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Non–LTE Line Formation for Fe I and Fe II in the Atmospheres of A–F Type Stars

Mashonkina L.

Institute of Astronomy, Moscow, Russia

Abstract. Non–local thermodynamical equilibrium (non–LTE) line formation for neutral and singly–ionized iron is considered for the A–F type stars ranging from the effective temperatures of 6500 K to 8500 K, the gravities of $\log g = 4$ and 3, and solar metallicity. A comprehensive model atom for iron is taken from Mashonkina et al. (2010). The departures from LTE lead to the systematically depleted total absorption in the Fe I lines and positive abundance corrections in agreement with the Rentzsch–Holm (1996) study. However, the predicted magnitude of the non–LTE effects is significantly smaller compared to the previous results due to the use of a rather complete model atom of Fe I. The non–LTE abundance corrections do not exceed 0.1 dex for the dwarf models and 0.20 dex for the giant ones. Non–LTE leads to the Fe II lines strengthening, however, the effect is small, such that the abundance correction is at the level of -0.01 to -0.03 dex over the whole range of stellar parameters being considered. No firm conclusion can be drawn with respect to whether or not the Fe I/Fe II ionization equilibrium is fulfilled in the atmosphere of the Sun and Procyon due to a large uncertainty in the available gf–values for the visible lines of Fe I and Fe II.

Key words: Atomic data – Line: formation – Stars: atmosphere

1 Introduction

Iron is the most popular chemical element in the studies of both non–magnetic and magnetic A and later type stars thanks to quite numerous lines of the neutral and singly–ionized species in the visible spectrum. Iron lines are used to determine the stellar parameters, such as effective temperature, $T_{\rm eff}$, surface gravity, $\log g$, microturbulence velocity, $V_{\rm mic}$, and, in the magnetic stars, also to investigate the magnetic fields. Therefore, the calculations of the iron lines have to be based on realistic line formation scenarios.

In the atmospheres with $T_{\rm eff} > 4500$ K, Fe I is a minority species. Number density of the minority of species can easily deviate from the thermodynamical equilibrium (TE) population due to a small deviation of the mean intensity of ionizing radiation from the Planck function. Since the beginning of the 1970s a number of studies have attacked the problem of the non–local thermodynamic equilibrium (non–LTE) line formation for Fe I in the Sun and late type stars (Tanaka, 1971; Athay & Lites, 1972; Boyarchuk et al., 1985; Takeda, 1991; Gratton et al., 1999; Thévenin & Idiart, 1999; Gehren et al., 2001; Shchukina & Trujillo Bueno, 2001; Collet et al., 2005). Here we list only the studies, where the original model atom was produced. The non–LTE effects in the hotter atmospheres were investigated only by Gigas (1986) and Rentzsch–Holm (1996). All these researches came to a common conclusion that Fe I is subject to overionization in the stellar atmospheres due to enhanced photoionization of the levels with ionization edges in the ultra–violet (UV), and Fe I lines are weakened compared to their LTE strengths. However, a consensus on the expected magnitude of non–LTE effects was not reached. For example, the surface gravity correction for cool metal–poor atmospheres was calculated, in some studies, at the level of 0.5 dex, while no significant departures from LTE were found by others. The discrepancies between different papers might be due to an incompleteness of the applied model atoms.

Mashonkina et al. (2010) constructed a comprehensive model atom for iron with more than 3000 measured and predicted energy levels, and showed that the departures from LTE for Fe I decreased significantly in the atmospheres of solar–type stars, in particular, in the metal–poor atmospheres compared to those calculated in the previous non–LTE studies. In this study, we revise non–LTE effects for the stellar parameter range characteristic of A–type stars. The paper is organized as follows. An introduction to the non–LTE approach is given in the following section. Sect. 3 describes briefly the method of non–LTE calculations for Fe I – Fe II. The results for the two reference stars, the Sun and Procyon, are presented in Sect. 4. Finally, we report on the departures from LTE depending on stellar parameters.

2 What is Meant by the Non–LTE Approach?

We assume that the particle velocity distribution is Maxwellian with a single kinetic temperature for various kinds of particles, i. e., for the electrons, atoms, and ions: $T_e = T_a = T_i$. We consider that the occupation number of any atomic level is determined from the balance between radiative and collisional population and de–population processes, such as photoexcitation, photoionization and their inverse processes, inelastic collisions with electrons, atoms, molecules, dielectronic recombination, charge exchange, i. e., from a statistical equilibrium (SE):

$$n_i \sum_{j \neq i} (R_{ij} + C_{ij}) = \sum_{j \neq i} n_j (R_{ji} + C_{ji}) \qquad i = 1, \ldots, NL. \tag{1}$$

Collision rate C_{ij} is defined by the local kinetic temperature T_e and collider particle number density. Collision processes tend to establish TE. Radiative rate R_{ij} depends on the radiation field, which is, in general, highly non–local in character. Radiative processes tend to destroy TE.

In the nature, each chemical species possesses a huge number of bound energy levels approaching infinity. In practice, the real atomic term structure is represented by the model atom with finite number of levels NL. To investigate the SE of an atom, a large amount of various atomic data is required, such as the energy levels, photoionization cross-sections for every level in the model atom, oscillator strengths (f_{ij}) for the entire set of allowed transitions, and collision excitation and ionization data for the entire set of transitions. For the past two decades, the situation with atomic data has significantly improved. A fairly extensive set of accurate atomic data on the photoionization cross–sections and oscillator strengths was calculated in the Opacity Project (Seaton et al., 1994) and has become available via the TOPBASE database. The IRON project is in progress and provides the data for the Fe group elements. Quantum–mechanical *ab initio* calculations exist for the electron impact excitation in a number of selected atoms and ions. However, for heavy elements beyond the Fe group, much data are missing, in particular, for the high–excitation states. Rough theoretical approximations are still used to evaluate inelastic collision cross–sections. The calculated SE of an atom depends on completeness of the adopted model atom and the accuracy of the atomic data used.

The excitation and ionization states of the matter are calculated from the solution of combined SE (1) and radiation transfer equations (2):

$$\mu \frac{dI_\nu(z, \mu)}{dz} = -\chi_\nu(z) I_\nu(z, \mu) + \eta_\nu(z) \tag{2}$$

Here, χ_ν and η_ν are the absorption and emission coefficients, respectively. The radiation transfer equations have to be solved at the frequencies of all the radiative transitions in the atom which makes the non–LTE calculations bulky. In non–LTE, atomic level population $n_i(d)$ at any depth point d depends on the physical conditions throughout the atmosphere: $n_i(d) = f(n_1, \ldots, n_{NL}, J_1, \ldots, J_{NF})$. Here, J_ν is the mean intensity. The models in which the Saha–Boltzmann equations are replaced by the physically more accurate SE equations are called the non–LTE models.

For comparison, in LTE the level populations are calculated from the Saha and Boltzmann equations and depend only on local temperature and electron number density. This implies simple numerical calculations and the need in atomic data only for the spectral line under investigation. The LTE assumption is valid if every transition in the atom is in detailed balance. This is not fulfilled in spectral line formation layers, where the mean–free path of photons is large and the intensity of radiation is far from being in TE. To evaluate the effect of the departures from LTE on line strengths and stellar parameters, derived from these lines, one needs to solve the non–LTE problem for a given chemical species.

3 The Method of non–LTE Calculations for Iron

The non–LTE calculations were performed using a revised version of the DETAIL program (Butler & Giddings, 1985) based on the accelerated lambda iteration (ALI) scheme.

Model atom of Fe I – Fe II. We applied the model atom treated by Mashonkina et al. (2010). It was constructed using the 958 energy levels of Fe I known from the experimental analysis of Nave et al. (1994) and also the levels, predicted from the calculations of the Fe I atomic structure by Kurucz (2009), 2 970 levels in total. The system of measured levels is nearly complete below $E_{\rm exc} \simeq 5.6$ eV. However, laboratory experiments do not see most of the high–excitation levels with $E_{\rm exc} > 7.1$ eV, which should contribute a lot to provide close collisional coupling of Fe I levels to the Fe II ground state. Neglecting the multiplet fine structure gives 233 levels of Fe I in the model atom. The predicted high–excitation levels were used to make up six super–levels. This is new compared to all the previous non–LTE studies for Fe I. In total, 11 958 allowed transitions occur in this model atom of Fe I. For Fe II, we use the 89 lowest terms with $E_{\rm exc}$ up to 10 eV. The ground state of Fe III completes the system of levels in the model atom.

Photoionization is the most important process deciding whether the Fe I atom tends to depart from LTE in the atmosphere of a cool star. Our non–LTE calculations rely on the photoionization cross–sections of the IRON project (Bautista et al., 1997). The hydrogenic approximation was used for the Fe II states. Radiative bound–bound (b–b) transition rates were computed using the gf–values from the Nave et al. (1994) compilation and Kurucz (2009) calculations. All the levels in our model atom are coupled via the collisional excitation and ionization by electrons. The collisional rates were calculated using the theoretical approximation of van Regemorter (1962) and Seaton (1962).

Model atmospheres. For the Sun and Procyon, the calculations were performed with plane–parallel and blanketed LTE model atmospheres computed with the MAFAGS–OS code (Grupp et al., 2009), which is based on the up–to–date continuous opacities and includes the effects of line–blanketing by means of opacity sampling. Small grid of model atmospheres with $T_{\rm eff} = 6500 - 8500$ K and $\log g = 3$ and 4 was taken from the Kurucz (2008) website to evaluate the departures from LTE depending on stellar parameters.

Statistical equilibrium of iron. The departure coefficients, $b_i = n_i^{\rm NLTE}/n_i^{\rm LTE}$, for the levels of Fe I and Fe II in the representative model atmosphere $T_{\rm eff}/\log g/[{\rm M/H}] = 8000/4/0$ are presented in

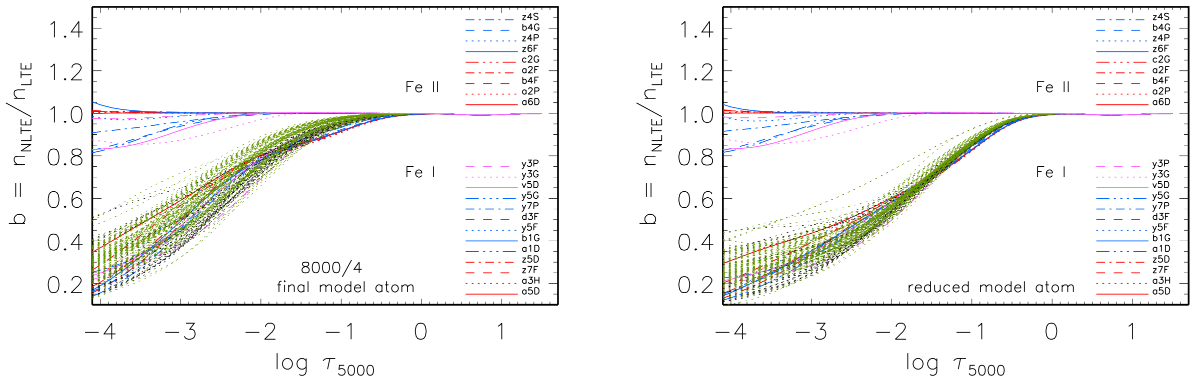

Figure 1: Departure coefficients, b, for the levels of Fe I and Fe II as a function of $\log \tau_{5000}$ in the model atmosphere 8000/4/0 from the calculations with our final model atom (left panel) and the reduced model atom which ignores the predicted levels of Fe I (right panel)

Fig. 1 as a function of $\log \tau_{5000}$. Here, $n_i^{\rm NLTE}$ and $n_i^{\rm LTE}$ are the statistical equilibrium and thermal (Saha–Boltzmann) number densities, respectively. The difference between two panels of Fig. 1 is in using two different atomic models, i. e., the final model atom from Mashonkina et al. (2010) in the left panel and the reduced model atom which ignores the predicted levels of Fe I in the right panel. Our calculations support qualitatively the previous results of Rentzsch–Holm (1996) for common stellar parameters.

- All the levels of Fe I are underpopulated in the atmospheric layers above $\log \tau_{5000} = -0.3$ due to the overionization caused by superthermal radiation of a non–local origin below the thresholds of the low excitation levels of Fe I.

- Fe II dominates the element number density over all atmospheric depths. Thus, no process seems to affect the Fe II ground–state and low–excitation–level populations significantly, and they keep their thermodynamic equilibrium values.

In this study, progress was made in establishing close collisional coupling of Fe I levels near the continuum to the ground state of Fe II, as a bulk of the predicted high–excitation levels of Fe I was included in the model atom. As a result, the populations of the Fe I levels obtained with the final model atom (Fig. 1, left panel) are closer to the corresponding TE populations in the line–formation layers ($\log \tau_{5000} = 0$ up to -3) than that for the reduced model atom (Fig. 1, right panel).

4 Fe I/Fe II Ionization Equilibrium in the Sun and Procyon

The non–LTE method was applied to analyze the Fe I and Fe II lines in the two stars with well–determined stellar parameters: the Sun and Procyon. The solar flux observations are taken from the Kitt Peak Solar Atlas (Kurucz et al., 1984). The spectroscopic observations for Procyon were carried out by Korn (2003) with the FOCES fibre–fed échelle spectrograph at the 2.2–m telescope of the Calar Alto Observatory, with the spectral resolving power of $R \simeq 60\,000$ and a signal–to–noise of $S/N \geq 200$.

In the solar spectrum, we selected 54 unblended lines of Fe I and 18 lines of Fe II, which cover a broad range of line strengths and excitation energies of the lower level. Despite the existence of many sources of gf–values for neutral iron, there is no single source that provides data for all the selected Fe I lines. We employ experimental gf–values from Bard et al. (1991), Bard & Kock (1994), Blackwell et al. (1979, 1982a, 1982b), Fuhr et al. (1988), O'Brian et al. (1991). Multiple sources of gf–values are available for each line of Fe II. We inspected 5 sets of data from Meléndez & Barbuy (2009, hereafter MB09), Moity (1983, hereafter M83), Raassen & Uylings (1998, hereafter RU98), Schnabel et al. (2004, hereafter SSK04), and the VALD database (Kupka et al., 1999). Van der Waals broadening of iron lines is accounted for using the most accurate data, available from the calculations of Anstee & O'Mara (1995), Barklem & O'Mara (1997), Barklem et al. (1998), and Barklem & Aspelund–Johansson (2005).

The Sun. With the solar model atmosphere 5780/4.44, the non–LTE effects are small for the Fe I lines and negligible for the Fe II lines, such that the non–LTE abundance correction amounts, on the average, to $\Delta_{\rm NLTE} = \log\varepsilon_{\rm NLTE} - \log\varepsilon_{\rm LTE} = +0.03$ dex for Fe I and smaller than 0.01 dex for Fe II. A depth–independent microturbulence of $0.9\,{\rm km\,s^{-1}}$ was adopted in the calculations. The iron abundance was derived from line profile fitting. For the Fe I lines, we obtained the mean non–LTE abundance $\log\varepsilon_{\rm FeI} = 7.56 \pm 0.09$. The statistical error which is defined as the dispersion in the single line measurements about the mean, $\sigma = \sqrt{\Sigma(\overline{x} - x_i)^2/(n-1)}$, is considerably too high. This is, most probably, due to the uncertainty in gf–values because the abundance scatter is largely removed in the line–by–line differential analysis of the solar type stars as shown by Mashonkina et al. (2010). For example, the Fe I based abundance $[{\rm Fe/H}]_I = 0.11 \pm 0.03$ for β Vir (6060/4.11). We find that the average Fe II–based abundance depends significantly on the used source of gf–values: $\log\varepsilon_{\rm FeII} = 7.41 \pm 0.11$ (SSK04), 7.45 ± 0.07 (VALD), 7.47 ± 0.05 (MB09), and 7.56 ± 0.05 (RU98, M83). It is worth noting that the most recent laboratory gf–values of SSK04 lead to the highest abundance scatter.

Large statistical errors and significant systematic discrepancies between different authors make the situation with oscillator strengths for the visible Fe I and Fe II lines unacceptable. Independent of either 1D or 3D modelling, no firm conclusion can be drawn with respect to whether or not the Fe I/Fe II ionization equilibrium is fulfilled in the solar atmosphere and how realistic the non–LTE calculations for iron are. The astrophysical community shall ask atomic spectroscopists for new accurate measurements.

With the cited gf–values for Fe I and the data of RU98 for Fe II, the ionization equilibrium between Fe I and Fe II is matched consistently with the solar $\log g = 4.44$. Is it possible to achieve a similar consistency for any other star using the same line list and the same atomic data?

Procyon. Procyon is among very few stars for which the whole set of fundamental stellar parameters except metallicity can be determined from the (nearly) model–independent methods. Allende Prieto et al. (2002) obtained $T_{\rm eff} = 6510 \pm 49$ K and $\log g = 3.96 \pm 0.02$. Microturbulence velocity of $V_{\rm mic} = 1.6\,{\rm km\,s^{-1}}$ was determined in this study from the requirement that the non–LTE iron abundance derived from Fe I lines must not depend on the line strength.

We find that the mean LTE abundance determined from the Fe I lines is 0.14 dex lower than that from the Fe II lines. The non–LTE abundances from the individual Fe I and Fe II lines are presented in Fig. 2 with the mean values of $\log\varepsilon_{\rm FeI} = 7.55 \pm 0.09$ and $\log\varepsilon_{\rm FeII} = 7.62 \pm 0.06$. Non–LTE partly removes the disparity between two ions and leads to abundances from two ionization stages, consistent within the error bars. But the abundance error is as large as for the Sun, and this leaves a space for speculations that either one needs to improve further the non–LTE line formation modelling, or revise upwards the $T_{\rm eff}$ (change in $T_{\rm eff}$ by 80 K fully removes the disparity between Fe I and Fe II), or to apply a new–generation model atmosphere based on hydrodynamic calculations.

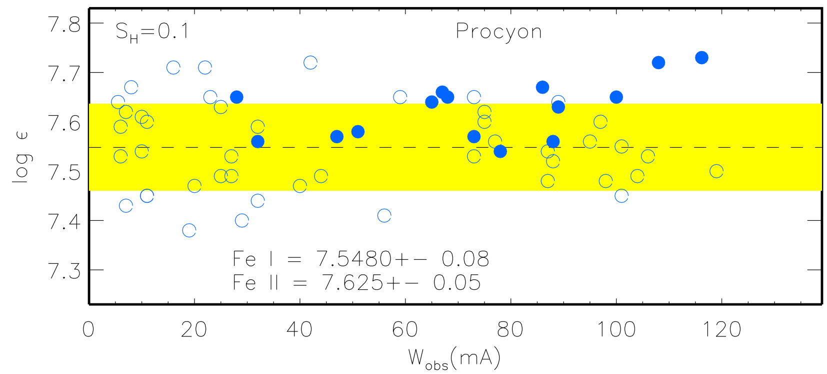

Figure 2: Non–LTE iron abundances from the Fe I (open circles) and Fe II (filled circles) lines in Procyon plotted as a function of W_{obs}. The dashed line indicates the mean abundance derived from the Fe I lines and the shaded grey area marks its statistical error. The Fe II, gf–values are adopted from Raassen and Uylings (1998).

5 Departures from LTE Depending on Stellar Parameters

The non–LTE calculations were performed for the small grid of model atmospheres with the stellar parameters characteristic of early F to late A–type stars: $T_{\rm eff} = 6500 - 8500$ K, $\log g = 3$ and 4. In this stellar parameter range, the general behavior of departure coefficients of the Fe I and Fe II levels is independent of the effective temperature and surface gravity and very similar to that shown in Fig. 1. Non–LTE leads to the weakening of Fe I lines and to the opposite effect for Fe II. Table 1 presents the non–LTE abundance corrections for the representative lines of Fe I and Fe II with various $E_{\rm exc}$.

Non–LTE effects are only minor for the Fe II, namely, the abundance correction does not exceed 0.03 dex in the absolute value. For the Fe I in the $\log g = 4$ models, ΔNLTE ≤ 0.12 dex and, on the average, it decreases towards higher $T_{\rm eff}$. For the lower gravity models, ΔNLTE ≤ 0.20 dex and, on the average, it grows towards higher $T_{\rm eff}$. It is worth noting that the non–LTE abundance correction is substantially different for different lines at any given temperature.

Our theoretical results were compared with non–LTE predictions of Rentzsch–Holm (1996) in the common stellar parameter range, $T_{\rm eff} = 7000 - 8500$ K, $\log g = 4$ and 3.5. There is no discrepancy for the Fe II lines, while the departures from LTE for Fe I are stronger in Rentzsch–Holm (1996) than in this study. For example, in the model 8500/4, Rentzsch–Holm (1996) gave the mean non–LTE correction of 0.17 dex, which is 0.1 dex larger than our value. In contrast to our results, the non–LTE correction from Rentzsch–Holm (1996) grows towards higher $T_{\rm eff}$ independent of the stellar surface gravity. In both studies, the departures from LTE grow towards lower gravity, however, with $\log g = 3$, we obtain smaller non–LTE corrections, than Rentzsch–Holm (1996) did with $\log g = 3.5$. The difference between two studies is in the use of different model atoms. Our model atom of Fe I is much more complete, than that of Rentzsch–Holm (1996), where only 79 terms of Fe I are included and most of high-excitation levels with $E_{\rm exc} > 6$ eV are absent. This explains why the overionization of Fe I is stronger in the Rentzsch–Holm (1996) calculations.

6 Conclusions

- Completeness of the model atom is important for the correct calculation of the statistical equilibrium of iron.

Table 1: Non–LTE abundance corrections (dex) for the selected lines of Fe I and Fe II. Multiplet numbers are indicated in the third string.

$T_{\rm eff}$	$\log g$	Fe I					Fe II			
		5434	4920	5282	5217	5367	4924	4583	5325	6247
		(15)	(318)	(383)	(553)	(1146)	(42)	(37)	(49)	(74)
6500	4	0.06	0.08	0.12	0.12	0.04	−0.02	0.00	0.00	-0.01
7000	4	0.06	0.06	0.10	0.10	0.03	−0.02	0.00	0.00	−0.01
7500	4	0.06	0.03	0.08	0.08	0.04	−0.02	0.00	0.00	−0.01
8000	4	0.05	0.01	0.06	0.07	0.05	−0.02	0.00	0.00	−0.01
8500	4	0.06	0.00	0.05	0.07	0.08	−0.02	0.00	0.00	−0.01
6500	3	0.01	0.10	0.14	0.12	0.01	−0.02	−0.01	−0.01	−0.02
7000	3	0.03	0.08	0.12	0.11	0.02	−0.02	−0.01	0.00	−0.02
7500	3	0.06	0.05	0.10	0.11	0.06	−0.02	0.00	0.00	−0.02
8000	3	0.10	0.06	0.11	0.14	0.14	−0.02	0.00	0.00	−0.02
8500	3	0.13	0.06	0.12	0.18	0.20	−0.03	0.00	0.00	−0.02

- In the stellar parameter range, characteristic of middle F to middle A–type stars, the LTE underestimates the element abundance derived from the Fe I lines by 0.02 – 0.1 dex for the dwarfs depending on the line and stellar temperature and by up to 0.20 dex for giants.
- LTE is as good as non–LTE for Fe II.
- The uncertainty in the available gf–values for the visible lines of Fe I and Fe II is uncomfortably too high, hence the solar and stellar iron abundances cannot be determined with the accuracy better than 0.1 dex. The astrophysical community shall ask atomic spectroscopists for new more accurate measurements.

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