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State-selective charge exchange from H(1s), H(n = 2), Li and Na targets by very highly charged ions

S Otranto[1] **and R E Olson**[2]

[1] CONICET and Departmento de Física, Universidad Nacional del Sur, 8000 Bahía Blanca, Argentina
[2] Physics Department, Missouri University of Science and Technology, Rolla, MO 65401 USA

E-mail: sotranto@uns.edu.ar

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Abstract
In order to provide information for charge exchange spectroscopy diagnostics in new, high temperature tokamak plasmas, n-level state-selective electron capture cross sections are presented for very highly charged ions with charge states $q \geqslant 10$. Fully stripped ions with charges of 10+, 18+, 26+, 54+ and 92+ are considered in order to provide scaling information over a broad range. The H(1s) and H($n = 2$) targets are evaluated at 1, 10 and 100 keV/amu, i.e. plasma core temperatures to those encountered during neutral beam heating. For use in pellet diagnostics, cross sections are given for Li and Na targets at 10 keV/amu. These latter targets also provide a means to experimentally test the accuracy of the H($n = 2$) results since they are pseudo-one-electron atoms with ionization energies close to that of excited hydrogen.

(Some figures in this article are in colour only in the electronic version)

Introduction

Charge exchange spectroscopy is routinely used as a diagnostic tool for tokamak plasmas [1]. The line emission from excited impurity ions that are formed after charge exchange with ground and excited state hydrogen (deuterium) can be used to determine plasma temperature via analysis of line broadening, plasma rotation via the Doppler shift of the lines and impurity ion concentrations via absolute magnitudes of the emission lines. Usual temperatures extend from tens to hundreds of eV at the plasma edge, to around 10 keV in the core region. In many cases the diagnostic is combined with neutral beam heating of the plasma, so that the energy range for study can extend up to 100 keV/u.

The basis for charge exchange spectroscopy is the state-selective electron capture reaction

$$A^{q+} + B \rightarrow A^{(q-1)+*} + B^{+}, \tag{1}$$

which is followed by decay of the excited ion via photon emission,

$$A^{(q-1)+*}(nl) \rightarrow A^{(q-1)+}(n', l') + h\nu. \tag{2}$$

Here, A is a plasma impurity ion and B is the neutral target which is usually deuterium, but may be other atoms that are seeded into the plasma for diagnostic purposes.

In this work we present n-level cross sections since the orbital angular momenta are statistically mixed by the electric and magnetic fields in the reactor. The classical trajectory Monte Carlo (CTMC) theoretical method is employed [2]. For these types of calculations it is well tested. Furthermore, it is not hindered by basis set limitations that make atomic- and molecular-orbital calculations impossible for the ion charge states considered here.

Previous work has largely been confined to studies of low charge state ions, primarily those of Be, C and O (for example, see Anderson *et al* 2000 [3]). Other recent studies have considered Ne^{10+} [4–6] and high charge state ions of Ar [7–10]. There is also a number of charge exchange studies which have considered high-Z projectiles (up to +26) on molecular targets of astrophysical interest [11–13]. However, in new and planned nuclear fusion reactors, longer run times and higher temperatures provide the need for charge exchange cross sections for ions with higher charge states. It is the purpose of this paper to try to meet this need, and to extend the ion charge state regime to very high charges

so that scaling rules can be confidently developed without unnecessary extrapolations. Moreover, the state-selective cross sections should give guidance as to the feasibility of using specific transitions for diagnostic purposes.

Hence, we have included ion charge states of 10+, 18+, 26+, 54+ and 92+. Ground state hydrogen (deuterium) is the principal target. However, during neutral beam injection, a residual 1–2% of the hydrogen is in the excited H($n = 2$) state. For this target the cross sections are much larger than those of the ground state and populate higher n-levels of the impurity ions. Thus, for charge exchange spectroscopy employing visible radiation which can only originate from high n-levels, the line emission from collisions with H($n = 2$) can exceed those from H(1s). This is especially true for the half and one-third energy components of the neutral beam [14, 15]. For these cases we provide state-selective charge exchange cross sections at energies of 1, 10 and 100 keV/amu.

Experimentally, it is impossible to test the calculated cross sections for excited hydrogen. However, the use of an MOT (magneto optical trap) experiment makes possible the study of Li and Na alkali atom targets [16]. These atoms are pseudo-one-electron targets that have ionization energies very close to that of H($n = 2$), so provide a good simulation of the latter atom. Lithium pellets are also sometimes seeded into the fusion plasma to provide unique line emission profiles used in diagnostics [17]. Thus, we provide state-selective charge exchange cross sections for the projectiles listed above with Li and Na to provide the eventual experimental test of our calculations. At present MOT data exist for 18+ ions on Na [18]. These data will be shown below and are found to be in excellent agreement with our calculations. A Li MOT has been recently included in a reaction microscope allowing photo-double ionization studies on Li($1s^2nl$) [19, 20]. Future measurements are also planned at GSI-Darmstadt that will eventually test our electron capture calculations for highly charged ions up to U^{92+}. The alkali-atom calculations are presented for 10 keV/amu since they are not associated with neutral beam injection energies.

Theoretical method

We have performed classical trajectory Monte-Carlo (CTMC) calculations of the cross sections for single electron capture [2]. Hamilton's equations were solved for a mutually interacting three-body system. Although the hydrogenic approximation has been used for decades as a fast and easy alternative to explore more complex systems (molecules, multielecronic atoms) with the CTMC model, we restrict the use of the hydrogenic approximation to the hydrogen atom only. For Li and Na we consider the active electron to evolve under the central potential model developed by Green *et al* from Hartree-Fock calculations [21], and later generalized by Garvey *et al* [22]. The CTMC method directly includes the ionization channel and is not limited by basis set size for the prediction of capture to very high-lying excited states.

Since the electron tends to be captured to high n-values with minimal contributions from the s-states, quantum defects play a minor role and the orbital energies for the captured electron are similar to those obtained with bare projectiles. We then represent the captured electron-projectile interaction by a Coulomb potential where the projectile asymptotic charge is considered. We note however that in a recent article we have shown that the consideration of the Garvey potential can modify the l-distributions of the captured electrons from that of an unscreened Coulomb potential, and is necessary for a quantitative description of the collision [23].

A classical number n_c is obtained from the binding energy E_p of the electron relative to the projectile by

$$E_p = -Z_p^2/(2n_c^2), \tag{3}$$

where Z_p is the charge of the projectile core. Then, n_c is related to the quantum number n of the final state by the condition derived by Becker and McKellar [24]:

$$[(n-1)(n-1/2)n]^{1/3} \leqslant n_c \leqslant [n(n+1)(n+1/2)]^{1/3}. \tag{4}$$

The cross section for a definite n-state is then given by

$$\sigma_n = N(n)\pi b_{\max}^2/N_{\text{tot}}, \tag{5}$$

where $N(n)$ is the number of events of electron capture to the n-level and N_{tot} is the total number of trajectories integrated. The impact parameter $b_{\max}$ is the value beyond which the probability of electron capture is negligibly small.

Results

H(1s) and H($n = 2$) targets

The results for 1 keV/amu are displayed in figure 1. The vertical dashed lines correspond to the predicted position for the most probable principal quantum number for capture given by the scaling relation

$$n_p = n_i q^{3/4}, \tag{6}$$

where n_i is the initial level of a hydrogen target and q the charge state of the projectile [4]. For the largest projectile charges here considered (+54 and +92) we note a small deviation of the respective n_p-values from the scaling law. We note that had the exponent been 0.76 instead of 0.75, then the agreement along the whole range of Z-charges here considered would have been perfect. This shows the limitation of such a simple exponent in equation (6) and suggests that further studies based on high-Z projectiles could lead to a more accurate power value. 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, not a factor of n^4 as would be predicted from the geometrical cross section of the electron orbits. This is because for the excited target, the partial cross sections for capture are spread over a larger range of final n-levels. It is for the same reason 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 generally depend on the observation of visible light. At 1 keV/amu such line emission from excited products formed via ground state H(1s) collisions will be very faint since the cross sections are extremely small. These transitions would correspond to roughly 11 → 10 for 10+,

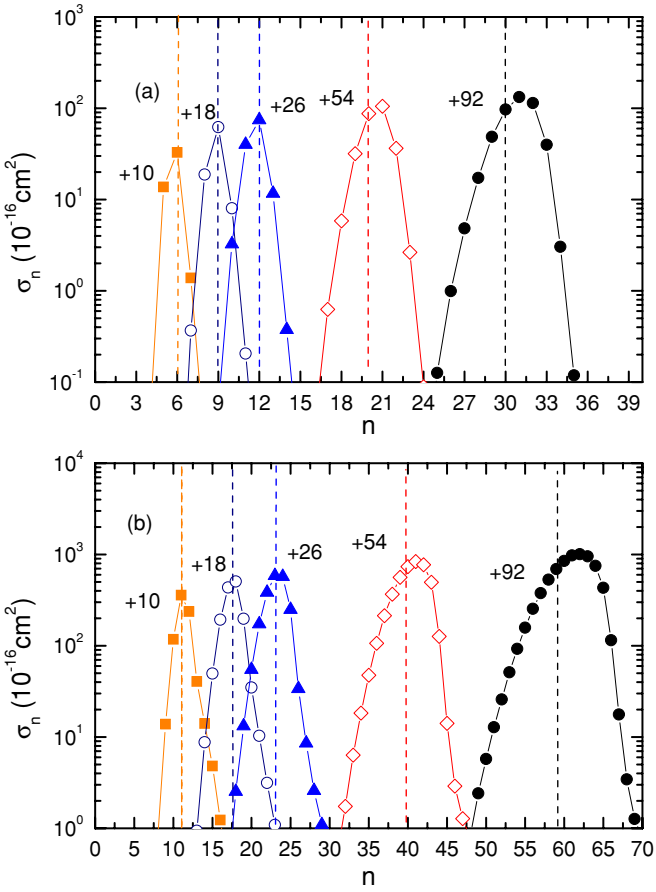

Figure 1. State-selective electron capture cross sections for 1 keV/amu collisions of fully-stripped ions A^{q+} on ground state H(1s), upper figure (a), and for the H($n = 2$) target, lower figure (b). The corresponding total cross sections are presented in table 1. The vertical dashed lines are the predictions of the maxima cross sections from equation (6).

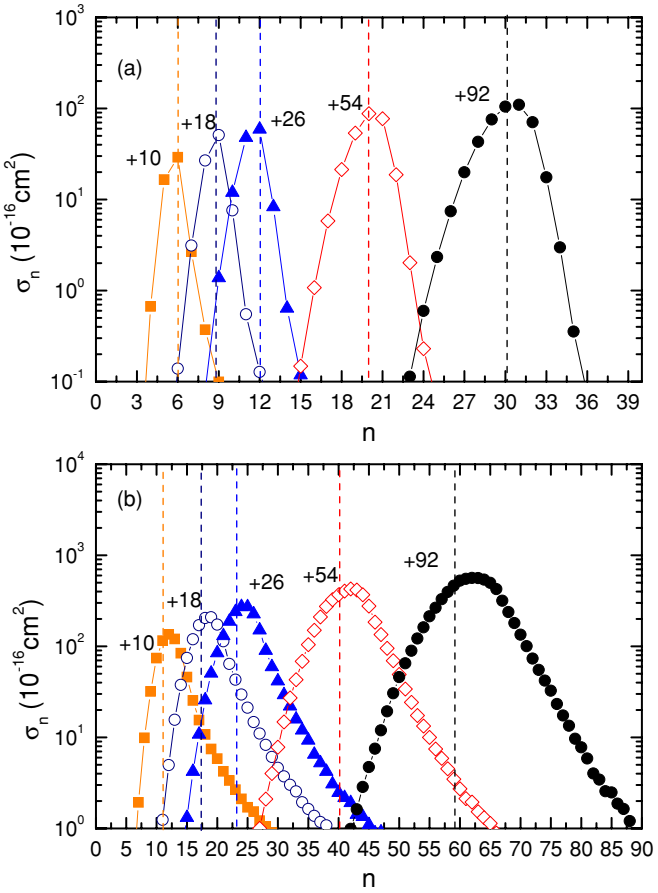

Figure 2. Same as for figure 1, but for 10 keV/amu.

20 → 19 for 26+, and the 45 → 44 line for 92+. However, even a 1% component of H($n = 2$) in the plasma would give rise to a very strong visible signal for these high charge state ions.

Proceeding to a central plasma core temperature of 10 keV/amu, figure 2, the same general trends as noted in the 1 keV/amu cases are noted. However, now the partial cross sections display more broadening with slight shifts to higher n-values. Even with these trends, visible-light-based charge exchange spectroscopy studies will still mainly observe transitions from collisions with the minor component of excited H($n = 2$) in the plasmas.

It is not until 100 keV/amu, figure 3, corresponding approximately to the main energy component of neutral beam injection do we find that collisions with ground state hydrogen dominate the visible line emission spectra for all ions between 10+ and 92+. This is due to two reasons. The first is that the n-level capture from H(1s) spreads over a large range in n's. The second is that the H($n = 2$) target cross sections now decline rapidly in magnitude because of the mismatch in velocity between the ion and the orbital speed of the bound-state electron, leading to the electron removal reaction being dominated by impact ionization rather than electron capture. We have used a log–log scale in this case to provide a better visualization of the distributions.

In table 1, we have tabulated the overall total charge exchange cross sections for the collision processes shown above.

Li(2s) and Na(3s) targets

One can use a variation of equation (6) above to predict the most probable principal quantum number for electron capture from non-hydrogenic targets. The equation can be generalized to other neutral targets by using hydrogenic scaling of the ionization potentials (IP) to yield

$$n_p = (13.6\ \text{eV}/IP)^{1/2}\, q^{3/4}, \tag{7}$$

where the ionization potential of the active electron is given in the energy units of electron volts. For Li(2s) targets, and incident ions with charge states less than 10+, equation (7) has been found to underestimate the n-level for the maximum cross section by approximately 20% [25]. A possible reason for such a deviation is due to the screening of the core electrons, so that the target electron does not see a well-defined charge as a function of distance from the nucleus. Thus, the hydrogenic relationship used in equation (7) can only be considered approximate. We note however, that the $q^{3/4}$ dependence is still valid for these targets.

Table 1. Total charge exchange cross sections (in cm^2) for 1 keV/amu, 10 keV/amu and 100 keV/amu collisions of A^{q+} projectiles on H(1s) and H($n = 2$).

	1 keV/amu		10 keV/amu		100 keV/amu	
q	H(1s)	H($n = 2$)	H(1s)	H($n = 2$)	H(1s)	H($n = 2$)
10	4.798×10^{-15}	7.884×10^{-14}	4.952×10^{-15}	7.116×10^{-14}	2.482×10^{-15}	2.953×10^{-16}
18	8.948×10^{-15}	1.441×10^{-13}	8.952×10^{-15}	1.353×10^{-13}	6.684×10^{-15}	1.197×10^{-15}
26	1.301×10^{-14}	2.085×10^{-13}	1.295×10^{-14}	1.977×10^{-13}	1.054×10^{-14}	2.891×10^{-15}
54	2.700×10^{-14}	4.313×10^{-13}	2.680×10^{-14}	4.168×10^{-13}	2.487×10^{-14}	1.974×10^{-14}
92	4.583×10^{-14}	7.314×10^{-13}	4.552×10^{-14}	7.170×10^{-13}	4.359×10^{-14}	9.590×10^{-14}

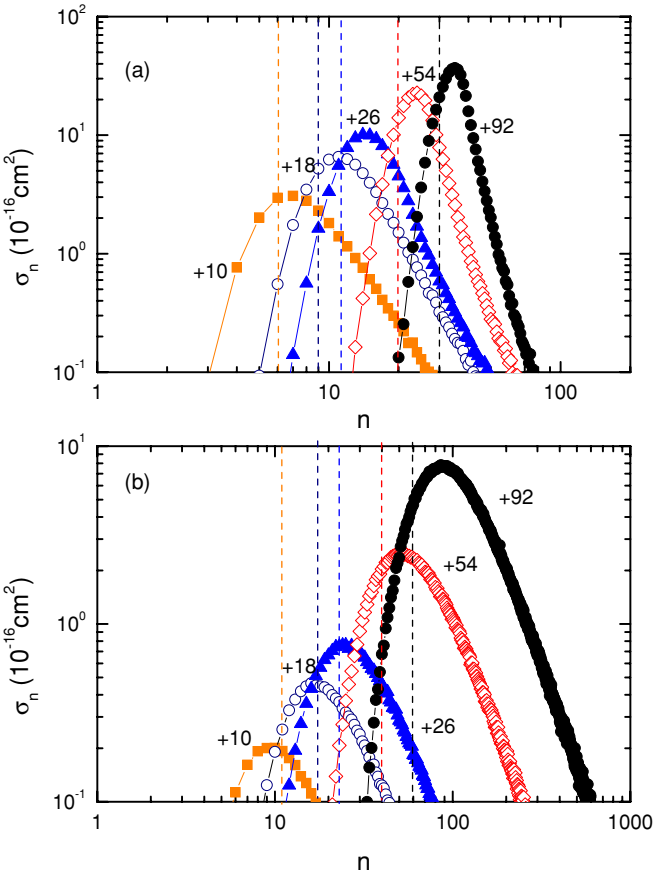

Figure 3. Same as for figure 1, but for 100 keV/amu.

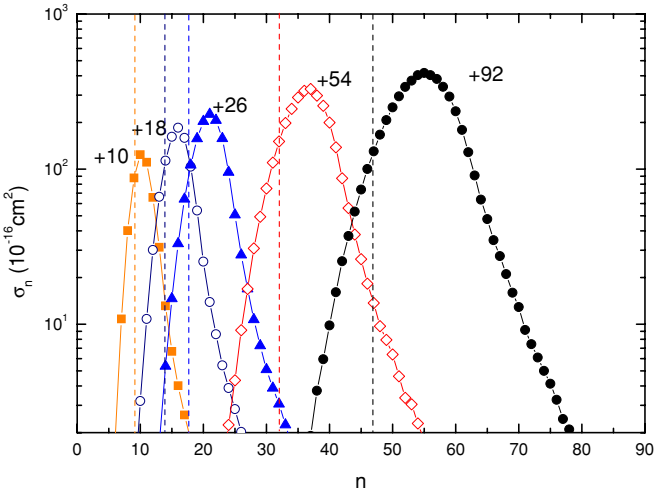

Figure 4. State-selective electron capture cross sections for 10 keV/amu collisions of fully-stripped ions A^{q+} on Li(2s). The corresponding total cross sections are presented in table 2. The vertical dashed lines are the predictions of the maxima cross sections from equation (7).

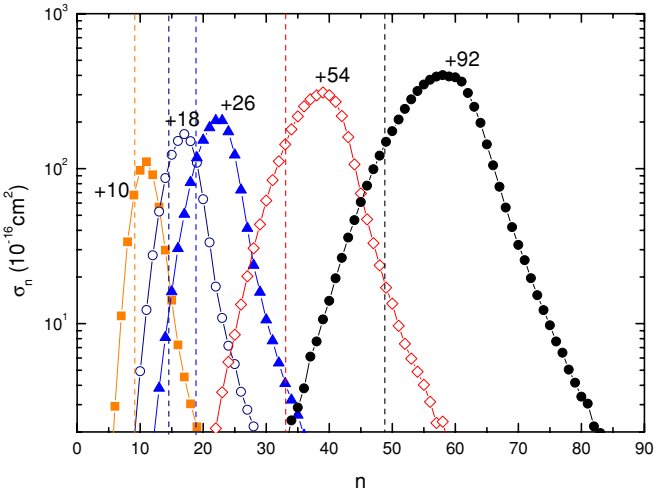

Figure 5. Same as for figure 4, but for the Na(3s) target.

In figure 4 are displayed the cross sections for a Li(2s) target at a collision energy of 10 keV/amu. Figure 5 shows the results for Na(3s). For both systems, equation (7), the dashed lines, underestimates the maxima positions in the state-selective cross sections by about 20%, similar to that previously found for low charge state ions.

It has always been assumed that Li and Na are good prototypes for the experimentally inaccessible H($n = 2$) atom. Comparing the results given for H($n = 2$) in figure 2 to those for the two alkalis, we find very close agreement between all systems, especially between H($n = 2$) and Na(3s). The peak position of these state-selective cross sections, along with their magnitudes and widths are in very close agreement up to charges of 26+. Even for 92+, the peak positions only differ by 10%. This is somewhat surprising in that the ionization potential of Na(3s) is 5.14 eV, significantly differing from that of 3.40 eV for H($n = 2$). However, the larger radial expectation value for Na(3s) versus that of H($n = 2$) compensates for the differing ionization energies.

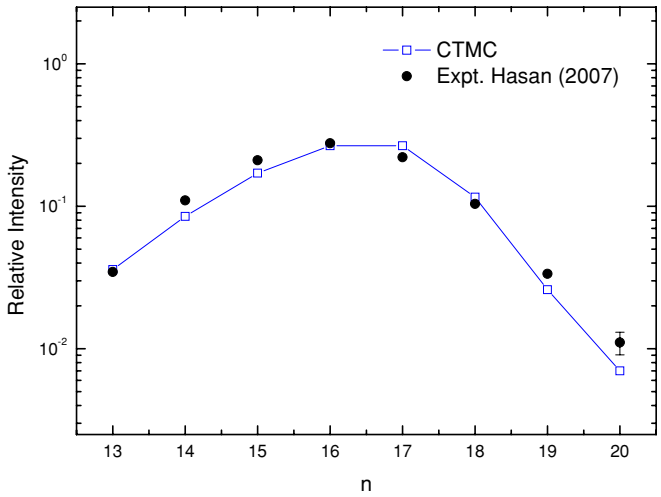

Figure 6. Calculated relative state-selective cross sections for 18+ ions colliding with Na(3s) at 2.23 keV/amu compared to the data of Hasan *et al* [7]. The calculated total cross section is given in table 2.

Table 2. Total single charge exchange cross sections (in cm^2) for 10 keV amu^{-1} collisions of A^{q+} projectiles on Li(2s) and Na(3s).

q	Li(2s)	Na(3s)
10	5.083×10^{-14}	5.426×10^{-14}
18	9.603×10^{-14}	1.045×10^{-13}
26	1.411×10^{-13}	1.554×10^{-13}
54	3.012×10^{-13}	3.377×10^{-13}
92	5.238×10^{-13}	5.914×10^{-13}

It is always difficult to assess the validity of various theoretical models. Our early work on line emission after collisions of 4+ to 8+ ions on Li(2s) revealed good agreement with experimental observations [26, 27]. However, experimental benchmarks to theory for ions with charge states above 8+ in the low keV/amu energy range were basically non-existent until very recently. Now there are available state-selective cross sections for higher charges from the pioneering work by the Hoekstra group in Groningen using an MOT [18].

In figure 6 we compare our calculations to the experimental data for 2.23 keV/amu collisions of Xe^{18+} on Na. Although the data are not absolute, we find extremely good agreement between theory and experiment regarding the peak position and width of the state-selective cross sections. Such a comparison lends credibility to the predicted H($n = 2$) cross sections presented above. The overall total cross sections for the alkali targets are presented in table 2.

Conclusions

State-selective electron capture cross sections have been presented for ions of very high charge states colliding with ground and excited H($n = 2$) targets. These calculations provide a base for extending scaling rules used in diagnostics of fusion plasmas. They also give guidance as to the feasibility of observing specific line radiation used in electron capture recombination spectroscopy applications. The energies given are meant to be representative of edge plasma temperatures—1 keV/amu, core plasma temperatures—10 keV/amu and for neutral beam heating studies—100 keV/amu.

Lithium and sodium targets are also considered since they have been used in pellet-based diagnostics. Further, as we have found, they provide a very good simulation of the H($n = 2$) target so that there may be further experimental tests of the calculations. We are very pleased that very recent MOT experiments with 18+ ions display excellent agreement with our calculations.

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