Electron capture and ionization in collisions of multiply charged ions with H(2s).

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Abstract. We present total cross sections for electron capture and ionization in collisions of B^{5+} and Ne^{10+} with H(2s), calculated using two methods: the semiclassical close-coupling molecular formalism and the eikonal-CTMC method. We have evaluated partial cross sections for capture into excited n-levels, required in plasma diagnostics.

1. Introduction.

Accurate electron capture cross sections are required in charge exchange recombination spectroscopy (CXRS) experiments, where a neutral hydrogen beam is injected into the plasma to measure characteristic plasma parameters such as ionic temperature and density. Although the proportion of excited hydrogen atoms in the diagnostic beam is small (around 0.5%) [1], the cross sections for electron capture by impurity ions from H($n = 2$) are one order of magnitude higher than those from H(1s), which makes their contribution to the total cross sections relevant [2]. In this work, we have considered the charge exchange reactions:

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

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

We present total and partial cross sections for population of Ne^{9+}(n=10-15) and B^{4+}(n=2-7) using two different formalisms, the semiclassical molecular close-coupling expansion and the eikonal-Classical Trajectory Monte-Carlo (CTMC) method, previously applied [3, 4] to ion-H(1s) collisions.

2. Semi-classical molecular expansion.

In this treatment the nuclei follow straight-line trajectories with constant velocity $\boldsymbol{v}$ and impact parameter $\boldsymbol{b}$ ($\boldsymbol{R} = \boldsymbol{v}t + \boldsymbol{b}$), while the electronic motion is described quantum-mechanically by means of the wavefunction Ψ, solution of the equation (in atomic units):

$$\left[\widehat{H} - \mathrm{i}\left.\frac{\partial}{\partial t}\right|_{\boldsymbol{r}}\right]\Psi(\boldsymbol{r}, t; v, b) = 0 \quad ; \quad \widehat{H} = -\frac{1}{2}\nabla^2 - \frac{Z_{\mathrm{A}}}{r_{\mathrm{A}}} - \frac{1}{r_{\mathrm{H}}} \tag{3}$$

with $Z_{\rm A}$ the nuclear charge of the ion, and $r_{\rm A,H}$ the electron distances to both nuclei. Ψ is expanded as a linear combination of molecular orbitals (OEDMs) $\{\chi_k\}$ in the form:

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

where the OEDMS are eigenfunctions of $\widehat{H}$ with energies $E_k(R)$ and U is a common translation factor [5], defined in terms of the switching function proposed in ref. [6].

Substitution of equation (4) in (3) leads to a set of first-order differential equations for the expansion coefficients $a_k(t;v,b)$, and capture and excitation cross sections are obtained by integrating the corresponding probabilities over the impact parameter:

$$\sigma_{nlm}^{\rm A,H}(v) = 2\pi \int |a_{nlm}^{\rm A,H}(t\to\infty;v,b)|^2\, b{\rm d}b = 2\pi \int P_{nlm}^{\rm A,H}(v,b) b\,{\rm d}b \tag{5}$$

where the superscripts A,H indicate that the electron is asymptotically bound to nucleus A (charge exchange) or H (excitation). The coefficients a_{nlm} are obtained from the solutions a_k after projection of the OEDMs on the atomic states with quantum numbers nlm.

3. Eikonal-CTMC formalism.

In this treatment, the nuclei follow rectilinear trajectories and the electron dynamics is described by the statistical phase space distribution which satisfies the classical Liouville equation:

$$\frac{\partial \rho(\boldsymbol{r},\boldsymbol{p},t;v,b)}{\partial t} = -[\rho(\boldsymbol{r},\boldsymbol{p},t;v,b), H] \tag{6}$$

This distribution can be discretized using $\mathcal{N}$ classical trajectories [7]:

$$\rho(\boldsymbol{r},\boldsymbol{p},v,b,t) = \frac{1}{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \delta(\boldsymbol{r}-\boldsymbol{r}_j(t))\delta(\boldsymbol{p}-\boldsymbol{p}_j(t)) \tag{7}$$

Substitution of eq. (7) in eq. (6) yields the Hamilton equations for the individual trajectories $\boldsymbol{r}_j(t)$, $\boldsymbol{p}_j(t)$.

The accuracy of capture and ionization cross sections basically depends on that of the initial spatial and momentum distributions. In previous works we have employed either the microcanonical or the hydrogenic distributions. In the former [7], all electronic trajectories have the energy of the initial quantum state $E = E_0$. The hydrogenic distribution [8], is obtained by means of a linear combination of N microcanonical distributions. with an average energy $< E >= E_0$ (e.g. [3]). For excited atomic states (H(n=2)) a better description is achieved, as shown in figure 1, by using an initial gaussian distribution:

$$\rho(\boldsymbol{r},\boldsymbol{p}) = 2^{-1/2}\pi^{-3} \int (-E)^{5/2} \rho(E)\delta(H-E){\rm d}E \tag{8}$$

with

$$\rho(n_c) = K_1 {\rm e}^{-K_2(n_c-2.2)^2} \quad ; \quad n_c(E) = Z_H/\sqrt{-2E} \tag{9}$$

and where the constants K_1 and K_2 are determined by the conditions of normalization and mean energy $< E >= E_0$. The initial distribution for H(2s) has been obtained by retaining only those trajectories with angular momentum l_c fulfilling $0 < nl_c/n_c < 1$ (see [9]).

We apply an energy criterion to evaluate ionization, capture and excitation cross sections. Namely, trajectories leading to ionization fulfill (the origin of the electronic coordinates is placed on the H nucleus):

$$E_{\rm H} = p^2/2 - 1/r > 0;\ E_{\rm A} = 1/2(\boldsymbol{p}-\boldsymbol{v})^2 - Z_A/|\boldsymbol{r}-\boldsymbol{b}-\boldsymbol{v}t_{\rm max}| > 0 \tag{10}$$

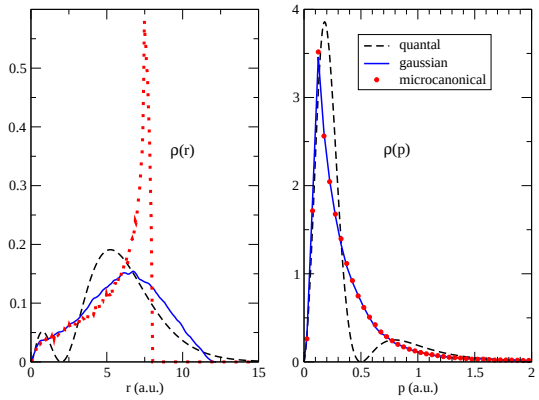

Figure 1. Comparison between microcanonical and gaussian distributions for the H(2s) state.

while for capture we have: $E_{\rm H} > 0, E_{\rm A} < 0$, and for excitation: $E_{\rm H} < 0, E_{\rm A} > 0$. The probability for a process X reads:

$$P_{\rm X}(v,b) = \int {\rm d}\boldsymbol{r} \int {\rm d}\boldsymbol{p}\, \rho_{\rm X}(\boldsymbol{r},\boldsymbol{p},t_{max}) = \mathcal{N}_{\rm X}/\mathcal{N} \tag{11}$$

where $\mathcal{N}_{\rm X}$ is the number of trajectories that lead to process X. Partial nl cross sections were obtained using the Becker and MacKellar criterion [9].

4. Results and discussion.

In the semiclassical calculations we have used large bases (223 OEDMs for B^{5+} + H(2s) and 210 for Ne^{10+} + H(2s)), in order to obtain accurate cross sections for capture into excited states, which lead to emission in the visible domain (e.g. B^{5+}(n=7) with λ(n=7→ n=6)=4946 Å , and Ne^{9+}(n=12) with λ(n=12 → n=11)= 6903 Å).

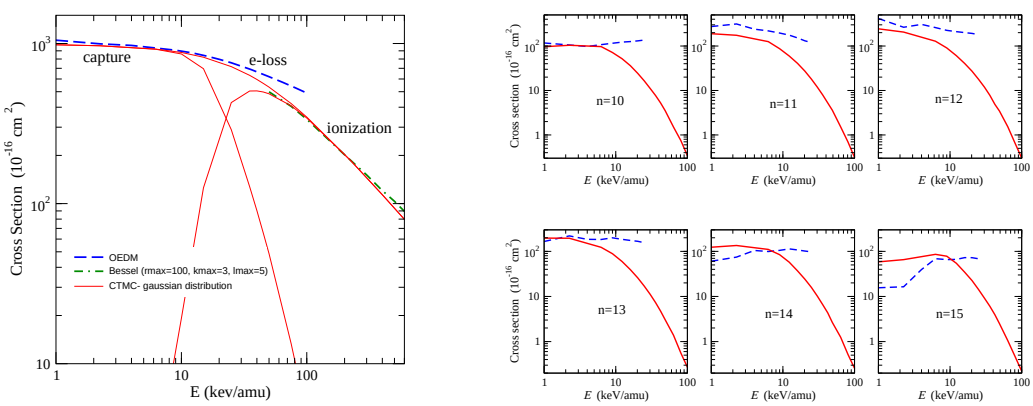

Figure 2. Electron capture and ionization cross sections for Ne^{10+} + H(2s) collisions (a) Total cross sections. (b) Partial semiclassical (- -) and classical-CTMC (—) cross sections for capture into Ne^{9+}(n=10 – 15).

Our results for reaction (1) (figure 2(a)) show that the semiclassical molecular formalism yields accurate total capture cross sections for energies $E < 15$ keV/amu; at higher energies, ionization starts to be competitive with charge exchange and the result corresponds to the

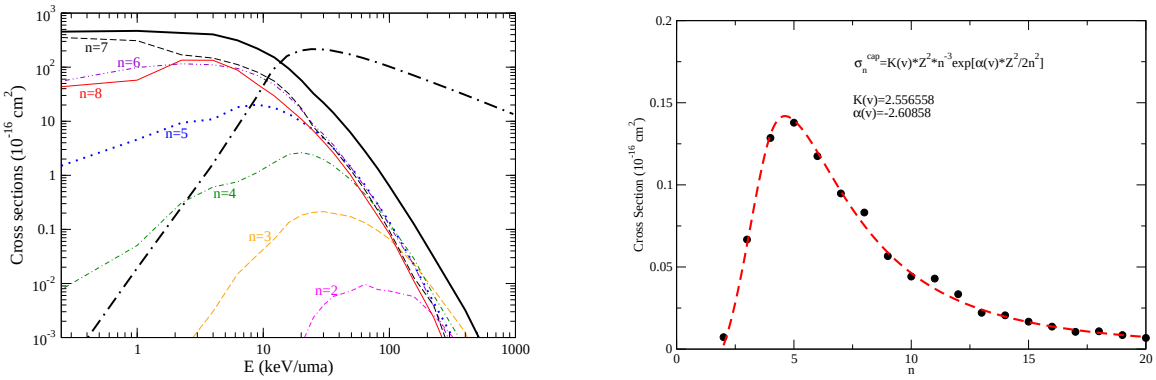

Figure 3. Electron capture and ionization cross sections for B^{5+} + H(2s)collisions: a) total capture (—-) and ionization (— · —) cross sections, together with the n-partial ($n = 2 - 8$) capture recommended cross sections as functions of the impact energy. (b) Fitting of the partial cross sections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

electron-loss cross section, i.e. the sum of capture and ionization ones. On the other hand, the CTMC results for capture and ionization are accurate for $E > 6$ keV/amu, and therefore we obtain a good agreement between both calculations at $E \approx 10$ keV/amu. A similar behaviour is found for the partial cross sections of fig. 2 (b), although the overlap between the two calculations is less satisfactory, mainly because the limitations of the molecular expansion when ionization starts to be sizeable, since the ionizing flux overpopulates the highest-lying capture states of the basis set.

Our results for reaction (2) are illustrated in figure 3. In this case, classical and semiclassical cross sections for populating $B^{4+}(n)$ levels, show good agreement in the region 6.25 keV/amu $< E <$ 15 keV/amu, which allows us to smoothly join both results, as shown in figure 3(a).

As for ion collisions with H(1s), we have employed the CTMC results to check (see figure 3 (b)) the n^{-3} Oppenheimer rule for high impact energies, where we have also checked that the partial capture cross sections are accurately reproduced by the expression $\sigma_n(v) = K(v)Z_A^2 n^{-3}\exp[-\alpha(v)Z_A^2/2n^2]$ where K and α are fitting parameters.

Acknowledgments

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