Numerical calculation of charge exchange and excitation cross sections for plasma diagnostics.

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Motivation

- Electron capture (EC) (Charge exchange) reactions:

$$A^{q+} + H \rightarrow A^{(q-1)+} + H^+$$

- Excitation

$$A^{q+} + H \rightarrow A^{q+} + H^*$$

- Cross sections required in plasma modelling and diagnostics.
- In this talk collisions with fully stripped ions (one-electron systems).
    - Be^{4+} specially relevant.
    - No experimental data.
    - Need of theoretical data. Several calculations available.

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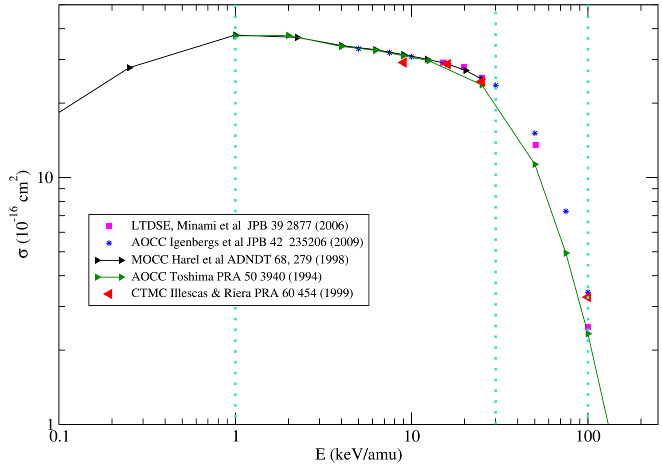
EC, total cross section



In this talk:

- $1 < E < 500$ keV/u. Semiclassical calculations.
- Numerical integration of the TDSE.
- Calculations of *n*-partial EC and excitation cross sections.
- Comparison with CC and CTMC calculations.
- Uncertainties of *n*-partial EC cross sections.
- See Jorge et al. Phys. Rev. A 94, 032707

Impact parameter method

In general valid for $E > 250$ eV/u

- Rectilinear nuclear trajectories $\boldsymbol{R} = \boldsymbol{b} + \boldsymbol{v}\,t$
- The electron wavefunction is a solution of the **TDSE** (in atomic units):

$$\left[H_{\rm el} - {\rm i} \left.\frac{\partial}{\partial t}\right|_{\boldsymbol{r}} \right] \Psi = 0$$

with

$$H_{\rm el} = -\frac{1}{2}\nabla_r^2 + V_{\rm P} + V_{\rm T}$$

MOCC

$$\Psi(\boldsymbol{r},t;b,v) = D(\boldsymbol{r},t)\sum_k a_k(t;b,v)\phi_k(\boldsymbol{r};R)\exp\left(-\mathrm{i}\int\epsilon_k(R)\mathrm{d}t\right)$$

where ϕ_k are **molecular** orbitals that fullfil:

$$H_{\mathrm{el}}\phi_k = \epsilon_k\phi_k$$

and $D(\boldsymbol{r},t)$ is a common translation factor.

AOCC

$$\begin{aligned}\Psi(\boldsymbol{r},t;b,v) = & \sum_k a_k(t;b,v)\phi_k^{\mathrm{P}}(\boldsymbol{r};R)\exp\left(-\mathrm{i}\epsilon_k^{\mathrm{P}}\right)D^{\mathrm{P}} + \\ + & \sum_l a_l(t;b,v)\phi_l^{\mathrm{T}}(\boldsymbol{r};R)\exp\left(-\mathrm{i}\epsilon_l^{\mathrm{T}}\right)D^{\mathrm{T}}\end{aligned}$$

where ϕ_k^{P}, ϕ_l^{T} are **atomic** orbitals that fulfill:

$$\left[-\frac{1}{2}\nabla_r^2 + V_{\mathrm{P}}\right]\phi_k^{\mathrm{P}} = \epsilon_k^{\mathrm{P}}\phi_k^{\mathrm{P}};\quad \left[-\frac{1}{2}\nabla_r^2 + V_{\mathrm{T}}\right]\phi_l^{\mathrm{T}} = \epsilon_l^{\mathrm{T}}\phi_l^{\mathrm{T}}$$

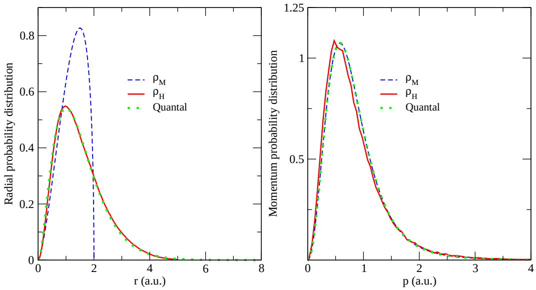
$D^{\mathrm{P,T}}$ are plane-wave translation factors.

In practice, **pseudostates** are added to represent the ionization continuum.

Eikonal CTMC Method

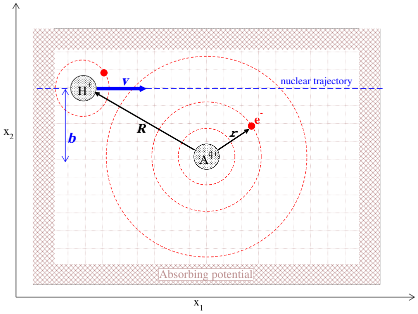
- Electronic motion is described by a **classical distribution function** $\rho(\boldsymbol{r}, \boldsymbol{p}, t)$[a]
- The projectile follows **straight-line trajectories**: $\mathbf{R} = \mathbf{b} + \mathbf{v}t$
- Initial distribution.

[a] Abrines & Percival, Proc. Phys. Soc. **88**, 861



Numerical integration of the TDSE

- Previous calculations of Minami *et al.* (JPB 39, 2877 (2006)) for Be^{4+} + H(1s). (LTDSE)
- New calculations using the program GridTDSE of Suarez *et al.* CPC 180, 2025 (2009).



TDSE

$$\left[H_{\mathrm{el}}(\boldsymbol{r}, t) - \mathrm{i} \left. \frac{\partial}{\partial t} \right|_{\boldsymbol{r}} \right] \Psi(\boldsymbol{r}, t; b, v) = 0$$

$$\Psi(\boldsymbol{r}, t_0) = \varphi^{\mathrm{H}}_{1s} \left(\boldsymbol{r} - \boldsymbol{R}(t_0) \right) \times$$

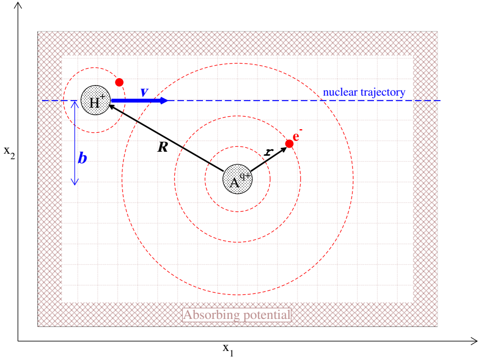
$$\exp\left(-\mathrm{i}\boldsymbol{v} \cdot \boldsymbol{r} - (\mathrm{i}/2) v^2 t_0 \right)$$

GridTDSE

The numerical solution of the TDSE has the form:

$$\boldsymbol{\Psi}(t + \Delta) = \boldsymbol{\Psi}(t - \Delta) - 2\mathrm{i}\Delta(\mathbf{T} + \mathbf{V})\boldsymbol{\Psi}(t).$$

The components of the vector $\boldsymbol{\Psi}$ are the values of the wavefunction in the grid points.



Grids

Box size: $-L_{\max} \leq x, z \leq L_{\max}$,

$0 \leq y \leq L_{\max}$, $L_{\max}$ =40 a_0

- G1 Δq= 0.2 a_0
- G2 Δq= 0.137 a_0
- G3 Δq= 0.1 a_0
- G4 Δq= 0.05 a_0

Mask function

$$M(\boldsymbol{r}) = \prod_{i=1,3} \begin{cases} \exp\left\{-\alpha(|q_i| - L_{\max} + \delta)^2\right\} & \text{if} \quad L_{\max} - |q_i| < \delta \\ 1 & \text{elsewhere} \end{cases}$$

Soft core

In practice:

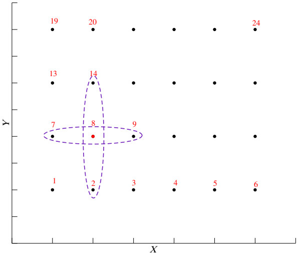
$$V_\mathrm{P}(\boldsymbol{r}) = -Z_\mathrm{P}\left[|\,\boldsymbol{r}\,|^2 + \epsilon_\mathrm{P}\right]^{-1/2}$$

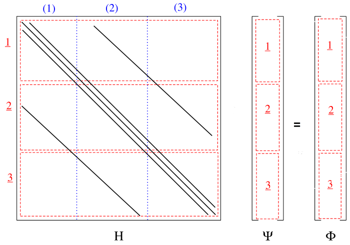
$$V_\mathrm{T}(\boldsymbol{r},t) = -Z_\mathrm{T}\left[|\,\boldsymbol{r}-\boldsymbol{R}\,|^2 + \epsilon_\mathrm{T}\right]^{-1/2} \quad , \quad \boldsymbol{R} = (b, 0, z_\mathrm{min} + vt)$$

Soft-core parameters ϵ_H, ϵ_Be employed for different grid densities

Δ_q (a.u.)	ϵ_H	ϵ_Be
0.2 (G1)	3.65E-03	5.40E-03
0.137 (G2)	1.70E-03	2.22E-03
0.1 (G3)	7.98E-04	1.08E-03
0.05 (G4)	1.75E-04	2.29E-04

- $\mathbf{V}$ is a diagonal matrix.
- Finite diferences with a stencil of n_s (15) points for calculating $\mathbf{T}$.
- $\mathbf{H}$ matrix highly sparse.
- In our calculation $\approx 10^8$ points. Memory allocation ≈ 256 GB.





Low energy, $E = 1$ keV/u

Total cross sections for Be^{4+}+ H(1s) → Be^{3+}(n=3) + H^+

Calculation	σ, 10^{-16}cm^2
MOCC-17[a]	34.7
MOCC-88[b]	34.5
MOCC-96[a]	34.4
AOCC-170[c]	34.4
gridTDSE (G1)	33.2

[a] Errea et al. JPB 31, 3527
[b] Harel et al. ADNDT 68, 279
[c] Igenbergs et al. JPB 42 35206

Total cross sections for Be^{4+}+ H(1s) → Be^{3+}(n=4) + H^+

Calculation	σ, 10^{-16}cm^2
MOCC-17[a]	2.45
MOCC-88[b]	3.17
MOCC-96[a]	3.11
AOCC-170[c]	3.10
gridTDSE (G1)	3.27

[a] Errea et al. JPB 31, 3527
[b] Harel et al. ADNDT 68, 279
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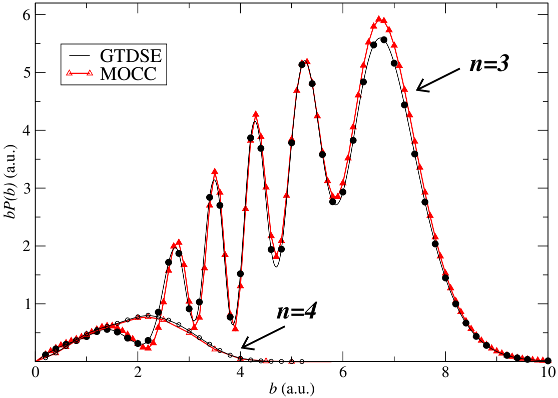
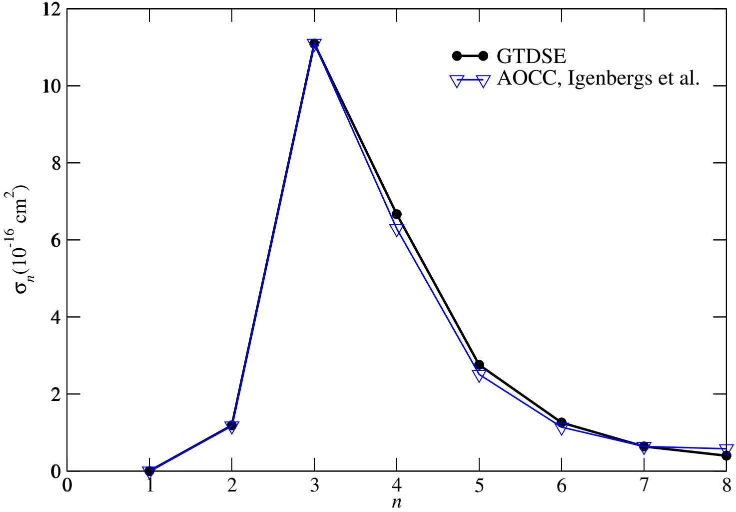
Transition probabilities, $E = 1$ keV/u



$$\sigma_k = 2\pi \int_0^{b_{\max}} bP_k(b)\mathrm{d}b$$

Intermediate energy, $E = 30$ keV/u



Intermediate energy, $E = 30$ keV/u

Total cross sections for Be^{4+} + H(1s) $\rightarrow Be^{3+}(n{=}3) + H^+$

Calculation	Cross section $10^{-16} cm^2$
gridTDSE (G3)	11.1
AOCC-170[a]	11.1

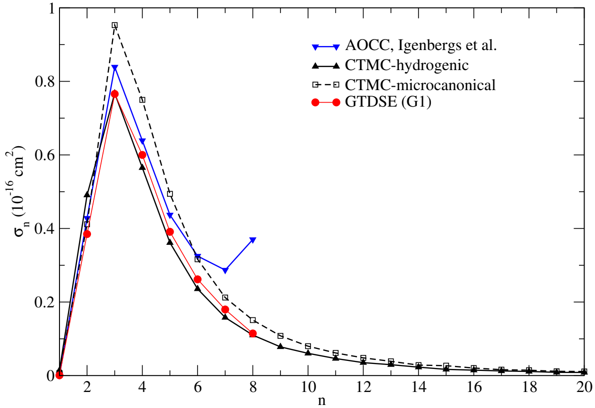
[a] Igenbergs et al. JPB 42 35206

Total cross sections for Be^{4+} + H(1s) $\rightarrow Be^{3+}(n{=}4) + H^+$

Calculation	Cross section $10^{-16} cm^2$
gridTDSE (G3)	6.67
AOCC-170[a]	6.29

[a] Igenbergs et al. JPB 42 35206

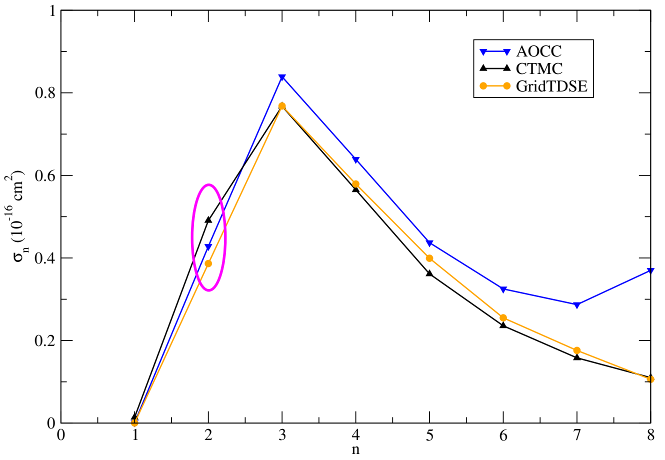
$E = 100$ keV/u, Total cross sections for $Be^{4+} + H(1s) \rightarrow Be^{3+}(n) + H^{+}$



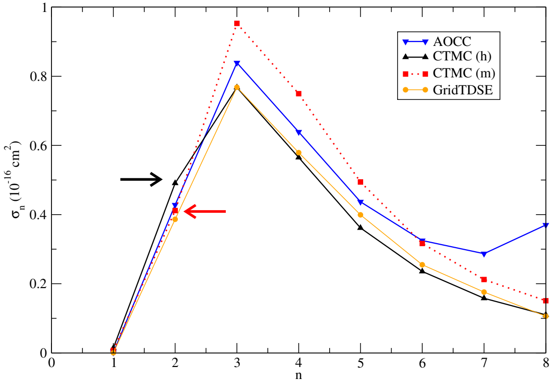
σ_n, 10^{-16} cm^2

n	CTMC (h)	GDTSE (G3)
2	0.49	0.38
3	0.77	0.77
4	0.57	0.60
5	0.36	0.39
6	0.23	0.26

$E = 100$ keV/u

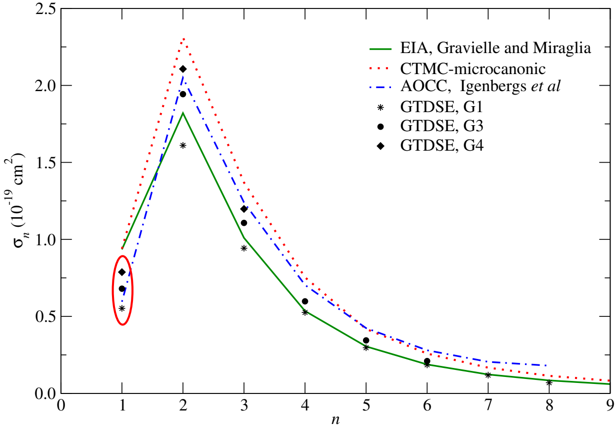


E = 100 keV/u, Be^{4+} + H(1s) → Be^{3+}(n=2) + H^+



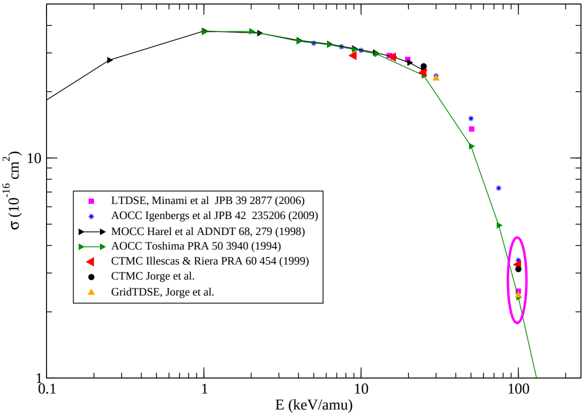
Calculation	Cross section 10^{-16} cm^2
gridTDSE (G3)	0.38
CTMC (m, 1×10^5 traj.)	0.41
CTMC (m, 5×10^5 traj.)	0.41

$E = 500$ keV/u

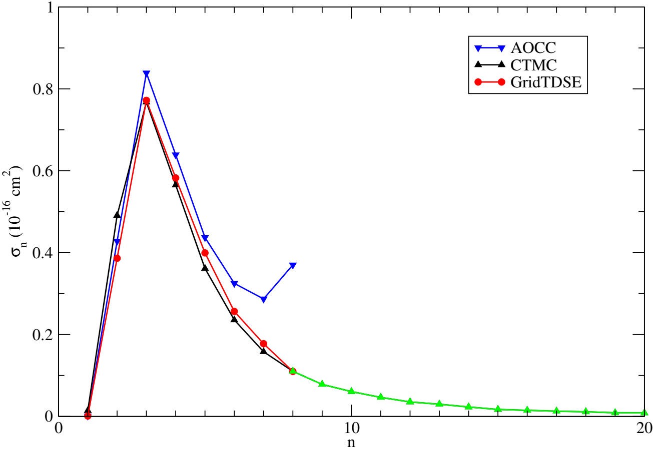


- Slow Convergence, in particular for small n.
- Vast computational resources required.

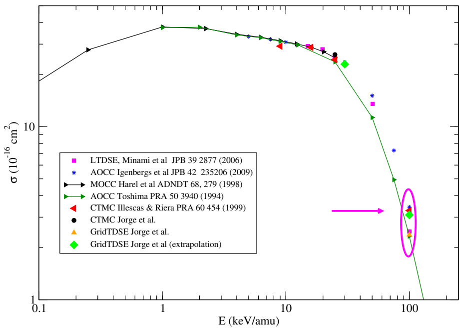
Total cross section



Total cross section, $E = 100$ keV/u



Total cross section



Calculation	σ, Å^2
CTMC (h, 1×10^5 traj.)	3.13
CTMC (h, 5×10^5 traj.)	3.14
GridTDSE (extrap.)	3.11

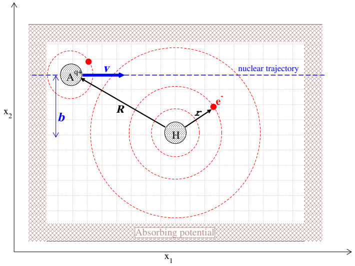
Uncertainties of the CTMC calculation, Å^2	Statistics	$n < 3$	Total
	1.5×10^{-2}	8×10^{-2}	$\approx 1 \times 10^{-1}$

Excitation and electron loss

$$\text{Excitation}: \quad Be^{4+} + H(1s) \rightarrow Be^{4+} + H(n = 2, 3)$$

$$\text{Ionization}: \quad Be^{4+} + H(1s) \rightarrow Be^{4+} + H^{+} + e^{-}$$

$$\text{Capture}: \quad Be^{4+} + H(1s) \rightarrow Be^{3+} + H^{+}$$



$$P_{\mathrm{EL}} = \lim_{t \to \infty} \left[1 - \|\Psi\|^2\right]$$

Excitation and EL cross sections

Total cross sections ($cm^2 \times 10^{-16}$), $E = 100$ keV/u

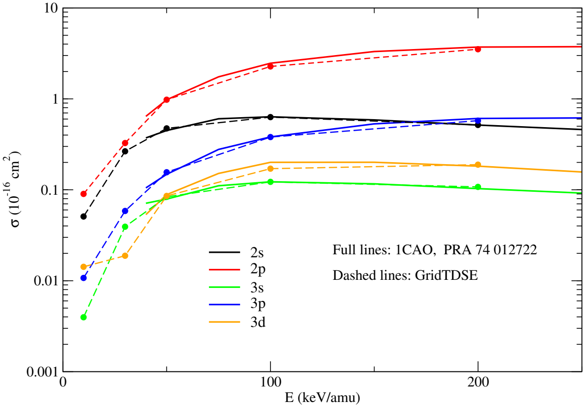
Calculation	$n = 2$	$n = 3$	EL
gridTDSE (G1)	2.96	0.68	15.7
1CAO	3.10	0.70	16.3

Total cross sections ($cm^2 \times 10^{-16}$), $E = 200$ keV/u

Calculation	$n = 2$	$n = 3$	EL
gridTDSE (G1)	4.26	0.89	9.86
1CAO[a]	4.23	0.84	10.6

[a] Errea et al. PRA 74,012722

Excitation cross sections



$E = 100$ keV/u

σ_{nl}, 10^{-16}cm^2		
	gridTDSE (G1)	1CAO
2s	0.63	0.63
2p	2.32	2.47
3s	0.12	0.12
3p	0.38	0.38
3d	0.17	0.20

$B^{5+} + H(1s) \rightarrow B^{4+}(n) + H^{+}$ (preliminary)

Total cross sections ($cm^2 \times 10^{-16}$), $E = 30$ keV/u

Calculation	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
gridTDSE (G1)	0.15	7.64	12.3	6.23	2.77	1.36
Recommended data	0.17	8.34	12.5	5.53	2.58	1.64

Total cross sections ($cm^2 \times 10^{-16}$), $E = 100$ keV/u

Calculation	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
gridTDSE (G1)	0.19	0.93	0.99	0.74	0.52	0.36
Recommended data[a]	0.22	1.03	1.28	0.71	0.49	0.34

[a] Errea et al. PPCF 48,1585

Summary

- Implementation of a lattice method to solve numerically the TDSE.
- Application to $Be^{4+} + H$ collisions. State resolved EC cross sections in a wide energy range.
- Convergence study.
- Comparison with other treatments. Estimation of uncertainties.

Coworkers

- TCAM group : **Alba Jorge**, **Jaime Suárez**, **Clara Illescas**, Luis Errea, Ismanuel Rabadán.
- Bernard Pons (CELIA, Bordeaux, France).

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