Non-LTE line formation for trace elements in stellar atmospheres,
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Mechanisms of departures from LTE

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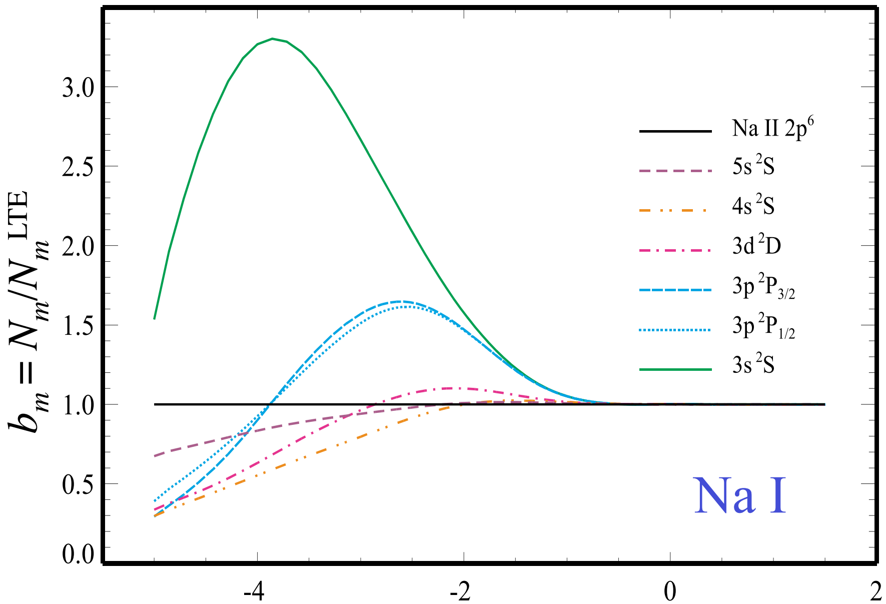
Outline

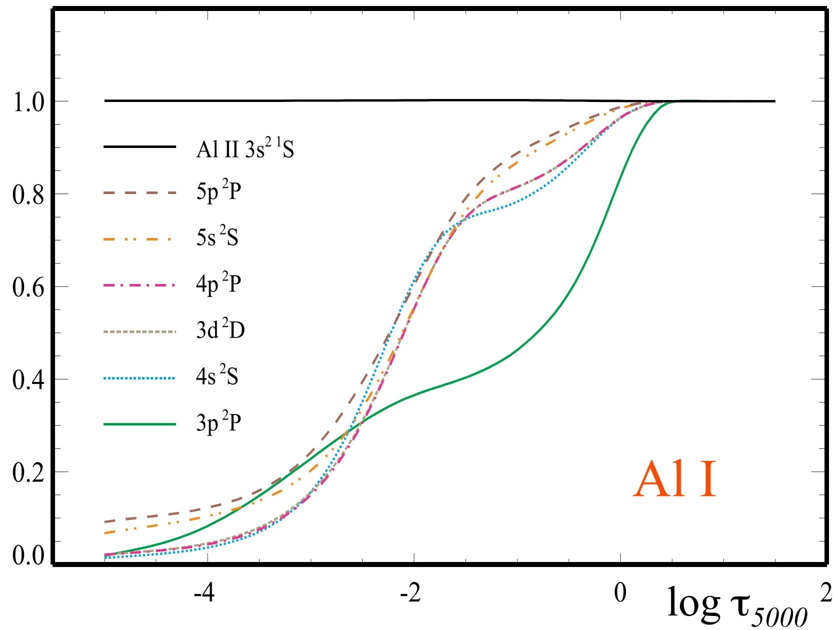
- Population and depopulation processes in atoms
- Non-LTE effects for spectral lines
- How is the statistical equilibrium of atoms achieved?

Departure coefficients $b_m = n_m / n^*_m$

for the selected levels of Na I and Al I in the solar atmosphere

Gehren et al. 2004





Na I: $b_{1,2} > 1, \quad n_{\rm NLTE} > n_{\rm LTE}$

overrecombination

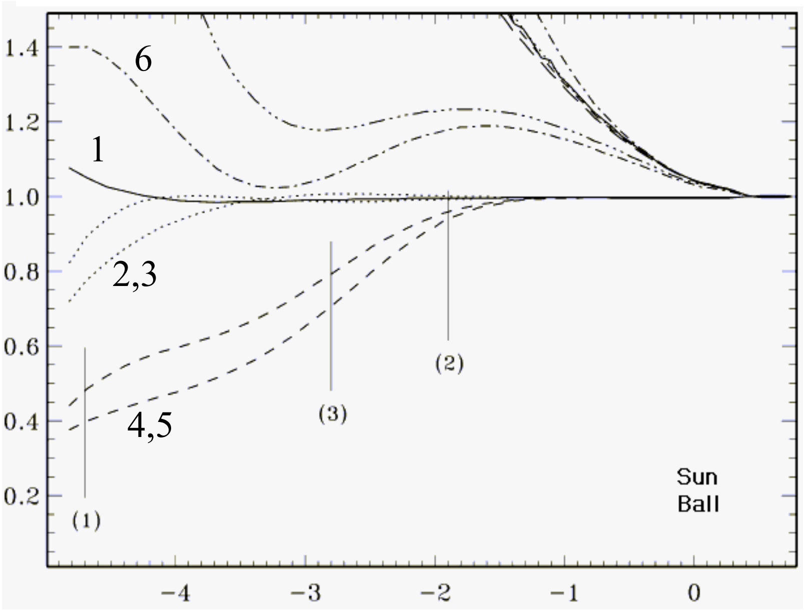
Al I: $b_i < 1, \quad n_{\rm NLTE} < n_{\rm LTE}$

overionization

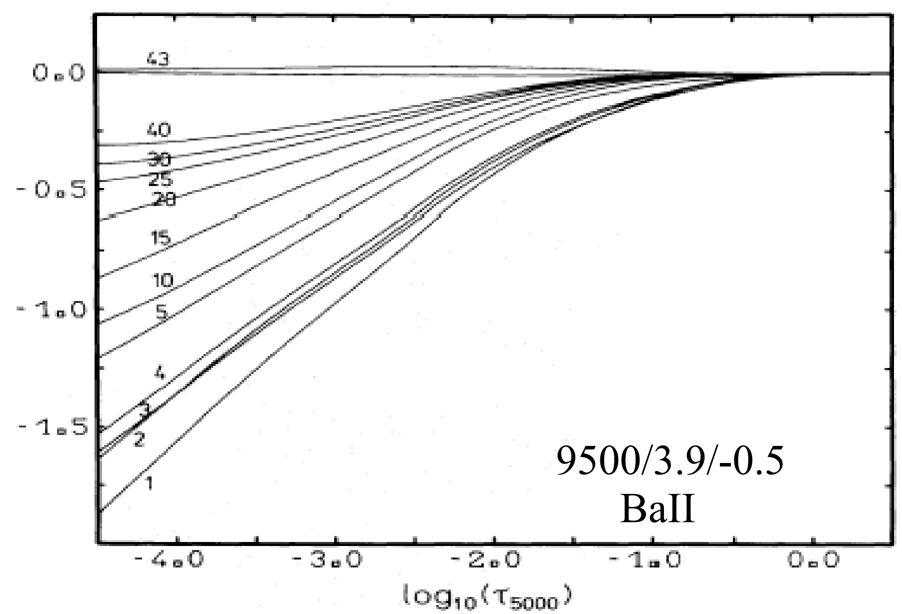
What is physics behind?

Departure coefficients for the selected levels of Ba II in the atmospheres of the Sun and Vega

Mashonkina et al. 1999



Gigas 1988



Ba II is the majority species

$n_{\mathrm{NLTE}}(\mathrm{BaII}) = n_{\mathrm{LTE}}(\mathrm{BaII})$

but $b_i \neq 1$ for excited levels

Ba II is the minority species

$b_i < 1$

$n_{\mathrm{NLTE}}(\mathrm{BaII}) < n_{\mathrm{LTE}}(\mathrm{BaII})$

overionization

Population and depopulation processes in atoms

UV overionization

is produced by superthermal radiation of non-local origin.

$R_{ik} \sim J_\nu\ (\lambda \leq \lambda_{thr})$ non-local

$R_{ki} \sim B_\nu\ (T)$ local

If $J_\nu\ (\tau_\nu < 1) > B_\nu\ (T)$

in the continuum of particular level, photoionization is so fast that recombination cannot keep up.

- Depopulation process

for low-lying levels in the atmospheric layers optically thin for ionizing radiation.

Bruls et al. 1992

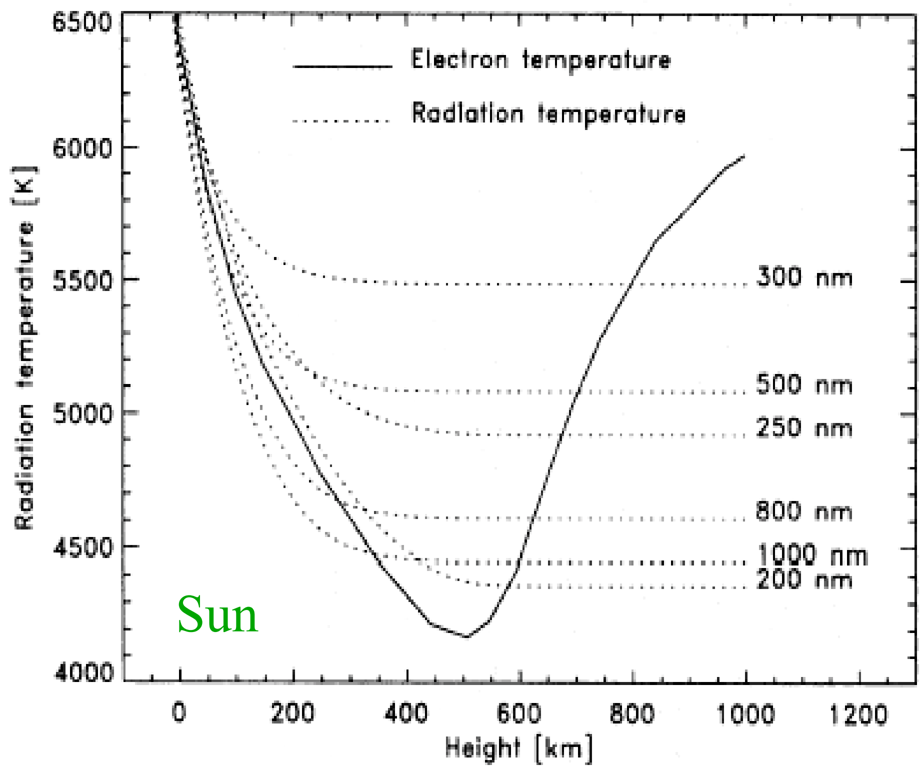


Fig. 3. Dotted: Equivalent black body radiation temperatures at different wavelengths. Solid: VAL3-C electron temperature

Solar photosphere (h < 500 km):

$T_R > T_e \rightarrow J_\nu > B_\nu\ (T)$ for $\lambda \leq 5000$A

$T_R < T_e \rightarrow J_\nu < B_\nu\ (T)$ for $\lambda \geq 8000$A

Photon pumping

is produced by superthermal radiation of non-local origin at line frequencies (*b-b* analogon of UV overionization).

- Overpopulation of the upper level out of the lower level of the pumping transition
  where $\tau_{core} > 1$ and $\tau_{wing} < 1$.

Photon loss

When $\tau_0 < 1$ in a transition,

photoexcitation is deficient and radiative decays result in

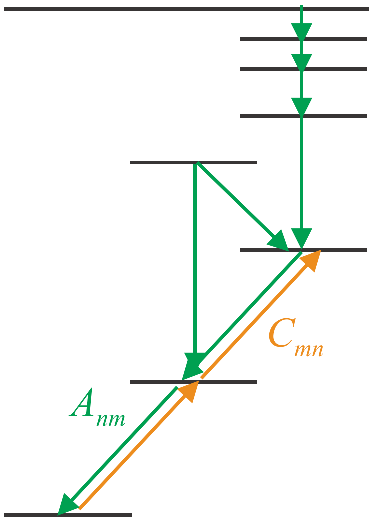
- overpopulation of the lower level out of the upper level (the reverse of photon pumping).

Resonance line scattering and photon loss

Photon loss is particularly important for the resonance lines.

Due to frequency redistribution in the scattering process a photon can escape in the line wings from the layers far below the location of $\tau_0 = 1$.

Photon suction



Photon losses in a sequence of downward transitions from close to the ionization limit down to the lower levels can siphon an efficient flow of electrons downward.

- Photon suction tends to overpopulate low-lying levels.

It works for the minority species where the next ionization stage is a large reservoir and collisional b-f transitions produce net recombination.

Important! The highest levels in the model atom have to be separated from the continuum by $\leq kT$.

NLTE effects for spectral lines

1) a change in the line opacity

$$\chi_\nu^l \sim n_i \left(1 - \frac{n_j}{n_i}\frac{g_i}{g_j}\right) \sim b_i \left(1 - \frac{b_j}{b_i} e^{-h\nu/kT}\right)$$

$$\chi_\nu^l \sim b_i$$

- if $h\nu/kT > 1$,

  $b_i < 1$ weakening compared to LTE

  $b_i > 1$ strengthening compared to LTE

$$\chi_\nu^l \sim b_i (1 - (1+\beta)(1-\delta))$$

- if $h\nu/kT = \delta < 1$,

  weakening can transform to emission if $b_j > b_i$!

NLTE effects for spectral lines

2) a change in the line source function

$$S_\nu^l = \frac{2h\nu_{ij}^3}{c^2} \frac{1}{\frac{n_i}{n_j}\frac{g_j}{g_i} - 1} = \frac{2h\nu_{ij}^3}{c^2} \frac{1}{\frac{b_i}{b_j}\left(e^{h\nu/kT} - \frac{b_j}{b_i}\right)}$$

- if $h\nu/kT > 1$, $S_\nu^l \approx B_\nu(T) b_j / b_i$

$b_j > b_i \rightarrow$ $S_\nu^l > B_\nu(T)$ $\rightarrow$ weakening compared to LTE

$b_j < b_i \rightarrow$ $S_\nu^l < B_\nu(T)$ $\rightarrow$ strengthening compared to LTE

- if $h\nu/kT = \delta < 1$, $S_\nu^l \approx B_\nu(T) b_j / b_i (1 - \beta / \delta)^{-1}$

Strong non-LTE effects for tiny populations divergences!

NLTE effects for spectral lines

- Changes in the line opacity and the line source function can work in one direction and in opposite directions.

- Non-LTE effects may be of opposite sign for the core and wings of a line because *b*-factors vary over atmospheric depths.

- A combined effect on the line strength may be either weakening or strengthening depending on b_i and b_j/b_i in line formation layers.

How is the statistical equilibrium of atoms achieved?

SE of an atom is a result of interaction and competition of all population and depopulation processes, and it depends on the conditions in atmosphere and atomic parameters.

Atoms in their minority ionization stage are particularly sensitive to non-LTE because any small change of ionization rates largely changes its population.

Atomic Properties

Ionization edges and threshold photoionization cross-sections:

Ion	Level	λ_0 [nm]	a_0 [MBarn]
H I	$n = 2$	364.7	15.84
Mg I	3s ^{1}S	162.1	0.2
	3p ^{3}P^o	251.4	15.8
	3p ^{1}P^o	375.7	80.0
Al I	3p ^{2}P^o	207.1	63.0
Ca I	4s ^{1}S	203.1	
7.8			
	4p ^{3}P^o	294.0	15.8
Fe I	a^{5}D	156.9	7.9
	a ^{5}F	176.0	5.6
Na I			
K I			

Fe I has a large number of additional *b-f* absorption edges between 200 and 300 nm, all of them large.

Photoionization-dominated atoms

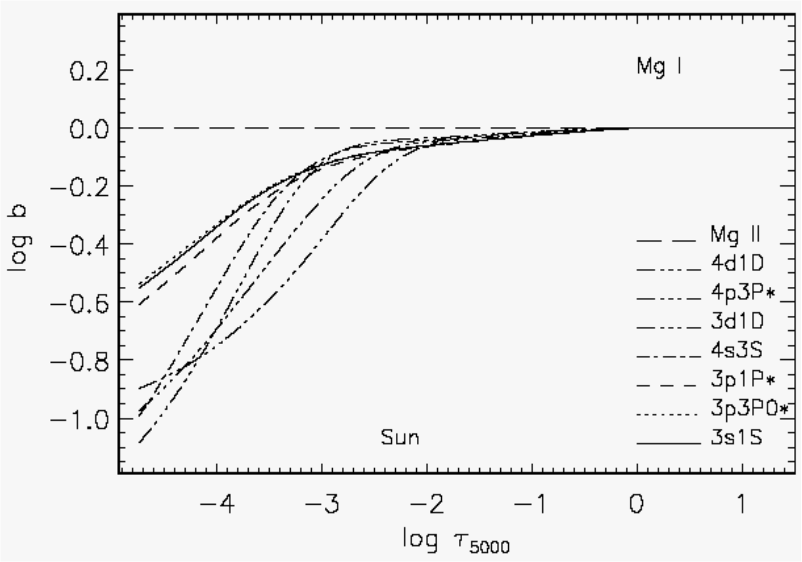
- Mg I (T_{eff} > 4500 K)

Main effect is overionization

of 3p $^3P^o$ and 3p $^1P^o$.

The population loss is redistributed over

many levels.



Photon losses in the strong lines lead to the stronger underpopulation of the upper level compared to that for the lower level.

$b_i < 1$,

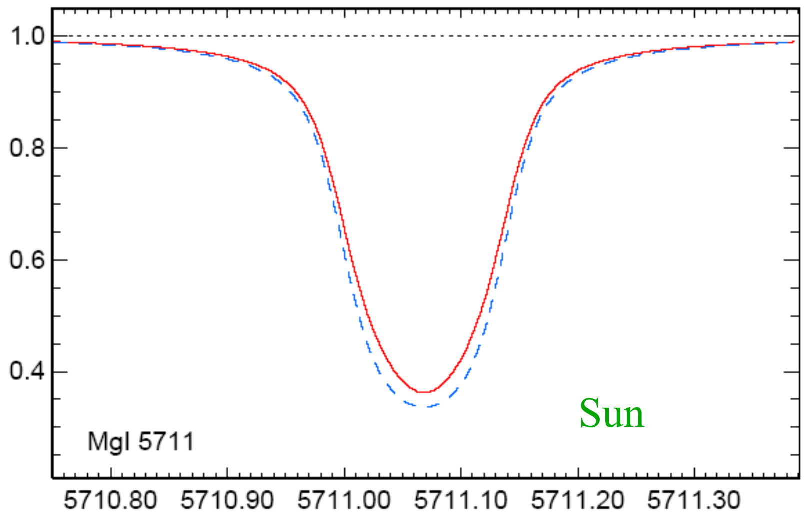
$b_j > b_i$ for weak lines,

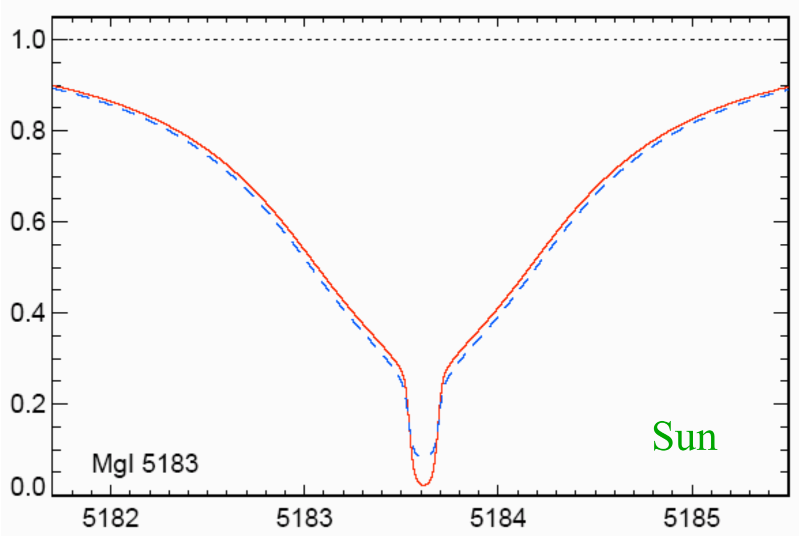
$b_j < b_i$ at $\log \tau < -2$.

- Al I, Si I, Ca I, Fe I show a similar behavior.
- At T_{eff} > 8500 K

  Ca II, Ba II, Sr II are photoionization-dominated ions.

Photoionization-dominated atoms. Effect on line profiles.





In non-LTE, the line is weaker due to $b_i < 1$ and $b_j/b_i > 1$.

The core is formed where photon loss defines $b_j/b_i < 1$.

The effects of overionization normally increase toward higher T_{eff} and lower log g and [Fe/H] due to strengthening the UV radiation.

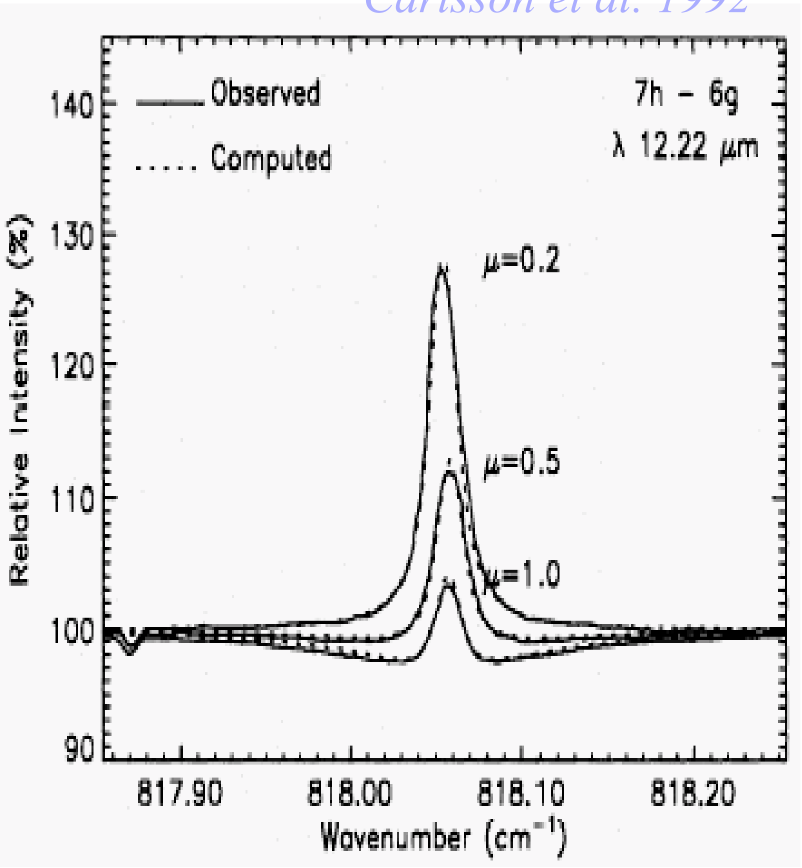
Non-LTE effects for the solar Mg I ~12 μm lines

$b_j/b_i > 1$ is a characteristic of the SE of photoionization-dominated atoms,

$h\nu_{ij}/kT < 1$ is a prerequisite to an appearance of emission line.

Non-LTE calculations for a standard 1-D model atmosphere without the chromosphere explain the formation of the emission lines of Mg~I in the solar spectrum near 12 μm

Carlsson et al. 1992



In the solar intensity spectra, Mg I ~12.2 μm is seen in emission

Alkalis are collision-dominated atoms

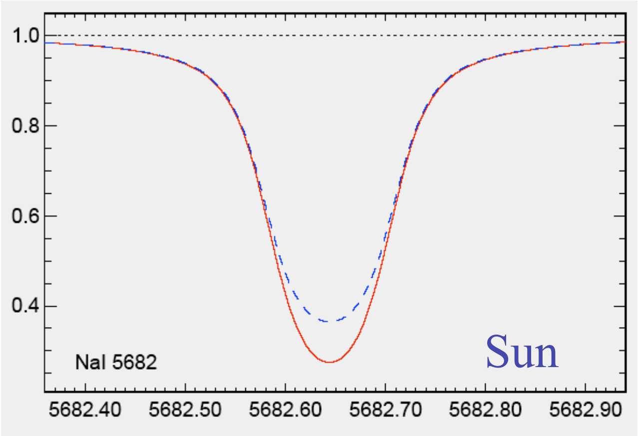
The SE of alkalis nearly does not depend on radiation field due to low photoionization cross-sections.

♦ Na I, K I ($T_{eff} > 4500$ K)

Photon suction → $b_{1,2} > 1$, $b_i < 1$ ($i \geq 3$)

- Photon suction is controlled by collisional thermalization.
- Non-LTE effects increase toward lower log g and [Fe/H].

In non-LTE, the lines are stronger due to $b_i > 1$ and $b_j/b_i < 1$.



Majority species: SE is controlled by *b-b* transitions.

♦ C I, N I, O I (cool stars).

Kiselman (1991, 1993):

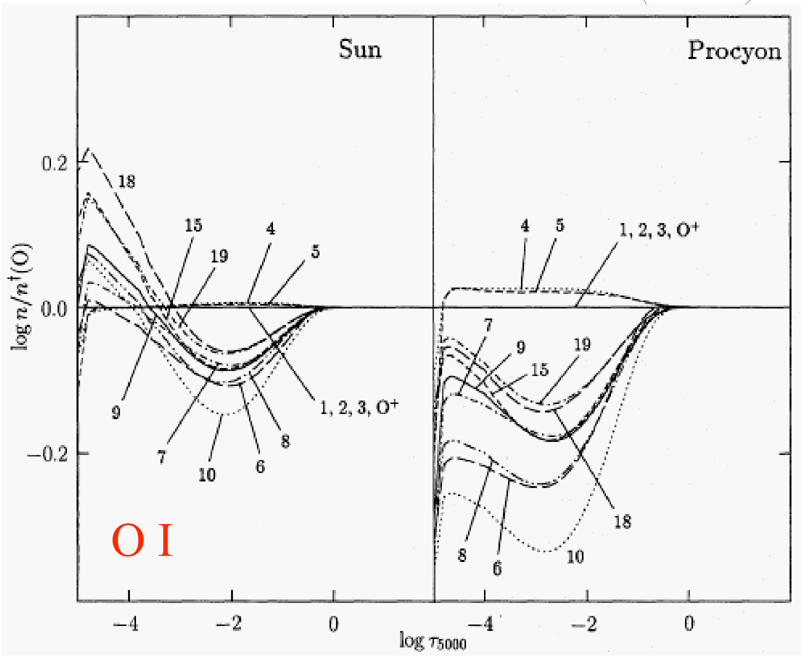
O I ~7770 A

(3s $^5S^o$ – 3p ^5P, 4 – 6)

– Photon loss in the line itself, $b_j < 1$.

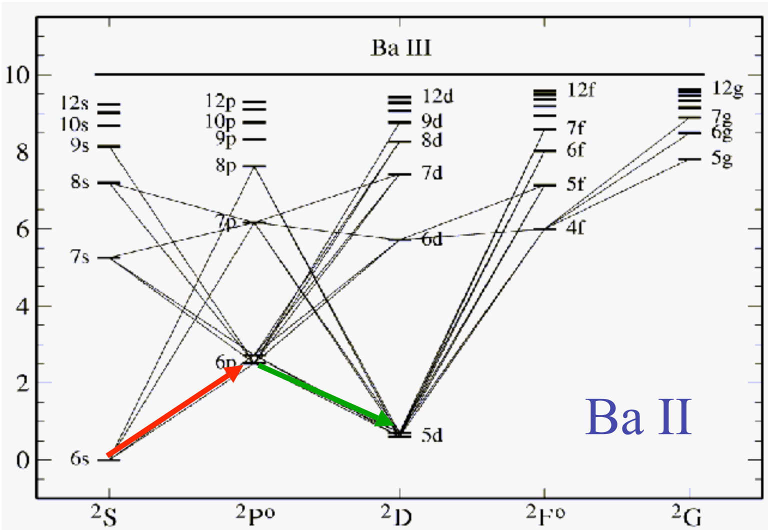
– O I 3s $^5S^o$ is metastable.

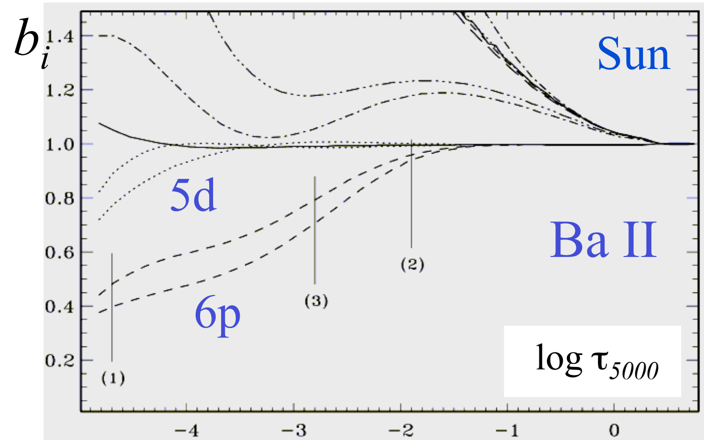
Takeda (1994)



Departure coefficients for the selected levels of O I in the atmospheres of the Sun and Procyon.

For the majority species, non-LTE effect depends on the line strength

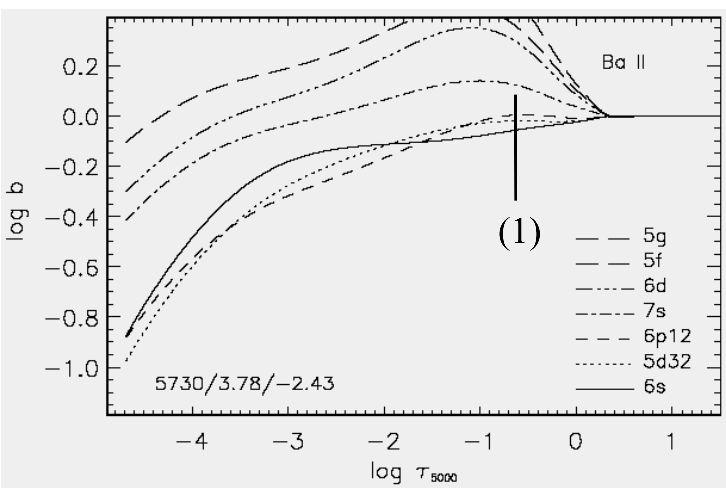




photon pumping in 6s – 6p competes with photon loss in 5d – 6p.

– Sun: photon loss depopulates 6p, lines are stronger in non-LTE.

– 5730/3.78/-2.43: photon pumping prevails over photon loss (b_j > b_1), lines are weaker in non-LTE.



Mashonkina et al. (1999)

Concluding remarks

- Combined effect of population and depopulation processes in atoms depends on

  the atomic *term structure*, *atomic data* and

  conditions in atmosphere.

- Departures from LTE in W_λ may be larger for the weaker lines compared to the stronger lines.

- Non-LTE effects for the lines of the majority species may be large enough.

- It is impossible to predict not only a value but sometimes also a sign of non-LTE effect in advance of SE calculations.