretically calculated and their relative contributions to the electron emission are analysed. In the present analysis, target ionization simultaneous with electron capture by the projectile, resulting in He2+ residual ions, has been neglected since its probability is small at the energies considered. In fact, total cross-sections for this process account for less than 0.04% of the total electron emission [20].

Atomic units (a.u.) are employed except where otherwise stated.

2. The experimental arrangement and procedures

Experimental data were measured with the 1.7 MV Tandem accelerator at Centro Atómico Bariloche. The experimental set-up is described in detail elsewhere [2, 21], so only details related to the present experiment will be given here. Lithium ion beams emerging from the accelerator with 440 keV/u are collimated in the transport section by two sets of four collimators to 0.60 × 0.60 mm², determining a beam divergence of 0.7 mrad (half-angle). Inside the collision chamber the projectiles collide with the effusive target at the focus of a cylindrical mirror spectrometer. The analyser rotates in a plane perpendicular to the gas flow direction, so it measures energy distributions of the electrons emitted in the collision for any selected angle between 0 and 180 degrees. After the collision, the beam is collected in a Faraday cup. The collected charge is used to normalize the electronic distributions to a constant number of projectiles.

The present data were taken under the same conditions as the ones described in [2]. The background pressure in the collision chamber was below 5 × 10⁻⁷ mbar, while the pressure in the transport section was lower than 4 × 10⁻⁶ mbar. The pressure in the collision chamber with the target gas was set to 4.4 × 10⁻⁵ mbar. The angular acceptance and energy resolution of the spectrometer were selected to be 2° and 6%, respectively.

Auxiliary data with a uniform gas target density in the collision chamber were taken to correct the distortions in the measured spectra due to the extended gas distribution established in the chamber from the localized effusive target. The relative normalization between different emission angles was estimated to have an uncertainty of ±15%. Statistical errors are relatively important at low counting rate, i.e. for high energy electrons and at backward emission angles.

DDCS for electron emission in collisions of 440 keV/u Li⁺ and Li²⁺ with helium atoms were determined from the electronic distributions [21]. They were measured at several emission angles, relative to the incident beam direction: θ = 0, 10, 20, 30, 40, 50, 70, 90, 120, 150 and 170 degrees.

Normalization to absolute values was done by using total cross-sections measured by Shah and Gilbody [22] and Woitke et al [20] for Li³⁺ + He. The discrepancies observed between these two sets of experimental data prevent us from using directly the data taken by Woitke et al for Li²⁺.

In order to determine absolute cross-section values, energy distributions for one selected angle were taken for Li⁴⁺ (q = 1, 2, 3) incident on He with the same energy and under the same experimental conditions. Numerical estimations of the beam charge fractions entering at the Faraday cup showed that the contributions of the beam contaminants were less than 0.04% for Li⁺ and 0.02% for Li²⁺ beams. Therefore, as the charge collected in the FC is determined only by the primary beam, the number of projectiles was obtained by dividing the collected charge by the charge state q. Then the distributions were normalized to the same number of projectiles. Using DDCS values already determined for Li³⁺ [2], absolute DDCS were calculated for the other projectiles. An uncertainty of
~20% was assessed from the disagreement between the available total cross-section (TCS) data.

3. Theory

In many-body collision systems with dressed projectiles, such as those investigated in this work, ionization may take place due to different identifiable physical mechanisms. The electrons play a dual role: on one hand, they screen the nucleus charge, while on the other hand, the direct electron–electron interaction influences the dynamics and may produce ionization. At high impact energies, the role of the interaction between target electrons and projectile electrons may be separated from the role of the electron–nucleus interactions, and they have been interpreted as two different mechanisms termed screening and antiscreening [23, 24]. In this context, antiscreening is associated with the collision of a quasi-free electron accompanying one centre with the bound electron in the other. Thus, such a clear distinction can only be accomplished in fast collisions, when the binding energy is negligible compared to the electron’s kinetic energy.

The measured spectra for the systems studied in the present work, obtained by electron spectroscopy, are the result of the combined contributions of electrons produced in target ionization (eTI), projectile ionization (ePI), and simultaneous ionization from both centres (PTI). In order to describe these channels we have performed theoretical calculations using two different quantum approximations, namely the CDW and the CDW–EIS models, and a classical approach using CTMC simulations.

3.1. Continuum distorted wave models for dressed ion impact single ionization of atoms

The electron emission process was studied by means of extensions of CDW and CDW–EIS models to describe ionization by dressed projectiles. Such extensions have been used previously to compute DDCS for several systems, combining different projectiles colliding with He targets at intermediate to high impact energies (see [3, 4]).

In order to treat multiple-electron systems within the independent electron model, we consider only one active electron and, following the procedure given in [16] (see also [1, 25]), the multielectronic Hamiltonian is reduced to

$$H_d = -\frac{1}{2} \nabla^2 + V_d(x) + V_p(s) + V_t(R)$$

where $x$ and $s$ are the positions of the active target electron in the target and projectile reference frames, respectively. $V_d(x)$ is a model potential taking into account the interaction of this electron with the remaining—partially dressed—target, $V_p$ is the interaction between the projectile and the active electron that, according to the work presented in [3, 4], is approximated with an analytical two-parameter GSZ potential:

$$V_p(s) = -\frac{q}{s} - \frac{1}{s} (Z_p - q) \left[ H(e^{i/d} - 1) + 1 \right]^{-1}$$

where $q$ is the net (asymptotic) charge of the projectile, $Z_p$ is its nuclear charge, and $H$ and $d$ are parameters that depend on $Z_p$ and $q$. $V_t(R)$ is the mean interaction of the projectile with the target nucleus and the passive electrons. This last potential depends only on the internuclear coordinate $R$ and thus, within the straight-line version of the impact parameter approximation, produces a phase factor which does not affect the electron dynamics. For both quantum approximations the initial bound state of the target was described by means of Roothaan–Hartree–Fock (RHF) wavefunctions [26].

Within the distorted wave framework, the transition matrix may be written in its prior or post version, depending on whether the perturbative operator acts on the initial-channel or the final-channel distorted wavefunction. The prior version of the CDW model presents well-known difficulties in its computation due to a logarithmic divergence near the binary encounter structure (see [27]). Consequently, in this work we employed the post version, where the initial and final distorted waves are given by:

$$\chi_i^+(x, t) = \Phi_i(x, t) L_i^+(s)$$

$$\chi_i^-(x, t) = \Phi_i(x, t) L_i^-(s)$$

Here $\Phi_i(x, t) = \phi_i(x) \exp(-i \epsilon_i t)$ and $\Phi_f(x, t) = \phi_f(x) \exp(-i \epsilon_f t)$ are the initial bound and final states which are solutions of the time-dependent Schrödinger equations:

$$\left[-\frac{1}{2} \nabla^2 + V_i(x) - i \frac{\partial}{\partial t}\right] \Phi_i(x, t) = \epsilon_i \Phi_i(x, t).$$

Also, $\epsilon_i$ and $\epsilon_f$ are the electron energies in the initial and final states, respectively. We used for $\Phi_i$ an RHF initial wave-function, and for $\Phi_f$ a continuum wavefunction corresponding to the effective Coulomb target potential $V_i(x) = -Z_{\text{eff}}/x$. Therefore, using the Belkić et al prescription [28], an effective charge $Z_{\text{eff}} = \sqrt{-2 n^2 \epsilon_n}$ is chosen in the residual target final continuum state, where $n$ is the principal quantum number of the $\Phi_i$ orbital. This effective charge partially considers the dynamics screening in the exit channel (see [29, 30]).

The initial distortion is proposed as

$$L_i^+(s) = N(\nu) \left[ F_i(\nu; 1; ivs + iv \cdot s) \right]$$

whereas the final distortion is chosen as

$$L_i^-(s) = N^*(\zeta) \left[ F_i(-i\zeta; 1; ivs - ivp \cdot s) \right]$$

where $v$ is the projectile velocity, $\nu = Z_p/v$, $\zeta = Z_p/p$, $p = k - v$ is the ejected electron momentum in the projectile reference frame, where $K$ is the ejected electron momentum in the target reference frame, $F_i$ is the confluent hypergeometric function, and $N$ is the corresponding normalization factor.
On the other hand, CDW–EIS results were obtained using the prior version of the transition matrix. The main difference from the CDW approximation case is that in the CDW–EIS case the initial distortion is proposed as

\[ \mathcal{L}_\epsilon'(s) = \exp(-i\epsilon \ln(\nu s + v \cdot s)) \] (8)

instead of that given in equation (6).

In order to calculate the electron loss from the projectile, the reaction is reversed and a reference frame transformation is applied from the projectile to the laboratory frame. The electron-loss DDCS as a function of the energy \( \epsilon \) and angle \( \theta \) of the emitted electron can thus be written in the laboratory reference frame as (see for example appendix B of [1])

\[ \frac{d\sigma(\epsilon, \theta)}{d\Omega} = \left( \frac{\epsilon}{\epsilon'} \right)^{1/2} \frac{d\sigma(\epsilon', \theta')}{d\Omega'} \] (9)

where the primed (unprimed) quantities are associated with the projectile (laboratory) reference frame. The transformation rules for energy and angle are easily derived:

\[ \epsilon' = \epsilon + T - 2(\epsilon T)^{1/2} \cos \theta, \] (10)

and

\[ \theta' = \arccos \left( \frac{\epsilon - T - \epsilon'}{2\sqrt{T\epsilon'}} \right), \] (11)

where \( T = v^2/2 \).

To investigate the simultaneous ionization (PTI), a four-body system with two active electrons should be considered, like in the CTMC calculations. There exist previous works on distorted wave models which deal with a four-body approximation of the ionization process [31, 32], but in those cases both active electrons are initially bound to the target and, accordingly, they are affected by the same perturbative potential. In contrast, in the case of PTI one of the two active electrons is initially bound to the projectile and the other to the target, the two aggregates thus being affected by different perturbative potentials, which complicates the computational solution of the problem. Hence, in order to simplify the calculation of the contribution of PTI, a probabilistic approach was considered using one-active-electron cross-sections, assuming that when an electron is ionized with a given momentum the other can be emitted independently with any energy and angle. The DDCS for the PTI was estimated as

\[ \text{DDCS}^{(PTI)} = \frac{\text{DDCS}^{(eTI)} \text{TCS}^{(ePI)}}{\text{TCS}^{(eTI)} + \text{TCS}^{(ePI)}} + \frac{\text{DDCS}^{(ePI)} \text{TCS}^{(eTI)}}{\text{TCS}^{(eTI)} + \text{TCS}^{(ePI)}}, \] (12)

In equation (12), \( \text{DDCS}^{(eTI)} \) and \( \text{TCS}^{(eTI)} \) stand for the DDCS and TCS for target ionization and projectile electron loss, respectively, at the given projectile velocity \( v \). In this rough estimation, we approximate the probabilities \( P^{(ePI)} \) and \( P^{(eTI)} \) of ionizing each collision aggregate by the total cross-section ratios shown in equation (12); that is,

\[ P^{(ePI)} \approx \frac{\text{TCS}^{(ePI)}}{\text{TCS}^{(eTI)} + \text{TCS}^{(ePI)}} \] (13)

Despite the simplicity of this approach, we have found that it gives a fair estimation of the contribution of the PTI to the total electron emission spectra [33]. This is also confirmed with our present findings, where the PTI cross-sections compare fairly well with those obtained in a four-body CTMC approach.

### 3.2. The CTMC approach

We have performed, additionally to the quantum calculations, four-body classical trajectory Monte Carlo (CTMC) simulations of the Li^+ + He ionization collisions. The CTMC method is well-known and has been extensively documented [1, 10, 34, 35]. We model the collision problem as a four-body system consisting of two centres, each with one electron. Both the lithium-ion projectiles and the helium targets are described as one-effective-electron systems, where the potentials produced by the two parent nuclei incorporate the screening due to ‘passive’ electrons. The interactions are represented by means of two-parameter GSW model potentials similar to those used in the quantum calculations.

The evolution of the system is obtained numerically for a large number of independent trajectories and the information is extracted by statistical methods [35–39]. The total process consists of three distinct stages: preparation of the system, evolution until convergence is achieved, and statistical analysis of the final state.

In the first step the system is prepared following a microcanonical ensemble. The initial position and velocity of the electron and the nucleus in the target are randomly chosen such that the energy is fixed to the helium binding energy \( \epsilon_f = -0.903 \) a.u., whereas the momentum distribution resembles the quantum-mechanical momentum probability density of the atom [35]. The helium target is modelled as an one-electron atom, where the core interacts with the active electron and the projectile through a non-Coulomb central potential, as given in [19]. The projectile initial velocity is fixed and determined by the collision energy, while its impact parameter is randomly chosen with a distribution that describes a uniform flux. The internal representation of the projectile Li^+ is prepared similarly to that of the target, using the experimental binding energy of the ion.

The classical evolution of the system is obtained by solving numerically Hamilton’s canonical equations by means of a modified middle-point code with an adaptive step-size control. When convergence is achieved within 0.02%, the velocities of the fragments in the final state are determined and the DDCS are evaluated by using the formula

\[ \frac{d\sigma}{d\Omega} = \frac{N_i(\Omega, E) \Delta E \Delta \Omega}{N \left( \frac{\pi b_{\text{max}}^2}{2} \right)} \]

Here \( N_i(\Omega, E) \) is the number of ionization events where the electrons have energy in a neighbourhood \( \Delta E \) of \( E \) and are emitted in a solid angle \( \Delta \Omega \) in the direction of \( \Omega \). The number of ionization events is normalized to the incident flux.
\( N/\pi b_{\text{max}}^2 \lambda \), where \( b_{\text{max}} \) is the maximum impact parameter evaluated, larger than the maximum impact parameter that produces ionization. In this work the number of trajectories obtained is approximately \( N = 1.5 \times 10^8 \) for each collision system. The acceptances \( \Delta \Omega \) in the solid angle and \( \Delta E \) in the energy bins were chosen to coincide at each point with those employed in the experiment.

### 4. Results and discussion

#### 4.1. Experimental data

Experimental absolute DDCS for electron emission in collisions of \( \text{Li}^+ \) and \( \text{Li}^{2+} \) with helium targets are shown in figures 1 and 2. For display purposes, the data are divided by different constant factors for the different emission angles, as indicated in the figures. In the spectra for \( 0^\circ, 40^\circ, 90^\circ, 150^\circ \), and \( 170^\circ \), we have included some bars representing the statistical error for different regions of emission energy.

A comparison among the total cross-section values for the different channels contributing to the total emission shows that the dominant process is eTI, which represents 73% of the total emission for \( \text{Li}^+ \) and 95% for \( \text{Li}^{2+} \) [20]. The remaining electron emission is produced by ePI and PTI. As was mentioned earlier, transfer ionization (electron capture simultaneous with target ionization) processes are negligible at this energy (<0.04%). The main structure observed at \( \theta = 0^\circ \) and centred at \( E_e \approx 240 \text{ eV} \) is formed by the superposition of target electrons captured to the continuum by the projectile (ECC) and electron loss from the projectile to the continuum (ELC). As is expected due to its lower ionization energy, the intensity of the electron-loss peak is much more important for incident \( \text{Li}^+ \) than for \( \text{Li}^{2+} \). For larger emission angles, the yield of the structure decreases and its maximum shifts to lower energies. This maximum corresponds to projectile electrons emitted in a binary-like collision with the target (PBE), and when plotted in an energy–angle space, forms a ridge located on a circle centred at zero velocity. The radius of this ring depends on the incident velocity \( v \), and, for fast collisions, is slightly smaller than the kinetic energy \( E_e \approx v^2/2 \).

At \( \theta = 0^\circ \) and \( E_e = 800 \text{ eV} \) another broad ridge structure is present. It is formed mainly by target electrons emitted in binary encounter collisions with the projectile (TBE). The position of this structure shifts to lower values for increasing emission angles, as is expected [1].

At small emission angles a set of peaks located at \( E_e \approx 560 \text{ eV} \) is observed for incident \( \text{Li}^+ \) projectiles only (figure 1). They are produced by auto-ionization emission from doubly excited \( \text{Li}^+ \) projectiles [40]. In the case of \( \text{Li}^{2+} \)

![Figure 1](image1.png)

**Figure 1.** Double-differential cross-section for electron emission in collisions of 440 keV u⁻¹ Li⁺ on He targets as a function of the electron energy. Emission angles are indicated in the figure. Different constant factors for each curve, shown in the figure, were applied to give a better display. Typical error bars are plotted for \( \theta = 0^\circ, 40^\circ, 90^\circ, 150^\circ \) and \( 170^\circ \).

![Figure 2](image2.png)

**Figure 2.** Same as figure 1, but for collisions of 440 keV u⁻¹ Li²⁺ with He targets.
projectiles, this process may occur only after single-electron capture, where the cross-section is small at the present collision velocity, so this is not visible in the experimental data. The effect of the initial projectile charge state on the DDCS varies depending on the energy range and the direction of the electron emission. In figure 3, electronic distributions for collisions of 440 keV/u Li\(^{+q}\) \(q = 1, 2, 3\), with He atoms are shown for four emission angles: \(\theta = 0^\circ, 10^\circ, 40^\circ\) and \(120^\circ\).

Figures 3(a) and (b) show the evolution of the ELC + ECC cusp for the three projectiles. As the only process contributing to the peak is ECC for incident Li\(^{3+}\), the evolution of the peak observed from \(0^\circ\) to \(10^\circ\), where the peak is transformed into a broad ridge, show the strong focusing of this effect in comparison with the EL structure angular dependence. The dependence of the cusp on \(q\) is remarkable.

In the case of emission in forward directions, fast electron distributions \((E_e \gtrsim E_{\text{Th}}}) show no dependence on the initial projectile charge state, which is consistent with the dominant low impact parameters of BE collisions. In contrast, in the backward direction there is a noticeable dependence on the projectile charge state, the largest emission occurring in Li\(^{+}\) + He collisions. The main contribution to the cross-section in this region comes from electrons ejected from the Li\(^{+}\) ions. Note that in a reference frame attached to the projectile, and considering the kinematically inverse collision—the helium atom impinging on the Li\(^{+}\) ions—the electrons from the projectile, emitted in binary-like collisions with the atom, are mainly directed in the forward direction. However, seen from the laboratory frame, with the helium atom initially at rest, these data correspond to emission angles in the backward direction. There is no noticeable difference between DDCS associated with Li\(^{2+}\) and Li\(^{3+}\).

On the other hand, the emission of low energy electrons is strongly dependent on \(q\), with larger emission probabilities for more highly charged projectiles. Since the release of slow electrons is dominated by long-distance interactions, the dominant parameter is the initial projectile’s charge state \((q = 1, 2, 3)\). However, for the systems under study here, the characteristic \(q^2\) dependence associated with the Born approximation is only valid for very low energy electrons. The emission of fast electrons is associated with close collisions. In this case the effective charge is in all cases \(q^2\), corresponding to the core Li\(^{+}\) charge. Thus, no dependence on the projectile initial charge is observed in the data.

The main contribution of projectile electrons to the total emission occurs mainly at the electron-loss peak and the PBE structure. This latter process becomes dominant when considering fast electrons ejected in the backward direction. However, in the case of Li\(^{2+}\), the contributions of ionization of projectile electrons are relatively small and the overall emission spectrum is similar to the one observed for Li\(^{3+}\). This may be attributed to the large value of the ionization energy of Li\(^{2+}\), \(\varepsilon = 122.4\) eV.

### 4.2. Comparison with theoretical results

Theoretical calculations and experimental results are compared in figures 4 and 5 for the two ions, Li\(^{+}\) and Li\(^{3+}\), and for three typical emission angles: \(\theta = 10^\circ, 52^\circ\) and \(150^\circ\). In each case, the contributions from electron target ionization (eTI),
Figure 4. Double-differential cross-sections for electron emission in collisions of 440 keV/u Li$^+$ on He targets as a function of the electron energy for three different emission angles: (a) $\theta = 10^\circ$, (b) $\theta = 52^\circ$ and (c) $\theta = 150^\circ$. •: experiment; ......: eTI; ——: ePI; −−−−: PTI; ———: total emission.
Figure 5. Double-differential cross-section for electron emission in collisions of 440 keV/u Li$^{2+}$ on He targets as a function of the electron energy for three different emission angles: (a) $\theta = 10^\circ$, (b) $\theta = 52^\circ$ and (c) $\theta = 150^\circ$. ●: experiment; ......: eTI; ——: ePI; ———: PTI; ———: total emission.
electron projectile ionization (ePI) and simultaneous ionization from the two centres (PTI) are shown.

4.2.1. Li⁺ projectiles. The three theoretical approximations reproduce the experimental data fairly well. They show similar qualitative behaviours as a function of the electron energy, but CDW–EIS calculations give a slightly better agreement with the experiment in the case of Li⁺ (figure 4) than the other two theories. In all cases the larger differences appear at small emission angles. Besides a slight overall overestimation of CTMC, the CDW and CDW–EIS approximations present a marked shoulder due to TBE processes, that is almost imperceptible in CTMC and appears appreciably milder in the experimental data. At intermediate and large angles the agreement of the theories with the experiment improves noticeably. The observed discrepancies may arise from the approximated theoretical treatment of the target and projectile as one-electron systems, and the corresponding complete neglect of correlations between electrons in the same centre. Additionally, the quantum theories do not include the interactions between electrons belonging to different centres.

The contributions to the total emission from the different channels included in the calculations depend strongly on the region of energies and angles investigated. For high energy electrons, eTI is the major contributor to the DDCS in the forward direction, while ePI and PTI are dominant for backward emission. For electrons emitted with velocities close to the incident velocity \(E_i \approx 240\,\text{eV}\) the main contribution in the forward direction comes from projectile electrons (ELC), ionized either by interaction with the core target or by electron–electron interaction. Note that at \(10^6\), the ECC peak is already almost completely washed out, appearing in the spectra as a small shoulder. Its contribution to the total emission cross-section is almost negligible as compared with that of the ELC cusp.

The three theories show that, other than in the ELC region, ePI contributes minimally, accounting for only approximately 10% of the total emission up to electron angles of 20°. This result is consistent with our previous analysis: besides ELC, electrons from the projectile are emitted in the PBE ridge, and its contribution is important in the backward direction, where the target ionization is very small. Thus, ePI and PTI dominate only the backward, high energy emission region.

The electron energy range where the eTI contribution is the most important consistently shrinks for increasing emission angles and, at 90°, the electron emission for \(E_i \gtrsim 200\,\text{eV}\) is dominated by ePI and PTI. In backward directions, as the electron energies considered increase, all the theories predict dominant contributions from PTI and ePI.

4.2.2. Li²⁺ projectiles. Figure 5 shows the comparison of experimental cross-section data with calculations for Li²⁺ projectiles. The conditions are the same as for Li⁺ in figure 4. As expected, due to the higher ionization energy, ePI and PTI are relevant only in the region of the ELC peak, but they become dominant for fast electrons in the backward direction. As in the Li⁺ case, the overall agreement between calculations and experiment, as well as between different theoretical approaches, is remarkably good. CTMC somewhat overestimates the DDCS at small angles, showing a TBE structure that is less pronounced than the one appearing in the experimental data. In contrast, CDW calculations present a more marked TBE structure than the data.

As in the case of Li⁺, the remarkable agreement between the three theories is observed not only for the total emission cross-sections but also for each of the processes contributing to the measured spectra. The two quantum theories show very similar behaviours of the double-differential cross-sections for target, projectile and simultaneous ionization. The energy dependences of CTMC DDCS are also very similar to the quantum results, but the simultaneous ionization is slightly wider at small angles, extending to higher emission energies.

It must be noted that in both quantum theories the interactions between the target active electron and those bound to the projectile are introduced via a projectile nuclear charge screening, as indicated by equation (2). On the other hand, in the CTMC calculations the interaction between the two active electrons (one of them bound to the target and the other to the projectile) is included separately from the screened nucleus interactions. However, the similarity of the spectra in the different theories suggests that the main effect of the electron–electron interaction is occurring as an effective screening of the nucleus. Explicit separation of simultaneous ionization spectra into two contributions, one considering only target ionization and the other only projectile ionization, confirms this result. Although these results are not shown, the contribution to PTI of electrons emitted from the target resembles single target ionization (eTI) spectra, while the contribution arising from projectile electrons is similar to that for ePI.
4.3. Total cross-sections

Results for total cross-sections of the different channels contributing to the total electron emission are shown in tables 1 and 2.

TCS values displayed in the first column are estimations from Woitke et al data [20] for 440 keV u\(^{-1}\) incident energy. Values obtained in the present experiment are shown in the second column. The errors were mainly due to the normalization process, since errors from other sources, like the integration method, are negligible by comparison. The other columns correspond to theoretical TCS values. As the theories include only one active electron per collision centre, tabulated experimental values for eTI, ePI and PTI from [20] do not include double electron emission from the same collision centre.

TCS values for electron emission obtained from the present measurements show good agreement with those obtained by Woitke et al considering the error bars. The present theoretical calculations show good agreement for Li\(^{2+}\) projectiles, but there is an overestimation for Li\(^{+}\) projectiles. This tendency is also observed in comparing with the TCS values obtained in the present experiment, though the agreement improves.

The comparison among all theoretical results is good for ePI and PTI channels, showing the main difference for eTI. There is a fair agreement between theories and tabulated values, with higher differences appearing for the PTI cross-sections, where factors of about 5 or 6 are observed. Also, the quantum calculations are systematically higher than the classical results.

5. Conclusions

We have investigated experimentally and theoretically electron emission in collisions between helium and dressed projectiles of lithium. Experimental data on double-differential cross-sections have been compared to a classical and two quantum-mechanical theories. The theoretical results are consistent with the present experimental data as well as with available published total cross-sections. For Li\(^{+}\) projectiles, the three theories show the most important discrepancies with the data in forward directions, where CDW–EIS gives a slightly better description. The CTMC approach gives a good qualitative description at small angles but shows an overall overestimation of the data. While at larger angles the agreement of the three theories improves considerably, the CTMC calculations produce the best results. For Li\(^{2+}\) projectiles, the best agreement for small emission angles is produced by CDW, while CDW–EIS underestimates the region of high electron energy. At small angles, for both projectiles, the target binary encounter ridge at about \(E_e = 900 \text{ eV}\) is much more marked for CDW than for CDW–EIS, and is the mildest for CTMC results. At larger angles the three theories perform similarly.

The very reasonable accord between experimental and theoretical DDCS for total electron emission, together with the general agreement among different theories, gives us confidence to draw conclusions on the relative importance of the different channels involved in the ionization collisions. The present findings show that the contributions of single target ionization, single projectile ionization, and simultaneous target–projectile ionization are different in different regions of energy and angle of the emitted electron. Notwithstanding the small differences between the different theories, they all predict similar contributions to the total emission DDCS from each of the mechanisms involved. In the case of Li\(^{2+}\), target ionization dominates the spectra, and only at high energies in the backward directions, where target ionization is negligible, do the projectile and simultaneous ionization contribute appreciably. For Li\(^{+}\), the ePI and PTI also dominate the spectra in the region of ELC for small emission angles. In all other regions of energies and angles, eTI is the main process of electron emission.

When comparing the target ionizations for the different projectiles, we observed that the cross-sections have the expected quadratic dependence on the projectile charge. However, the effective charge depends on the region of spectra investigated. For low energy electrons the ionizations take place due to far collisions and the effective charges are the asymptotic charges \(q = 1, 2, 3\). On the other hand, for high energy electrons, the close collisions are influenced by the core charge, which is the same, \(q_{\text{eff}} \sim 1\), for all three kinds of ions.

Acknowledgments

JMM and RDR acknowledge the Agencia Nacional de Promoción Científica y Tecnológica for financial support through the project PICT2011-2045. JF and PDF acknowledge support by the Consejo Nacional de Investigaciones Científicas y Técnicas (Grant PIP 112-200901-00166).
References

[1] Stolterfoth N, DuBois R D and Rivarola R D 1997 Electron Emission in Heavy Ion-Atom Collisions (Berlin: Springer-Verlag)

[2] Monti J M, Fregenal D, Suárez S, Fainstein P D, Rivarola R D, Bernardi G and Fiol J 2012 Experimental and theoretical results on electron emission from helium by the impact of bare Li\(^{+}\) ions J. Phys. B: At. Mol. Opt. Phys. 45 145202

[3] Monti J M, Rivarola R D and Fainstein P D 2008 Quantum interferences in swift highly-charged dressed-ion atom collisions J. Phys. B: At. Mol. Opt. Phys. 41 201001

[4] Monti J M, Rivarola R D and Fainstein P D 2011 Distorted wave theories for dressed-ion-atom collisions with GSZ projectile potentials J. Phys. B: At. Mol. Opt. Phys. 44 195206

[5] Schultz D R, Olson R E, Reinhold C O, Kelchb S, Kelchb C, Schmidt-Bocking H and Ulrich J 1990 Coincident charge state production in E\(^{in}\) + Ne collisions J. Phys. B: At. Mol. Opt. Phys. 23 3839–47

[6] Schultz D R, Meng L and Olson R E 1992 Classical description and calculation of ionization in 100 electrons and positrons with He and H\(_{2}\) J. Phys. B: At. Mol. Opt. Phys. 25 4601–18

[7] Cohen J S 1996 Quasiclassical-trajectory Monte Carlo methods for collisions with two-electron atoms Phys. Rev. A 54 757–86

[8] Wood C J and Olson R E 1999 Double electron removal and fragmentation model of the H\(_{2}\) molecule by highly charged ions Phys. Rev. A 59 1317–28

[9] Wood C J, Olson R E, Schmitt W, Moshammer R and Ulrich J 1997 Momentum spectro for single and double electron ionization of He in relativistic collisions Phys. Rev. A 56 3746–52

[10] Fiol J, Olson R E, Santos A C F, Sigaud G M and Montenegro E C 2001 Simultaneous projectile and target ionization in He\(^{+}\) + Ne collisions J. Phys. B: At. Mol. Opt. Phys. 34 503–9

[11] Geyer T and Rost J M 2003 Dynamical stabilization of classical multi-electron targets against autoionization J. Phys. B: At. Mol. Opt. Phys. 36 107–12

[12] Abbas I, Champion C, Zarour B, Lasti B and Hanssen J 2008 Single and multiple cross sections for ionizing processes of biological molecules by protons and \(\alpha\)-particle impact: a classical Monte Carlo approach Phys. Med. Biol. 53 N41

[13] Fiol J, Olson R E, Moshammer R and Ulrich J 2003 Dynamical electron-electron correlation in C\(_{2}\) + He simultaneous target-projectile collisional ionization J. Phys. B: At. Mol. Opt. Phys. 36 99–105

[14] Belkić Dž 1978 J. Phys. B: At. Mol. Opt. Phys. 11 3529

[15] Crothers D S F and McCann J F 1983 Ionisation of atoms by ion impact J. Phys. B: At. Mol. Opt. Phys. 16 3229–42

[16] Fainstein P D, Ponc V H and Rivarola R D 1988 A theoretical model for ionisation in ion-atom collisions. Application for the impact of multicharged projectiles on helium J. Phys. B: At. Mol. Opt. Phys. 21 287–99

[17] Green A E S, Sellin D L and Zachor A S 1969 Analytic independent-particle model for atoms Phys. Rev. 184 1

[18] Szydlík P P and Green A E 1974 Independent-particle-model potentials for ions and neutral atoms with Z \(\leq\) 18 Phys. Rev. A 9 1885–94

[19] Szydlík P P and Green A E 1975 Independent-particle-model potentials for atoms and ions with 36 < Z \(\leq\) 54 and a modified Thomas–Fermi atomic energy formula Phys. Rev. A 12 1144–60

[20] Woitke O, Závodský P A, Ferguson S M, Houck J H and Tanis J A 1998 Target ionization and projectile charge changing in 0.5 – 8 – MeV/q Li\(^{+}\) + He(q = 1,2,3) collisions Phys. Rev. A 57 2692–700

[21] Bernardi G, Suárez S, Fregenal D, Focke P and Meckbach W 1996 Measurement of doubly differential electron distributions induced by atomic collisions: apparatus and related instrumental effects Rev. Sci. Instrum. 67 1761–8

[22] Shah M B and Gilbody H B 1985 Single and double ionisation of helium by H\(^{+}\), He\(^{2+}\) and Li\(^{3+}\) ions J. Phys. B: At. Mol. Opt. Phys. 18 899–913

[23] McGuire H J, Stolterfoth N and Simony P R 1981 Screening and antiscreening by projectile electrons in high-velocity atomic collisions Phys. Rev. A 24 97–102

[24] Montenegro E C and Zouros T J M 1994 Relationship between the Born and impulse approximations for the antiscreening process Phys. Rev. A 50 3186–91

[25] Fainstein P D, Ponc V H and Rivarola R D 1991 Two-centre effects in ionization by ion impact J. Phys. B: At. Mol. Opt. Phys. 24 3091–119

[26] Clementi C and Roetti C 1974 At. Data Nucl. Data Tables 14 445

[27] Brauner M and Macek J H 1992 Ion-impact ionization of He targets Phys. Rev. A 46 2519–31

[28] Belkić Dž, Gayet R and Salin A 1979 Phys. Rep. 56 279

[29] Monti J M, Fojón O A, Hanssen J and Rivarola R D 2010 A Complete Postversion of the Three-Body Continuum Distorted Wave-Eikonal Initial State Approximation for Single Ionization of Multielectron Atoms J. At. Mol. Opt. Phys. 2010 128473

[30] Monti J M, Fojón O A, Hanssen J and Rivarola R D 2010 Influence of the dynamic screening on single-electron ionization of multi-electron atoms J. Phys. B: At. Mol. Opt. Phys. 43 205203

[31] Belkić D 1997 Electron detachment from the negative hydrogen ion by proton impact J. Phys. B: At. Mol. Opt. Phys. 30 1731–45

[32] Monti J M, Fojón O A, Hanssen J and Rivarola R D 2009 Ionization of helium targets by proton impact: a four-body distorted wave-eikonal initial state model and electron dynamic correlation J. Phys. B: At. Mol. Opt. Phys. 42 195201

[33] Monti J M, Fiol J, Fregenal D, Fainstein P D, Rivarola R D, Wolff W, Horsdal E, Bernardi G and Suárez S 2013 Experimental and theoretical results on electron emission in collisions between partially dressed ions with He targets Phys. Scr. T156 014031

[34] Olson R E and Salop A 1977 Charge-transfer and impact-ionization cross sections for fully and partially stripped positive ions colliding with atomic hydrogen Phys. Rev. A 16 531–41

[35] Reinhold C O and Falcón C A 1986 Classical ionization and charge-transfer cross sections for H\(^{+}\) + He and H\(^{2+}\) + Li\(^{+}\) collisions with consideration of model interactions Phys. Rev. A 33 3859–66

[36] Abrines R and Percival I C 1966 Proc. Phys. Soc. 88 861

[37] Hardie D J W and Olson R E 1983 Charge transfer and ionisation processes involving multiply charged ions in collision with atomic hydrogen J. Phys. B: At. Mol. Opt. Phys. 16 1983–96

[38] Fiol J, Courbin C, Rodríguez V D and Barrachina R O 2000 Classical description of threshold effects in ion-atom ionization collisions J. Phys. B: At. Mol. Opt. Phys. 33 5343–55

[39] Fiol J and Olson R E 2002 Three-body dynamics in the ionization of hydrogen by positron impact J. Phys. B: At. Mol. Opt. Phys. 35 1173–84

[40] Bruch R, Paul G, Andráj J and Lipsky L 1975 Autoionization of foil-excited states in Li and Li ii Phys. Rev. A 12 1808–24