PARTIAL AND TOTAL ELECTRON CAPTURE CROSS SECTIONS IN B^{5+},Ne^{10+}+H(2s) COLLISIONS FOR PLASMA DIAGNOSTICS

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One of the sticking points of the energy confinement in plasmas is the control of the impurities by means of the wall conditioning. One of this techniques is the first wall boronization as it has been done in TJ-II sterallator at Ciemat (Madrid) [1]. Very accurate cross sections are required to calculate emision lines in charge exchange recombination spectroscopy (CXRS) experiments when a neutral Hydrogen beam at 30 keV (main energy) is injected into the plasma to get characteristic plasma parameters such as ionic temperature or density [2].

Although excited hydrogen atoms in the diagnostic neutral beams are in much lower proportion than in the ground state (around 0.5% of the total [3]), the charge exchange cross sections between excited H($n = 2$) and fully stripped ions (impurities) are one order of magnitude higher which makes their contribution to the total CX cross sections relevant. Therefore, we study at intermediate impact energies the charge exchange reactions:

$$\mathrm{B}^{5+} + \mathrm{H(2s)} \rightarrow \mathrm{B}^{4+}(nlm) + \mathrm{H}^{+} \qquad 0.25keV/amu < E < 1MeV/amu \tag{1}$$

$$\mathrm{Ne}^{10+} + \mathrm{H(2s)} \rightarrow \mathrm{Ne}^{9+}(nlm) + \mathrm{H}^{+} \qquad 1keV/amu < E < 100keV/amu \tag{2}$$

using two different formalisms, the semiclassical molecular close-coupling expansion and the Classical Trayectory Montecarlo (CTMC).

Semi-classical Impact Parameter Method

In this treatment the nuclei follow classical straight-line trajectories with constant velocity $\vec{v}$ and impact parameter $\vec{b}$ ($\vec{R} = \vec{v}t + \vec{b}$), while the electronic motion is described quantum-mechanically through the solution of the time-dependent Schrödinger equation:

$$(H - i\partial_t|_{\vec{r}})\Psi(\vec{r},v,b,t) = 0 \quad ; \quad H = -\frac{1}{2}\nabla^2 - \frac{Z}{r_B} - \frac{1}{r_H} \tag{3}$$

Ψ is expanded in terms of bound $\{\chi_k\}$ molecular states OEDMs:

$$\Psi(\vec{r},v,b,t) = e^{iU(\vec{r},t)} \sum_k a_k(v,b,t)\chi_k(\vec{r},R)e^{-i\int_0^t E_k(t')dt'} \tag{4}$$

that are eigenfunctions of the nuclei fixed Born-Oppenheimer hamiltonian H_{BO}:

$$H_{BO}(\vec{r},R)\chi_K(\vec{r},R) = E_K(R)\chi_K(\vec{r},R) \tag{5}$$

and U is a common translation factor (CTF), introduced to account for the momentum transfer problem [4, 5, 6]. The time derivative in equation (3) is taken by keeping fixed the electron position $\vec{r}$ in the laboratory fixed frame.

Substitution of equation (4) in (3) leads to a set of single differential equations for the expansion coefficients $a_k(v,b,t)$, which are integrated up to very large time t_{max}. Capture and excitation cross sections are obtained by integration of the corresponding probabilities over the impact parameters [7]:

$$\sigma_{nlm}^{A,H}(v) = 2\pi \int |a_{nlm}^{A,H}(v,b,t \to \infty)|^2 b\mathrm{d}b = 2\pi \int P_{nlm}(v,b) b\mathrm{d}b. \tag{6}$$

CTMC formalism

The statistical phase space distribution satisfies the clasical Liouville equation:

$$\frac{\partial \rho(\vec{r},\vec{p},v,b,t)}{\partial t} = -[\rho(\vec{r},\vec{p},v,b,t),H] \tag{7}$$

This distribution can be discretized using $\mathcal{N}$ different classical trajectories [8]:

$$\rho(\vec{r},\vec{p},v,b,t) = \frac{1}{N}\sum_{j=1}^{N} \delta(\vec{r}-\vec{r}_j(t))\delta(\vec{p}-\vec{p}_j(t)) \tag{8}$$

Substitution of eq. (8) in (7) yields the Hamilton equations that rule the temporal evolution:

$$\dot{\vec{r}}_j(t) = \frac{\partial H}{\partial \vec{p}_j(t)} \qquad \dot{\vec{p}}_j(t) = -\frac{\partial H}{\partial \vec{r}_j(t)} \tag{9}$$

Thus, the quality of the final CX and ionization cross sections will basically depend on the accuracy with we describe the initial spatial and momentum quantal distributions. In previous $A^{q+} + H(1s)$ collisions we have employed either the microcanonical or the hydrogenic distributions. In the former [8], all electronic trajectories have the energy of the exact initial quantum state $E = E_0$. The hydrogenic distribution [9], is obtained (e.g.) using a linear combination of $\mathcal{N}$ microcanonical distribution. with an average energy $E = E_0$ (e.g. [10]).

For excited atomic states (H(2s)) a better description is achieved by using an initial gaussian distribution

$$\rho(n_g) = K_1 \mathrm{e}^{-K_2(n_g-1.2)^2} \quad ; \quad n_g(E) = Z_H/\sqrt{-2E} \tag{10}$$

with K_1 and K_2 normalization constants [11].

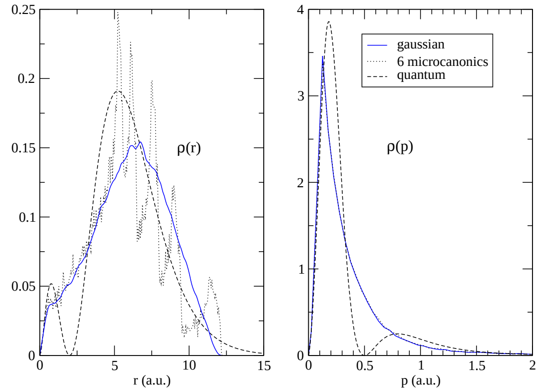

Figure 1: Comparison between different electronic distributions to reproduce the initial H(2s) state

In figure 1 we show the improvement obtained with the gaussian initial density distribution.

We apply an Energy criterion to differenciate ionization ($\{E_H = \vec{p}^2/2 - 1/r > 0$, $E_B = 1/2(\vec{p}-\vec{v})^2 - Z/|\vec{r}-\vec{b}-\vec{v}t_{max}| > 0\}$) from capture ($\{E_H > 0, E_B < 0\}$) and excitation ($\{E_H < 0, E_B > 0\}$). The probability for a process X reads as

$$P_X(v,b) = \int d\vec{r} \int d\vec{p}\, \rho_X(\vec{r},\vec{p},t_{max}) = N_X/N \quad (11)$$

where N_X is the number of trajectories that finish in the process X.

Partial nl cross sections were obtained using the Becker and MacKellar binning distribution [12].

Results

We have perfomed CTMC and semiclassical calculations for $B^{5+}, Ne^{10+} + H(2s)$collisions. Semiclassical calculations used large bases, 223 OEDMs for $B^{5+} + H(2s)$ and 210 for $Ne^{10+} + H(2s)$ in order to get accurate cross sections to (very) capture excited states of interest in plasma diagnostics (n=7 $\rightarrow$ n=6; λ =4946 Åãnd n=12 $\rightarrow$ n=11; λ =6903 Åf̃or B^{4+} and Ne^{9+} respectively).

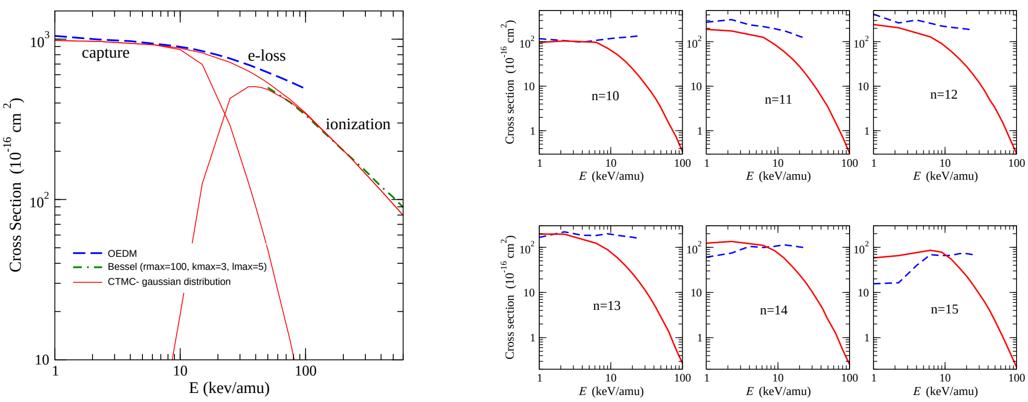

Figure 2: (a) Total capture and ionization cross sections for the Ne^{10+}+H(2s) collisions. b) Partial semiclassical(- -) and classical-CTMC(—) capture cross sections to n=10 – 15 states.

For reaction (2) we show in figure 2 a) that the semiclassical formalism yields accurate values of capture cross sections for energies ($E > 6keV/amu$) where ionization is negligible ($E <$

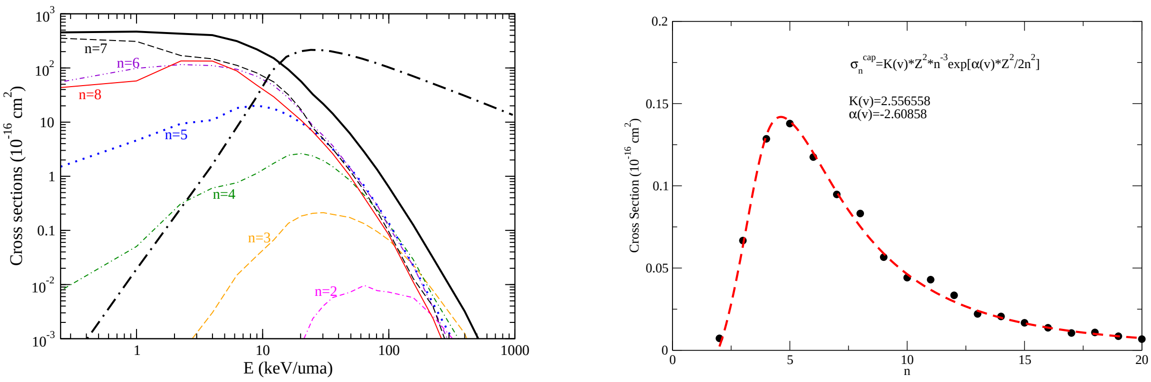

Figure 3: a) B^{5+}+H(2s) total capture (—-) and ionization (— · —) together with the n-partial ($n = 2-8$) capture recommended cross sections as a function of the impact energy. b) Oppenheimmer n^{-3} extrapolation law for $E \sim 100 keV/amu$.

$15 keV/amu$); on the other hand, capture and ionization CTMC results are accurate for ($E > 6 keV/amu$). The overlapping between this two methods is almost perfect in the $E \sim 10 keV/amu$ region, where ionization begins to be competitive with capture. A similar behaviour is found for n (fig. 2 b)) and nl partial cross sections (not shown here for space reasons).

Partial capture cross sections to $B^{4+}(n)$ are presented in figure 3 a); here both sets of results closely merge in the common region of accuracy, $6.245 keV/amu < E < 15.41 keV/amu$, allowing us to provide accurate recommended cross sections. We have also checked (see figure 3 b) for $E \sim 100 keV/amu$) the n^{-3} Oppenheimer rule for high impact energies in order to extrapolate our results to higher n capture cross sections.

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