Atomic and molecular physics for modelling of stellar spectra

PI: L. Tchang-Brillet (LERMA)

2 themes:

1. Contribution to the preparation of POLLUX:

LERMA: L. Tchang-Brillet, C. Balança, N. Champion; **LESIA**: C. Neiner, R. Monier
Collaborations: A. Meftah (Tizi Ouzou University, J. F. Wyat (Aimé Cotton)

2. Modeling of stellar atmospheres at the area of GAIA:

LERMA: N. Feautrier; **GEPI**: E. Caffau
Collaborations: A. Belyaev, S. A. Yakovleva, Y. V. Voronov (St Petersburg University)
M. Guitou, A. Mitrushchenkov (Paris-Est University)

Description of the project

- In parallel with the rapid advances in observations, analysis of the data and development of increasing sophisticated models,

need for atomic data to characterize the chemical and physical conditions of the observed stars

- We propose an interdisciplinary strategy, combining:

experimental and theoretical laboratory works in close collaboration with astrophysical teams

2 projects :

✧ contribution to the preparation of the POLLUX project

✧ non-LTE modelling of spectra: contribution of H-atom collisions

Contribution to the preparation of POLLUX

POLLUX project (C. Neiner, J. C. Bourret): high-resolution spectropolarimeter for the LUVOIR mission

Contribution of the LERMA team:

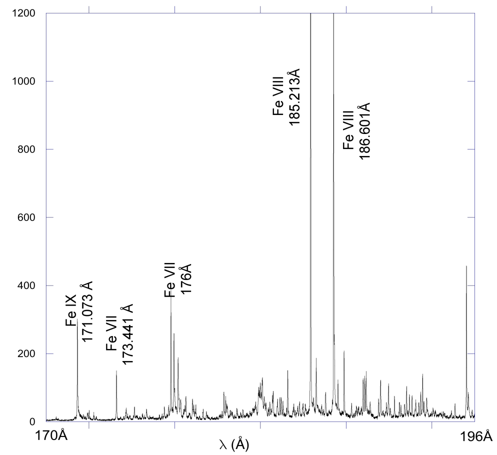
- acquisition of spectra with the high-resolution VUV 10m-Spectrograph (Meudon)

- recording of spectra (1200 – 1800 Å) using emission light produced by a deuterium lamp → transmitted I(λ) for 3 polarisations U, V and Q (calibration of the spectropolarimeter vs λ)

High resolution VUV normal incidence spectrograph Paris - Meudon Observatory

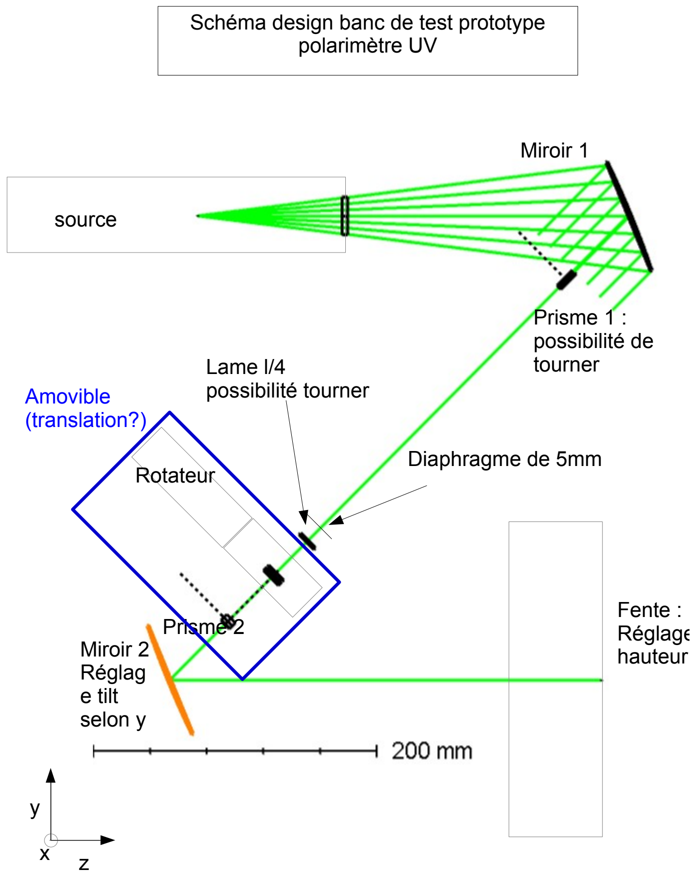
- Concave holographic grating focal distance 10.7 m, 3600 lines/mm, dispersion = 0.25 Å /mm first order
- Resolution ~ 150 000 (8mÅ, slit 30μm)
- One single exposure : 2 x 120Å on two photographic plates or image plates (IP) (2x100Å)
- Wavelength range : 400-3000 Å

Down to 170 Å with IP, overlapping the grazing incidence range



Current light sources :
High voltage vacuum sparks for atomic ions
Penning discharge for molecular spectra

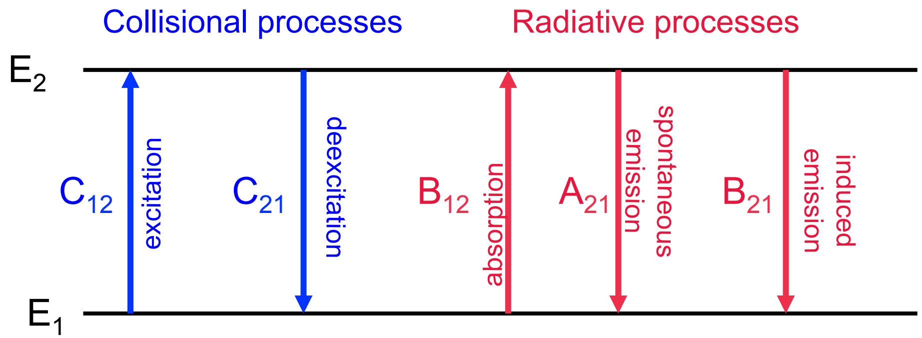
Schematic setup



→ VUV 10m spectrograph

Non-LTE modelling of spectra

• Non-LTE modelling implies competition between radiative and collisional processes for both excitation and ionisation



$$C_{21} = n_P \, k_{21}(T)$$

s^{-1} $\qquad$ $cm^3 s^{-1}$

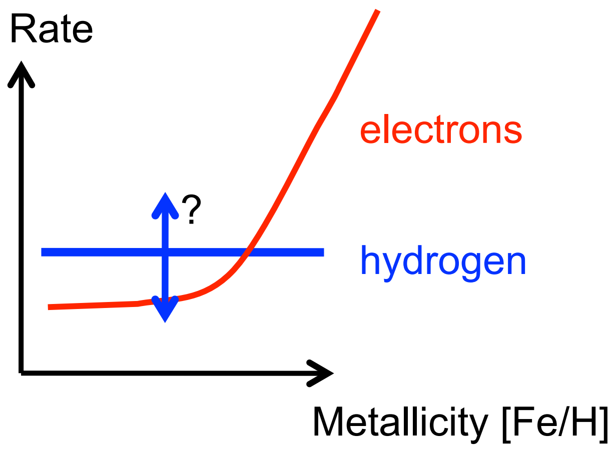
n_P: perturber density, k_{21} rate coefficient proportional to cross sections $\quad k_{21}(T) = \langle v\sigma \rangle_v$

- a priori, collisions should decrease the non-LTE effects on populations

Which collisions?

$N_H/N_e \sim 10^4–10^7$
• do numbers overcome efficiency?

$N_H/N_e \sim 1$
• protons can (probably) be neglected



→ Collisions with H-atoms are dominant for low-metallicity atmospheres

Collisional rates with H-atoms

Dealing with the collisional problem in two steps:

- During the collision the 2 atoms are getting closer to each other and form a quasi-molecule →
  Computing of: - interaction potentials
  - coupling terms between the potentials

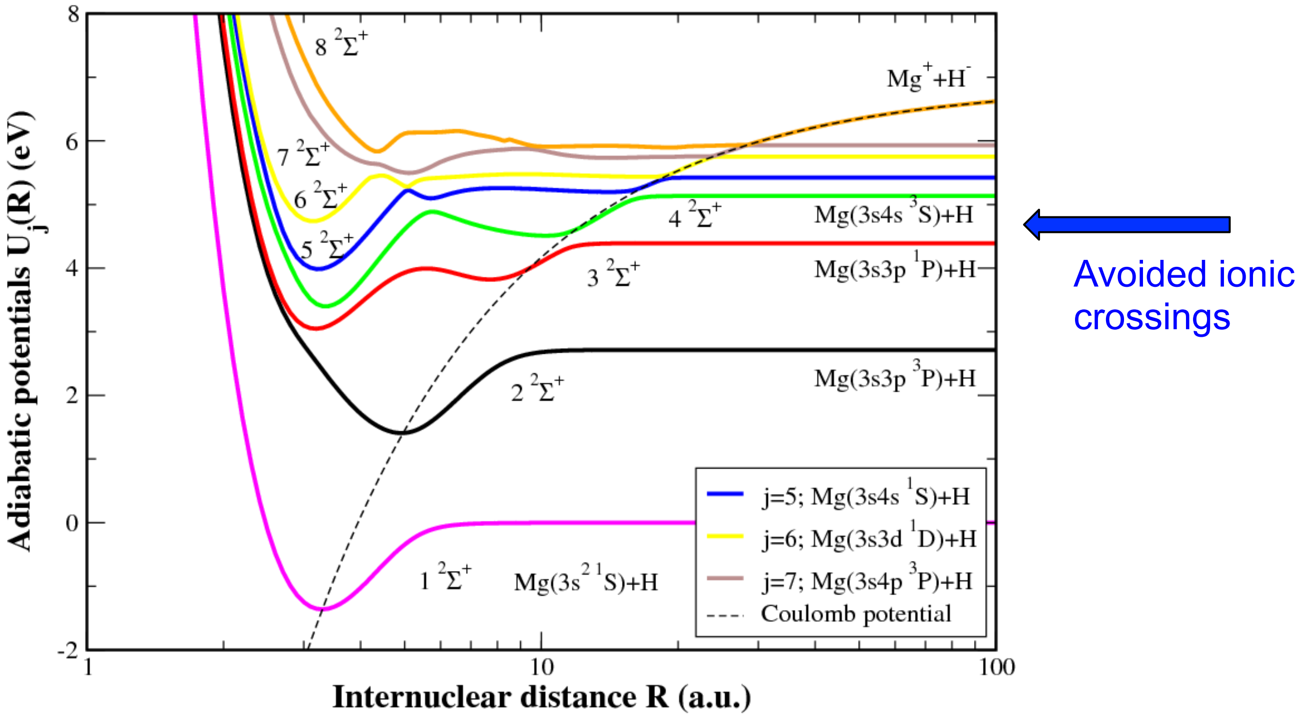
ab initio quantum chemistry increasingly difficult for high excited states

- Dynamical calculations using in these potentials and couplings
  quantum dynamics if possible

- Already done: Li+H, Na+H, Mg+H
  Under way: O+H, Ca+H

Main characteristics of the quasi-molecular problem: Mg+H several processes

$$Mg + H \underset{\text{désexcitation}}{\overset{\text{excitation}}{\rightleftarrows}} Mg^* + H \underset{\text{neutralisation}}{\overset{\text{ionisation}}{\rightleftarrows}} Mg^+ + H^-$$



Guitou, Spielfiedel, Feautrier,
Chem. Phys. Lett. 2010

Mg+H rate coefficients

T = 4000.00 K

initial/final states	3s ^{1}S	3p ^{3}Po	3p ^{1}Po	4s ^{3}S	4s ^{1}S	3d ^{1}D	ionic
3s ^{1}S		1.67e-17	9.32e-20	5.37e-20	2.14e-20	6.31e-21	5.05e-22
3p ^{3}Po	4.87e-15		2.76e-13	7.95e-14	2.07e-14	4.35e-15	1.47e-16
3p ^{1}Po	1.05e-14	1.07e-10		5.21e-11	7.88e-12	9.96e-13	1.84e-13
4s ^{3}S	5.26e-14	2.67e-10	4.52e-10		1.38e-10	1.18e-11	9.14e-12
4s ^{1}S	1.46e-13	4.83e-10	4.75e-10	9.56e-10		1.42e-09	8.64e-10
3d ^{1}D	2.23e-14	5.28e-11	3.12e-11	4.28e-11	7.41e-10		1.73e-10
ionic	2.42e-13	2.42e-10	7.84e-10	4.48e-09	6.10e-08	2.35e-09	

- For excitation: the dominant rate coefficient are those to the closest final state
- Large rates for transitions between excited states even for non-radiatively allowed transitions
- Important contribution of ionisation/mutual neutralisation

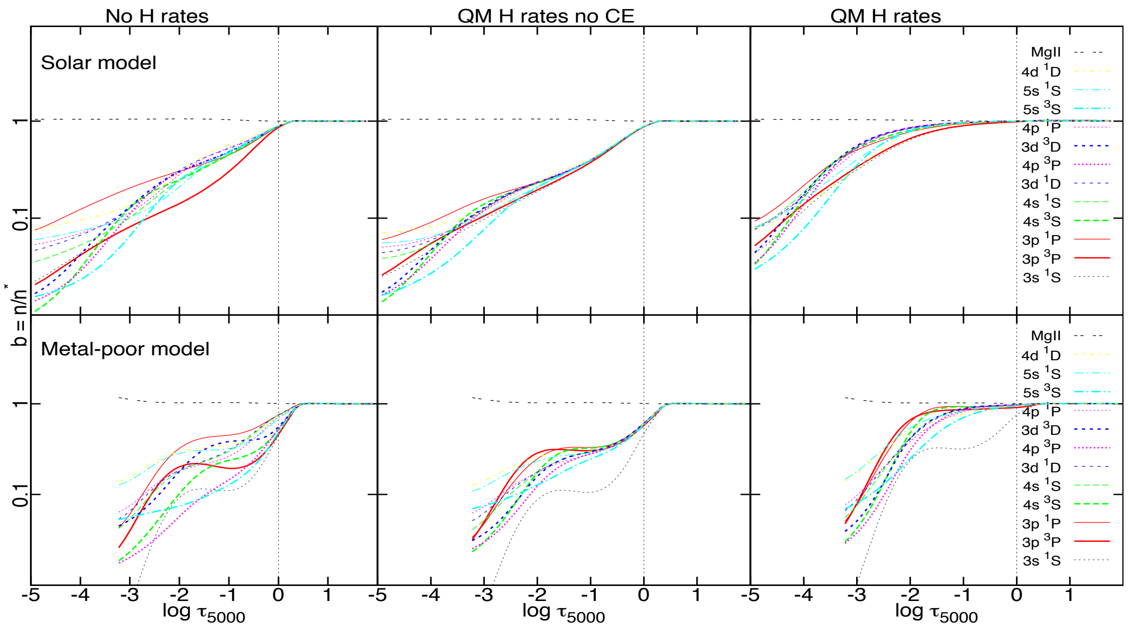
Guitou, Belyaev, Barklem, Spielfiedel, Feautrier, 2011

NLTE consequences

coll. F. Thévenin and T. Merle, Guitou et al. Chem. Phys. 2015

- Model for two atmospheres: Sun and HD122563 (metal poor):
- Statistical equilibrium + radiative transfer (MARCS model, code MULTI)
- Inclusion of radiative processes+ collisions (e, H with CE or not)

Without H with H, no CE with H and CE



NLTE departure coefficients $b_i=n_in_i^*$ vs log τ

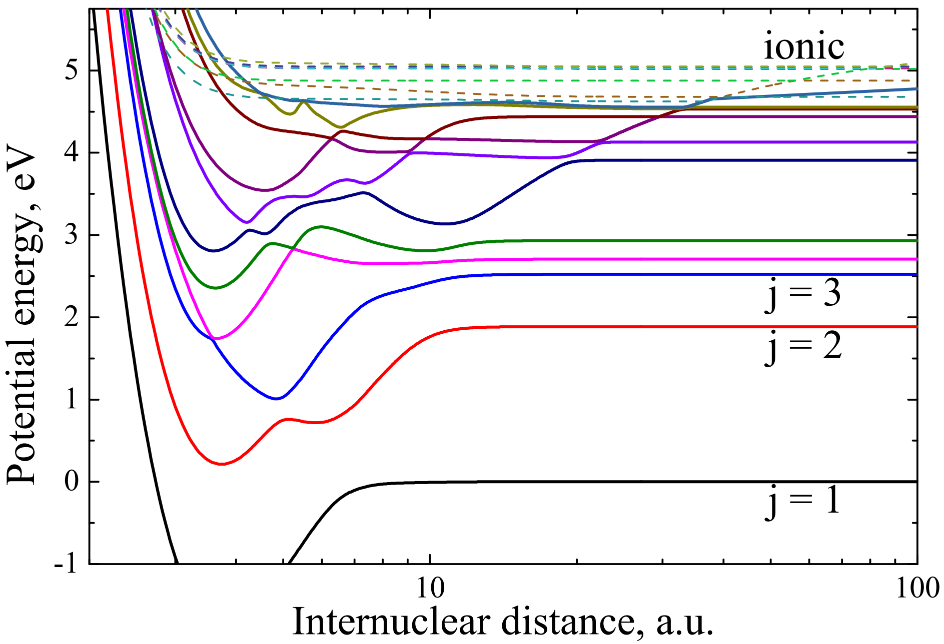
<-- Sun

<-- HD122563

- H-collisions reduce the departure coefficients for metal-poor atmospheres
- Importance of charge-exchange processes (CE)

Ca+H

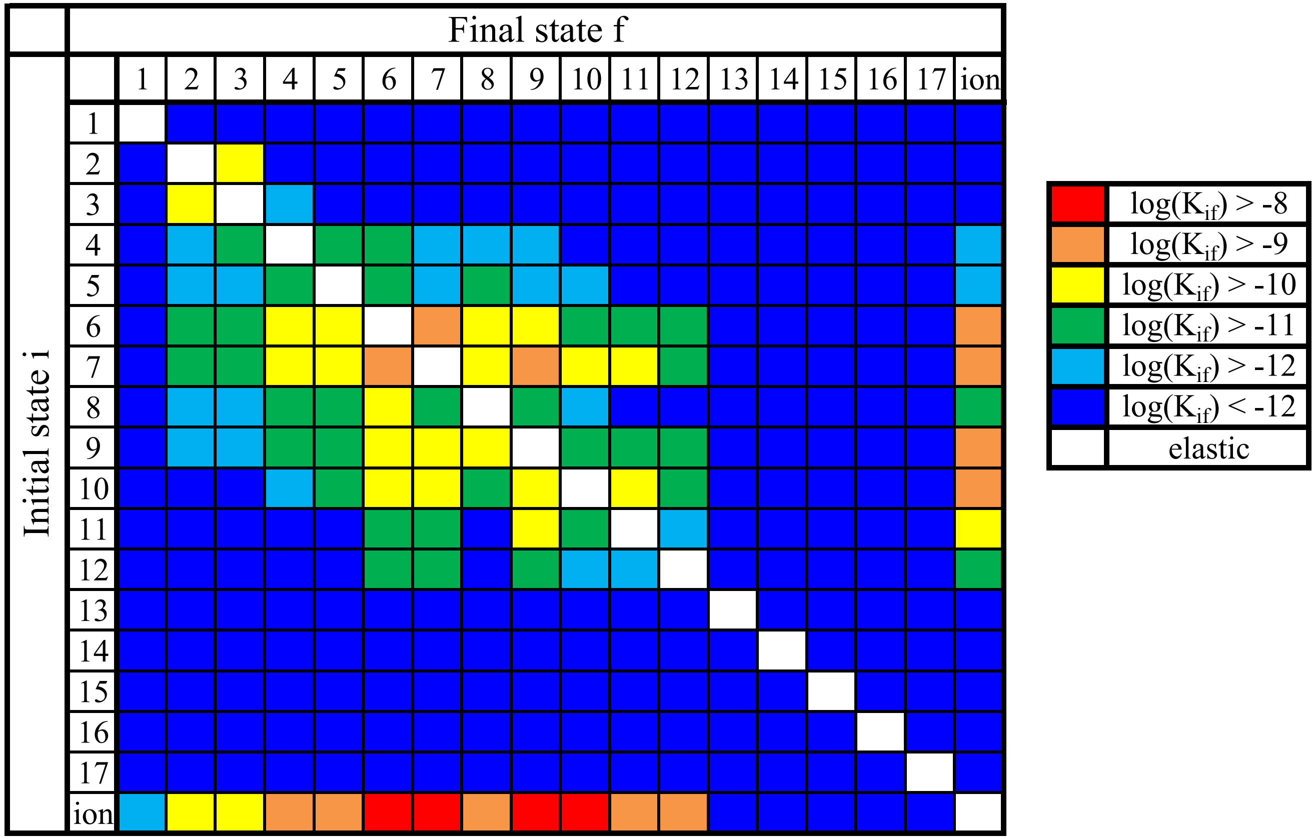
Ca + H —excitation→ / ←de-excitation— Ca* + H —ionisation→ / ←neutralisation— $Ca^+ + H^-$



j	Scattering channels
1	$Ca(4s^2\,{}^1S) + H(1s\,{}^2S)$
2	$Ca(4s4p\,{}^3P^\circ) + H(1s\,{}^2S)$
3	$Ca(3d4s\,{}^3D) + H(1s\,{}^2S)$
4	$Ca(3d4s\,{}^1D) + H(1s\,{}^2S)$
5	$Ca(4s4p\,{}^1P^\circ) + H(1s\,{}^2S)$
6	$Ca(4s5s\,{}^3S) + H(1s\,{}^2S)$
7	$Ca(4s5s\,{}^1S) + H(1s\,{}^2S)$
8	$Ca(3d4p\,{}^3F^\circ) + H(1s\,{}^2S)$
9	$Ca(4s5p\,{}^3P^\circ) + H(1s\,{}^2S)$
10	$Ca(4s5p\,{}^1P^\circ) + H(1s\,{}^2S)$
11	$Ca(4s4d\,{}^1D) + H(1s\,{}^2S)$
12	$Ca(4s4d\,{}^3D) + H(1s\,{}^2S)$
13	$Ca(3d4p\,{}^3P) + H(1s\,{}^2S)$
14	$Ca(4s6s\,{}^3S) + H(1s\,{}^2S)$
15	$Ca(3d4p\,{}^1F) + H(1s\,{}^2S)$
16	$Ca(4s6s\,{}^1S) + H(1s\,{}^2S)$
17	$Ca(4p^2\,{}^1D) + H(1s\,{}^2S)$
ionic	$Ca^+(4s\,{}^2S)+H^-(1s^2\,{}^1S)$

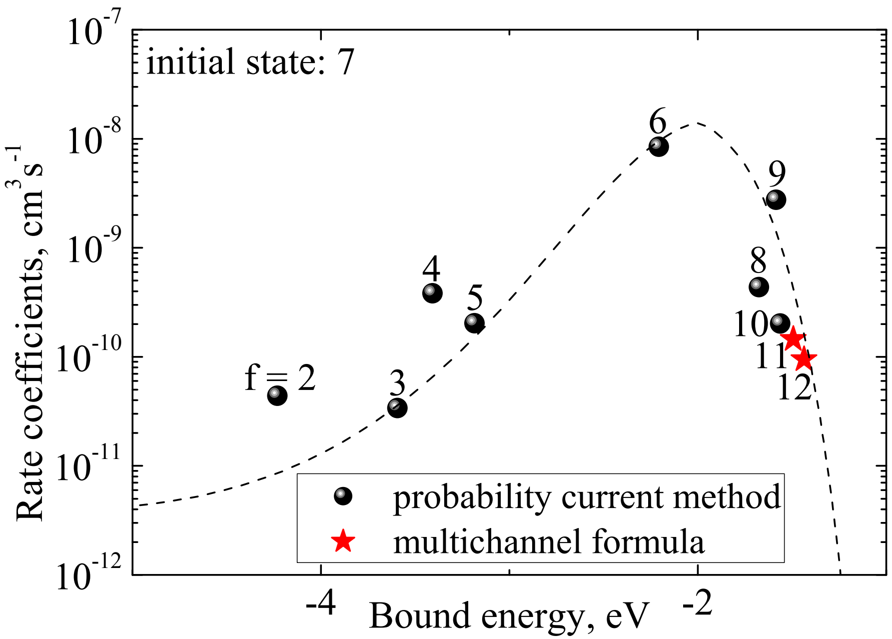
Mitrushchenkov et al.,JCP. 2016

Ca+H rate coefficients

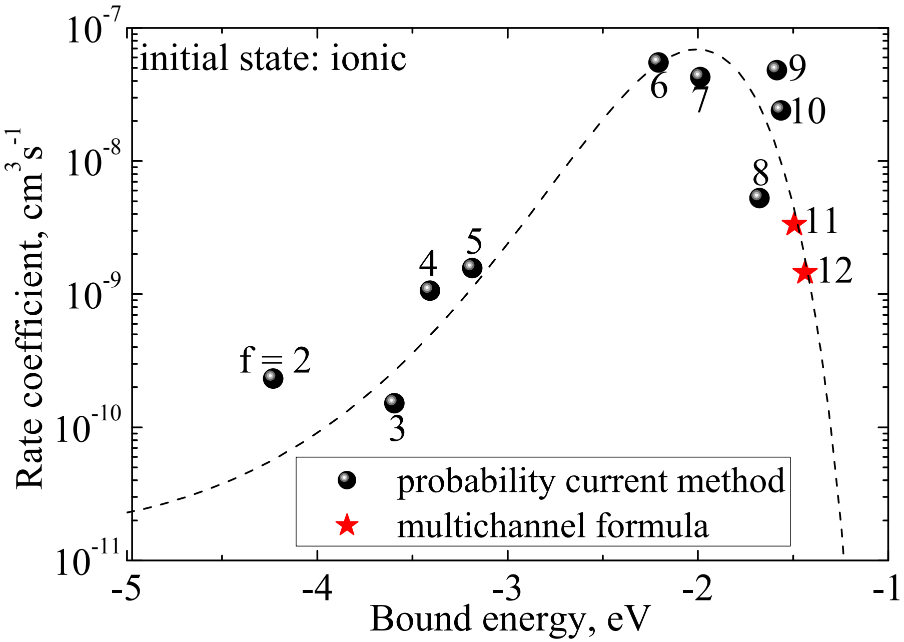


Ca-H rate coefficients

Excitation/de-excitation from
the Ca(4s5s^{1}S) state (j=7)



Mutual neutralisation
$Ca^+ + H^- \rightarrow Ca + H$



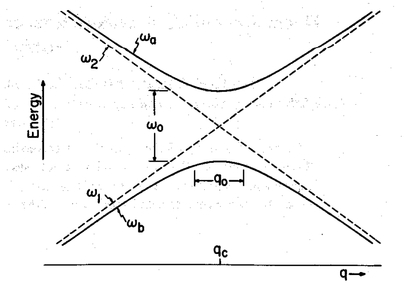
- Large rates for some transitions
- Importance of ionisation/neutralisation
- Similar trends for other systems: Li, Na, Mg

Belyaev et al. ApJ 2017

What is the physical origin of this trend?

the Landau Zener model

Transitions occur at avoided crossings between two potentials: the model



- 2 potentials V1 and V2 interacting through C_{12}

- Initial state 1: the atoms move along V1
- at the crossing: probability P_{12} to jump on V2

$$P_{12} \propto \frac{|C_{12}|^2}{\left(\frac{d(V1-V2)}{dR}\right)}$$

- the atoms approach each other and fly apart ➔ 2nd crossing

- for final state 2: **Total probability :** P_{12} **(1-**P_{12} **)**

➔P_{12} =0.5 **« optimal crossings » for the largest rates**

What is known about the H-rate coefficients?

1. The Drawin's formula is not reliable (no physical basis and inaccuracies by factors up to 10^5)

2. From « exact » quantum results for both interaction and dynamics (Li, Na, Mg, Ca) , with « optimum » relative position of the molecular interactions (avoided crossings and interatomic distance), the order of magnitude of the rates are:

~ 10^{-9}-10^{-10} cm^3/s for excitation/de-excitation

~ 10^{-8}-10^{-9} cm^3/s for charge exchange

3. The collisional mechanism is well idendified,

→ « model methods » could give reliable estimates of the rate coefficients

Our strategy: complementary directions

Investigation of new systems (complex atoms) by full quantum approaches : coll M. Guitou, A. Mitrushchenkov, Paris-Est) O I in progress

Developments of :

- asymptotic approaches for interactions of 2 atoms at large distances
- new theoretical models giving good estimates of rate coefficients for a large number of species (coll. A. Belyaev, St petersburg) Fe?

to be compared to « exact » results

Impact of the data on NLTE modelling investigated (coll. E. Caffau, F. Thévenin)

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