Non-LTE line formation for trace elements in stellar atmospheres,
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Accurate collision cross-sections: important non-LTE input

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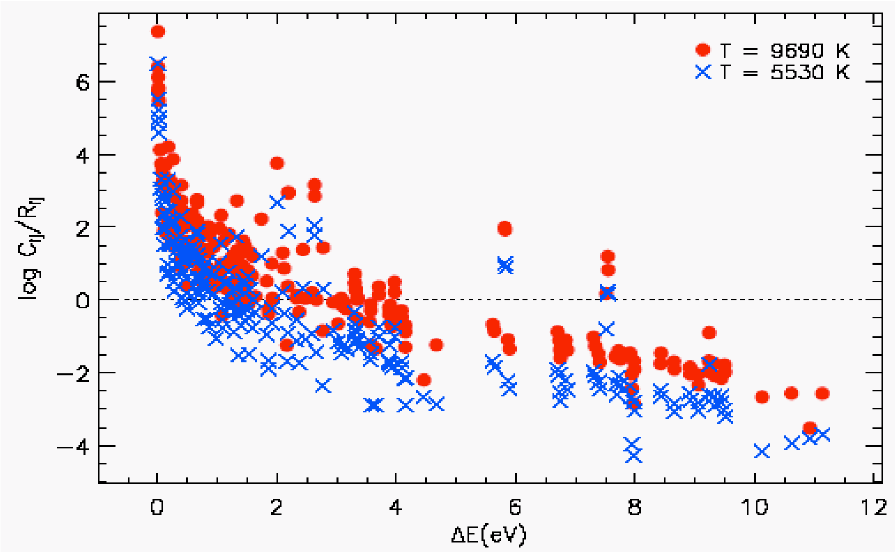
Inelastic collisions versus radiative processes in stellar atmospheres

ΔE > 5 eV, radiative processes dominate,

ΔE < 0.2 eV, strong collisional coupling,

0.2 eV < ΔE < 5 eV,

accurate collision cross-sections are particularly important.



C_{ij}/R_{ij} ratios for the Ca II transitions at log $\tau_{5000} \cong -0.5$ in the models 5780/4.44 (T = 5530K) and 9400/3.70 (T = 9690K)

Electron impact excitation and ionization

Among all particles the collision frequency is the highest for electrons, $\mathrm{v}_e / \mathrm{v}_\mathrm{A} = (m_A / m_e)^{1/2}$

Sources of cross-sections.

- Laboratory measurements: for the transitions mostly from the ground state of atoms.
- Quantum-mechanical calculations (the R-matrix method in the close-coupling approximation) of collision *excitation* cross-sections exist for the selected atoms and ions.

More data is expected from the Iron Project.

An accuracy is a few 10%.

• Approximation formulae for the majority of the transitions in atoms. Accurate to a factor of 2 to 10.

Collision excitation.

- *Sobelman et al.* (1981) cross-sections in the Born I approximation for neutrals,
- *van Regemorter* (1962) semi-empirical formula for allowed transitions,

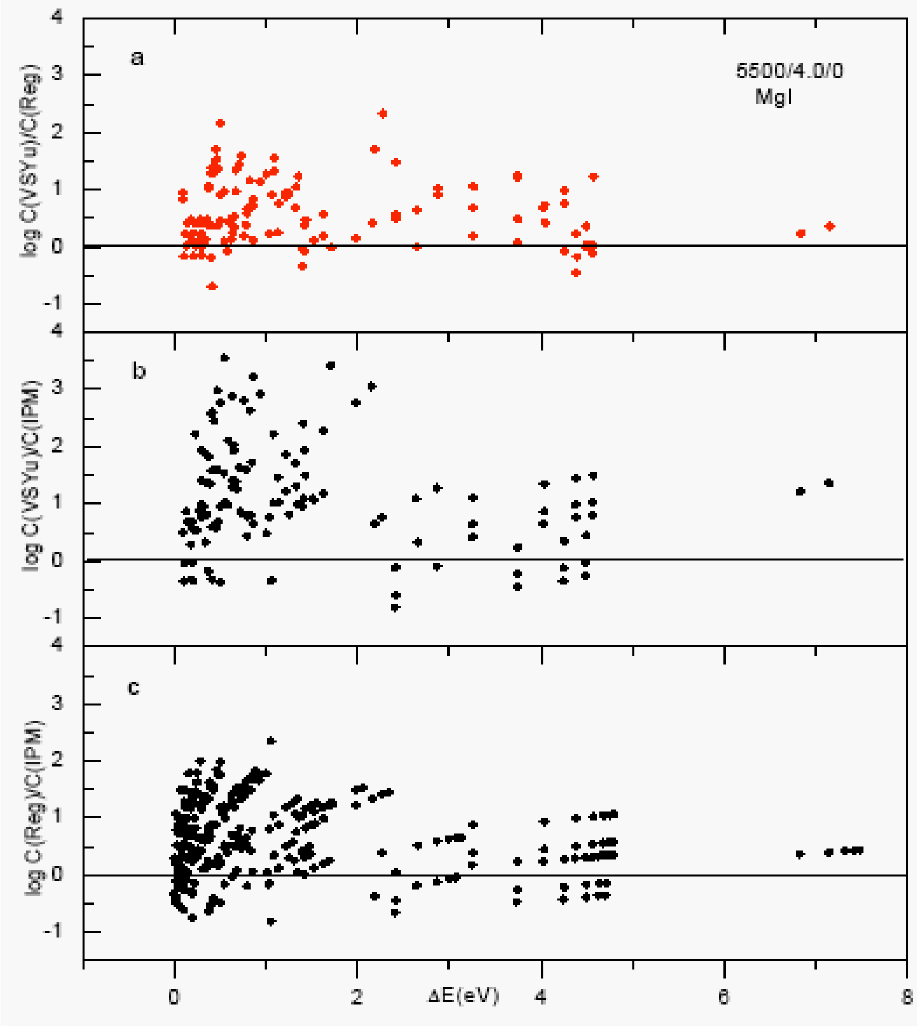
$$C_{ij} = n_e \times 3.2 \times 10^{-8} f_{ij} \left(\frac{Ryd}{\Delta E} \right)^{3/2} \beta^{1/2} e^{-\beta} P(\beta), \qquad \beta = \Delta E / kT$$

- the impact parameter method (IPM, *Seaton* 1962) for allowed transitions,
- the Eissner-Seaton formula for forbidden transitions

$$C_{ij} = n_e \times 8.631 \times 10^{-6} \frac{1}{g_i \sqrt{T}} e^{-\beta} \Omega_{ij}$$ with a collision strength $\Omega_{ij} = 1$.

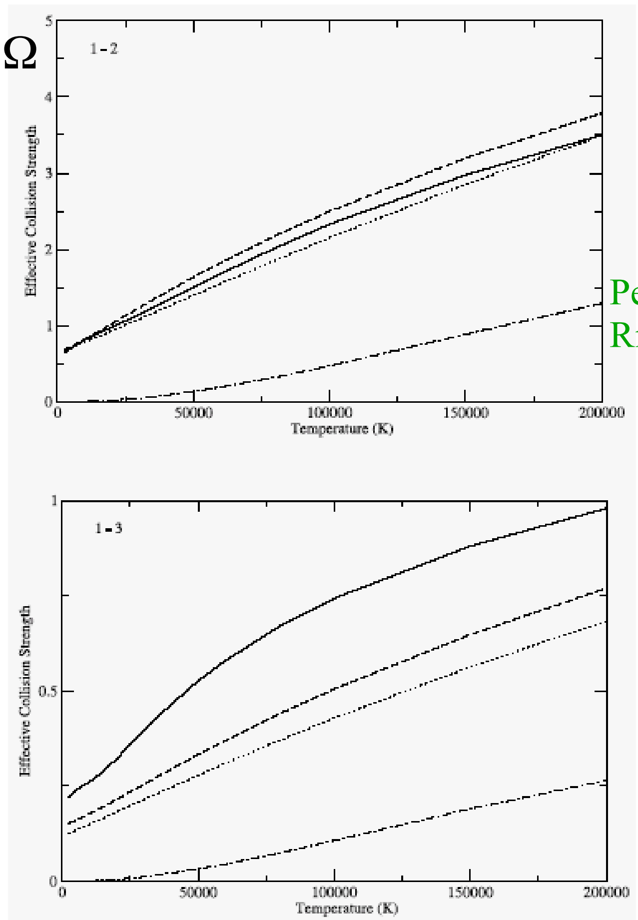
Comparisons among theoretical approximations

- The Born approximation leads to the larger rates compared to those from the van Regemorter formula,
- the van Regemorter rates are larger than the IPM rates



The rate ratios for the transitions in Mg I.

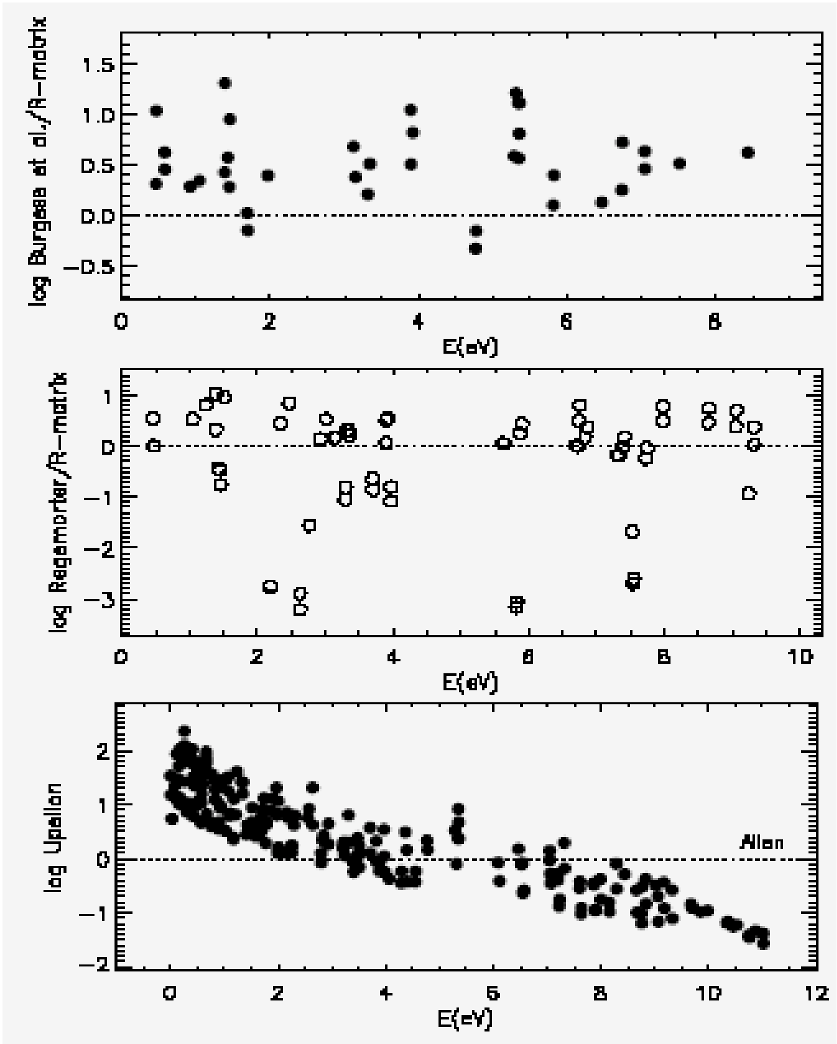
Comparisons of theoretical approximations with the R-matrix method predictions



Persival&
Richards 1978

H I, R-matrix method calculations
of Butler (continuous line).

Fig. 1 from Przybilla&Butler (2004).



Ca II, R-matrix method calculations
of Melendez et al. (2007)

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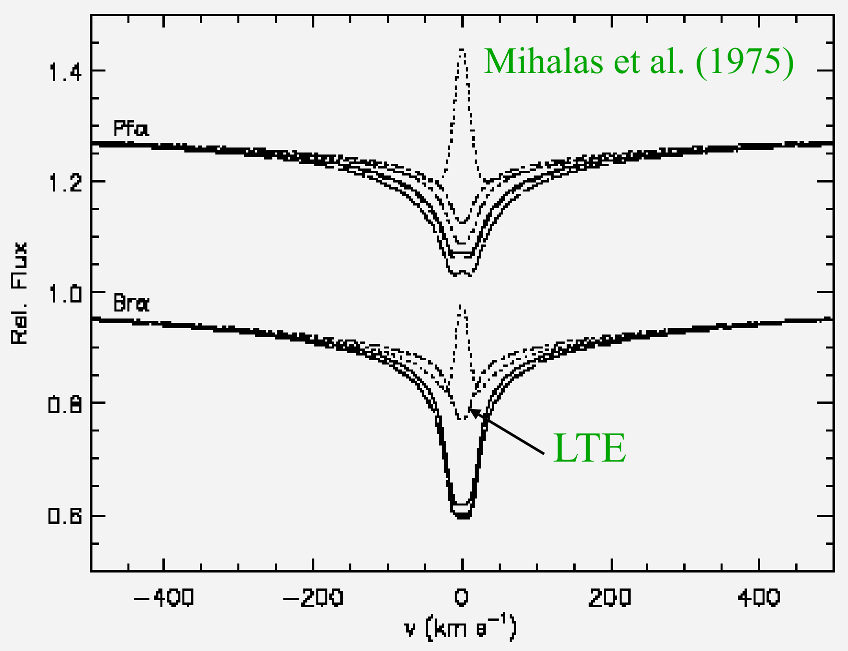
How do the uncertainties in the atomic data translate to uncertainties in the non-LTE modelling?

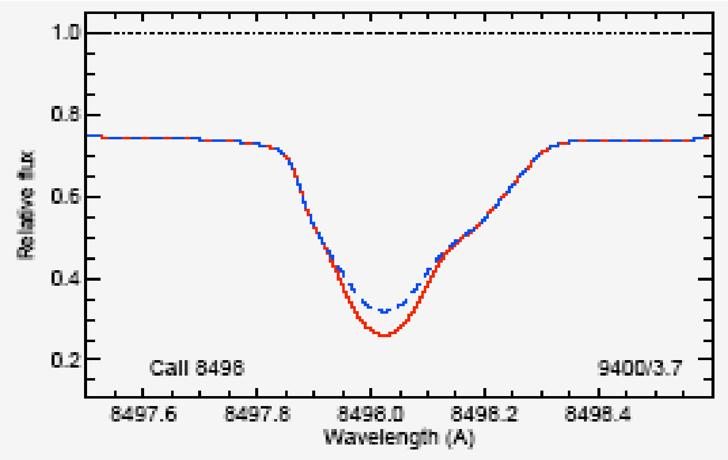


Theoretical profiles for

Pf_α and Br_α in Vega for various

electron collision rates.

(Przybilla & Butler 2004)



Non-LTE profiles for Ca II 8498 in the model 9400/3.7 for the R-matrix method data (continuous line) and approximation formulae (dashed line).

Effect on abundance determinations

The van Regemorter rates vs. the IPM rates

for T_{eff} = 6000 K, log g = 4.0, [Fe/H] = 0 to -3.

A change in $\Delta_{NLTE} = \log \varepsilon(NLTE) - \log \varepsilon(LTE)$:

$\leq$ 0.03 dex for different lines of Ca I,

0.07 dex to 0.14 dex for different lines of Ca II.

(Mashonkina et al. 2007a)

Collision ionization

For the excited levels:

semi-empirical formulae based on the classical Thomson theory.

They should provide data accurate to a factor of 2 or better.

The *Seaton* (1962) formula:

$$C_{ik} = n_e \times 1.55 \times 10^{13} \alpha_{i,thr} \frac{\overline{g_i}}{\beta \sqrt{T}} e^{-\beta}$$

Here, $\alpha_{i,thr}$ is the threshold photoionization cross-section,

$\overline{g_i}$ = 0.1, 0.2, and 0.3 for Z = 1, 2, and ≥ 3.

Inelastic collisions with hydrogen atoms

In the atmosphere of solar-type stars, $n_H/n_e \geq 10^4$.

Cross-sections ?

- Low-energy experimental data

  (for only the very lowest states of Na I, *Fleck et al.* 1991),
- quantum mechanical calculations

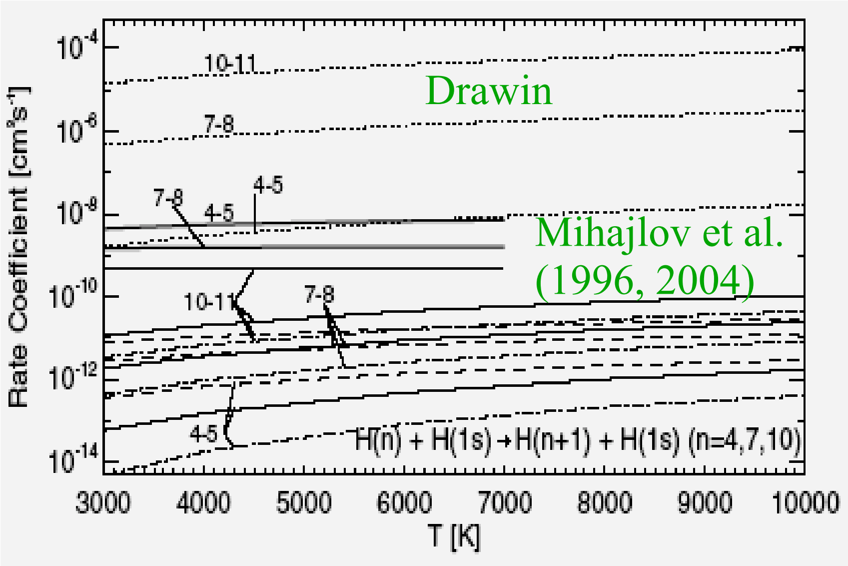
  (for the transitions between low-excitation levels in Li I, *Belyaev&Barklem* (2003) and Na I, *Belyaev et al.* (1999)),
- some theoretical approximations for the system H(n) + H(1s) (see review and detailed discussion in *Barklem*, 2007),
- the approximation formula of *Drawin* (1968,1969). This is a semi-empirical modification of the classical Thomson formula for ionization by electrons.

Data comparisons

- The Drawin's formula vs. experimental data and quantum mechanical calculations.

  The resonance transitions in Li I and Na I: the classical formula overestimates the cross-sections by 3 dex to 5 dex.

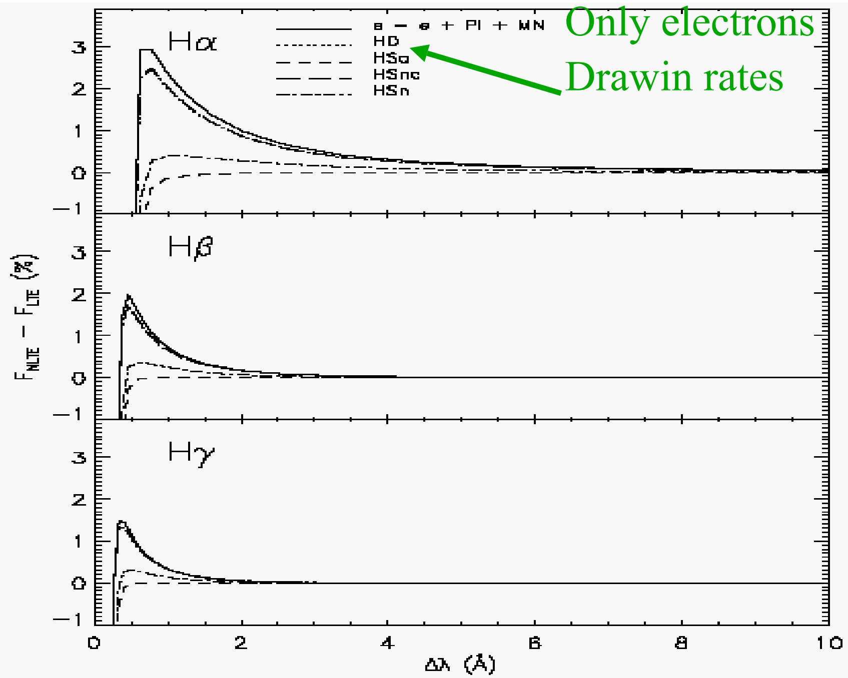
Barklem (2007)



Excitation rates for
the $n - (n+1)$ transitions in H I
from different approximations

- The Drawin's formula vs. the semi-classical data of *Mihajlov et al*. (1996, 2004) for H I.
  For the transition 4 – 5, a consistency within a factor of 2.
  A discrepancy increases up to 3 dex / 5 dex for n = 7 / n = 10.

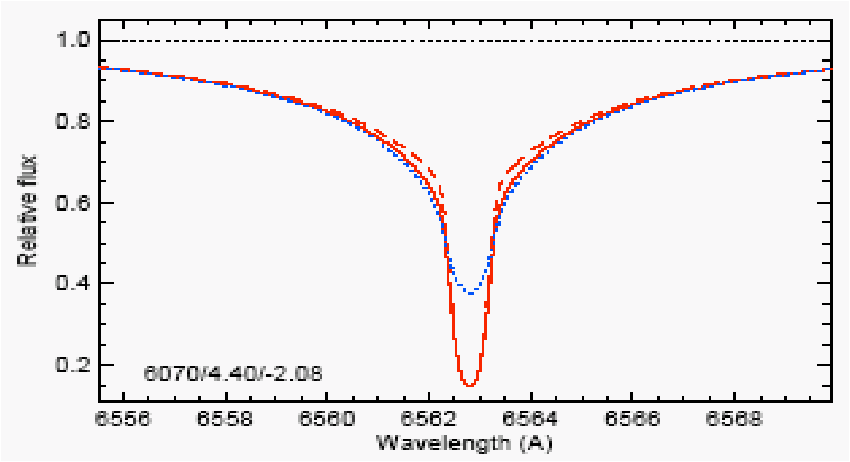
How do the uncertainties in the atomic data translate to the uncertainties in non-LTE modelling?



Barklem (2007): the differences between the non-LTE and LTE profiles for different collisional data, MACKKL solar model.

Hydrogen collisions à la Drawin are relatively unimportant for the SE of H in the Sun.

How do the uncertainties in the atomic data translate to the uncertainties in non-LTE modelling?



The effect of the inclusion of the Drawin hydrogen collisions (continuous curve) for the metal-poor model.
Dashed curve: only electronic collisions.
Dotted curve: LTE.
(Mashonkina et al. 2007b):

6070/ 4.4/-2.08:
The inclusion of the Drawin hydrogen collisions leads to a 100 K lower T_{eff} from H_{α}.

Experimental and quantum mechanical data predict a minor role of hydrogenic collisions in the SE of atoms.

What do observations say?

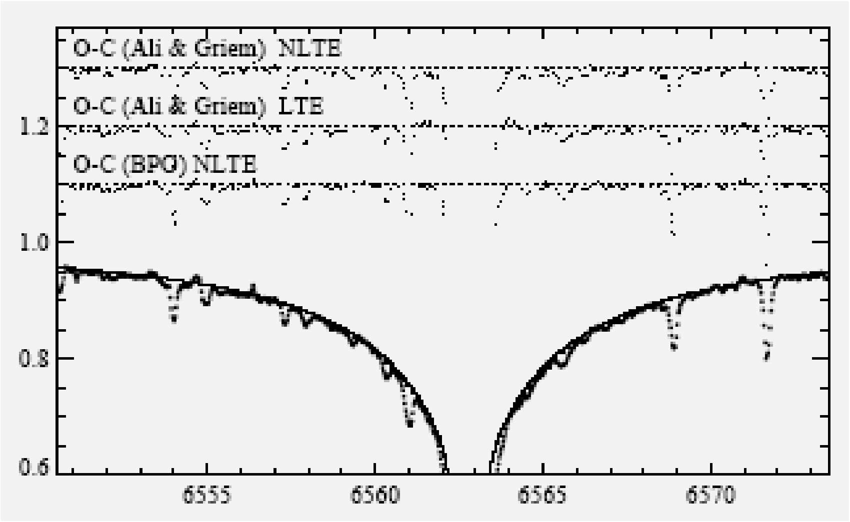
Empirical estimation of the efficiency of hydrogen collisions

It is represented by a scaling factor S_H applied to the Drawin's formula as described by Steenbock&Holweger (1984).

- H I: S_H can be estimated from achieving a consistency of T_{eff} derived from H_α and H_β.

Mashonkina et al. (2007b):
for four VMP ([Fe/H] < -2) stars,
S_H = 1 to 2.

Example: BD+3°740
(log g = 3.90, [Fe/H] = -2.65).
T_{eff} = 6340 K from H_β.
T_{eff} = 6440 K from H_α, $S_H = 0$.



H_α in BD+3°740 (bold dots).
LTE: T_{eff} = 6280 K,
non-LTE (S_H = 2): T_{eff} = 6340 K.

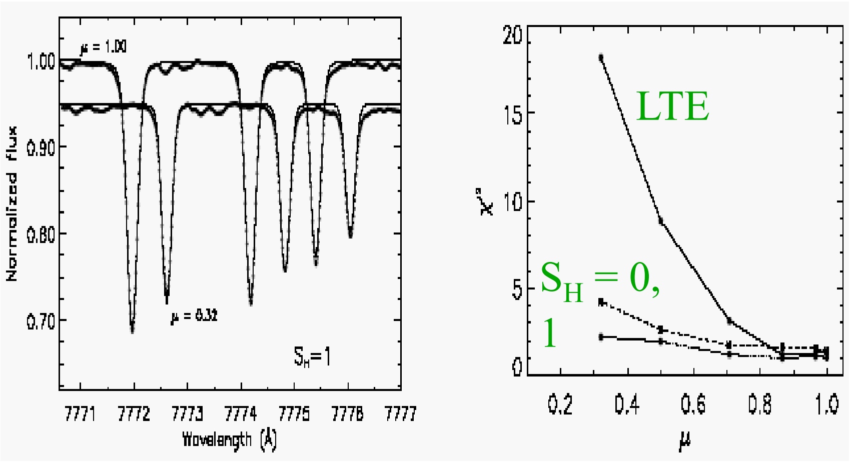
Empirical estimation of S_H

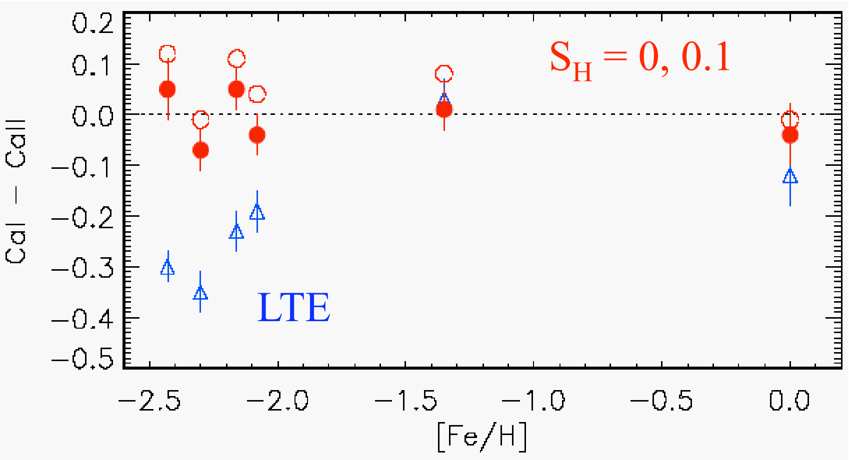
- from studying the center-to-limb variation of solar Na I 6160 and O I triplet ~7770 Å

(Allende Prieto et al. 2004)

- from the CaI/CaII ionization equilibrium in the Sun and selected metal-poor stars

(Mashonkina et al. 2007a)





$S_H = 1$ from O I ~7770 Å, $S_H = 0$ from Na I 6160

Variation in the quality of the fits

$S_H = 0.1$

Empirical estimation of S_H

- Solar line profile fitting.

  O I: $S_H = 1$ (*Takeda* 1995),

  Na I: $S_H = 0.05$ (*Gehren et al.* 2004),

  0.1 (*Takeda* 1995),

  Al I: $S_H = 0.002$ (*Gehren et al.* 2004),

  K I: $S_H = 0.05$ (*Zhang et al.* 2006),

  Sr II, Ba II: $S_H \cong 0$

  (*Mashonkina&Gehren* 2000, 2001)

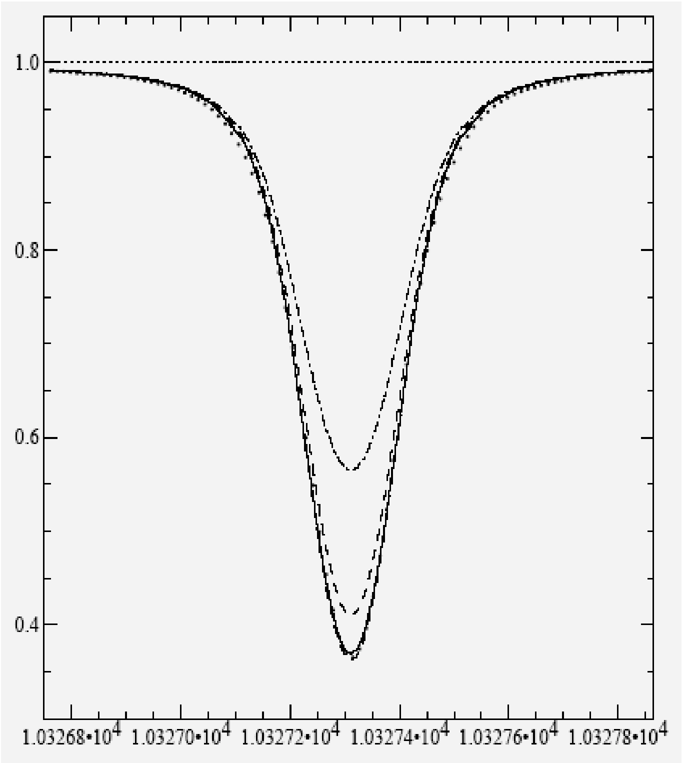
- Spectral analysis of RR Lyr type stars (*Gratton et al.* 1999).

  O I: $S_H = 3$,

  Na I: $S_H = 0.01$,

  Mg I: $S_H = 3$,

Mashonkina&Gehren (2001)



Sr II 10327 in the Sun (bold dots)
$S_H = 0$ (long-dashed curve),
0.01 (continuous curve),
0.1 (dashed curve), and
LTE (dash-dotted curve).

Concluding remarks

- Collisional data used in non-LTE calculations have various degrees of accuracy.
- A practice points to the existence in stellar atmospheres of some thermalization processes in addition to electronic collisions.
- The empirical estimates of the efficiency of hydrogen collisions are obtained to be rather different for different atoms.
- The collisional efficiency may well differ from element to element and transition to transition.
- A calibration may mean that any modelling deficiency (atmospheric structure, atomic data, stellar parameters, etc.) is simply hidden in S_H.