Theoretical studies of ionization, charge transfer and excitation in ion-H, He collisions in the energy range of 25-500 keV/amu

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Contents

Motivation

In the framework of this CRP on *Data for Atomic Processes of Neutral Beams in Fusion Plasmas* we are interested in calculating:

Fully (and partially) stripped impurity ions colliding with atomic hydrogen

The processes relevant to neutral beam diagnostics of fusion plasmas are:

- Target Ionization: $A^{q+} + H(nlm) \longrightarrow A^{q+} + H^{+} + e^{-}$
- Electron Capture: $A^{q+} + H(nlm) \longrightarrow A^{(q-1)+}(n'l'm') + H^{+}$
- Target Excitation: $A^{q+} + H(nlm) \longrightarrow A^{q+} + H(n''l''m'')$

Motivation

Purpose I.: Detailed data for atomic processes involving neutral hydrogen

Data found in ADAS[1] at 100 keV/amu

- Collisions with H($1s$): Several sets of data: A need to asses their uncertainties and to provide a well recommended data set.

$$Be^{4+} + H(1s) \rightarrow Be^{3+}(6lm) + H^{+}: \sim 33\%$$

- Collisions with H($n = 2$): Significant gaps, especially related to processes initiated from an excited state of the neutral atom.

$$C^{6+} + H(n = 2) \rightarrow C^{5+}(8lm) + H^{+}: \text{ 1 set of data}$$

[1] http://open.adas.ac.uk

Motivation

Methods to be employed:

- CTMC (Classical Trajectory Monte Carlo Method) [2]

  Wide experience in the treatment of one-active electron collisions with H($1s$)

  Stripped ions:[3] He^{2+}, Li^{3+}, Be^{4+}, B^{5+}, C^{6+}, N^{7+}, O^{8+}, Ne^{10+}

  Highly charged ions:[4] $Ar^{16+,17+,18+}$, Kr^{36+}, W^{60+}

- GTDSE (Grid Time Dependent Schrödinger Equation)[5]

  A complete study of state-selective cross sections of Be^{4+} + H($1s$) collisions[6]

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[2] R Abrines & I C Percival, Proc. Phys. Soc. **88**, 861 (1966)

[3] Phys. Rev. A **60** 4546 (1999), Phys. Rev. A **70** 052713 (2004), Eur. Phys. J. D. **68**, 227 (2014)

[4] J. Phys. B. **39**, L91 (2006), Phys. Scr. **T156** 014033 (2013)

[5] J Suárez *et al.*, Comput. Phys. Commun. **150** 2025 (2009)

[6] A Jorge *et al.*, Phys. Rev. A **94** 032707 (2016)

Motivation

Purpose II.: Detailed data for atomic processes involving neutral beams of helium and lithium.

Very scarce data

Proposed method: the Switching CTMC Approach

$\hookrightarrow$ implementation of a new approach especially designed to classically treat two-active electron systems[7]

[7] A Jorge *et al.*, Phys. Rev. A **94** 022710 (2016)

Method

In this talk,

Eikonal CTMC[8]

- The projectile follows **straight-line trajectories**: $\mathbf{R} = \mathbf{b} + \mathbf{v}t$
- The electronic motion is described by a **classical distribution function**

$$\rho(\mathbf{r}, \mathbf{p}, t) = \frac{1}{N} \sum_{j=1}^{N} \delta(\mathbf{r} - \mathbf{r}_j)\delta(\mathbf{p} - \mathbf{p}_j)$$

solution of the Liouville's equation:

$$\frac{\partial \rho}{\partial t} = -[\rho, H_{el}]$$

where H_{el} is the target electronic Hamiltonian and $N \approx 10^5$

[8] Illescas and Riera, Phys. Rev. A **60** (1999)

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[8] Illescas and Riera, Phys. Rev. A **60** (1999)

Method

Eikonal CTMC

- Hamilton's equations are solved for each electron trajectory:

$$\dot{\mathbf{r}}_j = \frac{\partial H}{\partial \mathbf{p}_j};\ \dot{\mathbf{p}}_j = -\frac{\partial H}{\partial \mathbf{r}_j}$$

- Including the total collision Hamiltonian:

$$H = \frac{p^2}{2} - \frac{Z_T}{r_T} - \frac{Z_P}{r_P}$$

- Energy criterion is applied at $t_{fin} = \frac{500 a.u.}{v}$ to select **ionized** ($E_T > 0$, $E_P > 0$), **captured** ($E_T > 0$, $E_P < 0$) or ($E_T < 0$) **elastic** or **excited** trajectories.

Method

- The classical phase space of captured (or excited, then referred to the target) electrons is partitioned into exclusive subspace[9]

$$[(n-1)\,(n-\frac{1}{2})\,n]^{1/3} \;<\; n_c \;\leq\; n\,(n+\frac{1}{2})\,(n+1)]^{1/3}$$

$$l \;<\; \frac{n}{n_c}\,l_c \;\leq\; l+1$$

with $n_c = Z_P/\sqrt{-2E_P}$ and $l_c = |(\mathbf{r}-\mathbf{b}-\mathbf{v}t)\wedge(\mathbf{p}-\mathbf{v})|$.

- Electron probabilities:

$$P^{i,c,e}(v,b) \;=\; \int d\mathbf{r} \int d\mathbf{p}\,\rho^{i,c,e}(\mathbf{r},\mathbf{p},v,b,t_{fin})$$

- Total cross sections:

$$\sigma^{i,c,e}(v) \;=\; 2\pi \int_0^\infty db\,b\,P^{i,c,e}(v,b)$$

[9] R L Becker & A D MacKellar, J. Phys. B **17** 3923 (1984)

Initial distributions: construction

Microcanonical (standard):

$$\rho_M(\mathbf{r},\mathbf{p},Z,E) = \frac{1}{K}\,\delta(H_{el}-E) = \frac{1}{8\pi^3}\,\delta\left(\frac{\mathbf{p}^2}{2}-\frac{1}{\mathbf{r}}+\frac{1}{2}\right)$$

All the particles have the same binding energy.

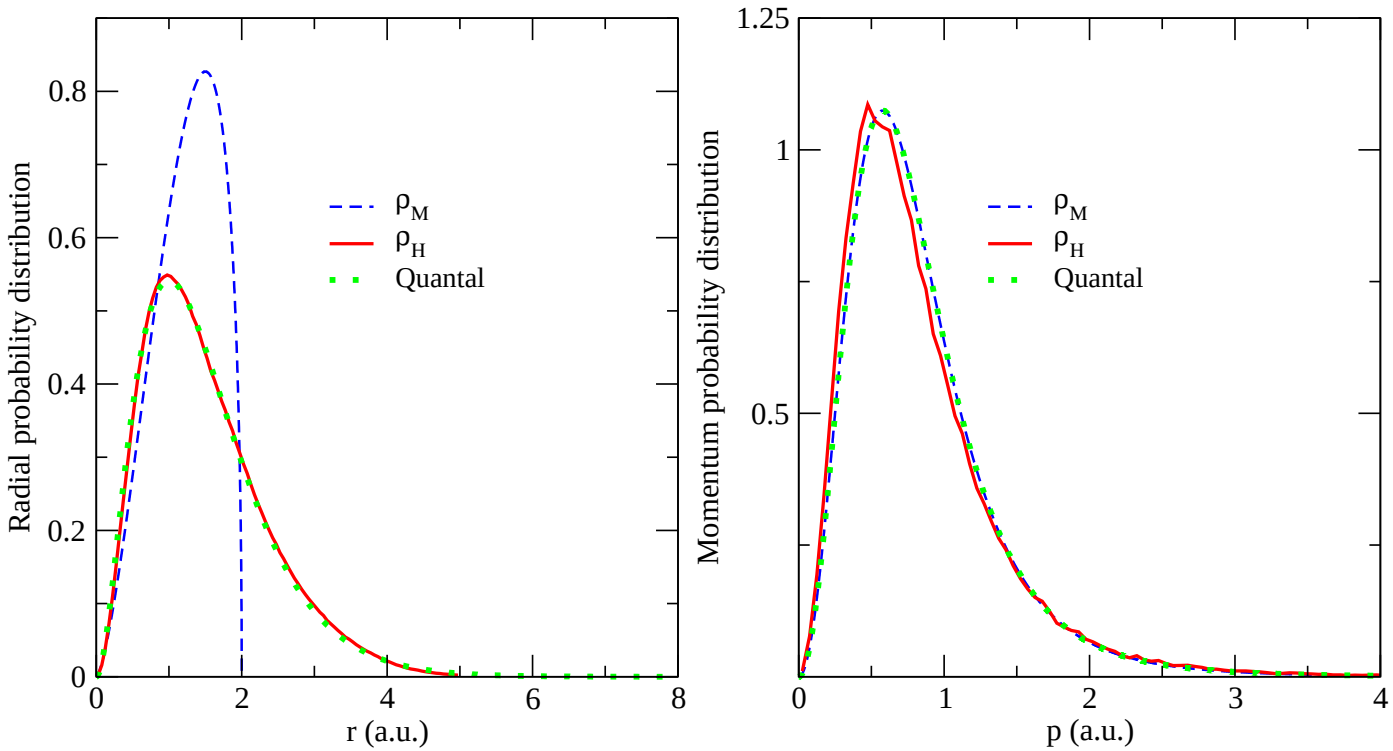
Hydrogenic[10]:

$$\rho_H(\mathbf{r},\mathbf{p},Z,\epsilon) = \sum_{k=1}^{\mathcal{M}} a_k\cdot\rho_M(\mathbf{r},\mathbf{p},Z,\epsilon_k) = \sum_{k=1}^{\mathcal{M}} \frac{(-2\epsilon_k^{5/2})}{8\pi^3}\,a_k\,\delta\left(\frac{\mathbf{p}^2}{2}-\frac{1}{\mathbf{r}}-\epsilon_k\right)$$

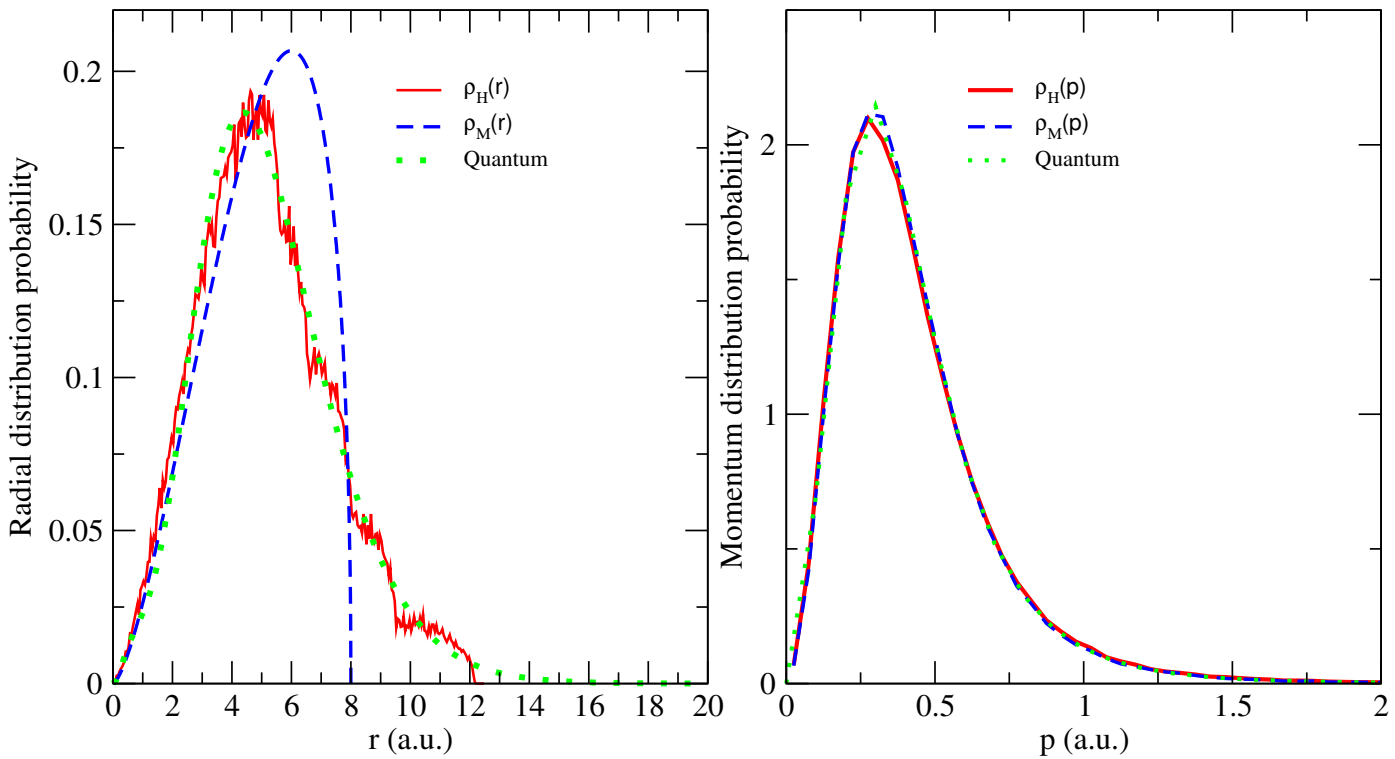
A linear combination of $\mathcal{M}$ microcanonicals with an averaged energy $<\epsilon>\simeq -\frac{1}{2}$.

[10] D J Hardie and R E Olson, J. Phys. B **16** 1983 (1983)

Phase space initial distributions for H(1s)



Phase space initial distributions for H(n =2)



Some CTMC results for A^{q+} + H collisions

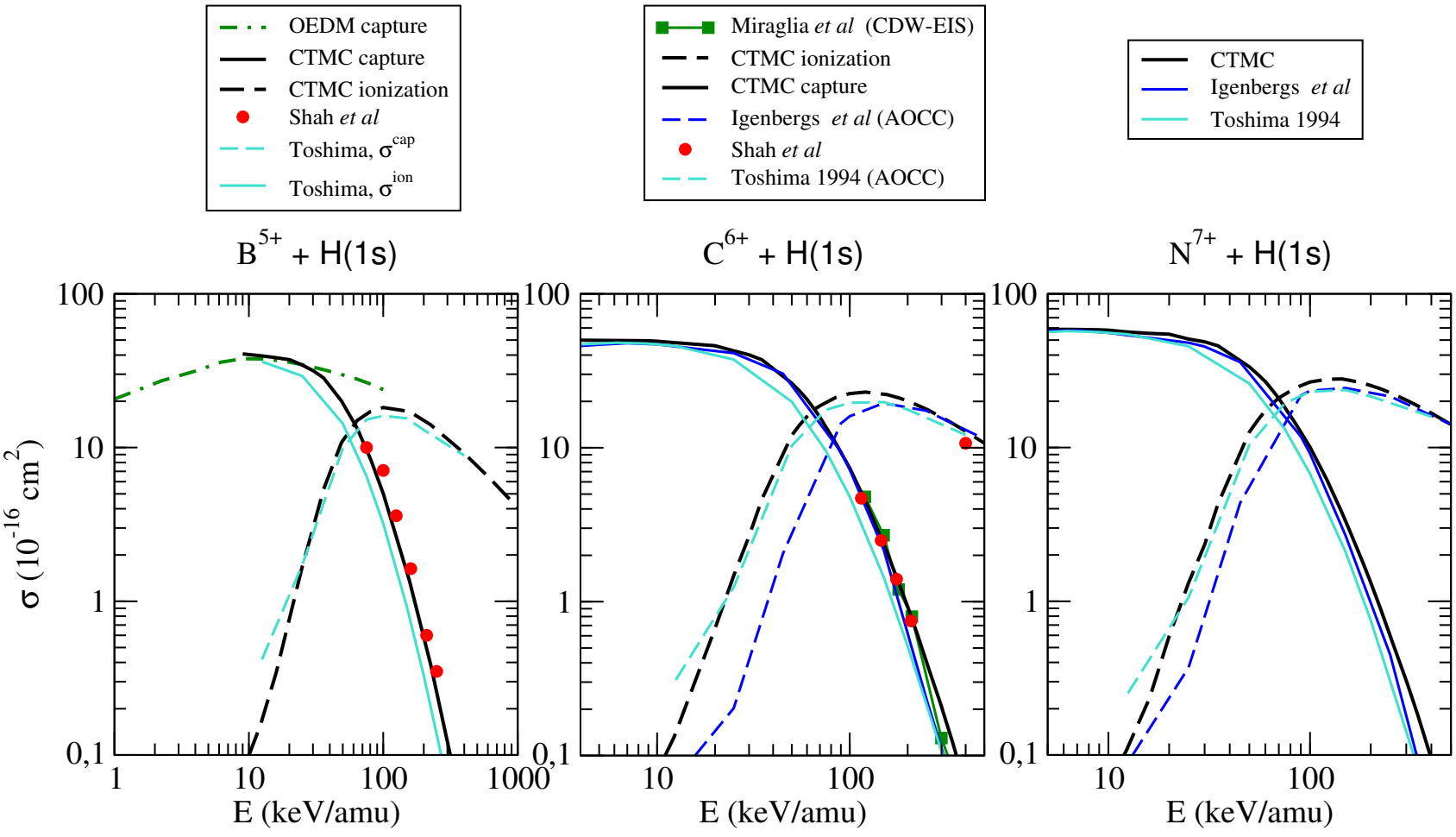
- B^{5+}, C^{6+}, N^{7+} + H($1s$) $\rightsquigarrow$ with neutral hydrogen.
- C^{6+}, N^{7+} + H($n = 2$) $\rightsquigarrow$ with excited hydrogen.

  Total and n-partial cross sections.

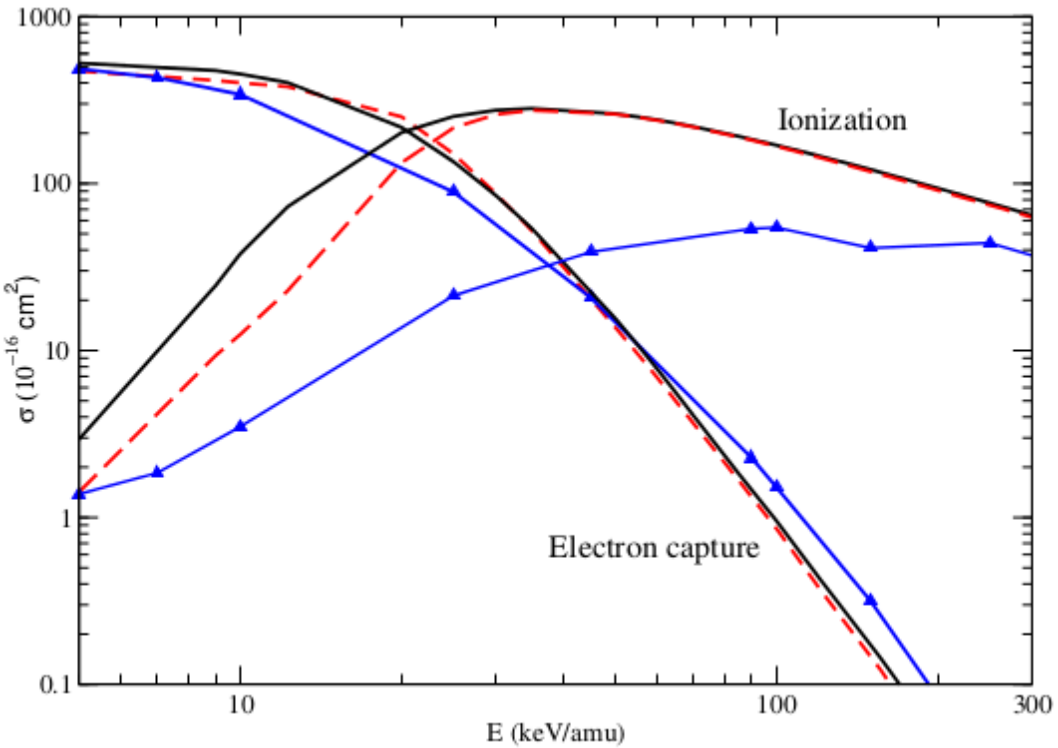
- $\rightsquigarrow$ Highly charged ions: $Ar^{16+,17+,18+}$, Kr^{36+}, W^{60+} + H($1s$)

  Total, n-partial and n, l-partial cross sections. Scaling.

Total cross sections for B^{5+}, C^{6+}, N^{7+} + H(n=1)



Total cross sections C^{6+} + H(n=2)

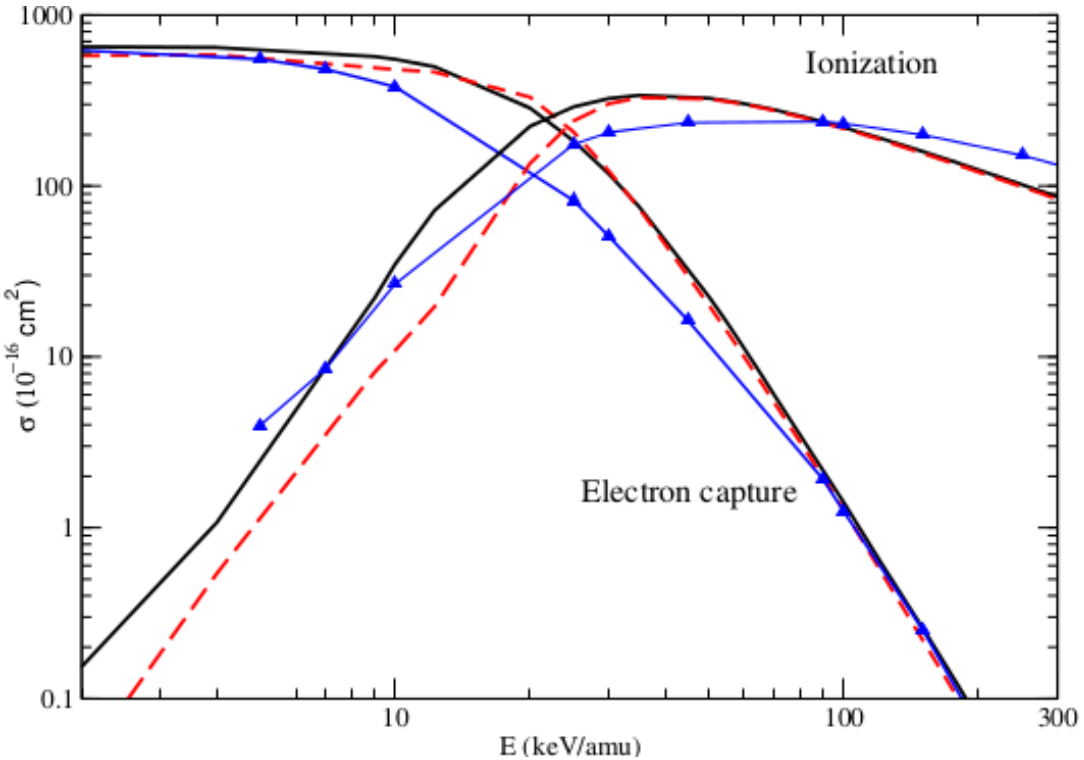


(——) **hydrogenic-CTMC**, (- - -) **microcanonical-CTMC** [11] and (—▲—) AOCC results from Igenbergs[12]

[11] A Jorge *et al.* EPJD **68** 227 (2014)

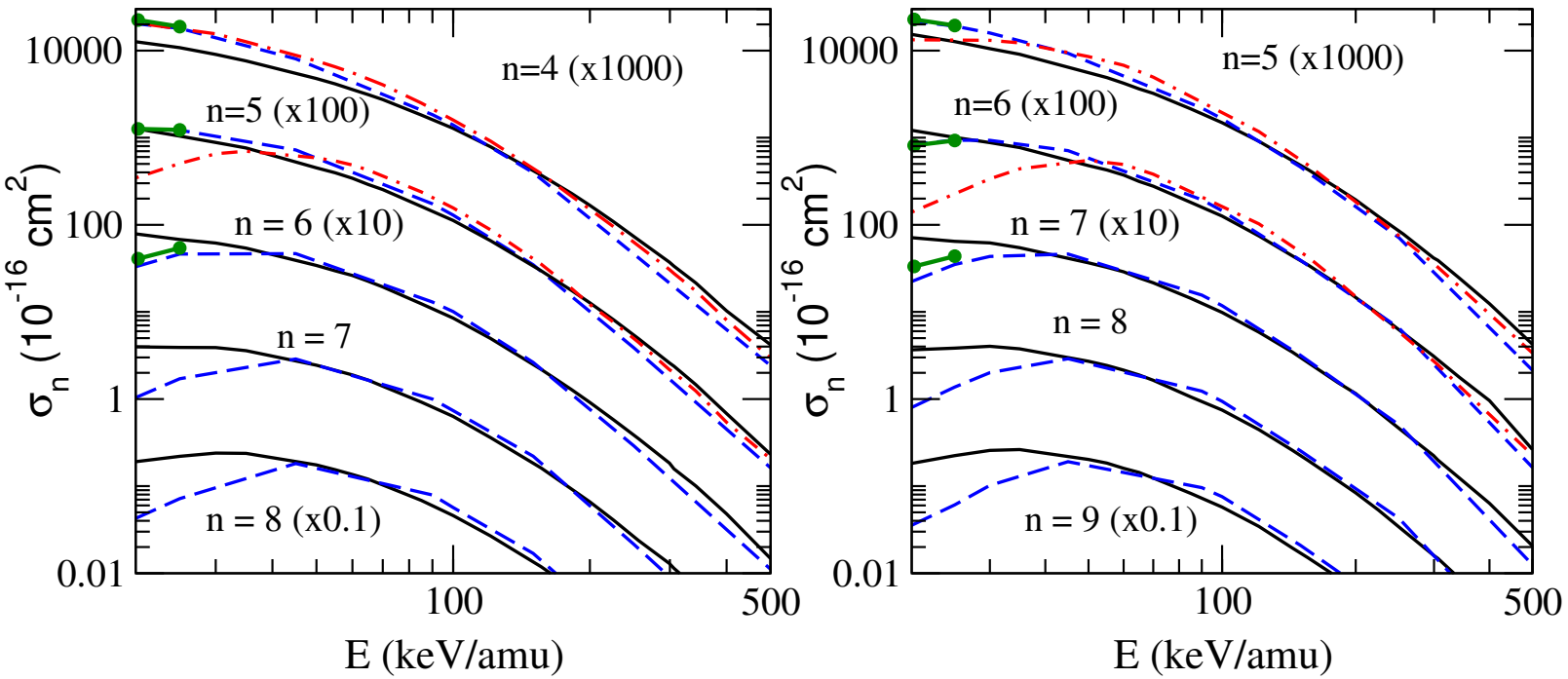
[12] K Igenbergs *et al.* J. Phys. B **45** 065203 (2012)

Total cross sections N^{7+} + H(n=2)



(——) **hydrogenic-CTMC**, (- - -) **microcanonical-CTMC** and (—▲—) AOCC results from Igenbergs.

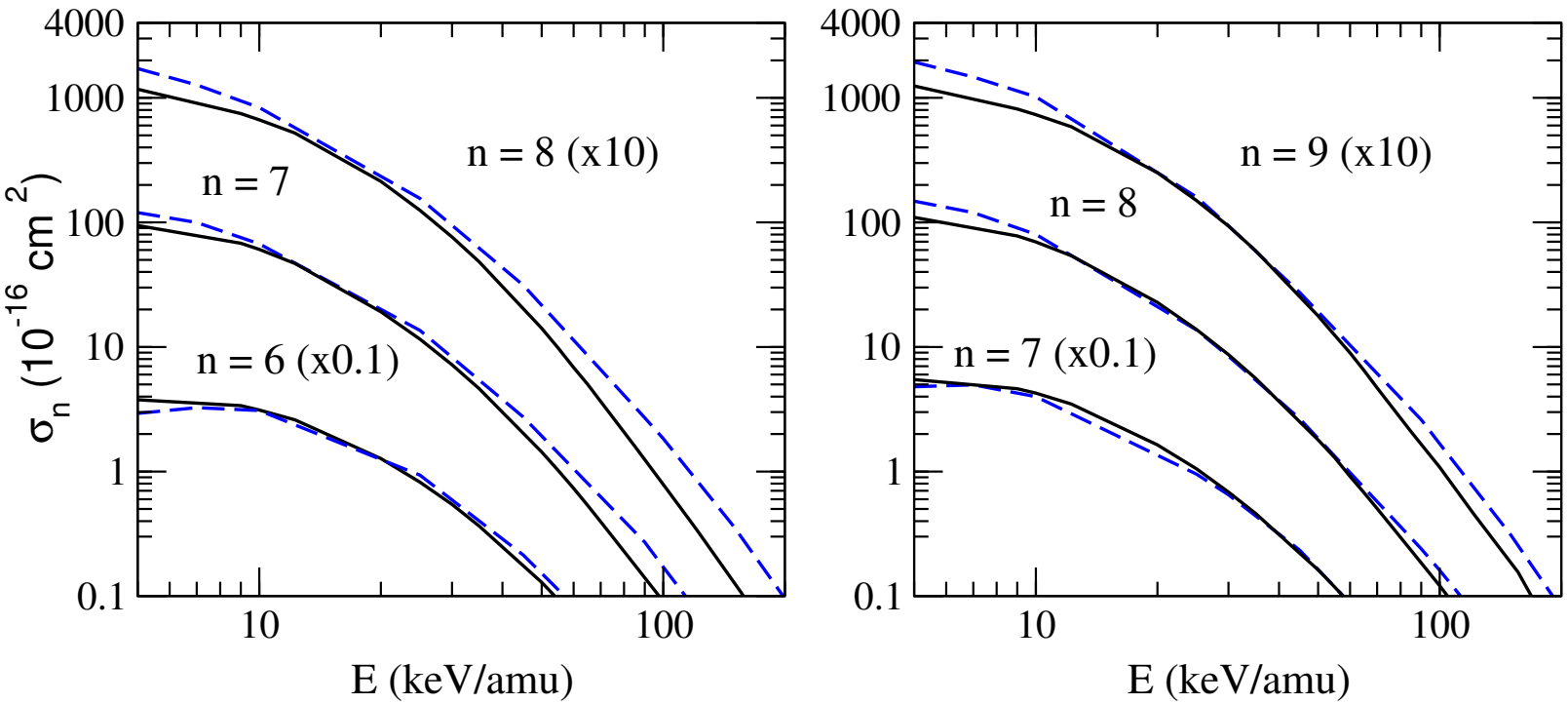
n-partial cross sections for C^{6+} and N^{7+} + H($n = 1$)



(——) **hydrogenic-CTMC**, (- - -) AOCC results from Igenbergs and (- • -) MOOC results[13].

[13] Harel *et al.*, At. Data. Nucl. Data Tables, **68** 279 (1998)

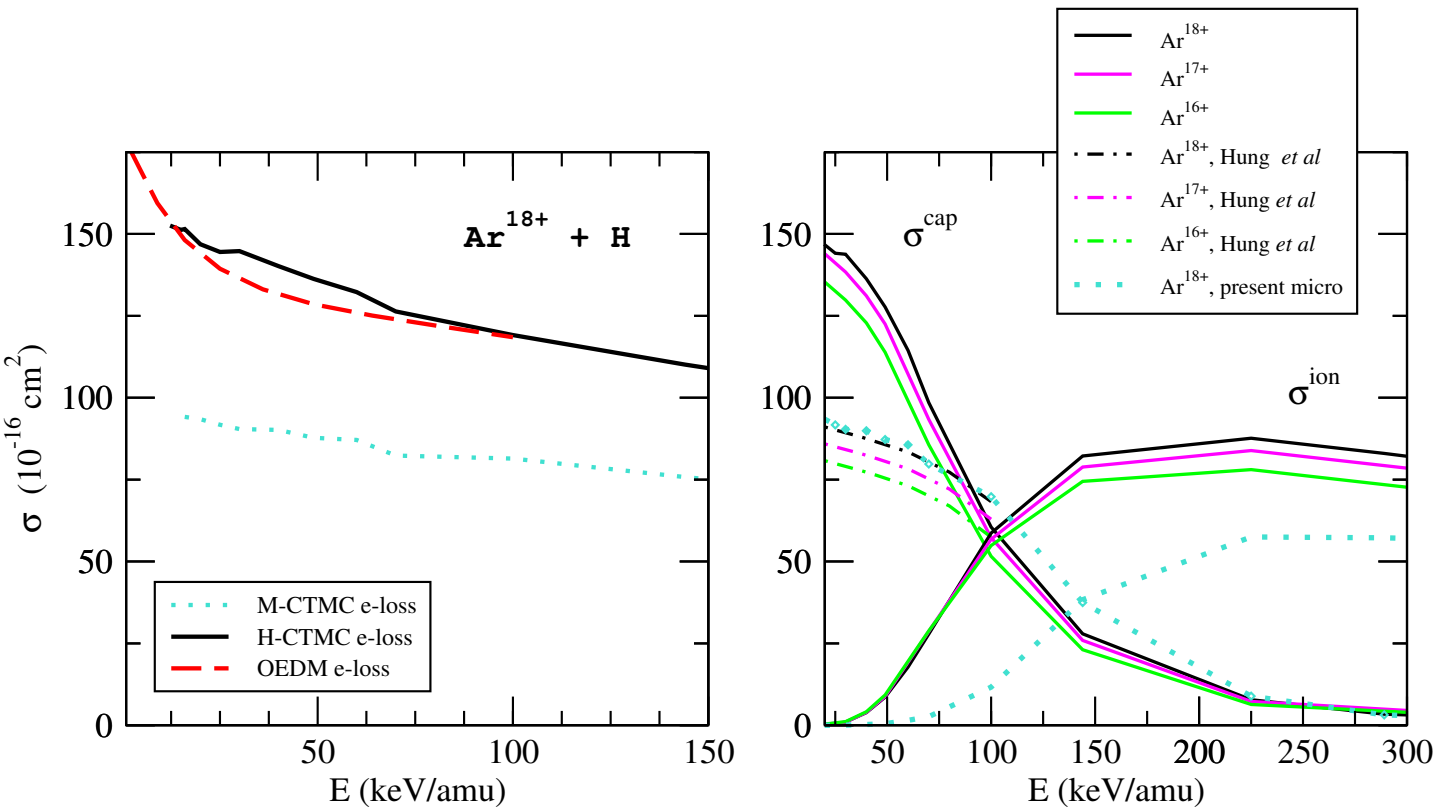
n-partial cross sections for C^{6+} and N^{7+} + H($n = 2$)



(——) **hydrogenic-CTMC** compared to (- - -) AOCC results from Igenbergs.

Ar^{q+} ions + H collisions: Total cross sections

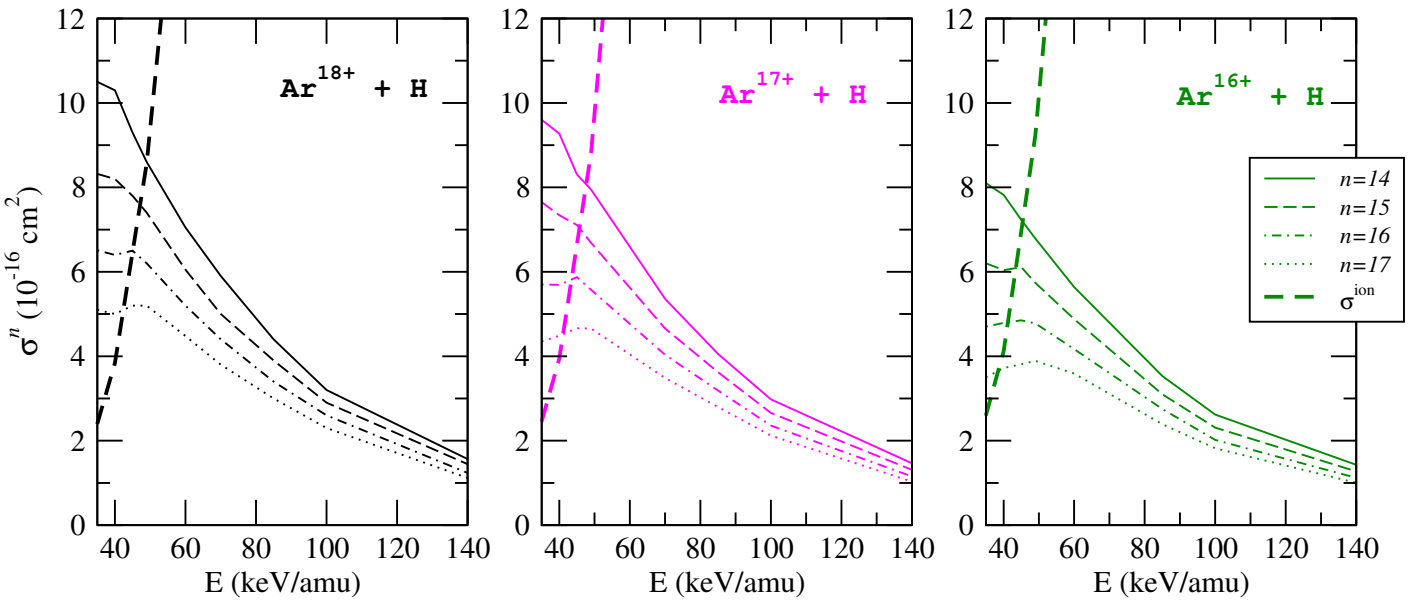
Hydrogenic *versus* **microcanonical** initial distribution: its importance in the TCS



In Errea *et al.* J. Phys. B **39** L91 (2006)

Ar^{q+} + H collisions: n-partial cross sections, σ^n

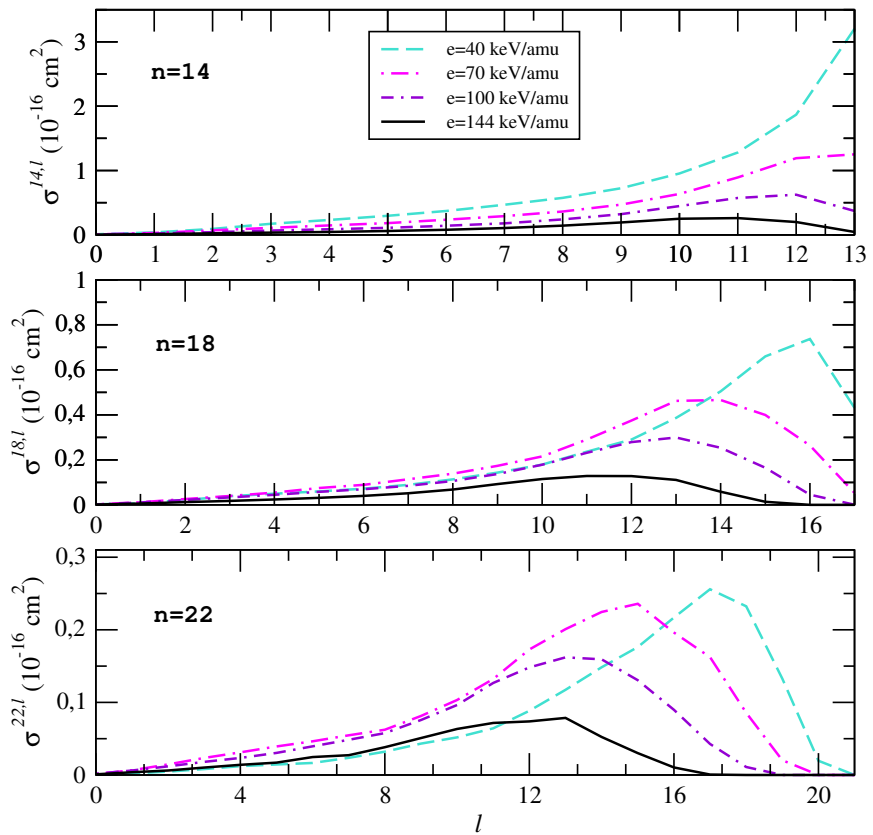
Focus on capture to very high-lying states of the projectile $n = 14 - 17$, triggering the visible radiative decay analysed in 2012 ASDEX diagnostic experiments.



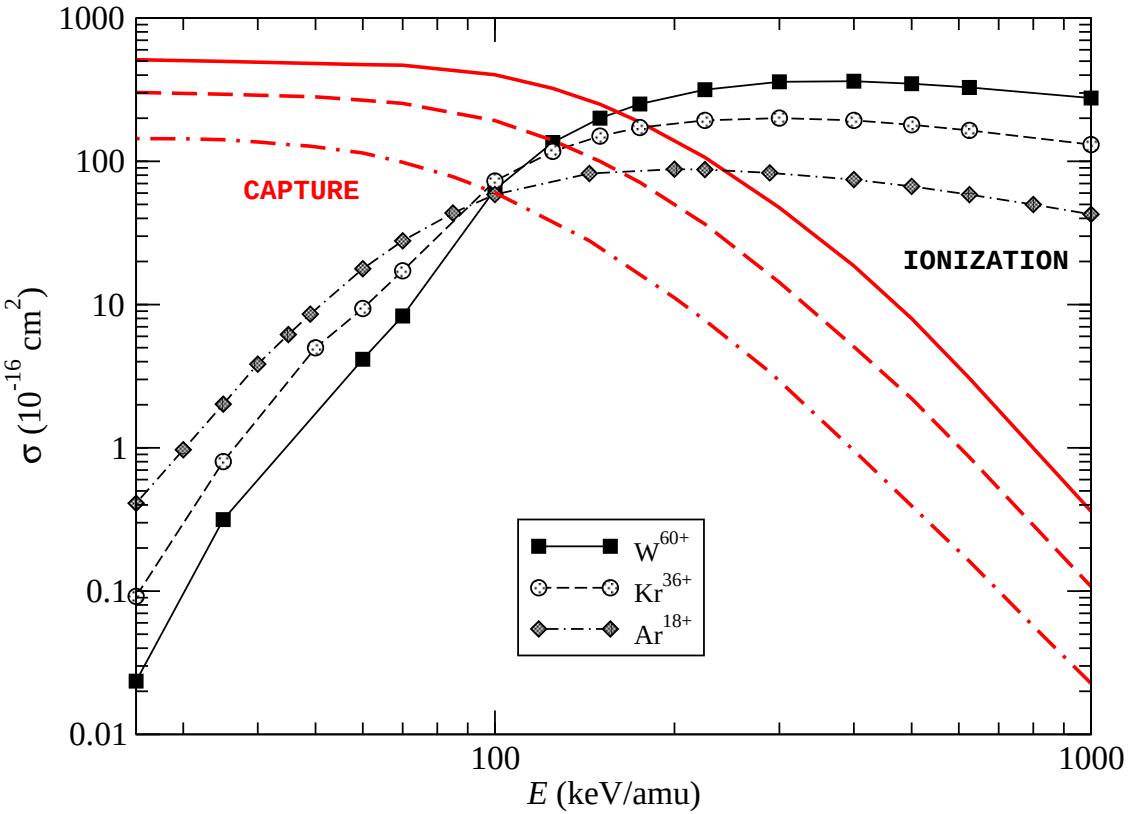
$\sigma^{n,l}$: ℓ distributions in Ar^{18+} + H collisions

E ranging from 40 to 144 keV/amu and 3 typical *n*-shells.

Capture to high-*n* shells $\Rightarrow$ captured orbits of large ℓ values. The shifts of $\sigma^{n,l}_{max}$ are larger as *n* and E increase.

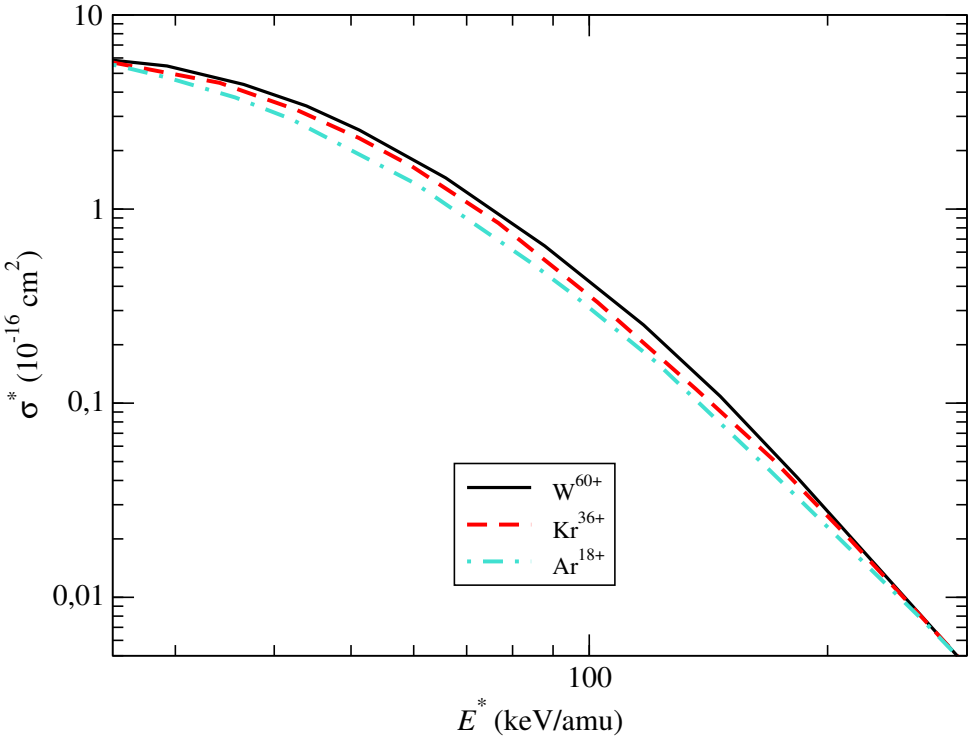


Ar^{18+}, Kr^{36+}, W^{60+} + H collisions: Total cross sections



In Illescas *et al.*, Phys. Scr. **T156** 014033 (2013)

Scaling for total electron capture cross sections



$$\sigma^* = \sigma\, Z^{-\alpha}$$

$$E^* = E\, Z^{-\beta},$$

with $\alpha = 1.05$ and $\beta = 0.30$

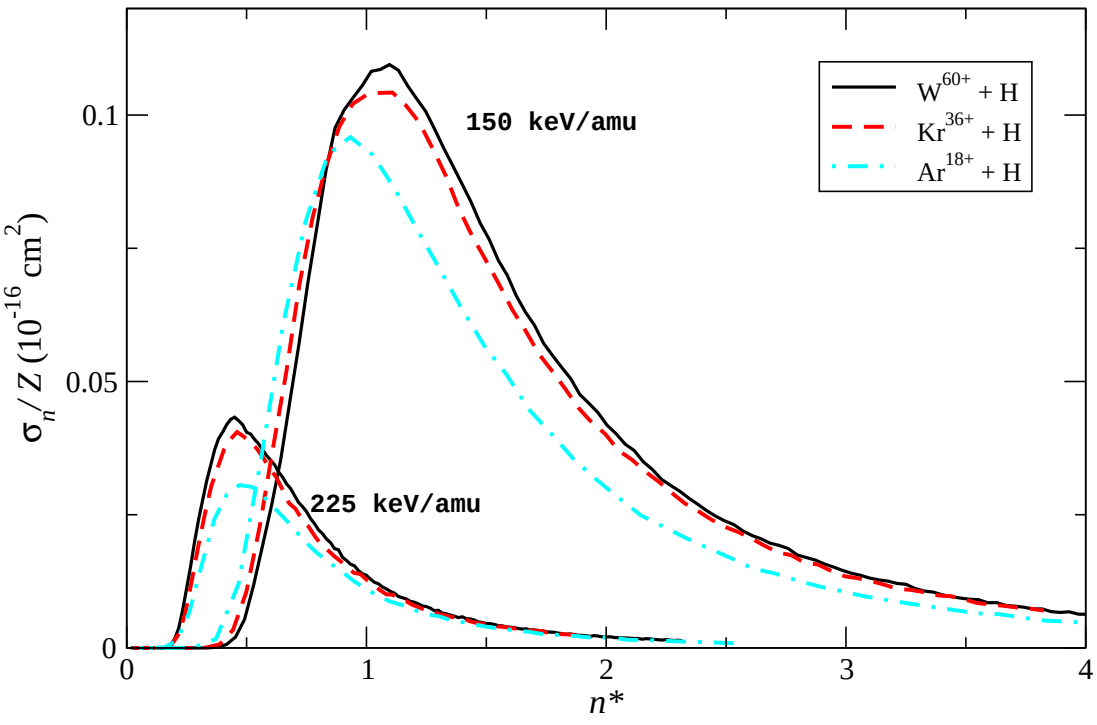
(Foster, PhD Thesis, 2008)

$\hookrightarrow$ Good agreement of our results with the empirical scaling law which allow to predict σ^{EC} for collisions of high Z without performing detailed calculations.

n-partial cross sections

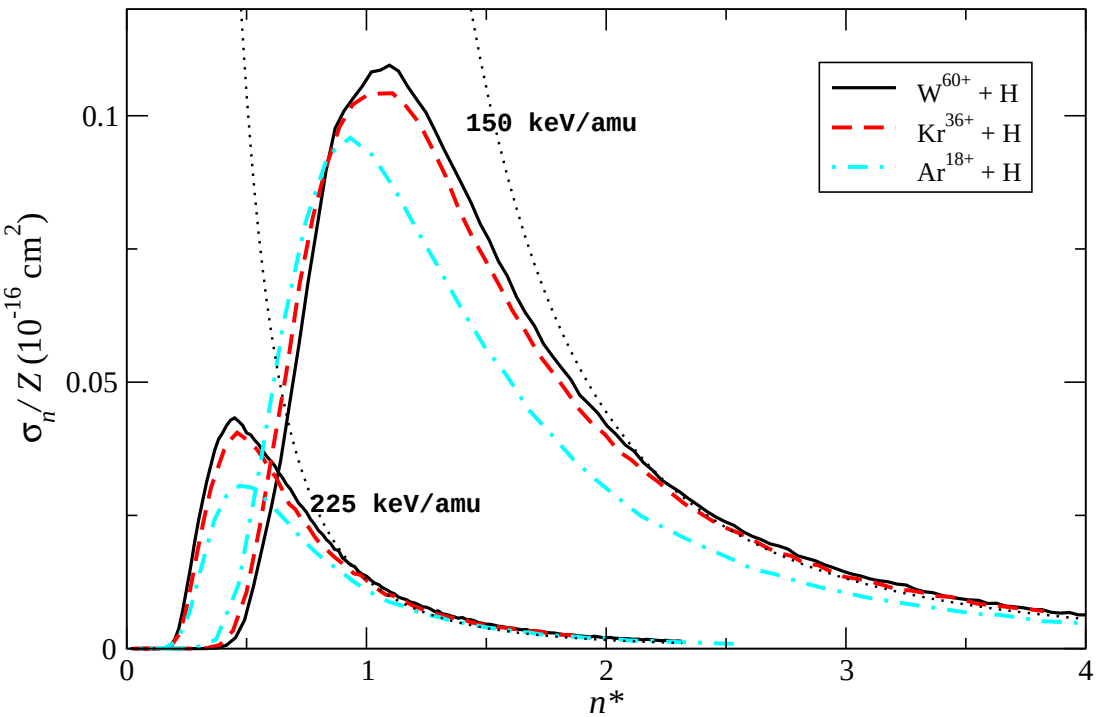
σ_n/Z as functions of scaled $n^* = n\,Z^{-\gamma(E^*)}$

γ= 0.8 for E = 150 keV/amu; γ= 1.0 for E = 225 keV/amu



n-partial cross sections exhibit a maxima at $n_{max} \approx Z/2$, as predicted by COBM.

n-partial cross sections



The Oppenheimer n^{-3} rule holds for $E > 100$ keV/amu for the three systems.

Four-body & Switching CTMC treatments

Two-active electrons and two-nuclei:

We have studied the most simple $2e^-$ systems:

- $H(1s) + H(1s) \longrightarrow$ Electrons initially in different centers
- $H^+ + H^-(1s, 1s) \longrightarrow$ Electrons initially in the same center

$\hookrightarrow$ Our idea: To apply these methods to explicitly treat e_1 and e_2

ion-He$(1s, 1s)$ collisions.

Two-active electron processes

$$H(1s) + H(1s) \rightarrow \begin{cases} H + H & \text{elastic/excitation} \\ H + H^+ + e & \text{target ionization} \\ H^+ + H + e & \text{projectile ionization} \\ H^+ + H^+ + 2e & \text{double ionization} \\ H^+ + H^- & \text{target electron capture} \\ H^- + H^+ & \text{projectile electron capture} \end{cases}$$

$$H^+ + H^-(1s, 1s) \rightarrow \begin{cases} H^+ + H^- & \text{elastic/excitation} \\ H + H & \text{mutual neutralization} \\ H + H^+ + e & \text{transfer ionization} \\ H^+ + H + e & \text{detachment} \\ H^+ + H^+ + 2e & \text{double ionization} \\ H^- + H^+ & \text{charge exchange} \end{cases}$$

Four-body CTMC method

- Classical initial distribution function:

  $\rightarrow$ The electronic motion of each electron is described by a **microcanonical** initial distribution, $\rho_M(\mathbf{r}, \mathbf{p}, Z, E)$, solution of the Liouville's equation.

  $\rightarrow$ The initial two electron distribution consists of the **product** of two microcanonical sets of $N = N_H \cdot N_H$

- We solve the Hamilton equations for each pair of electrons $\{e_1, e_2\}$:

$$\dot{\mathbf{R}}_j = \frac{\partial H_{2e}}{\partial \mathbf{P}_j}; \quad \dot{\mathbf{P}}_j = -\frac{\partial H_{2e}}{\partial \mathbf{R}_j}$$

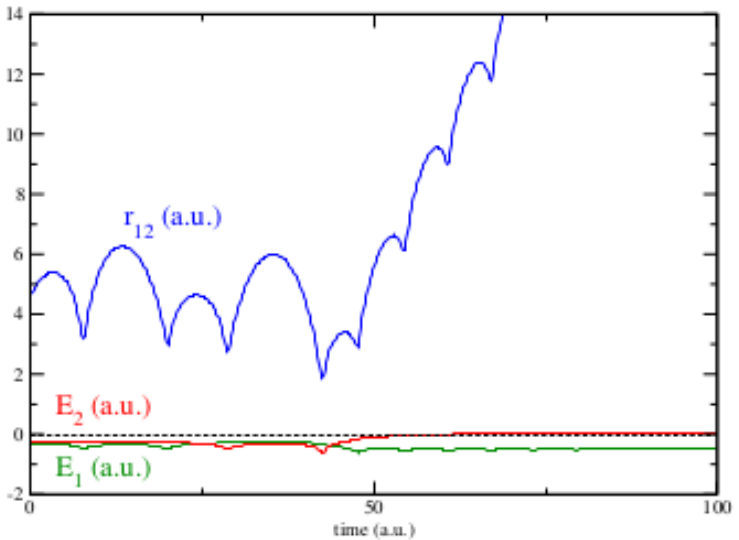
  using Jacobi coordinates $\{\mathbf{R}_1, \mathbf{R}_2, \mathbf{R}_3\}$ and $\{\mathbf{P}_1, \mathbf{P}_2, \mathbf{P}_3\}$.

Classical autoionization problem

An isolated classical H^- anion is described by the hamiltonian:

$$H = \frac{p_1^2}{2} + \frac{p_2^2}{2} + \frac{p_3^2}{2M} - \frac{1}{r_{e_1}} - \frac{1}{r_{e_2}} + \frac{1}{r_{12}}$$

The system is not classically stable due to the interelectronic repulsion[14]:



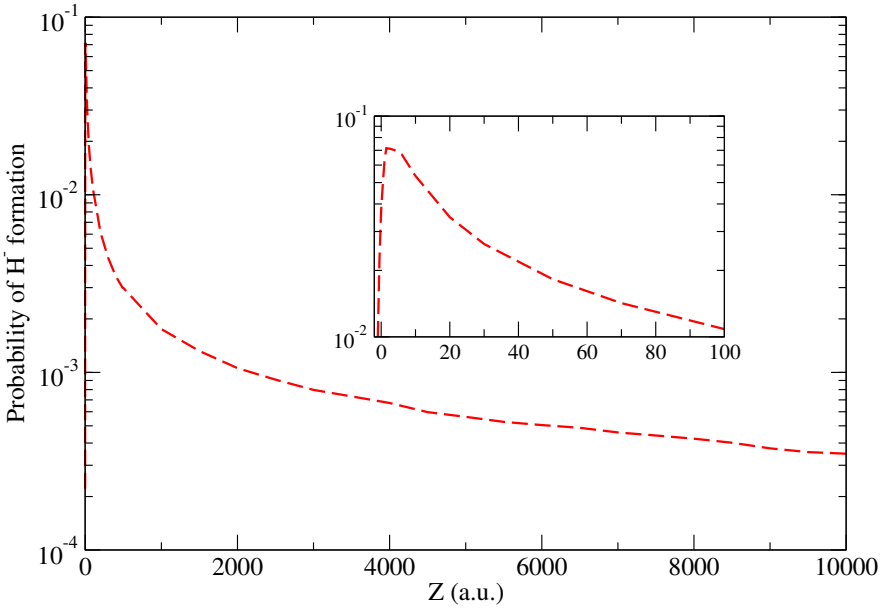
$$E_1 = \frac{p_{e_1}^2}{2} - \frac{1}{r_{e_1}}$$

$$E_2 = \frac{p_{e_2}^2}{2} - \frac{1}{r_{e_2}}$$

[14] See F. Guzman *et al.* Phys Rev. A **80** (2009)

Classical autoionization problem

H(1s) + H (1s) collisions: H^- formation



A Four-body CTMC calculation yields a H^- formation probability which depends on the final time of integration.

Processes such $\begin{cases} H^+ + H^- \\ H^- + H^+ \end{cases}$ are <u>understimated</u> while the others are overestimated.

How can we describe a H^- anion?

We propose **two independent systems** to describe the H^-, **one for each electron**[15]:

$$H^-(e_1, e_2) \begin{cases} e_2 & \text{interacting with } \{H^+ + e_1\} \equiv \alpha \longrightarrow V_{\text{mod}}^{H^+ - e_1} \\ e_1 & \text{interacting with } \{H^+ + e_2\} \equiv \beta \longrightarrow V_{\text{mod}}^{H^+ - e_2} \end{cases}$$

$$V_{\text{mod}}^{H^+ - e} = -\frac{(1+\alpha r)\exp(-2\alpha r)}{r}$$

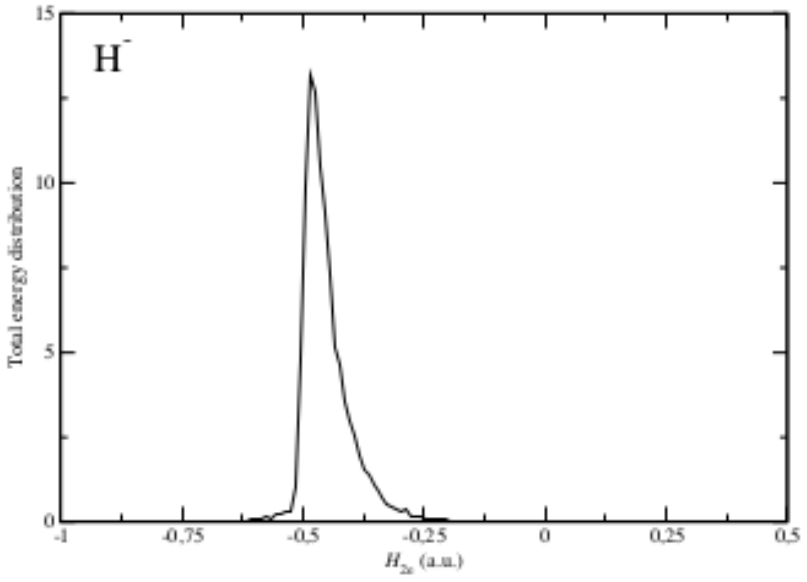
$\hookrightarrow$ is a model potential which represents the nucleus and one frozen electron.

The parameter α has been fitted to $\alpha = 0.65$ (a.u.)$^{-1}$([16])

[15] A Jorge *et al.*, Phys. Rev. A **94** 022710 (2016)

[16] J D Talman, Comput. Phys. Commun. **54** 85 (1989)

A classical stable description of the H^- anion



The construction of H^- is performed by using two ρ_M:

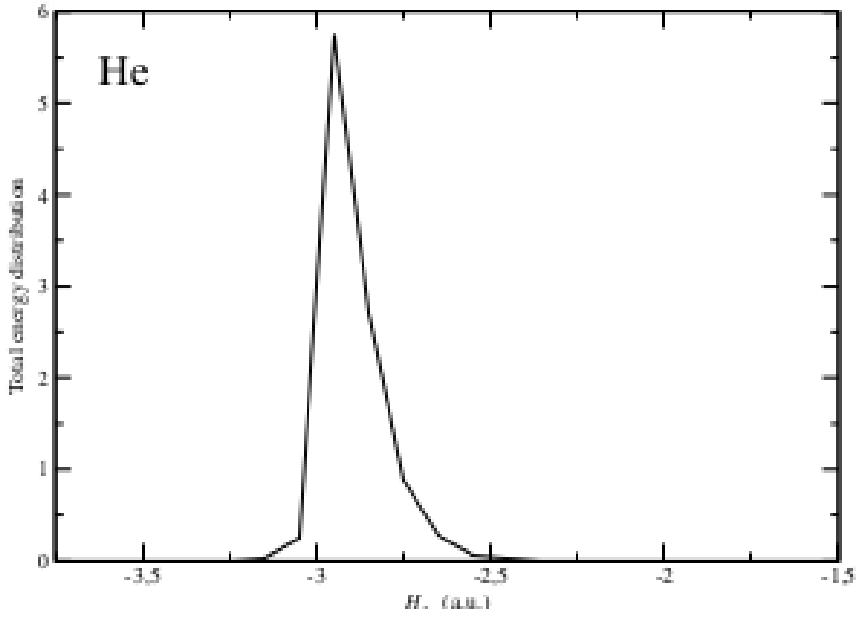
- U_{ion}= -0.027 a.u.
- $\ell = 0$
- $V_{mod}^{H^+-e}$

Under no external perturbation, we let the electron evolve in time and we calculate the total energy from the full hamiltonian: $H = \frac{p_1^2}{2} + \frac{p_2^2}{2} + \frac{p_3^2}{2M} - \frac{1}{r_{e_1}} - \frac{1}{r_{e_2}} + \frac{1}{r_{12}}$

We obtain $\langle H \rangle^{H^-} = 0.450$ a.u. close to $\epsilon_{exp}^{H^-} = 0.503$ a.u.

A classical stable description of the He atom

Similarly, we can describe the He atom with two active electrons:



We obtain $\langle H \rangle^{\mathrm{He}} =$ -2.89 a.u. very close to $\epsilon_{\mathrm{exp}}^{\mathrm{He}} =$ -2.90 a.u.

A classical stable description multielectronic atoms

This same approach has been applied to other atoms: Li, Be, B and C,

where each electron is represented by a different initial distribution

[different $V_{\mathrm{mod}}^{\mathrm{H^+-e}}$, ℓ and U_{ion} values]

$\hookrightarrow$ Good description with this approach

	Obtained value	HF value	CI value[15]
H^-	-0.450	-0.487	-0.526
He	-2.890	-2.861	-2.909
Li	-7.238	-7.405	-7.490
Be	-14.373	-14.751	-14.618
B	-24.038	-24.532	-24.596
C	-36.622	-37.690	-37.777

HF and CI values from NIST, `https://www.nist.gov`

The Switching CTMC Approach

Application to collisions: a combined 4-body and 2x3-body CTMC

We propose to perform the time evolution of:

- The 4-body system if the electrons are not bound to the same nucleus:

$$V_{4b} = -\frac{Z_T}{r_{Te_1}} - \frac{Z_T}{r_{Te_2}} - \frac{Z_P}{r_{Pe_1}} - \frac{Z_P}{r_{Pe_2}} + \frac{1}{r_{12}}$$

- Two 3-body systems if the electrons are bound to the same nucleus:

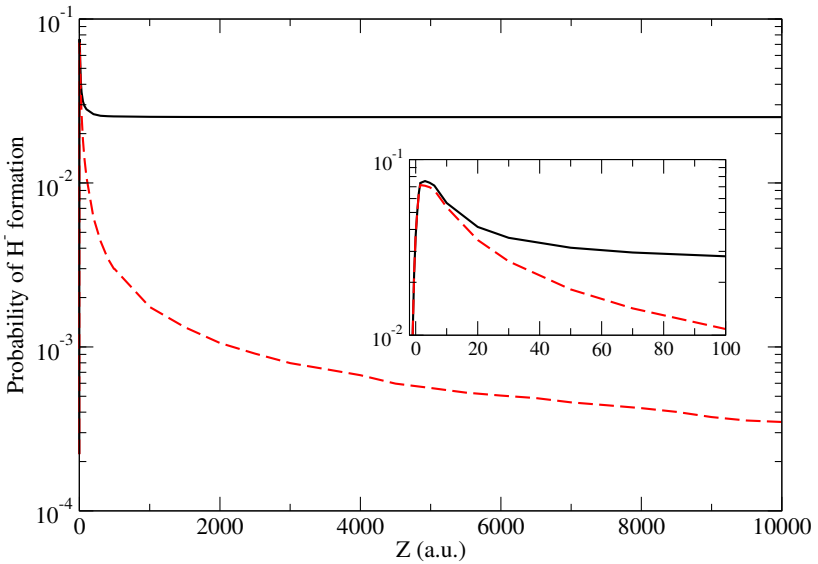
$$\text{Target} \begin{cases} V_{3b}^{e_1} = -\frac{Z_P}{r_{Pe_1}} - \frac{(Z_T-1)}{r_{Te_1}} - \frac{(1+\alpha r_{Te_1})}{r_{Te_1}} \exp(-2\alpha r_{Te_1}) \\ V_{3b}^{e_2} = -\frac{Z_P}{r_{Pe_2}} - \frac{(Z_T-1)}{r_{Te_2}} - \frac{(1+\alpha r_{Te_2})}{r_{Te_2}} \exp(-2\alpha r_{Te_2}) \end{cases}$$

or

$$\text{Projectile} \begin{cases} V_{3b}^{e_1} = -\frac{Z_T}{r_{Te_1}} - \frac{(Z_P-1)}{r_{Pe_1}} - \frac{(1+\alpha r_{Pe_1})}{r_{Pe_1}} \exp(-2\alpha r_{Pe_1}) \\ V_{3b}^{e_2} = -\frac{Z_T}{r_{Te_2}} - \frac{(Z_P-1)}{r_{Pe_2}} - \frac{(1+\alpha r_{Pe_2})}{r_{Pe_2}} \exp(-2\alpha r_{Pe_2}) \end{cases}$$

The Switching CTMC Approach

H(1s) + H(1s) collisions: correct H^- formation



(——) Switching calculation

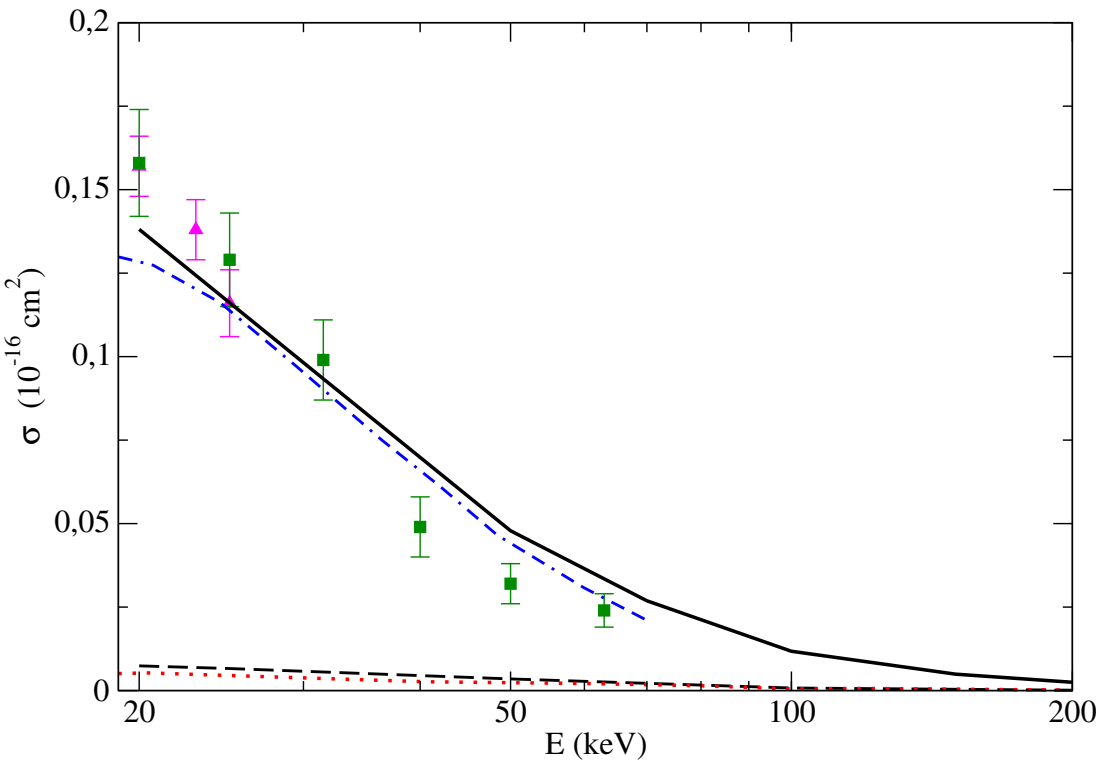
(- - -) Four-body CTMC

⇓

converged probability after

$t \sim 200$ a.u.

Results for H(1s) + H(1s) collisions: Projectile H^- formation



(——) **Switching**, (- - -) **4-body**, (- - -) 4-body CTMC[17], (- - · - - -) AOCC[18]. Measurements: (■)[19] and (▲)[20].

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[17] K Dimitriu *et al.*, J. Phys. IV (France) **10** 299 (2000)

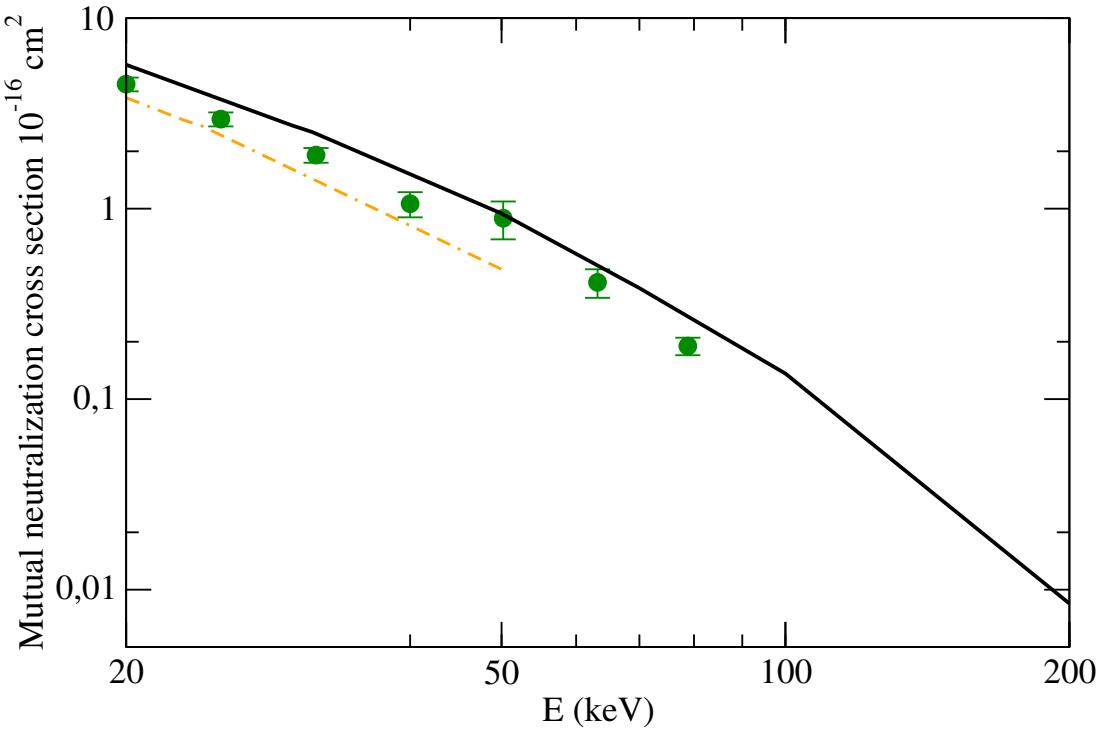
[18] J Wang *et al.*, J. Phys. B **33** 241 (2000)

[19] G W McClure, Phys. Rev. **166** 22 (1968)

[20] J Hill *et al.*, J. Phys. B **12** 3341 (1979)

Results for $H^+ + H^-$ collisions

$$H^+ + H^-(1s^2) \rightarrow H(nlm) + H(n'l'm')$$



(——) **Switching CTMC** and (- - · - -) Coupled-channel calculations[21]. Measurements. (●) from Schön *et al.*[22].

[21] R Shingal and B H Bransden, J. Phys. B **23** 1203 (1990)

[22] W Schön *et al.*, J. Phys. B **20** L759 (1987)

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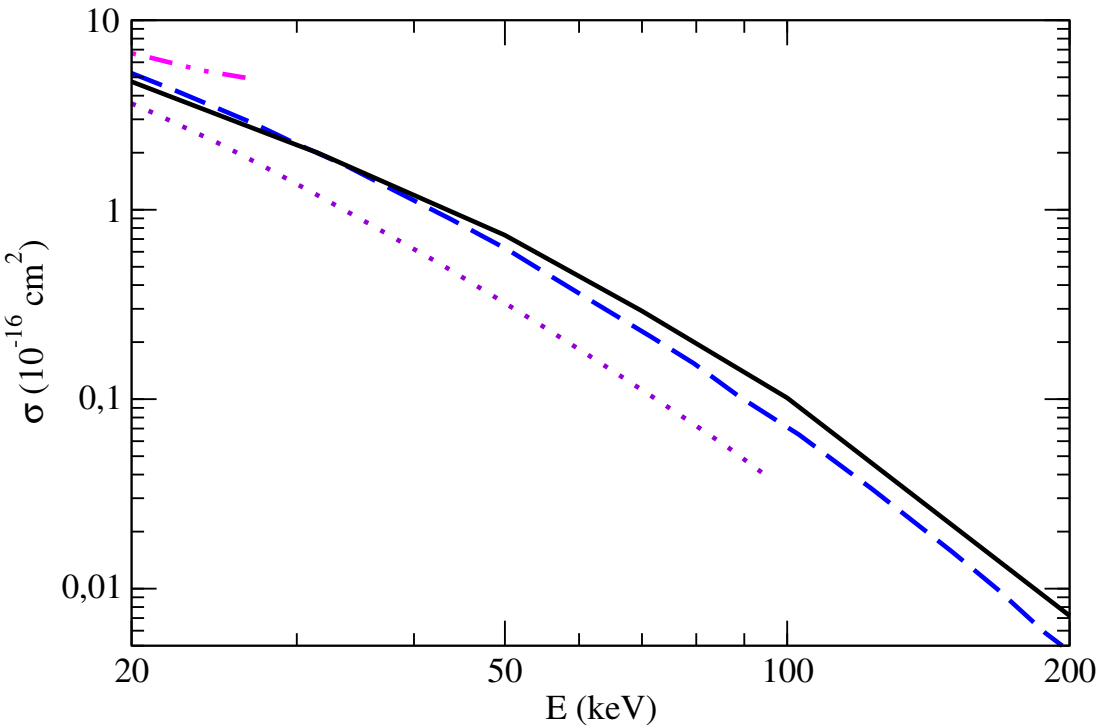

(——) **Switching CTMC**, (- - - - -) AOCC[23], (· · ·)[24] and (- - - - -) CB1-4B calculations from Mancev *et al.*[25]

[23] J Wang *et al.*, J. Phys. B **33** 241 (2000)

[24] L Ling and J Wang, Chin. Phys. Lett. **24** 3115 (2007)

[25] I Mancev *et al.*, Europhys. Lett. **103** 23001 (2013)

Final remarks

- CTMC methods for treating one- and two-active electron collisions at impact energies of interest in fusion research.
- Obtaining of accurate total and $n, \ell-$partial CROSS SECTIONS in low- and highly charged ions in collision with H.
- New Switching CTMC Approach which improves the computed cross sections for electron capture processes when two electron are involved.
  1. Classical stable description of multielectronic atoms through: independent potentials
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Coworkers

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