Role of input atomic data in *spectroscopic analyses of the Sun and metal-poor stars*

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Concepts

- Our goal is to determine effective temperature, gravity, chemical composition of a star using its observed spectrum
- How a spectrum is formed? → stellar atmosphere
- Methods: describe accurately a physical state of a stellar atmosphere
- → to construct a model, which is able to reproduce observed stellar fluxes and describe the properties of spectral lines for a unique set of (T_{eff}, log g, [Element/H], …)

A stellar atmosphere

- is a complex system, because both macro- and micro-scopic phenomena determine its *state:*

- macro: convection, pulsations, expanding envelopes, …

- micro: interactions on (sub)atomic scales

  photon - electron – atom - molecule

It is not possible at present to model all these phenomena simultaneously. Need *simplifications*.

Object definition

Focus is on late-type (FGK) stars with mass ~ 1 $M_\odot$

4000 < $T_{eff,\odot}$ < 6500 K

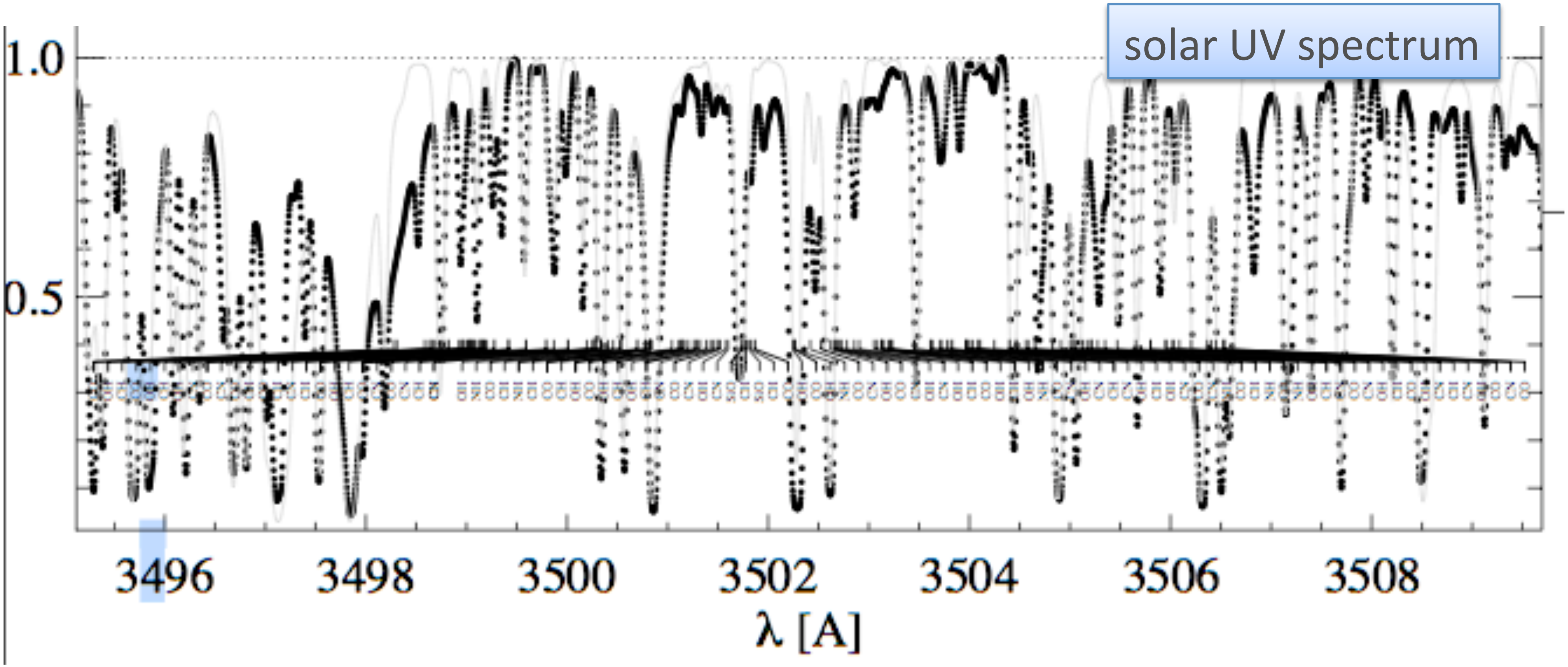
3 < $\log g_\odot$ < 5 , … < [Fe/H] < …

- *Low-mass stars*: very slow evolution on the MS
- Their atmospheres carry the same chemical composition as that of ISM, from which the stars formed
- Constraints on Galactic chemical evolution: *stellar populations (halo, disk), nucleosynthesis (SN II, SN Ia), IMF, mixing in the ISM, …*

Atmospheres late-type stars

- *Cool: rich atomic and molecular absorption* spectra (Fe I, Fe II, ...) possible to study different elements (Li, C, N, O, α – group, Fe-peak, r-, s-process)

- Convective envelopes, line blending, NLTE effects (change with stellar parameters)



Late-type stars: modelling & input atomic data

Construct a model atmosphere and use it to compute emergent stellar spectrum for comparison with observations

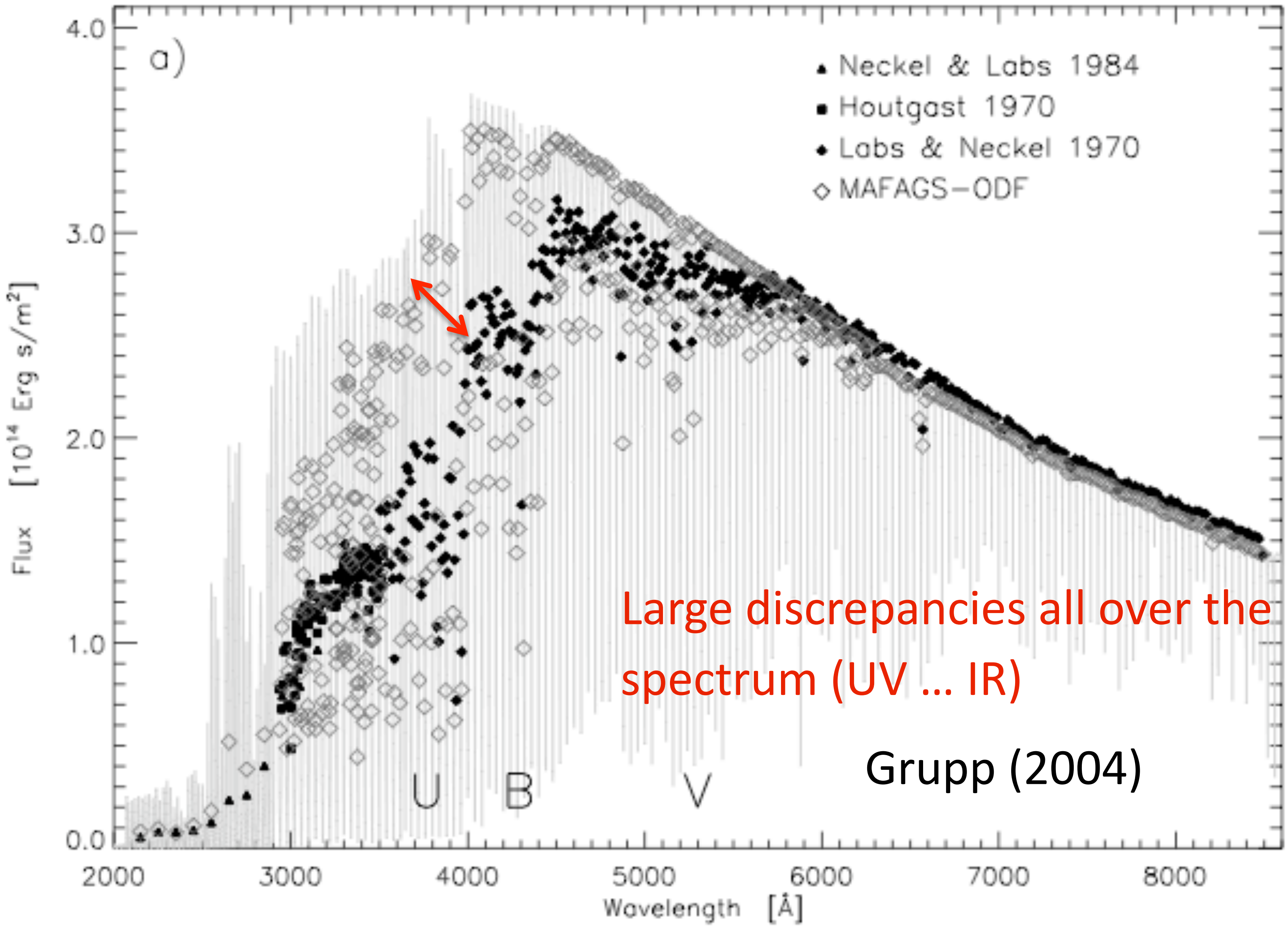
- b - b, b - f, f - f cross-sections (atoms, molecules, ions)

H^-, …

C, N, O, Mg, Al, Si, Ca, Fe (neutrals)

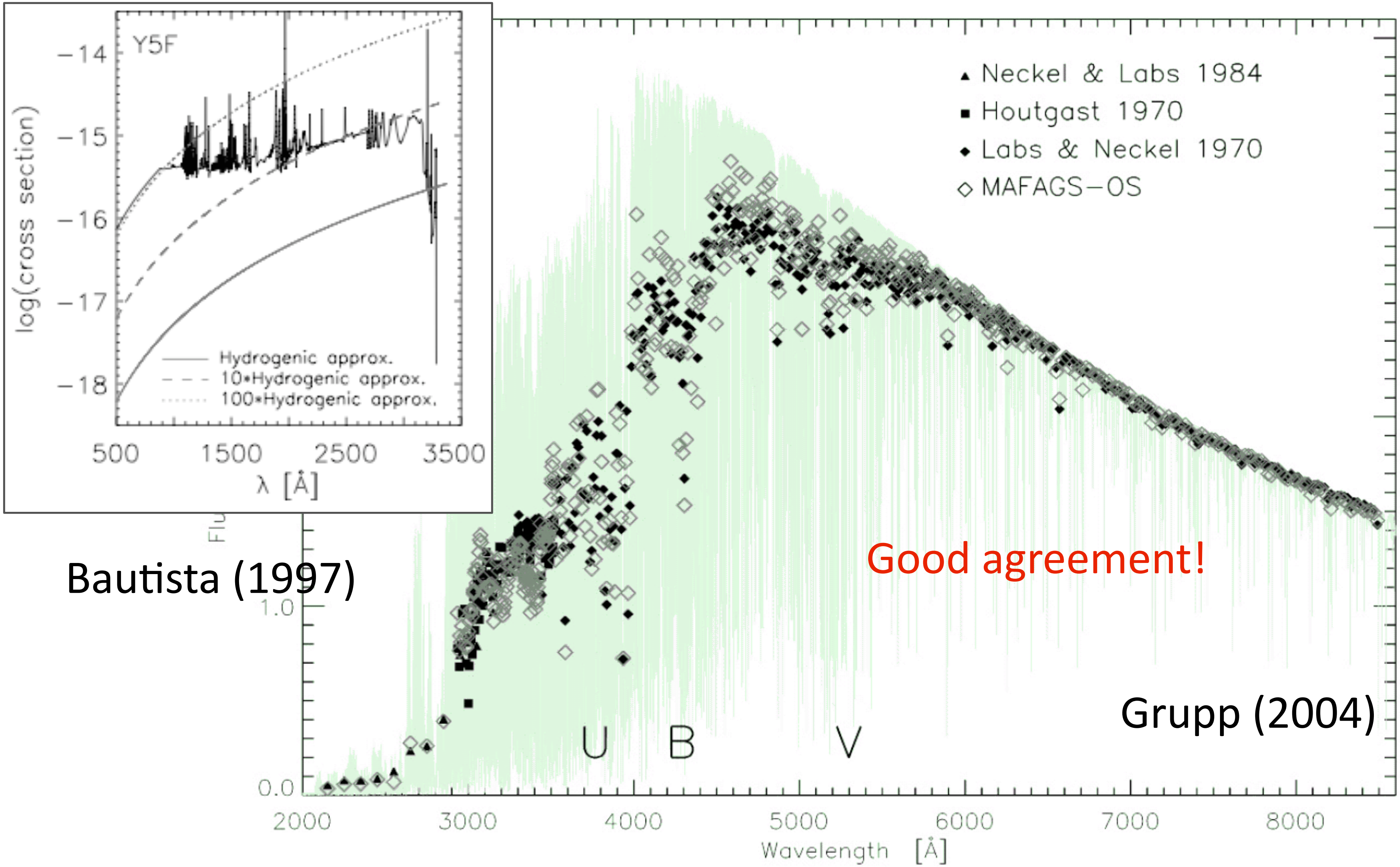
Tests of model atmospheres. I

Sun: theoretical emergent flux vs. observations (black dots)



Tests of model atmospheres. I

Sun: theoretical emergent flux with new bf cross-section for Fe I



Late-type stars: modelling & input atomic data

Construct a model atmosphere and use it to compute emergent stellar spectrum for comparison with observations

- b-b, b-f, f-f cross-sections (atoms, molecules, ions, electrons)
- for *each individual spectral line:* wavelengths, energies, oscillator strengths, line broadening parameters, hyperfine structure and isotopic shift (laboratory, if available)

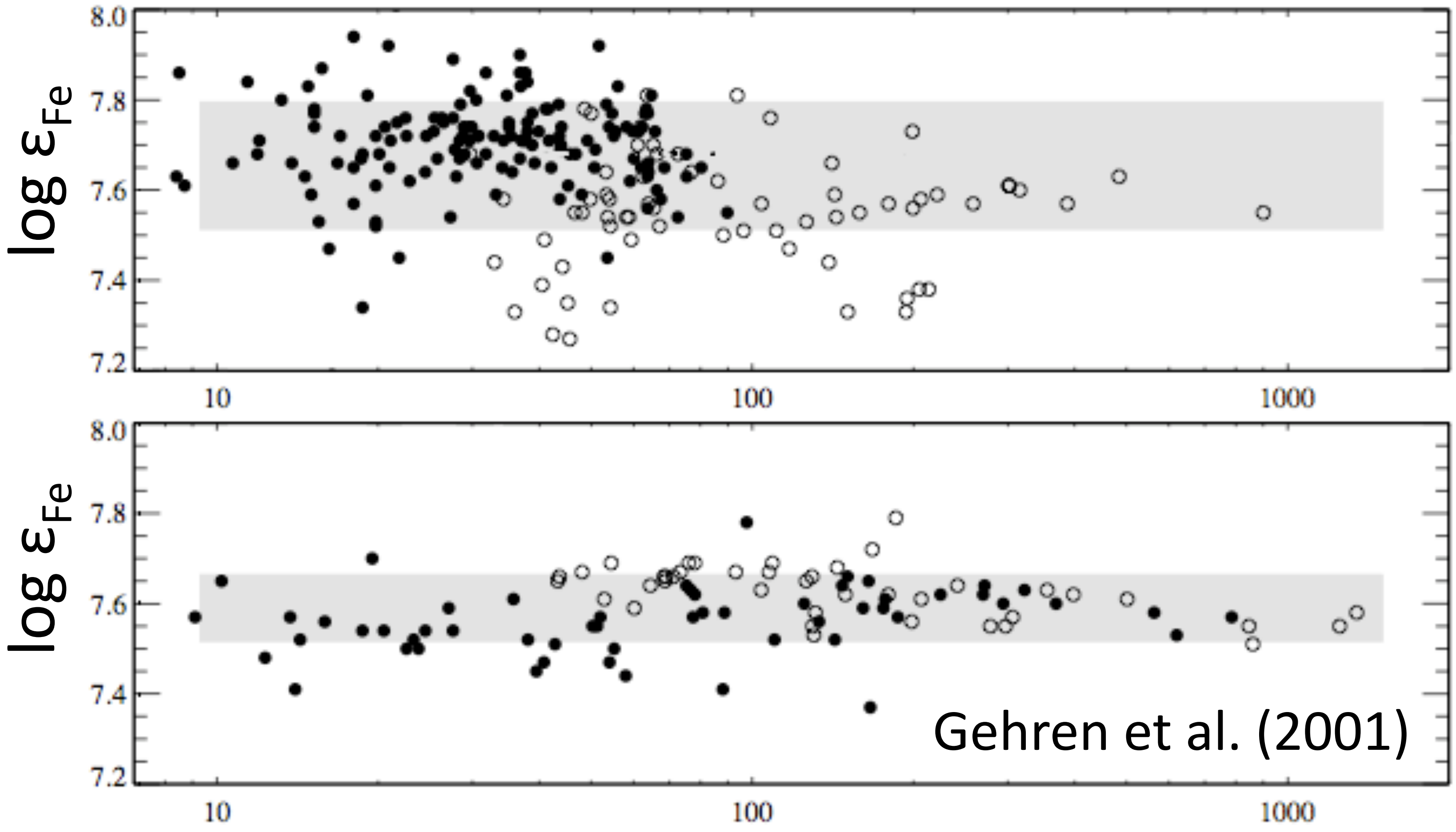
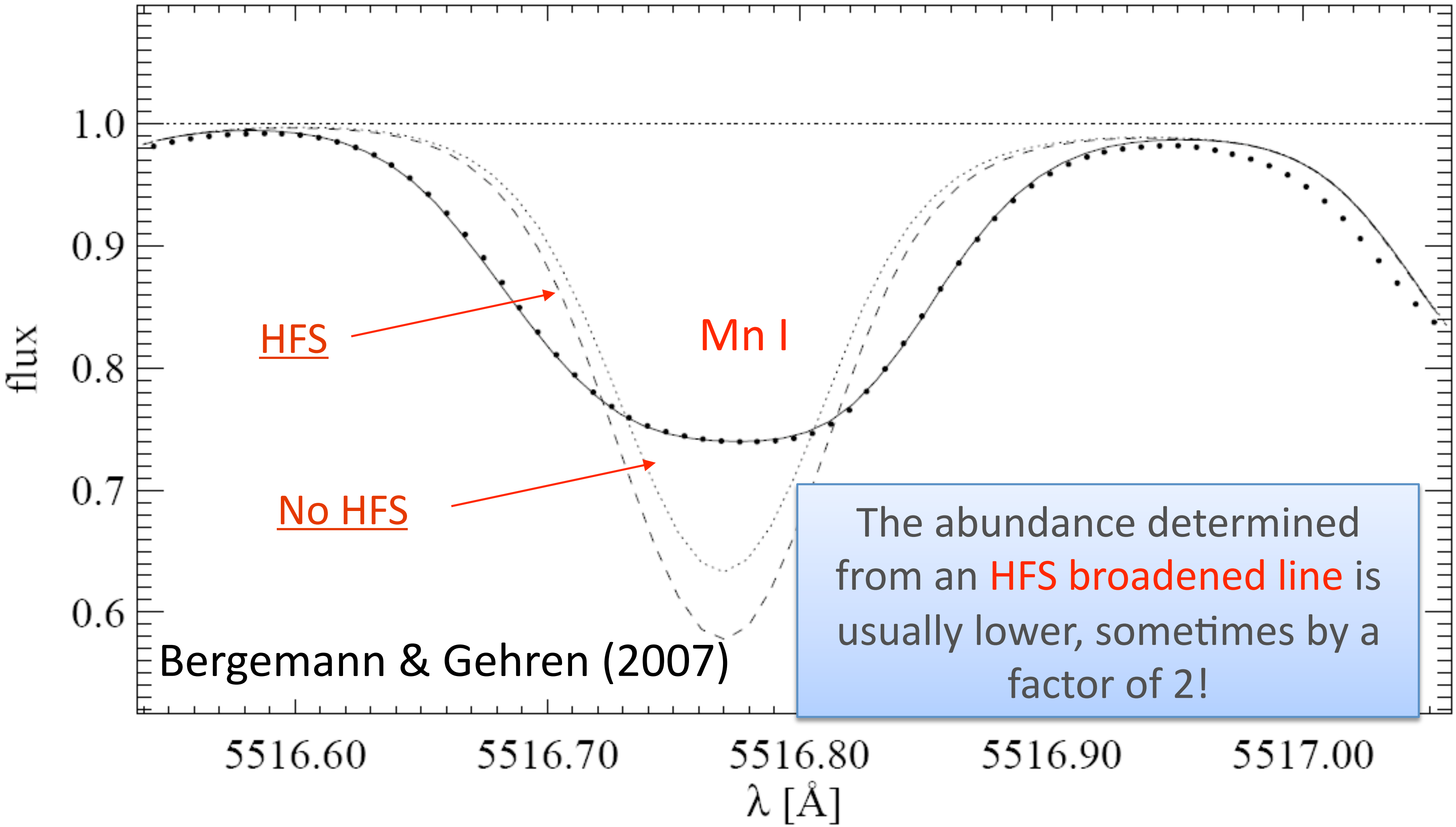


Fig. 8. Logarithmic solar abundances as a function of equivalent width in mÅ determined with the HM solar model in LTE and $\xi = 1.0$ km s^{-1}. *Top*: oscillator strengths from May et al. (1974, filled circles) and from O'Brian et al. (1991, open circles). *Bottom*: f-values from the Hannover group (sources p, q of Table 2, filled circles) and from the Oxford group (sources

Hyperfine structure

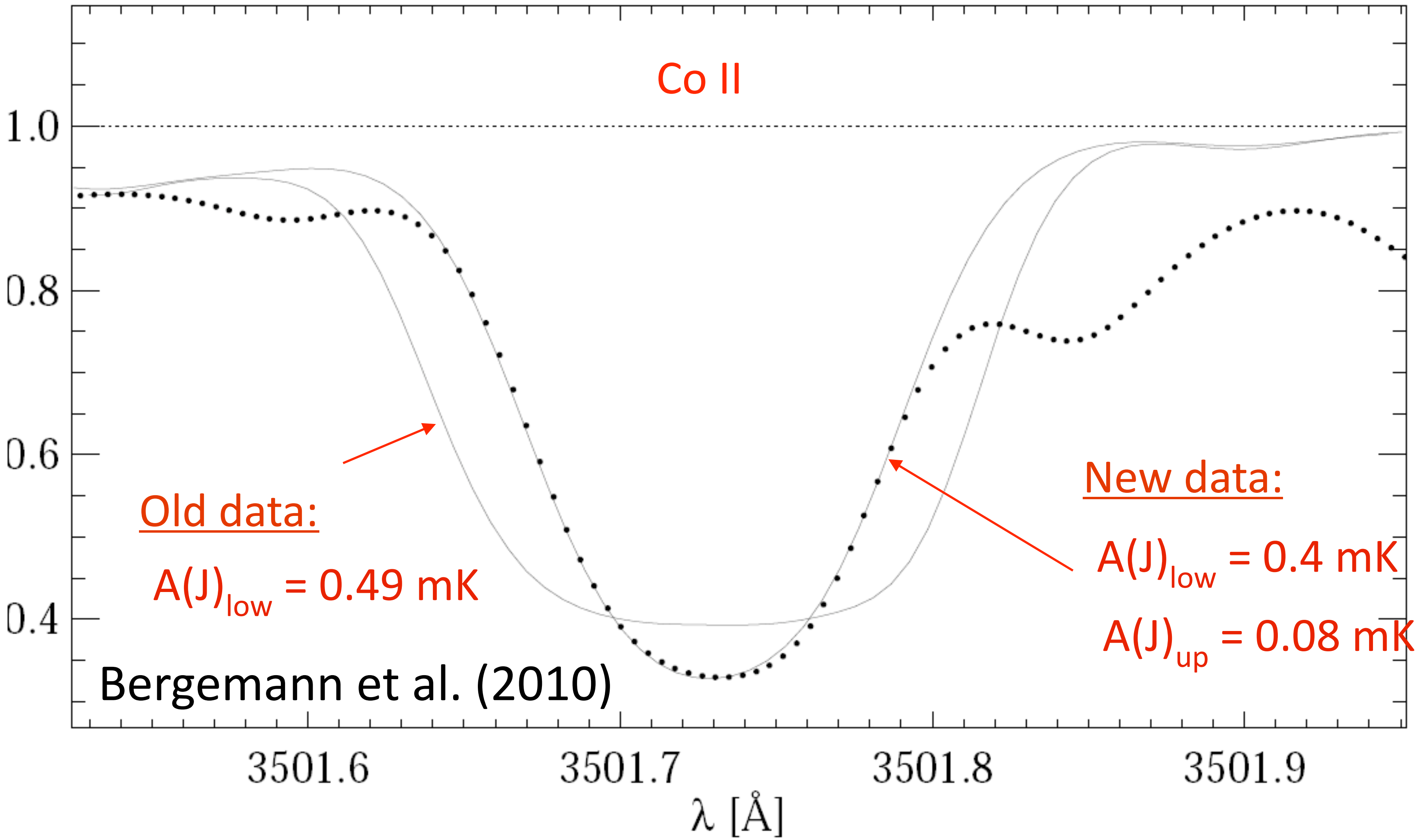
The effect of hyperfine structure is to desaturate a spectral lines.



The abundance determined from an HFS broadened line is usually lower, sometimes by a factor of 2!

Hyperfine structure

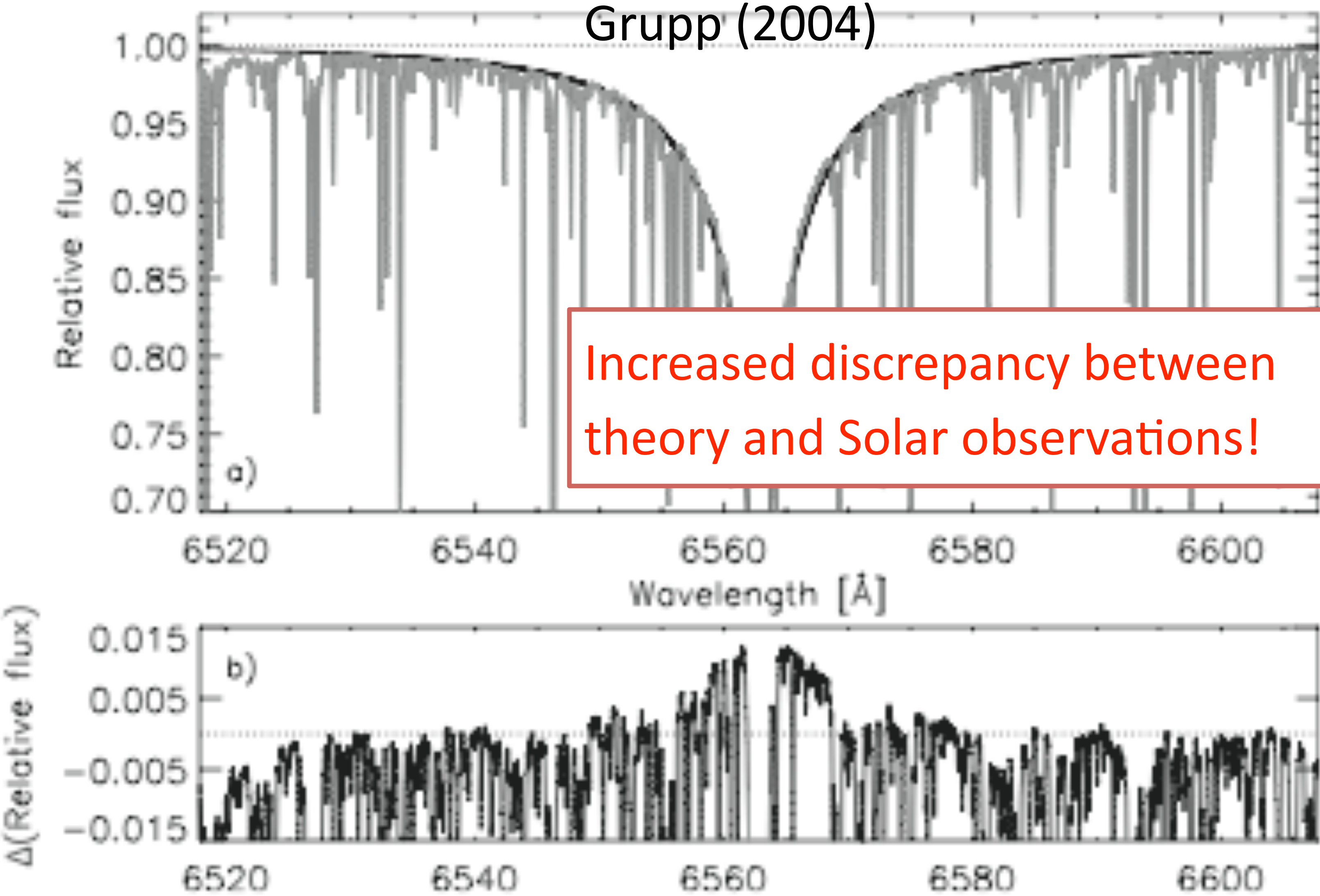
Solar abundances from Co II and Co I lines (NLTE) agree!



Tests of model atmospheres. II

Solar H_a line computed with Barklem et al. (2003) theory for the H self-broadening gives $T_{eff,\odot} \approx 5700 \ldots 5720$ K

Grupp (2004)



Increased discrepancy between theory and Solar observations!

Late-type stars: modelling & input atomic data

Construct a model atmosphere and use it to to compute emergent stellar spectrum for comparison with observations

- b-b, b-f, f-f cross-sections (atoms, molecules, ions, electrons)
- for *each individual spectral line:* wavelengths, energies, oscillator strengths, line broadening parameters, hyperfine structure and isotopic shift (laboratory, if available)
- In addition, under NLTE: energy levels, wavelengths of transitions, cross-sections for various b-b and b-f transitions (radiative: f-values, photoionization; collisional: electrons, H I atoms, etc).

Non-local thermodynamic equilibrium

Under NLTE, equations of *statistical equilibrium* determine the *rates* C_{ij}, R_{ij} with which atomic energy levels i, j are populated and depopulated:

$$N_i \sum (C_{ij} + R_{ij}) = \sum N_j (C_{ji} + R_{ji}) \qquad i = 1, \ldots, NL$$

$$J_\nu = f(N_i)$$

LTE if $J_\nu = B_\nu(T)$
or $C_{ij} \gg R_{ij}$
(in all transitions)

If radiation field J_ν is non-Planckian and collision rates C_{ij} are small large *deviations from LTE* occur.

NLTE effects

- *are not very important for the atmospheric structure* of solar-type stars

- are crucial for *modelling spectral lines*:

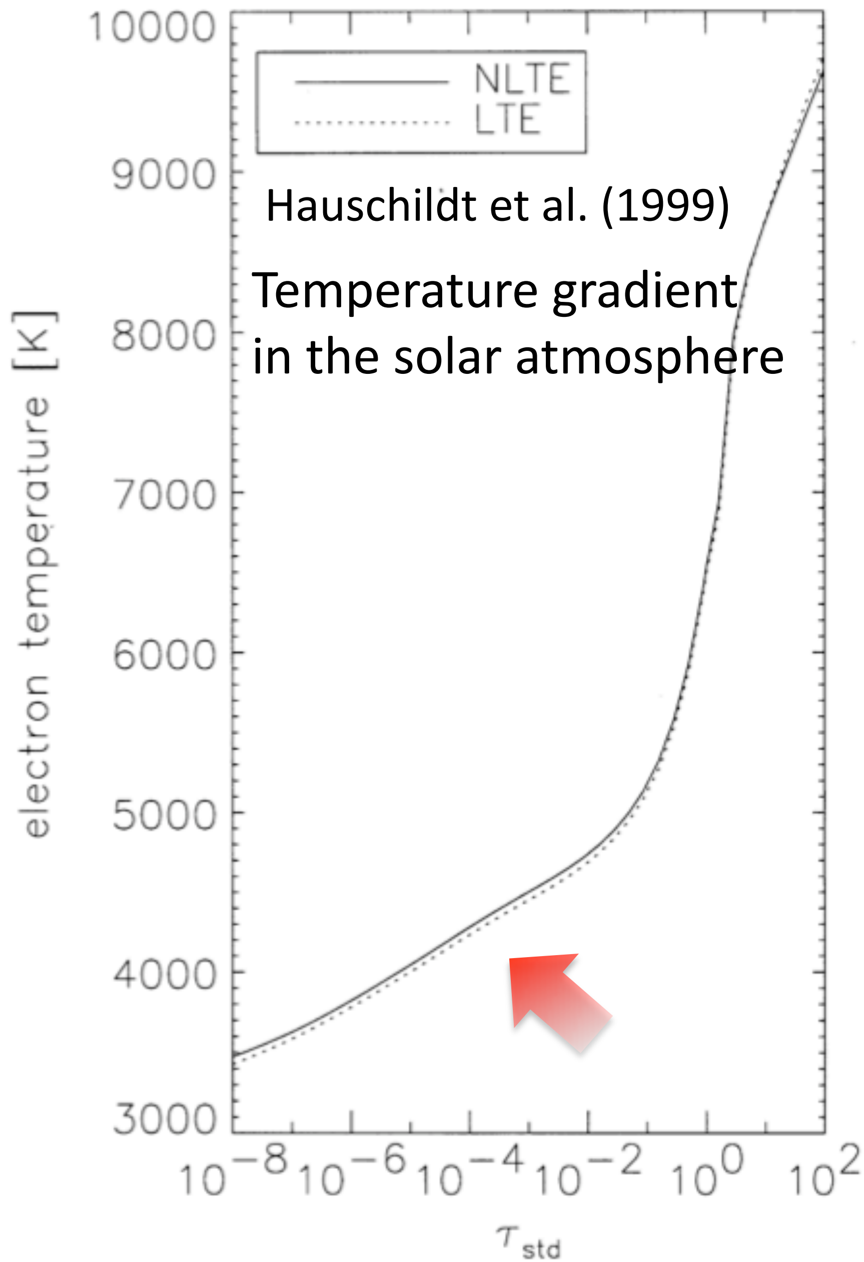
  H (Przybilla & Butler 04, …)

  Li, C, N, O (Asplund et al. 05)

  Na, Mg, Al, Si (Gehren et al. 06; Shi et al. 08)

  Cr, Mn, Fe, Co, Ni (Korn et al. 03, Bruls et al. 93, Bergemann et al. 09, Bergemann & Cescutti 10)

  Ba, Eu, Sr, Pr (Mashonkina et al. 08)



NLTE

The type and magnitude of NLTE effects are determined by *atomic structure of an element* *(thus, to physical conditions in the atmosphere)*:

- ionization energy, which gives relative abundances [Fe I/ Fe II/ …] depending on the temperature/gravity **+**
- characteristics of energy levels in the atom +/-
- number of transitions (allowed, forbidden) +/-
- magnitude of cross-sections for *particle & photon interactions* *?*

Models of simple atoms

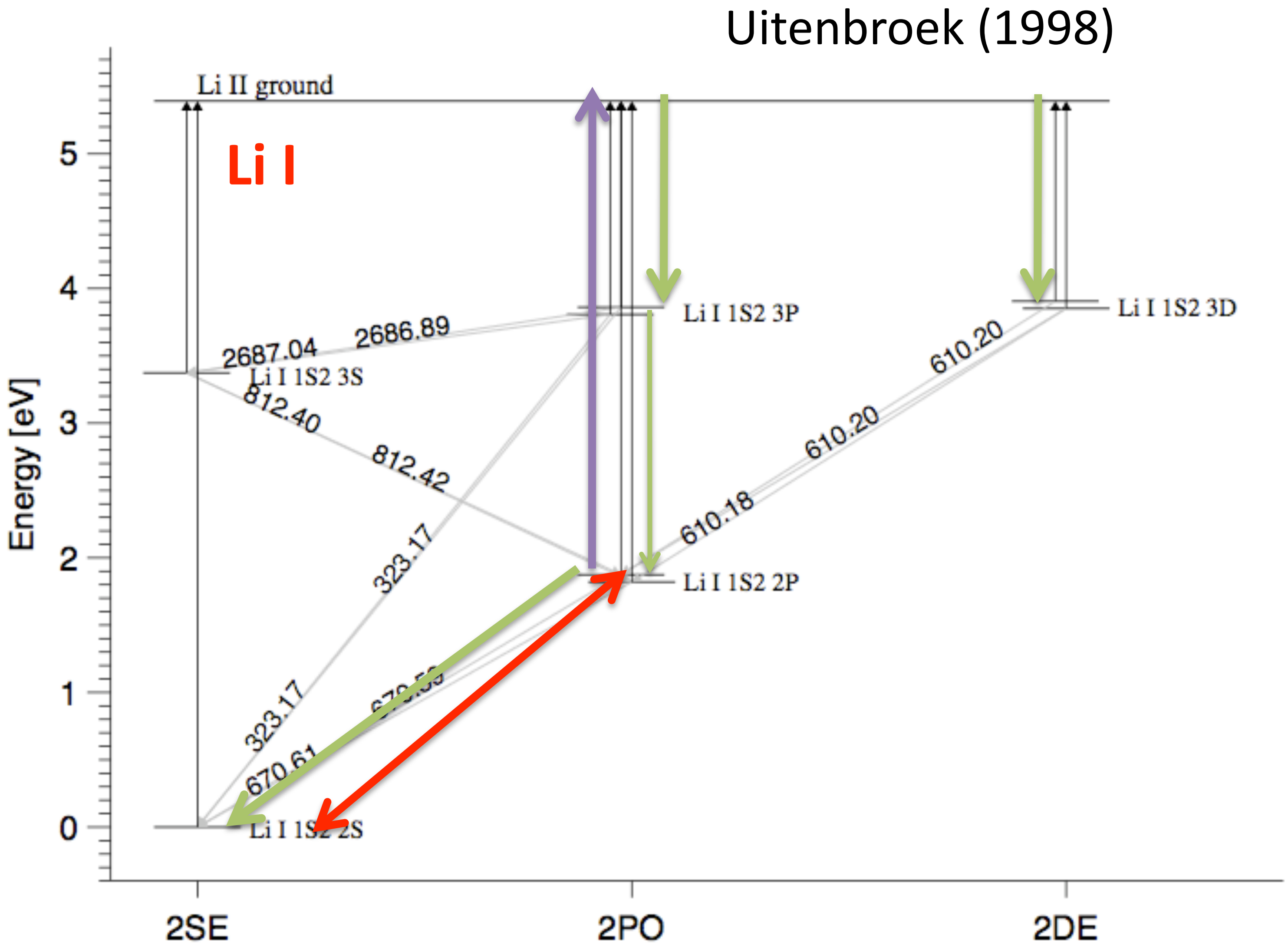
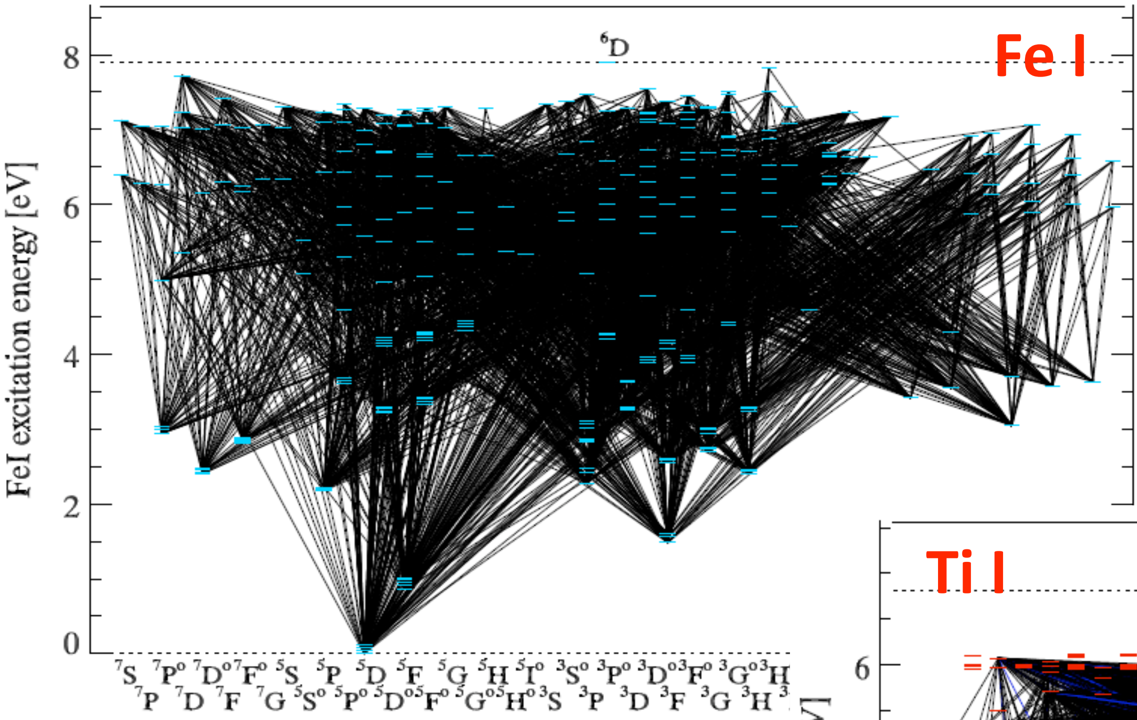


FIG. 4.—Term diagram of the lithium model atom

Models of complex atoms



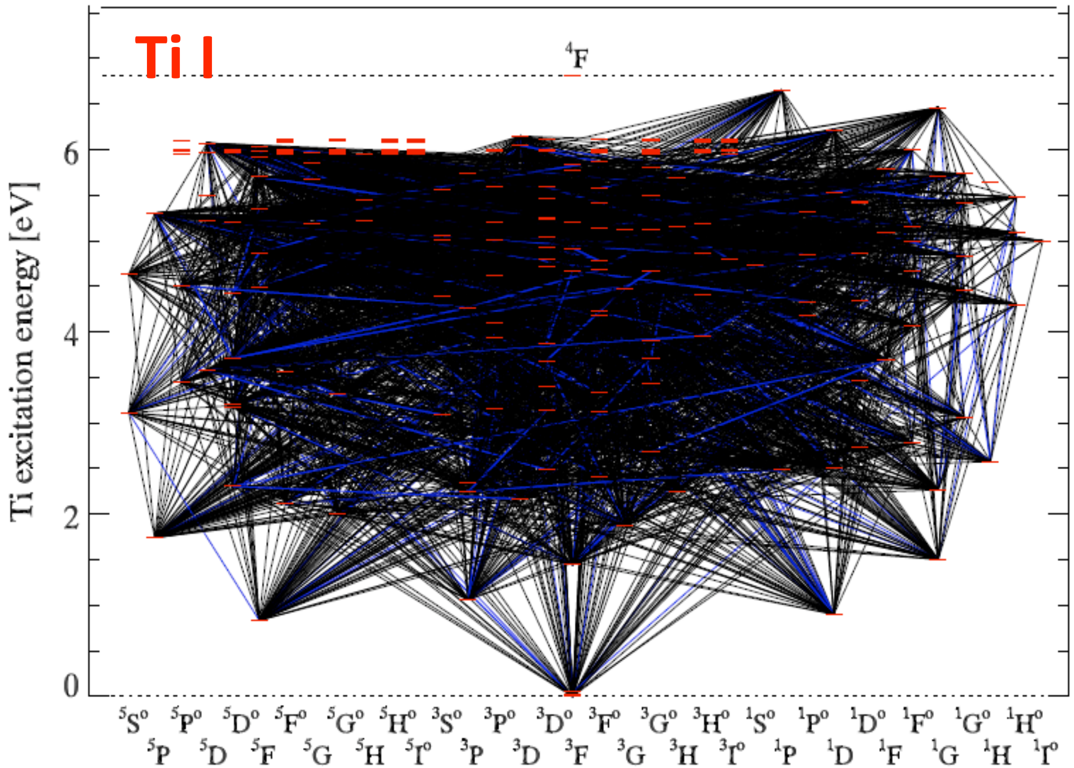
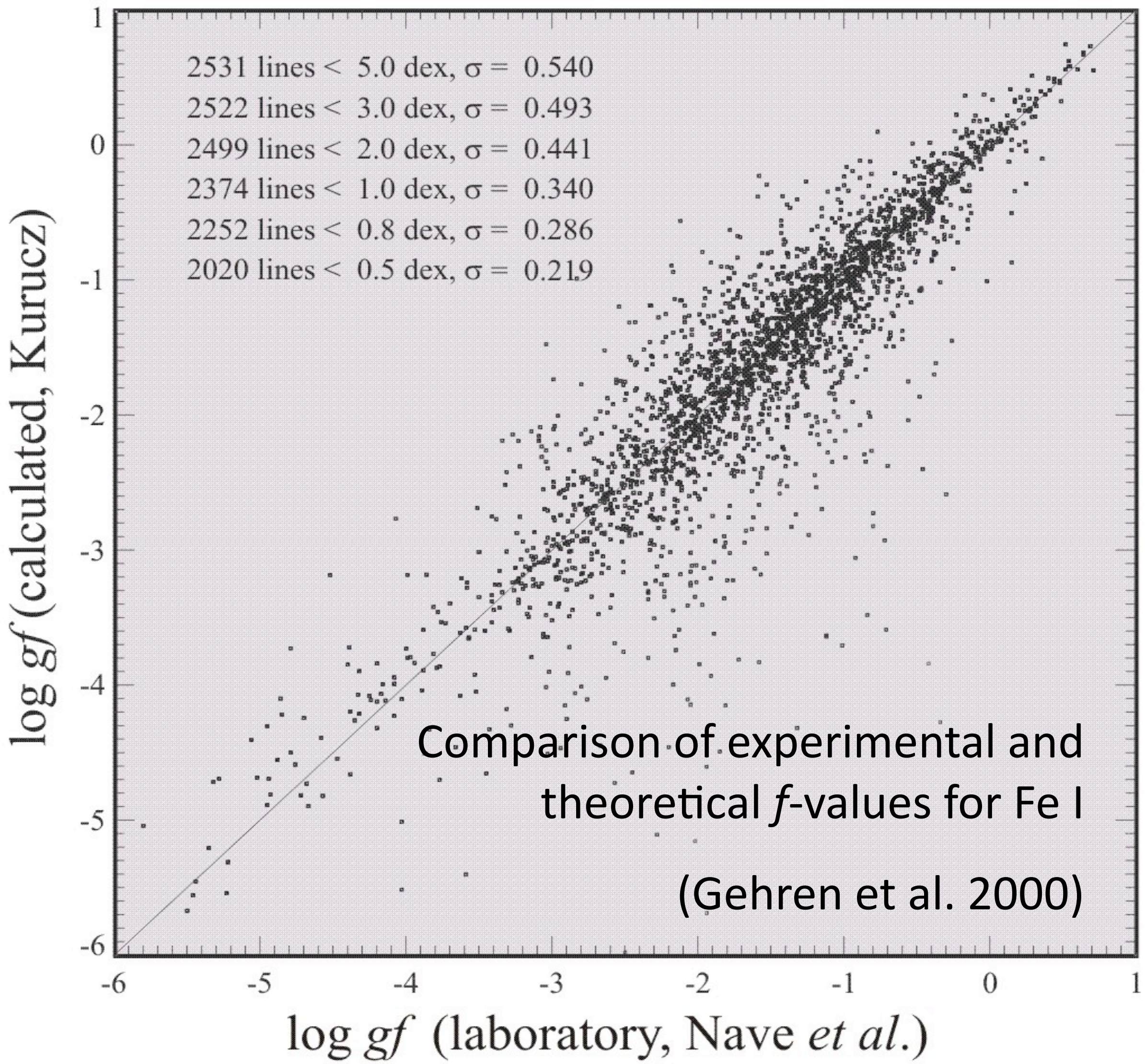


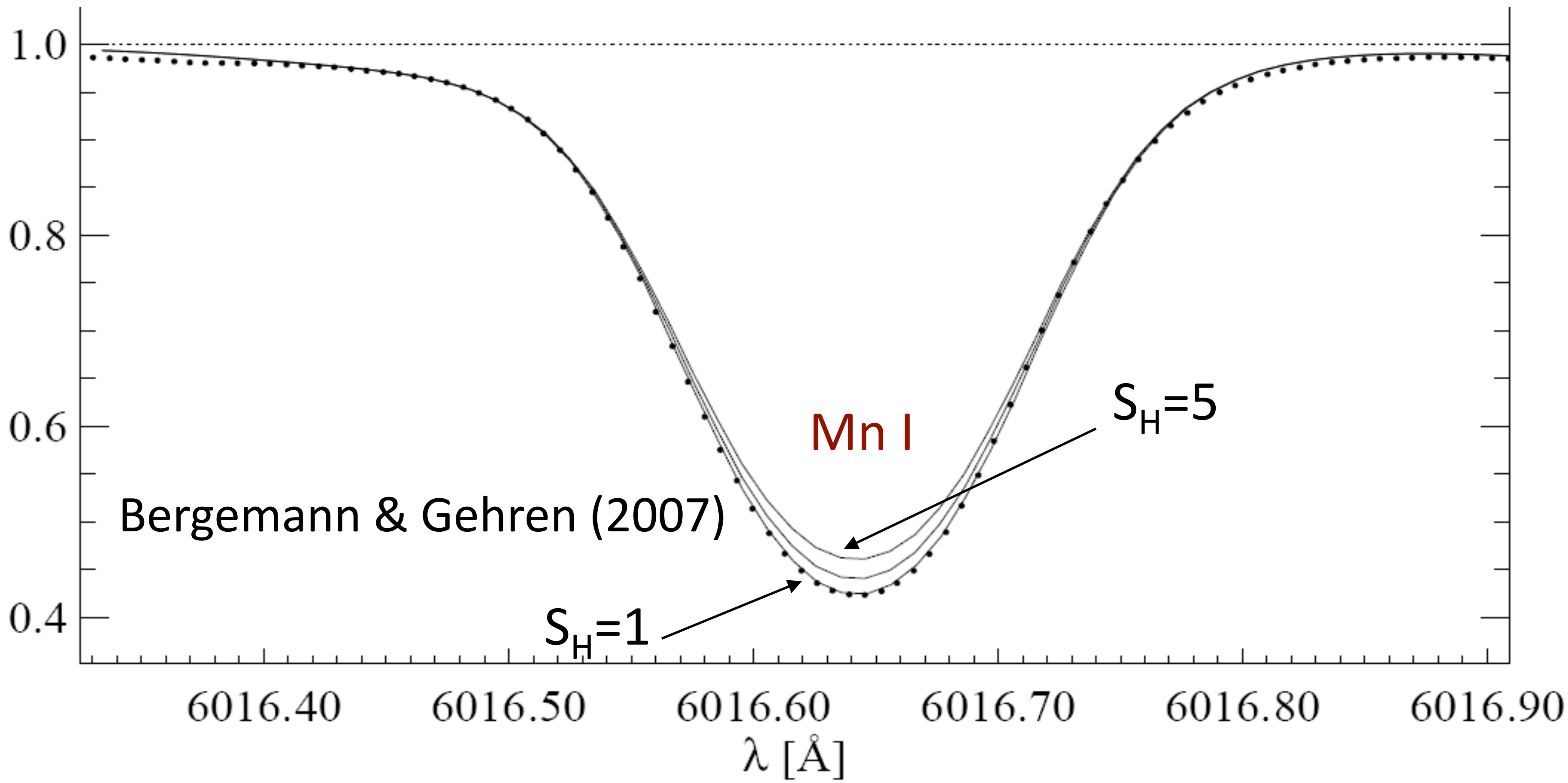
Photo-excitation

The *accuracy* of a single f-value is not important in calculations of statistical equilibrium of an element.



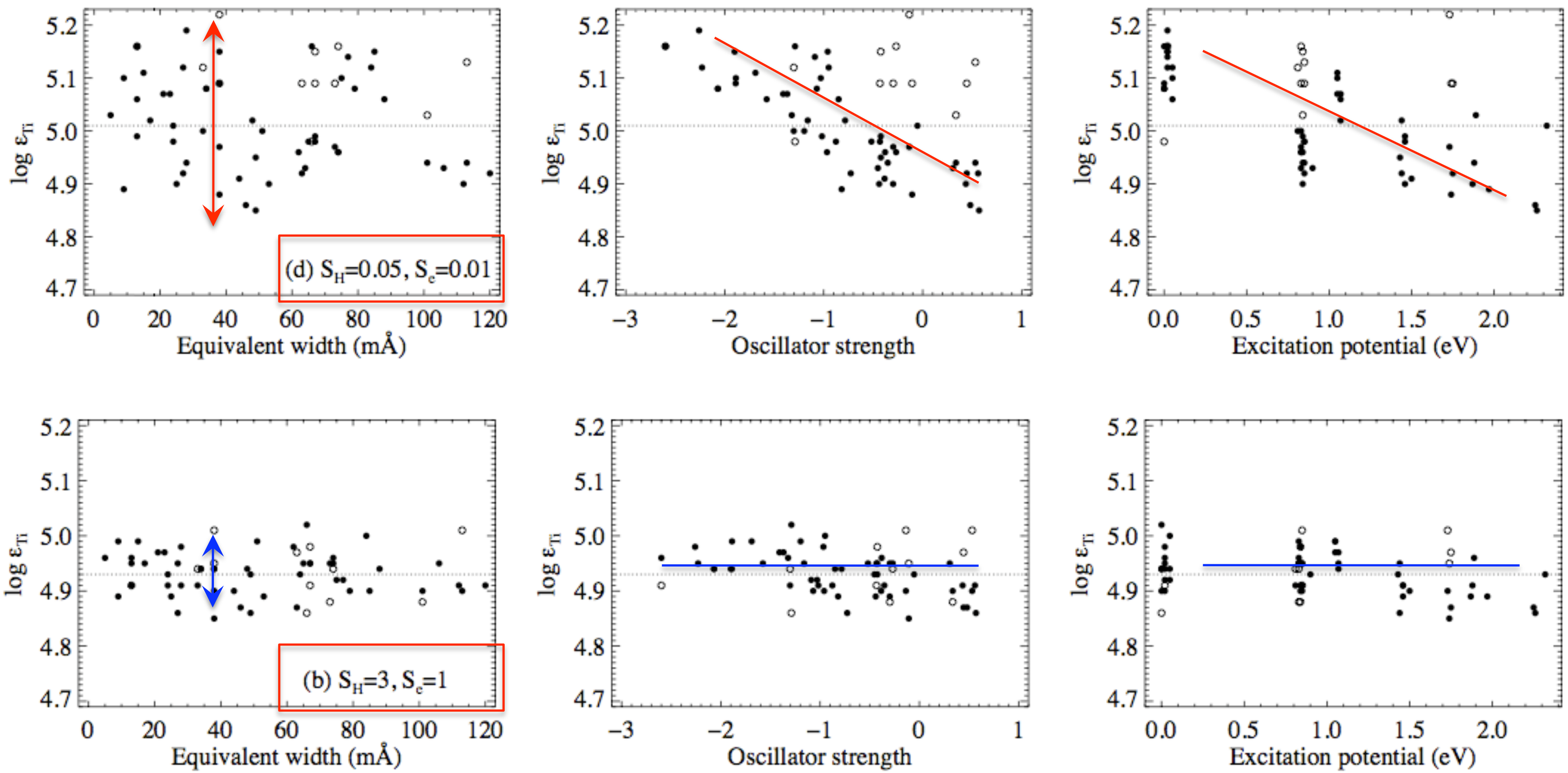
Inelastic collisions with H I

At present, we rely on the g-bar approximation (Drawin 1968, 1969), but this is by far insufficient to obtain realistic estimates of NLTE effects for neutral atoms of Fe-peak elements –> use scaling factors S_H to Drawin's cross-sections.



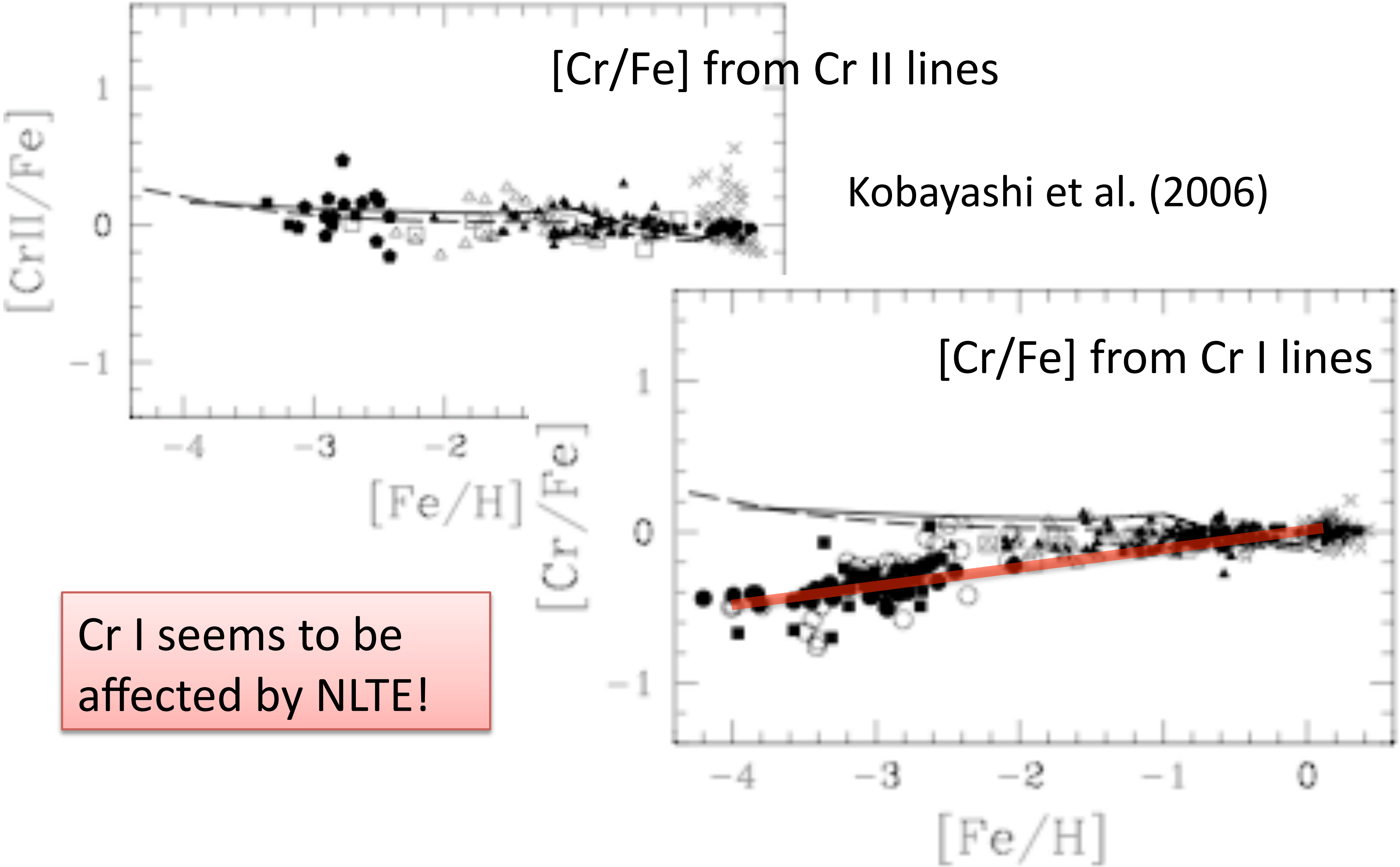
Inelastic collisions with H I

In fact, accurate choice of the scaling factor S_H to Drawin's cross-sections may produce satisfactory results (e.g. abundances).



Bergemann (2010), submitted

“Observations” and Galactic Chemical Evolution

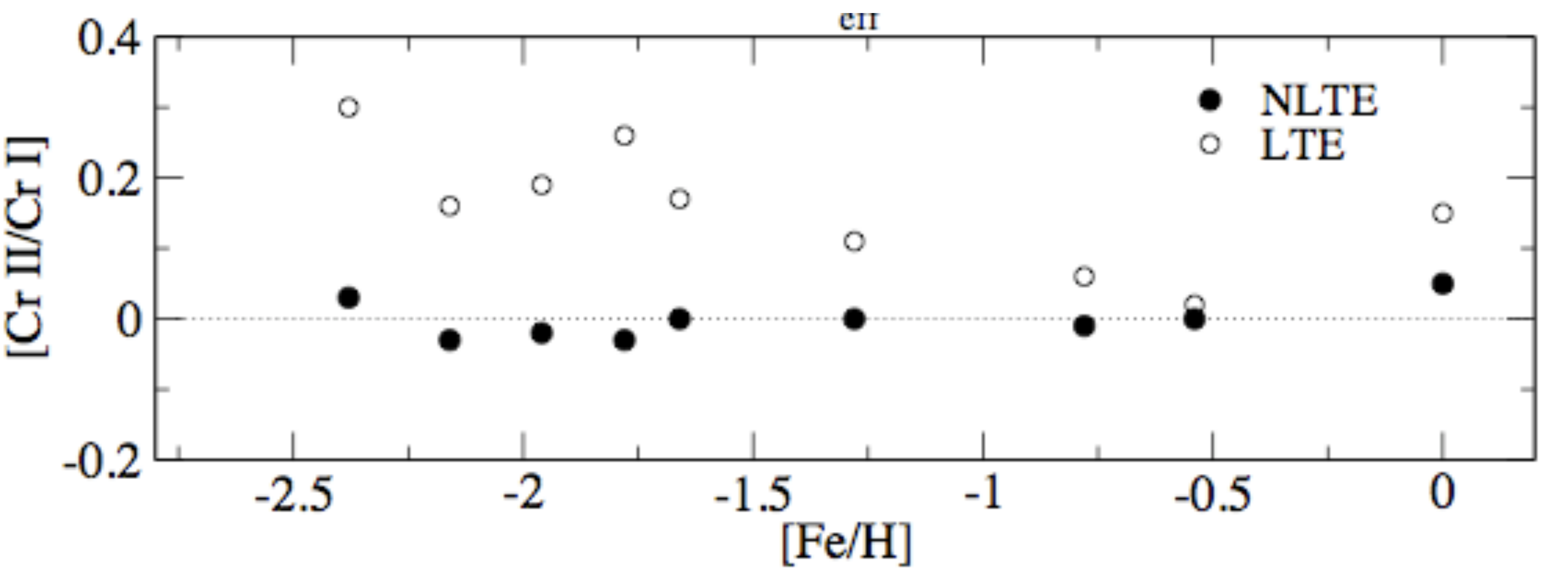


Kobayashi et al. (2006)

Cr I seems to be affected by NLTE!

NLTE and abundances

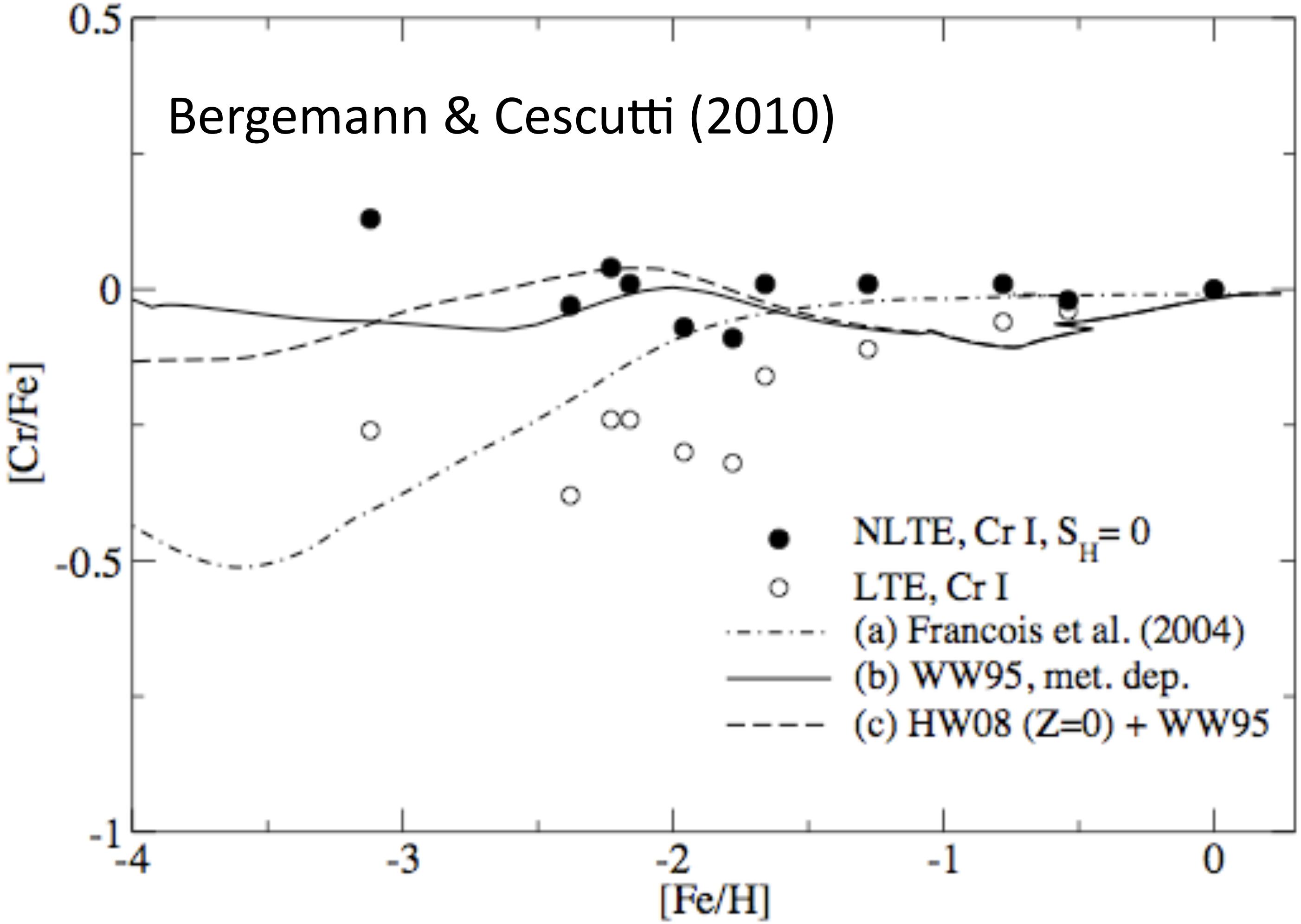
Application of NLTE to Cr using QM Cr I photoionization cross-sections from Nahar (2009) removed strong disagreement between lines of two ionization stages, Cr I and Cr II, for stars with any metallicity.



Bergemann & Cescutti (2010)

Implications for Galactic chemical evolution

We showed that the tendency of Cr to become deficient with respect to Fe in metal-poor stars is an artifact caused by the neglect of NLTE effects in the line formation of Cr I, and has no relation to any peculiar physical conditions in the Galactic ISM or deficiencies of nucleosynthesis theory.



SUMMARY

- Research on Galactic chemical evolution requires spectroscopic abundances with accuracies of ~ 0.1 dex
- This can only be achieved using NLTE line formation codes in connection with radiative hydrodynamics, if possible
- Accuracies of certain types of atomic data are insufficient to produce realistic estimates of NLTE effects for many chemical elements detected in spectra of late-type stars → this is very important for both electron and hydrogen collisions, and photoinization!