Classical and semiclassical calculations for ion-atom collision systems of relevance to neutral beams in fusion plasmas.

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Motivation

Purpose I.: Calculation of total and *n*, *l*-partial cross sections for excitation, electron capture and total ionization of collisions of Be^{4+} ions with neutral hydrogen atoms. Three collision energies were selected: 20, 100, and 500 keV/u.

Purpose II.: Code Comparison Workshop with regards to the accuracy of the cross sections.

The group at UAM has been working in Be^{4+} collisions with:

- H(2s), H(1s) employing the CTMC[1] and GTDSE[2] methods.
- H(2p) employing the CTMC method.

[1] Classical Trajectory Monte Carlo

[2] GridTDSE, numerical solution of the Time Dependent Schrödinger Equation

Reactions and processes considered:

1. Electron capture: $Be^{4+} + H \longrightarrow Be^{3+}(nl) + H^{+}$
2. Excitation of the target: $Be^{4+} + H \longrightarrow Be^{4+} + H(nl)$
3. Ionization: $Be^{4+} + H \longrightarrow Be^{4+} + H^{+} + e^{-}$

H (1s)			
processes	1	2	3
CTMC	✓	✓	✓
GTDSE	✓	✓	

H (2s)			
processes	1	2	3
CTMC	✓	✓	✓
GTDSE	✓	✓	

H (2p)			
processes	1	2	3
CTMC	✓	✓	✓
GTDSE			

Both initial dristributions, **microcanonical** and **hydrogenic**, have been considered in the CTMC calculations.

Impact parameter approximation

At the energies considered (E $\geq$ 1 keV/u), IPA is valid.

- The projectile follows rectilinear trajectories $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}t$
- The electronic hamiltonian is: $\mathrm{H}_{\mathrm{el}} = -\frac{1}{2}\nabla_r^2 + V_{\mathrm{H}} + V_{\mathrm{Be}}$

CTMC: Classical Trajectory Monte Carlo method

- The electronic motion is described by a classical distribution function $\rho(\boldsymbol{r}, \boldsymbol{p})$:
  - **Microcanonical** (standard): exact energy of the quantum one.
  - **Hydrogenic**: linear combination of $\mathcal{N}$ microcanonicals with average energy close to the quantum.
- The Hamilton equations are integrated for each electron trajectory $[N \approx 2 \cdot 10^6]$.
- The energy criterion is applied at t_{fin} to disclose each process: i, c, e
- Becker & McKellar binning to partion the classical phase space into exclusive subespaces $\{n, l\}$
- Electron probabilities: are obtained from the asymptotic values of the classical distribution function: $P^{i,c,e}(v, b) = \int d\boldsymbol{r} \int d\boldsymbol{p}\, \rho^{i,c,e}(\boldsymbol{r}, \boldsymbol{p}, v, b, t_{fin})$
- Total cross sections: $\sigma^{i,c,e}(v) = 2\pi \int_0^\infty db\, b\, P^{i,c,e}(v, b)$

GTDSE: Grid time-dependent Schrödinger equation method

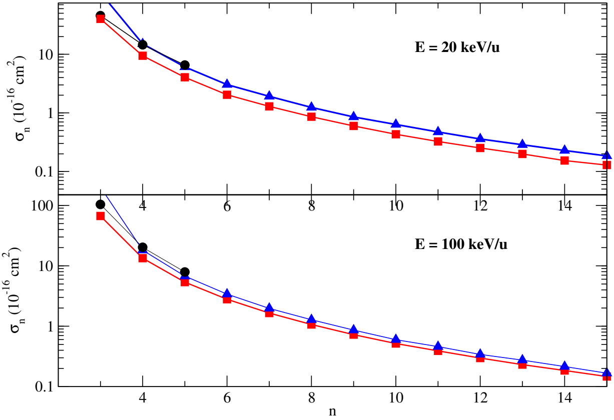
- Numerical solution of the time-dependent Schrödinger equation: Ψ is evaluated at the points of a 3D cartesian lattice.
- The spatial integration is obtained by applying finite-difference method and time integration by iteratively applying the second-order difference method (SOD).
- Grid densities: $\Delta_q = q_{i+1} - q_i$ for testing precision: Δ_q = 0.2 -0.05 (a.u.)
- The extension of the grid is a broad box: $-L_{max} \leq x, z \leq L_{max}$ and $0 \leq y \leq L_{max}$ [L_{max} = 40 or 80 a_0 depending of the target].
- Electron probabilities: $P_{nlm} = P_{nlm}^{\mathrm{H,Be}} = \lim_{t\to\infty} \left| < \Phi_{nlm}^{\mathrm{H,Be}} | \Psi > \right|^2$
- The integral cross sections for excitation and capture: $\sigma_{nlm} = 2\pi \int_0^\infty b P_{nlm} \mathrm{d}b$,

Be^{4+} + H(2s) collisions

Recent publications:

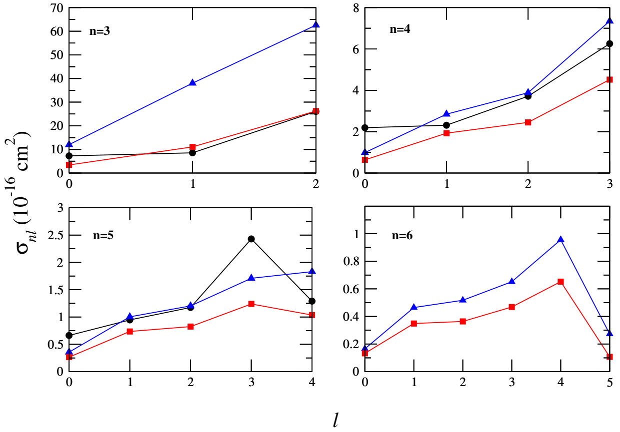
- Jorge *et al.*, Phys. Rev. A **105** (2022) → **h,m-CTMC** and **GTDSE** *nl*-partial EC and EXC.
- Ziaeian & Tökési, Eur. Phys. J. D. **75** (2021) → **m-CTMC** and **QTMC-KW** H(2*lm*) targets, EC.
- Igenbergs *et al.*, J. Phys. B **42** (2009) → **AOCC** *nl*-partial EC.

n-partial **excitation** cross sections: $Be^{4+} + H(2s) \rightarrow Be^{4+} + H(n)$



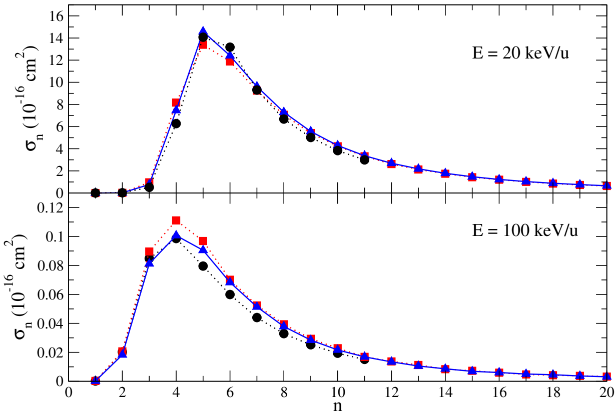
(— • —), GTDSE calculations [$n_{max} = 5$]; ■ m-CTMC; ▲, h-CTMC.

n, *l*-partial **excitation**: $Be^{4+} + H(2s) \rightarrow Be^{4+} + H(nl)$ **E=20 keV/u**



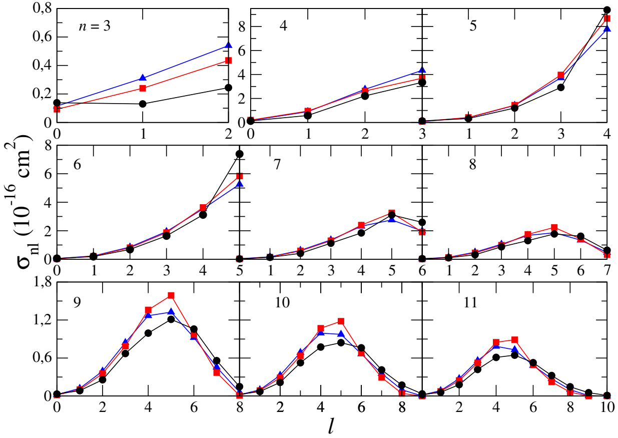
(— ● —), GTDSE; ■, m-CTMC; ▲, h-CTMC.

n-partial **electron capture** cross sections: $Be^{4+} + H(2s) \rightarrow Be^{3+}(n) + H^+$



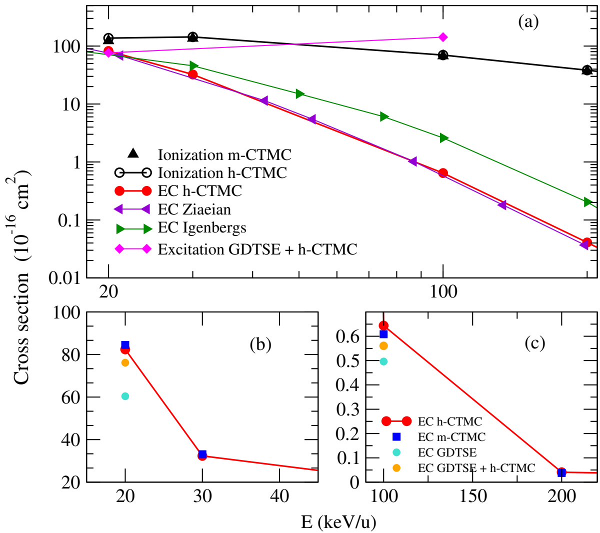
(— • —), GTDSE calculations [$n_{max} = 11$]; ■, m-CTMC; ▲, h-CTMC.

n, *l*-partial **electron capture**: $Be^{4+} + H(2s) \rightarrow Be^{3+}(nl) + H^{+}$ **E = 20 keV/u**

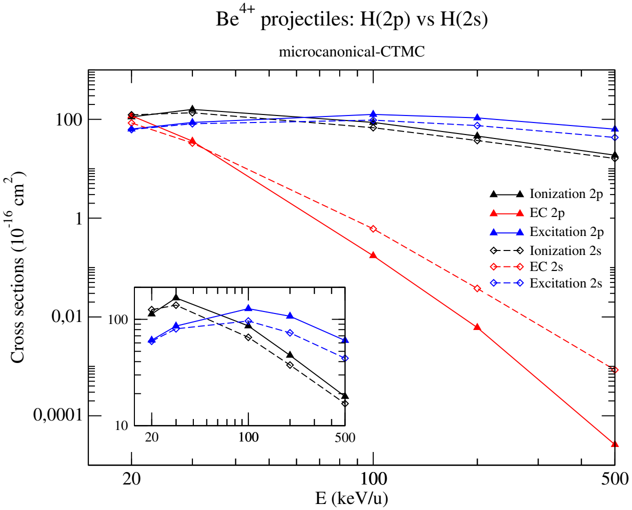


(— ● —), GTDSE; ■, m-CTMC; ▲, h-CTMC.

Total cross sections for excitation, capture and ionization in Be^{4+} + H(2s)



Total cross sections for excitation, capture and ionization in Be^{4+} + H(2p)

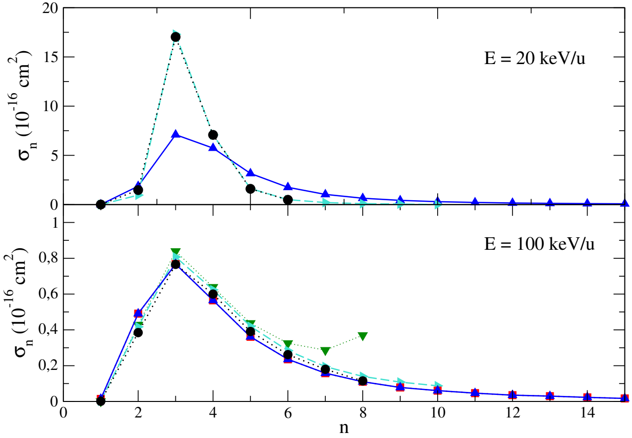


Be^{4+} + H(1s) collisions

Recent publications:

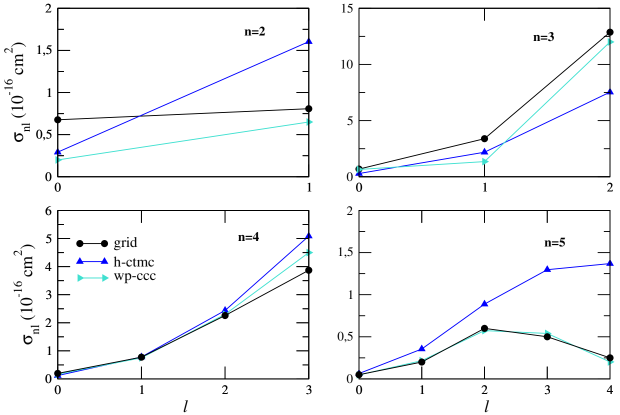
- Jorge *et al.*, Phys. Rev. A **94** (2016) → **h,m-CTMC** and **GTDSE** *nl*-partial EC.
- Ziaeian & Tökési, Atoms **8** (2020) → **m-CTMC** and **QTMC-KW** 2*l*-partial excitation.
- Antonio *et al.*, J. Phys. B **54** (2021) → **WP-CCC** *nl*-partial and total EC.
- Delibasic *et al.*, Atomic Data and Nuclear Data Tables **139** (2021) → **CDW** *nl*-partial and total EC.

n-partial **electron capture** cross sections: $Be^{4+} + H(1s) \rightarrow Be^{3+}(n) + H^+$



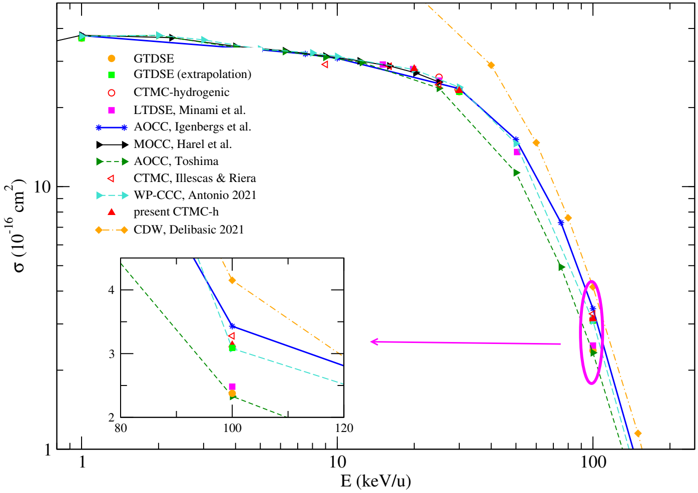
(— ● —), GTDSE; ▲, h-CTMC; ▶, WP-CCC; ▼, AOCC.

n, *l*-partial **electron capture**: $Be^{4+} + H(1s) \rightarrow Be^{3+}(nl) + H^{+}$ **E = 20 keV/u**

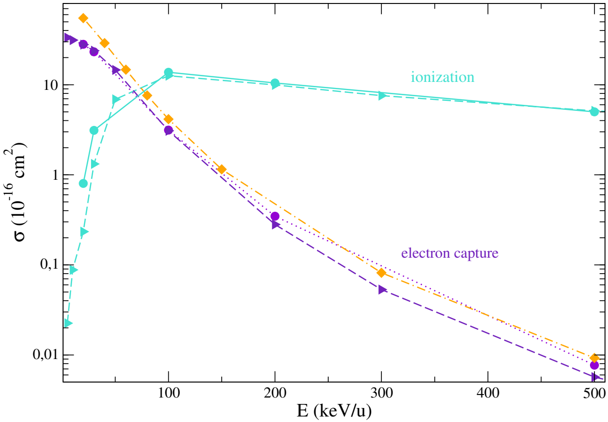


(— ● —), GTDSE; ▲, h-CTMC; ▶, WP-CCC.

Total cross sections for electron capture in Be^{4+} + H(1s)



Total cross sections for ionization and electron capture in Be^{4+} + H(1s)



(· · ● · ·), h-CTMC; (— ▶ —), WP-CCC from Antonio *et al.* J Phys. B **54** (2021); (—◆—) CDW TEC from Delibasic *et al.*, Atomic Data and Nucl. Data Tables **139** (2021).

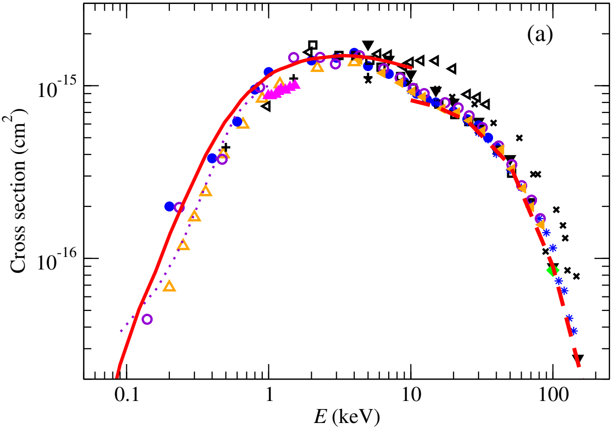
H^+ + Ar collisions

Study of collisions of protons with neutral argon beams[a]

- We have implemented a new approach: the switching-CTMC method designed to classically treat two-active electron systems[b] to calculate SI, SC and DC cross sections for $E \geq 10$ keV.
- We have applied a semiclassical method with an expansion in terms of molecular functions (MFCC) to calculate SC and DC cross sections.

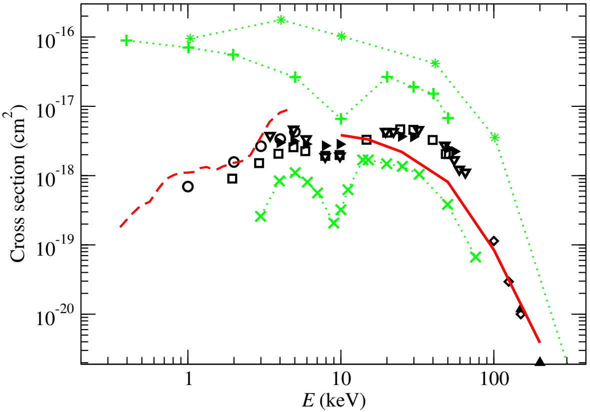
[a] Jorge *et al.*, J. Phys. Chem A **122** (2018)
[b] Jorge *et al.*, Phys. Rev. A **94** (2016)

Single electron capture: $H^+ + Ar \longrightarrow H + Ar^+$ **H formation**



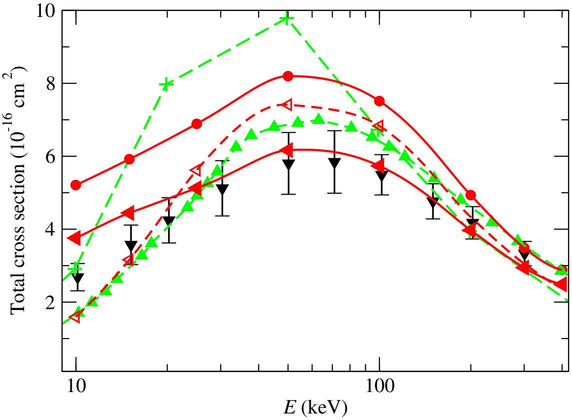
Our results: (——), MFCC (semiclassical Molecular Functions) and (- - - -), switching-CTMC with IEVM interpretation compared with different sets of experiments.

Double electron capture: $H^+ + Ar \longrightarrow H^- + Ar^{2+}$ **H^- formation**



(- - - -), MFCC results; (——), s-CTMC with IEVM interpretation. Experimental results: (▶), Afrosimov *et al.*; (□), Williams *et al.*; (◇),Toburen *et al.*. Previous calculations: (× · · ·), Martinez *et al.*, Phys. Rev. A 78,062715 (2008); (∗ · · ·) Wang *et al.* Phys. Lett. 375, 3290 (2011); (+ · · ·) Fremont J. Phys. B 49, 065206 (2016).

Total cross sections for **electron production** in $H^+ + Ar$ collisions



Switching-CTMC calculations for electron production (SI+DI+TI): (—●—), IEVM interpretation; (—◀—), IP2 interpretation; (– ◁ –), one-electron IPM-CTMC. Experimental results of Rudd *et al.*: (▼). Previous calculations: (- -▲- -), BGM-IPM, Kirchner *et al.* Phys. Rev. A (2002); (- + -), standard CTMC, Fremont J. Phys. B (2016).

Final remarks

- Calculation of accurate total and $n, \ell-$partial cross sections employing GTDSE and CTMC methods.
- Satisfactory agreement of CTMC and GTDSE results for electron capture with H(2s) targets. h-CTMC shows better agreement for excitation into H(n=4,5), which supports the application of this method for excitation into high n-lying excited levels (very difficult to compute with CC or grid treatments).
- Good agreement of h-CTMC (better than m-CTMC) and GTDSE with other nonperturbative EC in collisions with H(1s).
- The CTMC method yields accurated ionization cross sections in the 10-500 keV/u energy range.
- In $H^+ + Ar$ collisions, H and H^- formation cross sections calculated by our MFCC and s-CTMC models are in good agreement with the experiments.

Coworkers

- A. Jorge
- L. Méndez
- I. Rabadán

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THANK YOU FOR YOUR ATTENTION!