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Iron in Non-LTE – Pitfalls and Prospects

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Abstract. Apart from photo-ionization rates, the efficiency of collisions with hydrogen atoms constitutes the main unknown in statistical-equilibrium studies for cool stars.

Here we give details on a procedure carried out to calibrate the strength of hydrogen collisions S_H. It employs the most metal-poor local stars with significant HIPPARCOS parallaxes, as they display larger non-LTE effects than the Sun. The calibration succeeds in reproducing the HIPPARCOS parallaxes for stars in different evolutionary stages with a single value of S_H.

Areas in which previous studies (Gratton et al. 1999, Thévenin & Idiart 1999) were unsatisfactory, are discussed. In addition, future tests and applications of the current calibration are given.

1. Introduction

Accurate and unbiased stellar parameters are a fundamental first step towards interpreting the elemental signatures encoded in stellar spectra. The purely spectroscopic approach of Fuhrmann (1998 & 2000) has been extremely successful in reproducing the constraints of astrometry: the resulting spectroscopic distance scale for 100 stars agrees with the HIPPARCOS parallaxes to within 2 % $\pm$ 5 % (1σ). This scatter translates into uncertainties in *physical* gravities of 0.05 dex or 100 K in $T_{\rm eff}$.

While Balmer line profiles can be used as a temperature indicator at any metallicity, the pressure-broadened lines of Mg Ib cease to be strong enough to contain gravity information below 1/200 ([Fe/H] < -2.3) the metallicity of the Sun. Therefore, a different plasmadiagnostic tool has to be employed in the analysis of more metal-poor halo objects.

The ionization equilibrium of Fe I/II can serve as a gravity indicator down to [Fe/H] $\simeq -4$ and beyond. However, applying it to stars using LTE has been shown to yield results in conflict with the HIPPARCOS astrometry, in the sense that evolutionary stages are predicted which have not been reached. In other words, gravities are underestimated by up to 0.5 dex resulting in discrepancies as large as 50 % with respect to the astrometric result. Extreme examples are HD 140283, *the* halo subgiant, and Procyon, *the* standard F star (cf. Fig. 1).

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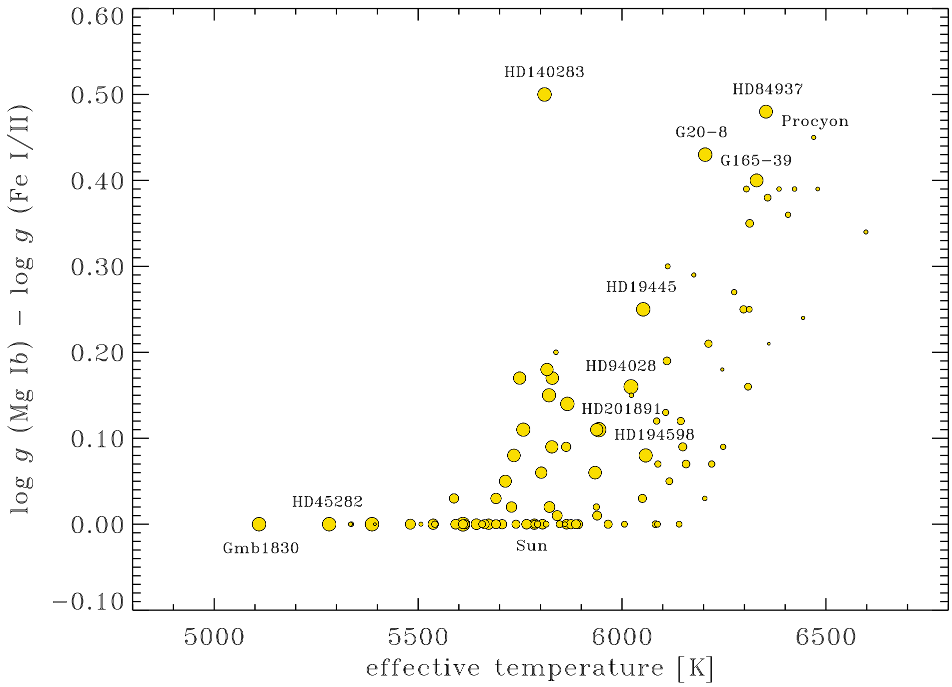

Figure 1. A selection of stars from Fuhrmann (1998 & 2000) showing the systematic deviation of Fe I/II gravities from the Mg Ib ones which are fully compatible with the HIPPARCOS astrometry (see text). Predominantly hot, metal-poor and/or evolved stars seem to be affected.

We investigate whether or not non-LTE in Fe I is the sole cause of this systematic effect. If so, analyses of halo objects would be subject to significant revisions, since in a consistent analysis the temperature, gravity and metallicity scale would all be affected.

2. Modelling Iron in Non-LTE

Since the 1970s many scientists have attempted to model the kinetic equilibrium of iron in the atmospheres of cool stars. During those past 30 years, the necessary atomic input physics has improved considerably. The current state of knowledge about the Fe I term system is summarized by the compilation of Nave et al. (1994): 236 terms and nearly 10 000 lines between them have been observed in the laboratory. Additionally, computations by Kurucz & Bell (1995) indicate the existence of hundreds of thousands of lines arising from levels close to the ionization energy of 7.87 eV.

A crucial ingredient comes from the IRON PROJECT: quantum-mechanical calculations by Bautista (1997) indicate that the photo-ionization cross sections for Fe I are significantly larger than the simple hydrogenic approximation by factors between 10 and 1000. Coupled with the enhanced UV fluxes in metal-poor stars, this makes departures from LTE quite a likely scenario.

The name of the game of non-LTE is, however, to model all important interactions entering the rate equations. As far as thermalizing processes are concerned, one can not be certain about the unimportance of collisions with hydrogen atoms: Although they are roughly a factor of 40 slower than electrons, they outnumber the latter by a factor of typically 10 000 in cool-star atmospheres. It is therefore paramount to know the ratio of the cross sections $\sigma_e/\sigma_{\rm H}$. If this ratio is close to 1, hydrogen collisions will dominate as a thermalizing mechanism.

The only theory which treats excitation and ionization due to interactions with hydrogen atoms is that of Drawin (1968, 1969). At best it gives an order-of-magnitude estimate for the efficiency of these interactions. No experimental verification is available in the relevant energy domain (thermal energies of a few tens of an eV). At higher energies (15 eV and above), the Drawin formula seems to overestimate the cross section by two orders of magnitude (Fleck et al. 1991).

Our model atom of Fe I and Fe II was presented in Gehren et al. (2001ab). We highlight the most important points below:

- 236 terms of Fe I with 4084 *bb* transitions between them
  267 terms of Fe II with 10 824 *bb* transitions between them
- photo-ionization of Fe I according to Bautista (1997)
  photo-ionization of Fe II hydrogenic (not a crucial ingredient)
- UV line blocking according to Kurucz & Bell (1995)
- electron collisions according to van Regemorter (1962), Allen (1973) and Seaton (1962)
- hydrogen collisions according to Drawin (1968, 1969) using a scaling factor $\rm S_H$ (*main free parameter of the modelling*)
- forced relative thermalization among terms above 7.3 eV. This simulates missing levels and compensates for increasing incompleteness.

3. Calibration of $\rm S_H$

In Gehren et al. (2001a) the results for strong solar lines of Fe I and Fe II were presented for different choices of $\rm S_H$ ($0 \leq \rm S_H \leq 5$). In Gehren et al. (2001b) weak lines of Fe I were included to refine our choice of $\log \rm C_6$ values. In contrast to Korn & Gehren (2001), the current calibration uses the damping constants of Anstee & O'Mara (1991 & 1995) modified by -0.15 dex. This correction minimizes trends of abundance with line strength for the Sun (cf. Gehren et al. 2001b).

It became clear that non-LTE effects in the Sun are too small to determine $\rm S_H$ uniquely. Part of the problem arises from the large scatter of gf values coming from sources incompatible with one another. In the end, we restricted our analysis to lines from the Oxford ("Blackwell") and Hannover ("Holweger")

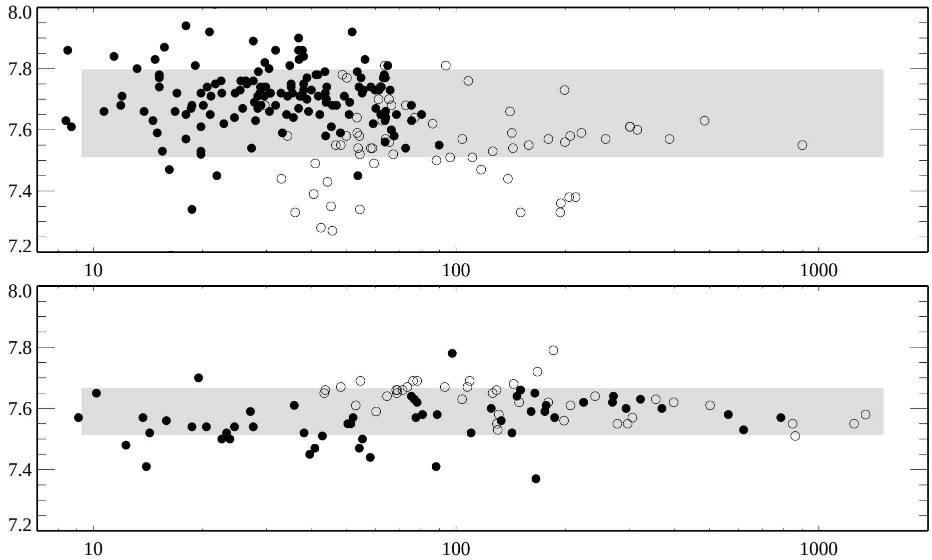

Figure 2. Solar Fe I line abundances as a function of line strength (in mÅ). *Upper panel*: gf values from May et al. (1974, bullets) and O'Brian et al. (1991, circles). *Lower panel*: gf values from the Hannover (bullets) and Oxford group (circles). The shaded area indicates the scatter around the mean value ($\pm 1\sigma$). (from Gehren et al. 2001b)

groups. The 1σ scatter is 0.08 dex for the combined set. Other sources show a larger dispersion and/or are not on the same scale (cf. Fig. 2).

While there are no halo stars for which we know T_{eff} and $\log g$ from fundamental observations, the HIPPARCOS parallaxes can be used to infer their gravities *on a given temperature scale*. Masses (VandenBerg et al. 2000), bolometric corrections (Alonso et al. 1996) and interstellar reddening (Hauck & Mermilliod 1998) enter the equation as well, but play only a minor rôle.

We chose to observe some of the most discrepant cases from the list of Fuhrmann (1998 & 2000): HD 19445 (main sequence), HD 84937 (turnoff) and HD 140283 (subgiant). We also include HD 103095 (= Groombridge 1830) for which no discrepancy was found between Mg Ib and Fe I/II (cf. Fig. 1).

Spectra of excellent quality (R = 60 000, peak S/N ≃ 300 at Hα) were obtained with FOCES (Calar Alto Observatory, Spain) between 1999 and 2001. The low blaze residuals of this fibre-fed échelle spectrograph make it the ideal instrument for analysing strong lines like Balmer profiles (Korn 2002b).

The calibration proceeds as follows: With an initial guess for the stellar parameters T_{eff} (from Balmer line profiles), [Fe/H] (from Fe I in LTE) and [O/Fe] (from the IR triplet lines in non-LTE, cf. Reetz 1999), the mass M is interpolated in a grid of evolutionary tracks. Here, the [α/Fe] ratio is important to know, especially in terms of oxygen, as it dominates the morphology change via the mean molecular weight. Alongside an estimate for the bolometric correction BC and the interstellar reddening A_V, these quantities enter the equation

$$\log \pi_{\rm HIP} = 0.5\,([g] - [M]) - 2\,[T_{\rm eff}] - 0.2\,(V + {\rm BC} + A_V + 0.25)$$

which can be solved for the logarithmic gravity $[g]$. This procedure is iterated until convergence is achieved. With the complete set of stellar parameters the value of S_H can be sought which fulfills the constraint of the non-LTE ionization equilibrium.

The results are presented in Table 1. The parameters given are calculated with S_H set to 3 which results in an – albeit marginal – offset with respect to HIPPARCOS.

Table 1. Stellar parameters derived using Fe I/II in non-LTE as a gravity indicator with $S_H = 3$. $\Delta_{\rm HIP} = 100\,(d_{\rm spec} - d_{\rm HIP})/d_{\rm HIP}$. Choosing $S_H = 0$ instead, would yield $\Delta(\text{Fe I} - \text{Fe II}) = 0.43$ dex for HD 140283, irreconcilable with the astrometric constraint.

object	$T_{\rm eff}$ [K]	log g	[Fe/H] NLTE	[O/Fe] NLTE	mass [$M_\odot$]	A_V [mag]	BC [mag]	$d_{\rm spec}$ [pc]	$d_{\rm HIP}$ [pc]	$\Delta_{\rm HIP}$ [%]
HD 103095	5070	4.66	−1.36	+0.63	0.62	0.00	−0.32	8.86	9.16	−3.2
HD 19445	6032	4.40	−2.08	+0.68	0.67	0.00	−0.21	38.80	38.68	0.3
HD 140283	5806	3.68	−2.43	+0.71	0.79	0.13	−0.23	56.60	57.34	−1.3
HD 84937	6346	4.00	−2.16	+0.59	0.79	0.11	−0.18	80.34	80.39	−0.1

The largest non-LTE effects are encountered for HD 84937 and HD 140283 where gravity corrections reach +0.1 dex. This value is much smaller than the 0.5 dex seemingly needed to bring Fe I/II in concordance with Mg Ib (cf. Fig. 1). The solution to this apparent contradiction is found in the significantly larger C_6 values used here: They enter in the derivation of the differential gf values in the analysis of the solar iron spectrum. Wrong C_6 values affect the product $gf\varepsilon$ determined by fitting solar lines in a systematic fashion.

4. Successes

The success of this calibration procedure is twofold:

- The offset between Fe I/II and Mg Ib can be removed in LTE by going from the Unsöld approximation C_6 values to those of Anstee & O'Mara (1991 & 1995). This results in spectroscopic distances accurate to more or less 10 %.
- Residual offsets can be removed by taking into account non-LTE. The scatter can also be significantly reduced (cf. Fig. 3). This is because non-LTE effects in HD 103095 are smaller than in the Sun which results in an opposite sign for the gravity correction in the framework of a differential analysis. The unanimous reproduction of the HIPPARCOS distances for the four calibration stars is noteworthy, as they are in different evolutionary stages and require corrections ranging from 0 to 0.5 dex (cf. Fig. 1).

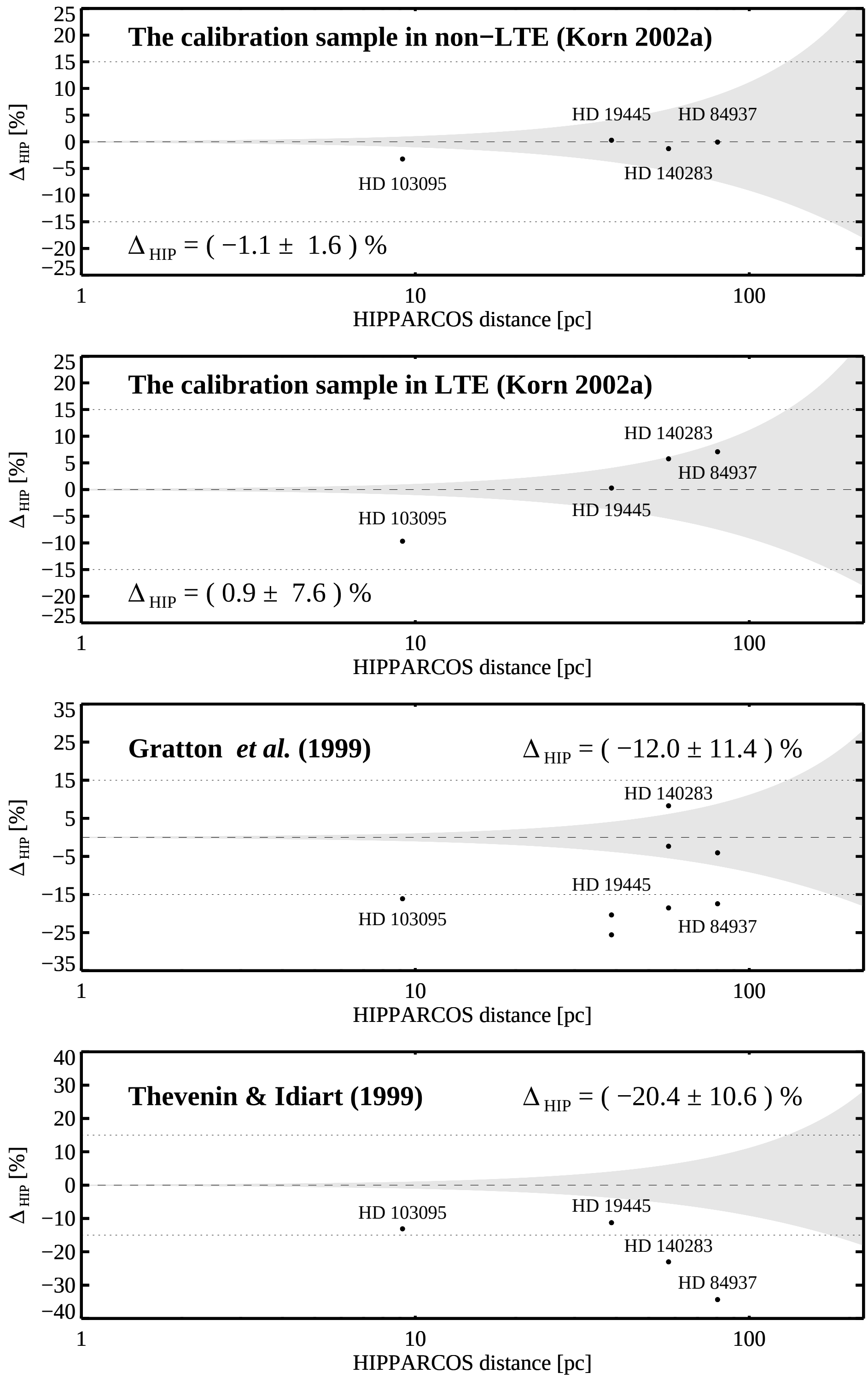

Figure 3. The ability to reproduce the HIPPARCOS distances serves to “separate the wheat from the chaff“.

5. Failures

For many stellar astrophysicists $S_H = 3$ is an unexpected result. We cannot rule out that H collisions are this efficient. We can neither rule out that this is a mere artifact of our modelling: Asplund (these proceeding) stresses that the temperature structures for metal-poor stars as derived from 3D hydrodynamical models are significantly cooler at low optical depth than their 1D static counterparts (adiabatic cooling dominates over radiative heating).

Cooler temperatures in the upper photosphere would predominantly affect neutral species like Fe I. Their lines would be strengthened allowing for larger overionization by photo-ionization respectively less efficient thermalization by collisions to reproduce a given observed profile. The "3D" results for HD 140283 presented by Shchukina, Trujillo Bueno & Vasil'eva (these proceeding) point in this direction, a quantitative verification like ours is still lacking.

Thévenin & Idiart (1999) presented a similarly comprehensive model atom for Fe I. Unfortunately, they fail to account for hydrogen collisions and line opacities in the UV. They do, however, implement the detailed photo-ionization cross-sections of Bautista (1997). All these choices go in the direction of aggravating departures from LTE. On their temperature scale (which is significantly cooler than our Balmer profile temperatures and the IRFM temperature scale of Alonso et al. 1996) gravities are thus overestimated by 0.2 dex on average (cf. Fig. 3).

Gratton et al. (1999) build their calculations on the simple Fe I model atom of Takeda (1991) which is no longer up-to-date. Photo-ionization is treated more or less hydrogenically, line blocking in the UV is accounted for empirically. The calibration of S_H is done with RR Lyrae stars and leads to thermal populations for cool stars of all metallicities ($S_H = 30$!). Therefore the results of Carretta et al. (2000) are based on LTE gravities.

Since they work on an IRFM temperature scale in excellent agreement with our spectroscopic one, it is surprising to see that their LTE Fe I/II gravities are not too low. While we cannot single out a reason for this fact, it signifies the importance of calibrating one's methods against standards, both in LTE and non-LTE. More disturbing than the offset of 10 % is the large scatter, e.g. among the three analyses of HD 140283 which amounts to nearly 30 %.

6. Application

The Fe I/II ionization equilibrium turns out to be applicable to stars significantly more metal-poor than what is within reach of Mg Ib as a gravitiy indicator (see Introduction). For example, we have successfully applied it to extremely metal-poor stars like CD $-38°$ 245 at [Fe/H] $\simeq -4$ and HE 0107 5240 at [Fe/H] $\simeq -5.4$ (Christlieb et al. 2002). Since these stars are giants, non-LTE correction to $\log g$ are much larger reaching 0.4 dex in CD $-38°$ 245. Since non-LTE effects in Fe I are a clear function of gravity, these model predictions can be put to the test by analysing globular cluster giants.

Thus stars over the whole range of metallicities encountered in the Galaxy can now be analysed in a homogeneous way with reduced methodological biases.

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