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State-selective charge exchange processes between fully stripped ions with H(1s) and H*(*n*=2)

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INTRODUCTION & AIM

Charge exchange spectroscopy is a powerful diagnostic tool of current use to analyze tokamak Plasmas [1,2]. This technique is based on the analysis of the photonic emission that follows charge-exchange processes between impurity ions and the D(n=1) and D*(n=2) components of the plasma. Observations are restricted to the visible range due to the implementation of fiber optics, thus limiting the range of photon energies that are useful for diagnostics to 1.771-3.1eV.
In what follows, we will refer to H(1s) and H*(n=2) instead of deuterium since from the collisional point of view the resulting cross sections are expected to be the same. As it has been previously pointed out in the literature [3], charge exchange cross sections from excited hydrogen are orders of magnitude greater than those obtained for the ground state. As a result, even a minor fraction of excited hydrogen (compared to the ground state proportion present in the plasma) could provide a strong signal for diagnostics.
Since charge-exchange experiments cannot be performed with H*(n=2) at the laboratory scale, theoretical cross sections are needed to calculate effective emission coefficients for the spectral lines.
In this poster, we show state-selective and total charge-exchange cross sections during collisions of bare ions with H(1s) and H*(n=2). The classical trajectory Monte Carlo method in its Z-CTMC version is employed [4], and is contrasted against theoretical and experimental data previously reported where available.

METHOD

The classical trajectory Monte Carlo (CTMC), is a non-perturbative method based on the classical simulation of a large number of trajectories for a given collisional system. This method, in different variants, has been employed with success for more than 5 decades to describe collisions between heavy/light particles and atoms/molecules.
One of the most visible limitations of the method in its three-body formulation is represented by the radial distribution of the target electron. In contrast to the quantum mechanical formulation, which predicts an exponentially decreasing behavior, classical mechanics predicts a sharp cut-off at the classical return point.
Noticing that the classical return point is determined by the binding energy E_0 and the target nuclear charge Z, an expansion either over energies (E-CTMC) or nuclear charges (Z-CTMC) can be used to improve the radial distribution. The Z-CTMC method is in this case provided by the following expansion on Z:

$$\rho(r) = \sum_{i=1}^{N=10} \alpha_i \; \rho(r, Z_i) \, .$$

Since the radial distributions are normalized to 1, the expansion coefficients fulfill the condition $\sum_i \alpha_i = 1$.

For H(1s) the expansion coefficients are obtained via a least-squares fitting procedure over the quantum H(1s) radial distribution. For H*(n=2), on the other hand, we fit an effective quantum mechanical radial distribution built upon the H(2p) and H(2s) distributions using a statistical proportion of 75% and 25% respectively.

The final state analysis is performed by determining in first place a classical n_c number via the hydrogenic energy relationship:

$$E_{eP} = -\frac{Z_P^2}{2n_c^2}$$

The (*n*,*l*) state is obtained by using the Becker-MacKellar binning procedure:

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

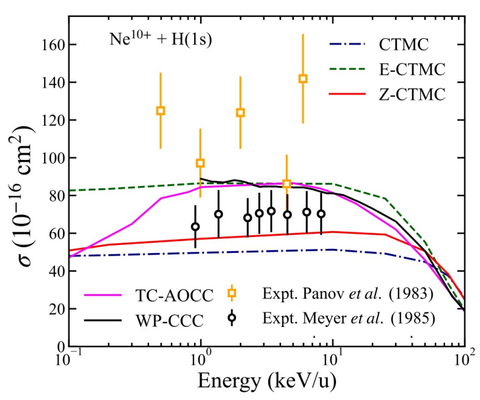
$$l \leqslant l_c \leqslant l+1 \qquad\qquad l_c = (n/n_c)(\vec{r} \times \vec{k})$$

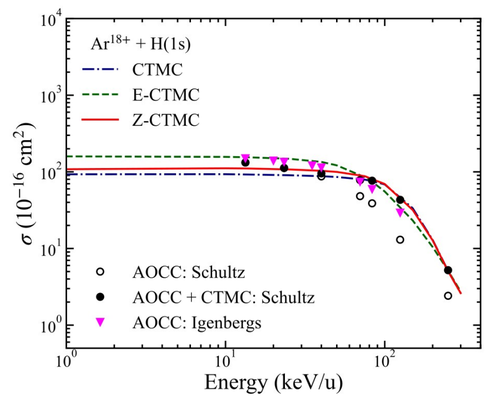
Here, l_c is the captured electron angular momentum and $\vec{r}$ and $\vec{k}$ are the electron position and momentum relative to the projectile respectively. The (*n*,*l*)-state selective charge exchange cross section is obtained by taking into account the geometrical area defined by the maximum impact parameter at which charge-exchange takes place and the fraction of trajectories that lead to that specific final state:

$$\sigma^{\mathrm{cap}} = \frac{N(n,l)}{N_{\mathrm{tot}}} \, \pi b_{\mathrm{max}}^2$$

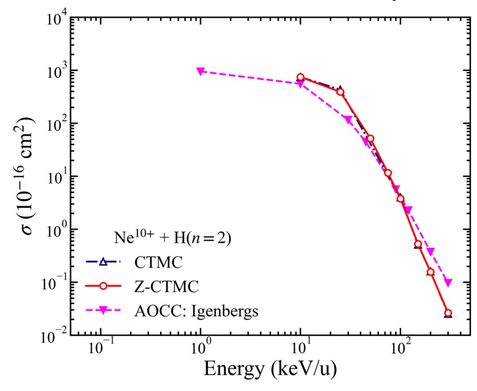
RESULTS & DISCUSSION

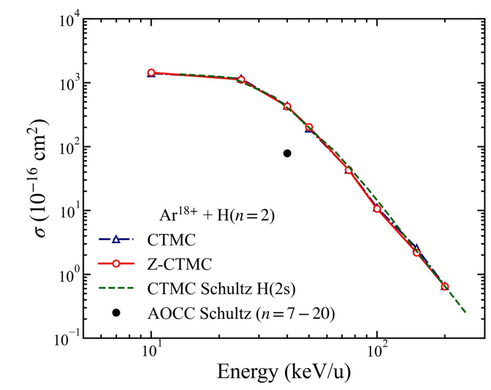
In the first place, we show the total charge-exchange cross sections for Ne^{10+} and Ar^{18+} on H(1s). For the former, experimental data reported by Panov and Meyer are available for comparison. No data has been reported for the latter as far as we are aware. The classical theoretical predictions of the standard microcanonical CTMC, the E-CTMC and the Z-CTMC methods are contrasted to those reported by using the Atomic Orbital Close Coupling (AOCC), the Two Center-AOCC and the Wave Packet-Convergent Close Coupling (WP-CCC) quantum mechanical numerically intensive methods.



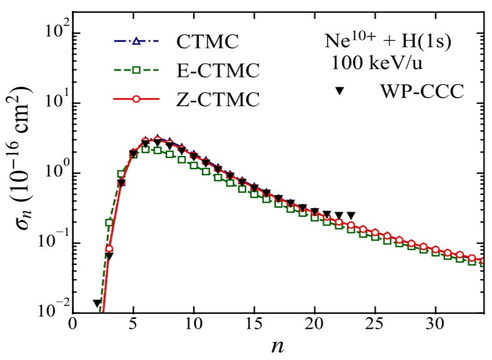


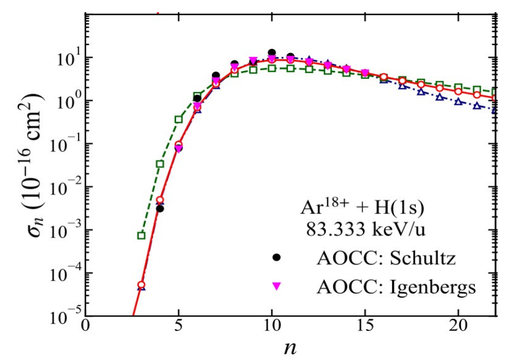
Next, we show the total charge-exchange cross sections for Ne^{10+} and Ar^{18+} on H*(n=2). The classical theoretical predictions of the standard microcanonical CTMC and the Z-CTMC methods are contrasted to those reported by the AOCC.

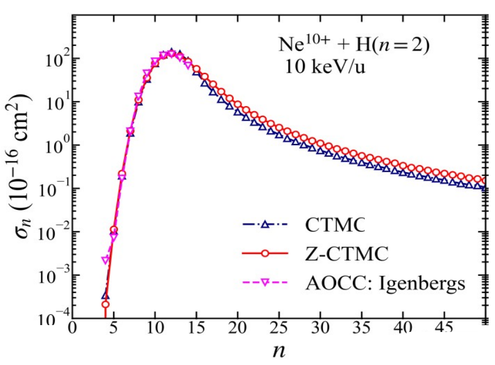


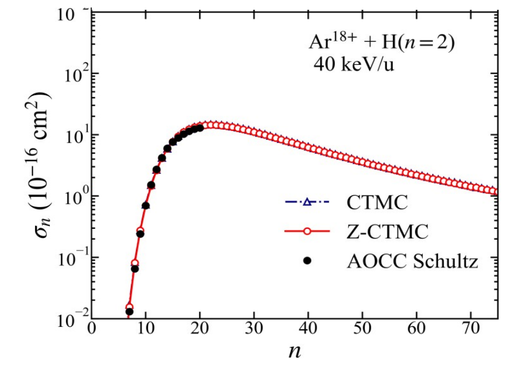


Below, we show a similar comparison a the *n*-state selective level.









Punctual collision energies for which data reported by the WP-CCC and AOCC models were available have been chosen in this case.

CONCLUSION

Charge-exchange between highly charged bare ions and H(1s) and H*(n=2) atoms have been analyzed by implementing a classical trajectory Monte Carlo method that improves the description of the radial electronic distribution in the target compared to the standard microcanonical formulation. The present data compares well with the available experimental data and those reported with numerically intensive quantum mechanical methods such as AOCC and WP-CCC.

REFERENCES

[1] R. C. Isler, Plasma Phys. Controlled Fusion 36, 171 (1994).
[2] R. Hoekstra *et al*, Plasma Phys. Controlled Fusion 40, 1541 (1998).
[3] I. Blank *et al*, Phys. Rev. A 85, 022712, (2012)
[4] N. D. Cariatore, S. Otranto, R. E. Olson, Phys. Rev. A 91, 042709 (2015); Phys Rev. A 93, 066702 (2016).
[5] A. M. Kotian *et al*, J. Phys. B: At. Mol. Opt. Phys. 55 115201 (2022).
[6] L. Liu, Y. Wu, J. Wang and R. Janev, At. Data Nucl. Data Tables 143 101464, (2022).
[7] D. R. Schultz, T. G. Lee and S. D. Loch S J. Phys. B: At. Mol. Opt. Phys. 43 144002 (2010).
[8] K. Igenbergs, PhD Thesis, Technische Universität Wien (2011).