Charge exchange processes involving highly charged ions and targets of interest in astrophysics and fusion plasmas

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Abstract. Renewed interest in charge exchange processes involving highly charged ions arises because of their crucial role in the planned ITER reactor as well as to recent X-ray observations in the astrophysical context. In this work, the classical trajectory Monte Carlo method (CTMC) is used to calculate state selective single charge exchange n-level cross sections and line emission cross sections pertinent to both fields. These are contrasted to recent laboratory data from KVI for the Xe18+ + Na(3s) collision system and NIST/BERLIN-EBIT data for the Ar18+ +Ar system.

1. Introduction
Starting in the 1970s, the tokamak fusion reactor program stimulated the study of charge exchange processes as a possible tool to indirectly estimate the impurity ion concentrations, the plasma temperature and its rotation. Typical collision systems involved multiply charged ions of C, N and O with atomic hydrogen at collision energies ranging from 1-80 keV/amu [1].

Charge exchange processes have yet to face another role at the planned construction of a large high temperature tokamak fusion (ITER) reactor in Cadarache, France [2]. In order to extract power from such reactor, the potential risk of hot plasma touching the facing walls must be avoided. In this sense, it is proposed that by injecting heavy rare gases into the divertor region, charge exchange by highly charged ions followed by photon emission will uniformly heat the facing walls avoiding the possibility of burn-through.

Our present knowledge on collision systems involving highly charged ions of Ar and Xe and H or D atoms is rather scarce. Furthermore, metastable H*(n=2) or D*(n=2) atoms provide a high fraction of the photon flux even though they reside as only 1% compared to the H and D atoms in the ground state. This is because of their much larger charge exchange cross section.

Since it is not feasible to provide experimental cross sections for H*(n=2) targets, alkali atoms provide very good substitutes to benchmark theoretical methods due to their similar cross sections and ionization potentials. The KVI group has recently published benchmark state-selective data for the Xe18+ +Na(3s) collision system using the MOTRIMS (magneto optical trap recoil ion momentum spectroscopy) method [3] at collision energies in the order of 1 keV/amu.

Concerning the astrophysical context, the first observation of X-ray emission from comet Hyakutake by the ROSAT satellite in 1996 led to surprise in the astrophysical community. Up to then, cold cometary environments were not expected to be a potential source of X-rays. Additionally, the fact that most of the emission was located 10⁴-10⁵ km ahead of the nucleus towards the Sun resulted in
an array of proposed physical mechanisms (see [4] for a review). It was only 4 years later when the Chandra X-ray Observatory (CXO) was in orbit that it was recognized charge exchange between the solar wind ions and the cometary gases at the cometary coma was the relevant mechanism for the cometary X-ray emission. Since then, it has been also established the role of charge exchange processes in X-ray emissions detected in planetary atmospheres.

Such a discovery prompted laboratory experiments on the Earth which tried to replicate the astrophysical conditions (solar wind ions, collision energies and cometary coma gaseous components). Two different experimental techniques have been used: a) The more traditional consists in using an accelerator together with SiLi and Ge detectors to collect the x-ray emissions from charge exchange collisions. This is the approach employed by the JPL group [5]; b) EBIT traps operated either in the magnetic trapping mode (LLNL and Berlin-EBIT groups) [6,7] or as ion sources (NIST and Berlin-EBIT groups) [7,8]. For the latter, the produced ions are extracted, filtered and directed onto a target gas in a separate collision chamber.

Significant discrepancies in the emission cross sections for Ar\textsuperscript{18+} + Ar collisions measured \textit{in situ} with those obtained once the beam is extracted have been recently reported by the Berlin-EBIT group [7]. A proper analysis of this situation from the experimental side is yet to be published. This work provides a theoretical insight of this problem and will hopefully stimulate further analysis from the experimental side.

The present work is organized as follows: in section II, we describe the two CTMC models hereafter used. For the alkali targets, a 3-body code will be used while for the Ar\textsuperscript{18+} + Ar system we introduce a 5-body model which incorporates the multiple capture channel neglected in previous studies by the authors. In section III, we present the calculated state selective capture cross sections and the emission cross sections for the collision systems under study and describe the main physical trends that we infer from the present data. Conclusions and outlook are drawn in section IV.

2. Theoretical Model

The classical trajectory Monte Carlo method has been widely used during the last 30 years and its applications in collision studies involving atoms and molecules are well documented in the literature [9-11].

To study highly charged ion collisions on Na(3s) and Na\textsuperscript{*}(3p) we use a 3-body code for which the interaction between the active electron and the parent nucleus is represented by the potential model developed by Green \textit{et al} from Hartree-Fock calculations and later on generalized by Garvey \textit{et al} [12]. The use of this potential form instead of the pure Coulombic representation accounts for the screening of the inner electrons. This quasi-hydrogenic picture of the Na valence orbital is expected to be reliable provided the differences in terms of binding energy among the valence and inner electrons.

The Na(3s) and Na\textsuperscript{*}(3p) states are distinguished not only through their respective ionization potentials. In addition, the classical angular momentum restriction \( l^2 < 1 \) and \( 1 < l^2 < 4 \) is imposed.

For the Ar\textsuperscript{18+} + Ar collision system, we consider a 5-body code which considers 3 active electrons. These electrons are initialized through their sequential binding energies over the quantum mechanical momentum distributions corresponding to the Ar(3p), Ar\textsuperscript{*}(3p) and Ar\textsuperscript{**}(3p) states for which we use the Clementi-Roetti expansions [13]. Coulomb potentials are used to represent the interaction of each electron with the corresponding parent nucleus with effective charges that are selected in order to provide the closest possible agreement to the quantum mechanical radial distribution [14]. As can be inferred from Figure 1, such a procedure clearly improved the respective radial distributions by adding the nodal structure which cannot be reproduced with the standard microcanonical sorting procedure.

In all cases, the charge exchange events are classified according to the classical number \( n_c \) that is obtained from the binding energy \( E_b \) of the electron relative to the projectile. Then, \( n_c \) is related to the quantum number \( n \) of the final state by the Becker and McKellar condition [15].

Multiple capture events are separated in the present 5-body model as coming from three different channels:
a) **Autoionizing double capture:** This channel is fed by double capture events to levels $n_1$ and $n_2$ for which $|n_1 - n_2| \leq 1$ [13]. The term “transfer ionization” is also used to denote this mechanism.

$$Ar^{18+} + Ar \rightarrow Ar^{16+*}(n_1l_1, n_2l_2) + Ar^{2+}$$
$$\rightarrow Ar^{17+*}(n, l) + e + Ar^{2+}$$  \hspace{0.5cm} (1)  

In our procedure, the electron with the greater $n_c$ value is considered to autoionize with zero energy. Conserving energy the inner electron falls to a deeper $n$-value and its $l$-value is modified by preserving the orbital eccentricity. The resultant argon ion is singly charged, just as in true single electron capture. However, the line emission after the Auger process arises from a lower $n$ value than in true single capture.

b) **Radiative double capture:** This channel considers events for which $|n_1 - n_2| > 1$,

$$Ar^{18+} + Ar \rightarrow Ar^{16+*}(n_1l_1, n_2l_2) + Ar^{2+}$$
$$\rightarrow Ar^{16+}(l^2) + h\nu_1 + h\nu_2 + Ar^{2+}$$  \hspace{0.5cm} (2) 

In our procedure, the decay routes of both electrons are explicitly considered. As a result, two sequences of line emission are obtained, one from the lower $n$ value and one from the larger $n$ value. The electronic energy structure corresponds to that of $Ar^{16+}$. The most notable feature is that instead of obtaining a Ly- line at 3306 eV like in single charge exchange or autoionizing double capture, the successive decays lead to a shoulder that is located on the low energy side of the dominant $Ar^{17+}$ $(2p_{1s})$ transition peak.

c) **Three electron capture:** For three electron capture, we have observed that most of the events correspond to two electrons bound with nearly equal $n$-values while the third one is bound to a greater $n'$-value. We have assumed these events decay according to the following scheme: the two electrons with the greatest $n_c$-values are emitted to the continuum (autoionize) with zero energy while the third inner one falls to a deeper $n$-level preserving orbital eccentricity and conserving energy:

$$Ar^{18+} + Ar \rightarrow Ar^{15+*}(n_1l_1, n_2l_2, n_3l_3) + Ar^{3+}$$
$$\rightarrow Ar^{17+*}(n, l) + e_1 + e_2 + Ar^{3+}$$  \hspace{0.5cm} (3) 

In all cases the emission cross sections are obtained following a similar procedure to that given in ref. [15].

3. **Results**

3.1. **State-selective charge exchange from $H(1s), H(n=2), Li$ and $Na$ target by highly charged ions**

In Figure 2 we show the $n$-state selective charge exchange cross sections for bare projectiles of charge $Z_p = 10+, 18+, 26+$ and $54+$ colliding with $H(1s)$ and $H^*(n=2)$ at an impact energy of 10 keV/amu. Vertical lines are added on the most probable principal quantum number for capture derived from the scaling relation [16],

$$n_p = n_i Z_p^{3/4},$$  \hspace{0.5cm} (4) 

where $n_i$ is the initial level in which the active electron is found in the hydrogen target. In both cases we observe good agreement, although for the largest projectile charge under consideration ($54+$) we notice a small deviation in the maximum of the distribution compared to the scaling law. We note that the magnitudes of the $H^*(n = 2)$ partial cross sections are approximately an order-of-magnitude larger than those of the ground state. Based on the geometrical cross section of the electron orbits one would expect the cross sections to increase like $n'$ 3. We have verified that this scaling is valid at the total cross
Figure 1. Radial distributions for Ar(3p), Ar⁺(3p), and Ar²⁺(3p). Solid line: quantum mechanical result; line+squares: present CTMC model.

Figure 2. State-selective electron capture cross sections for 10 keV/amu collisions of bare ions on a) H(1s) and b) H*(n=2). The vertical dashed lines represent the predictions of the scaling law shown in equation (4).

section level. However, for the excited target, the partial cross sections for capture are spread over a larger range of final \( n \)-levels and the \( n^4 \) scaling is not fulfilled. Similarly, it can be noticed that the cross section magnitudes do not increase proportional to linear in charge state as do the overall total cross sections.

Charge exchange recombination spectroscopy diagnostics in fusion reactors usually depend on the observation of visible light. At 10 keV/amu, visible light emitted from excited products formed via H(1s) collisions will be faint since the cross sections are small but even a 1% component of H*(n=2) would lead to a strong visible signal for highly charged ions.

As the impact energy increases the distributions shown in Figure 2 broaden and at impact energies around 100 keV/amu, we observed that collisions with ground state hydrogen dominate the visible line emission spectra. At this energy, the velocity mismatch between the impinging projectile and the bound electron for the H*(n=2) target implies that electron loss is dominated by ionization rather than charge exchange.

We now turn our attention to the alkali targets, which are good substitutes for the inaccessible H*(n=2) atom. In Figures 3 and 4 we show the state selective electron capture cross sections for 10 keV/amu collisions of bare ions with Li(2s) and Na(3s) respectively. For neutral targets the following extension of the hydrogenic scaling provided by equation (4) is usually recalled,

\[ n_p = \sqrt[3/4]{13.6eV/IPZ_p^{3/4}}, \]  

(5)
Figure 3. State-selective electron capture cross sections for 10 keV/amu collisions of bare ions on Li(2s). The vertical dashed lines represent the prediction of the scaling law shown in equation (4).

Figure 4. State-selective electron capture cross sections for 10 keV/amu collisions of bare ions on Na(3s). The vertical dashed lines represent the prediction of the scaling law shown in equation (4).

where $IP$ is the ionization potential of the target under consideration. It can be seen that for Li(2s) and Na(3s) the proposed scaling does not work well. It could well be that the screening of the core electrons affects the charge seen by the active electron leading to differences with the hydrogenic case.

As a side note, multiplying Eq. 5 by a factor of 1.2 leads to acceptable agreement with the calculations.

We note that the peak positions of the state selective cross sections as well as their magnitudes and widths are in very good agreement with those calculated for H*(n=2) for the projectiles under consideration.

Very recently, in an experimental breakthrough, state-selective data have been measured for Xe$^{18+}$ ions colliding with Na(3s) using the MOTRIMS method [3]. In Figure 5, we benchmark our CTMC calculations against these data at impact energies of 0.55 keV/amu, 2.23 keV/amu and 3.35 keV/amu. The relative experimental data have been normalized to our peak values. Good overall agreement can be inferred based on the present results, although the contributions from the higher levels seem to be underestimated at 0.55 keV/amu and 3.35 keV/amu.

3.2. State-selective charge exchange and x-ray emission cross sections following Ar$^{18+}$+Ar collisions

In the last few years, several charge exchange studies were performed from both the theoretical and experimental sides in order to reproduce the cometary x-ray data from the Chandra satellite - CXO. From the experimental side, the EBIT group at LLNL connected their EBIT trap to the spare microcalorimeter spectrometer of the Suzaku mission achieving an unprecedented resolution of about 8 eV [17]. Although cryogenic problems with the mission once in orbit did not allow any high resolution astrophysical x-ray spectral measurements, these Earth-based studies formed the grounds of the already planned missions to put microcalorimeters in orbit in the near future.

Two main limitations associated with the EBIT when operating in the magnetic trapping mode are: a) the range of collision energies accessible (10-25 eV/amu) is far below the typical solar wind energies (1-3 keV/amu) and b) the reported uncertainty for the collision energy is about 50% [6,7]. A very interesting and challenging issue was recently raised by the Berlin-EBIT group. They contrasted their x-ray line emission cross sections obtained in situ for the Ar$^{18+}$+Ar system with those obtained
by performing the collisions in a separate chamber, using the EBIT as an ion source. In this latter case, the extracted ions can be further accelerated to reach typical solar wind energies at the expense of losing the chance to measure forbidden transitions which are long lived compared to the typical dimensions of the collision chambers.

The results published by the Berlin-EBIT group showed a dramatic discrepancy among the results obtained by employing both experimental techniques and have not been reconciled as far as we know.

In order to theoretically explore this collision system, we first consider the charge exchange distributions as a function of the impact parameter which we show in Figure 6 a). A 3-body CTMC code with the same initialization used for the 5-body code (i.e. only one active electron with radial distribution equal to that shown in Figure 1 for Ar(3p)) is used to check the role of the multiple capture channels. As can be seen, for impact parameters larger than about 12 a.u., the 3-body and 5-body results are coincident, clearly indicating that the registered events correspond to the single charge exchange channel. As the impact parameter decreases, the 3-body code leads to single charge exchange hiding the multiple capture dynamics. Furthermore, we notice that by adding up the different multiple capture channels to the one of single capture, the total cross section at 1 keV/amu is 15% larger than that predicted by the 3-body code. In Figure 6 b) we show the n-state selective cross sections, noticing the two-peak structure obtained for the double radiative decay channel which clearly illustrates the decay route of both electrons.

Now moving to the line emission cross sections, in Figure 7 the present CTMC data are contrasted to the experimental data of Allen et al (2008) [7] (at 5 eV/amu, 218 eV/amu and 2.14 keV/amu), and
Figure 7. Line emission cross sections for 5 eV/amu, 218 eV/amu, 2.14 keV/amu (experimental data from Allen et al (2008) [7]), and 4 keV/amu (experimental data from Tawara et al (2006) [8]).

to the data of Tawara et al (2006) [8] (at 4 keV/amu). Both sets of measurements were obtained by EBIT traps used in the extraction mode. It can be seen that the present results are in good agreement with the extracted beam data. We have tried to reconcile our CTMC data with the magnetic trapping mode results by studying the possible dependence either on the collision energy or in possible electric field related alignments. No significant changes in the cross sections were found for reasonable field strengths. In principle, the only experimental variable left unstudied was the magnetic field inherent to the in situ measurements.

A possible source of discrepancy could be related to analysis of the in situ data. When investigating the line emissions from collisions with bare ions, the ion spectra for lower charge states are manually subtracted from the data. This procedure implies that possible contributions from the double radiative decay channel are artificially removed, lowering the Lyman→ peak signals, and thus raising the hardness ratio. This particular issue should be experimentally explored with great care.

4. Conclusions

In this work we have presented charge exchange studies involving collisions of highly charged projectiles with atomic targets of interest to the ITER reactor as well as studies closely related to astrophysical studies. The present theoretical results are more than encouraging. We have shown that lithium and sodium targets provide a close estimation of how even a very minor fraction of H*(n=2)
present in a tokamak should reveal itself in the visible light signal. In particular, for Na the recent data from KVI show that a more complete understanding of such collisions systems is at hand.

Concerning the Ar^{18+} + Ar collision system, we have not been able to reconcile the line emission cross sections measured in situ with those obtained by extracting the beam from an EBIT and performing the collision in a separate chamber. An important point we raise, alludes to the data analysis procedure performed when the EBIT is operated in the magnetic trapping mode.

A more detailed experimental analysis of this topic, which remained elusive during the last five years, is clearly needed and would represent a step forward for our future understanding of these collision processes.

Acknowledgments
The author would like to thank Professor R. E. Olson for critically reading this manuscript. Work at UNS supported by PGI 24/F049, PICT-2007-00887 of the ANPCyT, and PIP 112-200801-02760 of CONICET (Argentina).

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