NLTE effects on Fe I/II in the atmospheres of FGK stars and application to the abundance analysis of their spectra

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Abstract. We describe the first results from our project aimed at large-scale calculations of NLTE abundance corrections for important astrophysical atoms and ions. In this paper, the focus is on Fe which is a proxy of stellar metallicity and is commonly used to derive effective temperature and surface gravity. We present a small grid of NLTE abundance corrections for a sample of Fe I lines and discuss how the NLTE effects influence the determination of effective temperature, surface gravity, and metallicity for late-type stars.

1. Introduction
Iron is a key element in stellar astrophysics. The very complex atomic structure of its lowest ionization stages, Fe I and Fe II, gives rise to a wealth of spectral lines all across the spectrum of a typical late-type star. This atomic property, coupled to a relatively large abundance makes Fe a reference for spectroscopic estimates of stellar parameters using the method of excitation-ionization balance.

The classical implementation of this method in spectrum analysis codes involves three assumptions: local thermodynamic equilibrium (LTE), hydrostatic equilibrium, and 1-D geometry. These approximations strongly reduce the complexity of the problem, thus permitting analysis of very large stellar samples in short timescales. Yet, in conditions when the breakdown of 1-D static LTE models occurs the inferred stellar parameters suffer from large systematic biases. To assess the latter, more physically realistic modeling is necessary.

Studies of NLTE effects on the Fe I/Fe II level populations for FGK stars trace back to Athay & Lites (1972). Since then, vast amounts of work have been performed in the field, demonstrating that NLTE effects on the excitation-ionization balance of Fe I/Fe II are significant and cannot be ignored even for analyses of solar-type stars (Mashonkina et al. 2011 and references therein). Yet, despite major efforts aimed at understanding how non-local thermodynamic equilibrium affects the line formation of Fe, there has never been an attempt to accurately quantify these deviations in a systematic way for a wide range of stellar parameters, and to apply them to a large stellar sample.

We present a new NLTE model atom for Fe I/Fe II applied in large-scale calculations of NLTE abundance corrections of late-type stars. We discuss NLTE effects influencing atomic level populations at typical conditions in the atmospheres of late-type stars and provide a small grid of the NLTE corrections for Fe I lines. The model has been tested on a number of well-studied
stars with independently-determined parameters, including metal-poor giants and turnoff stars. These tests performed with classical 1-D hydro-static model atmospheres and averages of 3-D hydrodynamical simulations of stellar convection will be presented in Bergemann et al. (in preparation). A complete grid of NLTE abundance corrections computed with the multi2.3 statistical equilibrium code will be presented in Lind et al. (in preparation).

2. Methods

2.1. Model atmospheres and codes

The calculations presented here were performed with the 1-D LTE plane-parallel mafags-odf models (Fuhrmann et al. 1997, Grupp 2004). In these models convective energy transport is accounted for using the mixing-length theory of Böhm-Vitense (1958), with the mixing length parameter \( \alpha_{\text{mlt}} \) set equal to 0.5. Line opacity is represented for all chemical elements up to Ni, and for various diatomic molecules (\( \text{H}_2 \), CH, CO, Mg\( \text{H} \), etc). This accounts for nearly 20 million atomic and molecular lines. The reference solar abundances were compiled from various literature sources, giving preference to the determinations by the Munich group. The model atmospheres provide the partition functions and the partial pressures of all relevant atoms and molecules.

The NLTE statistical equilibrium of Fe was computed with a revised version of the detail code (Butler & Giddings 1985), which solves the multi-level NLTE radiative transfer for a given static 1-D model atmosphere. The latest version of the code is based on the Accelerated Lambda Iteration (ALI) method. LTE and NLTE line formation calculations with the departure coefficients from detail were performed with a revised version of the spectrum synthesis code SIU (Reetz 1999). The major update in the code relates to the automated computation of NLTE abundance corrections\(^1\), which generally proceeds by constructing the grids of LTE and NLTE line equivalent widths for a range of stellar parameters and interpolating the corresponding curves-of-growth for the input observed equivalent widths or abundance values.

2.2. Model atom

The NLTE model atom of Fe was constructed using all available atomic data from the Kurucz\(^2\) database, which also includes laboratory data from the NIST compilation\(^3\). All predicted energy levels of Fe\( \text{I} \) with the same parity above \( E_{\text{low}} \geq 5.1 \text{ eV} \) were grouped into super-levels. Transitions between the components of the super-levels were also grouped. The total transition probability of a super-line is a weighted average of the \( \log g_f s \) of individual transitions. Thus, in the final atomic model, the number of energy levels is 296 for Fe\( \text{I} \) and 112 for Fe\( \text{II} \), with the uppermost excited levels located at 0.03 eV and 2.72 eV below the respective ionization limits of 7.9 eV and 16.19 eV. The model is closed by the Fe\( \text{III} \) ground state. The total number of radiatively-allowed transitions is 16 207 (13 888 Fe\( \text{I} \) and 2 316 Fe\( \text{II} \)).

The photoionization cross-sections for 136 states of Fe\( \text{I} \) were taken from Bautista (1997) and the hydrogenic approximation was adopted for all other levels. The rates of transitions induced by inelastic collisions with electrons (\( e^- \)) and H\( \text{I} \) atoms were computed using different recipes. The electron cross-sections from states with allowed bound-bound and bound-free transitions were computed with the formulas of van Regemorter (1962), respectively, Seaton (1962). These states were also coupled by inelastic H\( \text{I} \) collisions using Drawin’s formula (Drawin 1969) in the version of Steenbock & Holweger (1984). All the other states are connected by forbidden transitions induced by inelastic collisions with \( e^- \) and H\( \text{I} \) atoms. These are computed using the

\(^{1}\) the NLTE abundance correction is defined to be the difference in the abundances required to match NLTE and LTE line profiles or equivalent widths

\(^{2}\) http://kurucz.harvard.edu/atoms.html

\(^{3}\) http://www.nist.gov/pml/data/asd.cfm
formulae of Allen (1973) and Takeda (1994). Quantum-mechanical calculations exist only for e\textsuperscript{−}-induced forbidden transitions between the 16 lowest Fe ii energy levels (Ramsbottom et al. 2007). These data are compared with Allen’s (1973) recipe in Fig. 1.

The influence of e\textsuperscript{−} and H i collisions on the statistical equilibrium of Fe was carefully investigated by performing test calculations with various scaling factors to the above-mentioned formulae. Furthermore, the NLTE synthetic profiles were compared with observed spectra of well-studied stars to check how well the test model atoms satisfy the constraint of ionization-excitation balance of Fe i/Fe ii under the restriction of different stellar parameters. The final choice of the scaling factors will be discussed in Bergemann et al. (in preparation).

3. Statistical equilibrium of Fe

3.1. NLTE effects

Figure 2 shows level departure coefficients\textsuperscript{4}, $b_i$, as a function of continuum optical depth \( \log \tau_{9000} \) for a number of model atmospheres computed with different stellar parameters. The latter are representative of stars typically used in Galactic chemical evolution studies. Only selected energy levels of Fe i and Fe ii typical for their depth-dependence are included in the plot: $^5\zeta$ (the ground state of Fe i), $^2\zeta$ (2.4 eV), $^5\zeta$ (5.4 eV), $^3\zeta$ (the ground state of Fe ii), and $^4\zeta$ (5.5 eV). All these levels give rise to radiatively-permitted transitions, which are used in the detailed abundance analysis of the Sun and of a number of metal-poor stars in Bergemann et al. (in preparation).

The common result for all the models shown in Fig. 2 is that in the optically thin atmospheric layers the majority of the Fe i levels are underpopulated compared to LTE, $b_i < 1$. The Fe ii number densities remain close to LTE values, $b_i \approx 1$, and a minor overpopulation of the Fe ii ground state develops only close to the outer atmospheric boundary.

Deviations from LTE in the distribution of atomic level populations arise because the mean radiation field, $J_\nu$, at different depths and frequencies is not equal to the Planck function, $B_\nu(T_e(\tau))$, which is defined by the local temperature $T_e(\tau)$ at each depth. For Fe i, an excess of the mean intensity over the Planck function in the UV continua leads to over-ionization, which sets in as soon as the optical depth in the photoionization continua of the low-excitation Fe i

\textsuperscript{4} Departure coefficient is defined to be the ratio of NLTE to LTE atomic level populations, $b_i = n_i^{\text{NLTE}}/n_i^{\text{LTE}}$. 

\begin{figure}
\centering
\includegraphics[width=\textwidth]{figure1}
\caption{Left-hand panel: Grotrian diagram of the Fe i atom. Right-hand panel: comparison of the quantum-mechanical rate coefficients for e\textsuperscript{−}-induced forbidden transitions between the lowest energy levels of Fe ii (Ramsbottom et al. 2007) with the classical Allen’s (1973) recipe.}
\end{figure}
Figure 2. The departure coefficients of selected Fe I and Fe II levels for a number of model atmospheres from the grid; stellar parameters are indicated in each figure.
levels falls below unity, i.e. \( \log \tau_{5000} \sim 0 \). In the outer layers, the ionization balance is dominated by the \( \text{Fe}^1 \) levels with excitation energies of \( 4 - 5 \) eV. In the infra-red continuum, \( J_\nu < B_\nu \) leads to over-recombination, which is very efficient in our atomic model with only a \( 0.03 \) eV energy gap between the upper \( \text{Fe}^1 \) levels and the ground state of \( \text{Fe}^2 \).

Due to an extremely tight radiative and collisional coupling of the atomic energy levels, the excitation balance of \( \text{Fe}^1 \) is also affected by radiative imbalances in the line transitions. These include radiative pumping by a super-thermal UV radiation field of non-local origin at the line frequencies, as well as photon suction driven by photon losses in the large-probability transitions between highly-excited levels. These processes leave a characteristic imprint on the behavior of \( b_\lambda \)-factors in the outer atmospheric layers. In Fig. 2, this is seen as the onset of deviations from the relative thermal equilibrium between the \( \text{Fe}^1 \) levels, which occurs, depending on the model metallicity, at \( \log \tau_{5000} \sim -1... -2 \). The NLTE effects on the line formation are different for the strong and weak \( \text{Fe}^1 \) lines. The former are mostly shaped by deviations of their source function from the Planck function, which yields a clear effect in the line cores. Weak lines are pre-dominantly controlled by their opacity, thus the major change is due to the shift of their optical depth scale in NLTE.

### 3.2. NLTE abundance corrections

We computed NLTE abundance corrections, hereafter \( \Delta_{\text{NLTE}} \), to \( \text{Fe}^1 \) lines for a small grid of model atmospheres covering the metallicity range \(-3.6 \leq [\text{Fe/H}] \leq +0.3\). The results are presented in Fig. 3 for parameters representative of giants (left-hand panel) and dwarfs (right-hand panel). Our sample of \( \text{Fe}^1 \) lines includes the transitions between 0 to 5 eV levels, and line equivalent widths \( W_\lambda \) that range from 5 m\( \text{A} \) to a few \( \text{A} \) depending on the stellar parameters. We used 30 to 130 lines per model.

In the plot, each symbol corresponds to a mean \( \Delta_{\text{NLTE}} \) obtained by averaging individual NLTE corrections for all \( \text{Fe}^1 \) lines in the sample, and the errorbars correspond to the line-to-line variations in \( \Delta \) for each model atmosphere. The former quantity roughly demonstrates how much the Fe I/Fe II ionization balance, and thus, the determination of the surface gravity, is affected by NLTE, whereas the latter helps to assess the influence of NLTE on the excitation balance and the determination of the effective temperature.

![Figure 3](image-url)  
**Figure 3.** NLTE abundance corrections for different stellar parameters. Right-hand panel: all model atmospheres adopt \( \log g = 4.6 \).

The NLTE corrections increase with decreasing \([\text{Fe/H}]\) and \( \log g \), thus the ionization balance achieved assuming LTE leads to progressively underestimated gravities and metallicities. In particular, at \( T_{\text{eff}} = 5000 \) K (Fig. 3, left-hand panel), the mean NLTE corrections are twice as
large in the log $g = 2.2$ model compared to the log $g = 3.4$ model, reaching $+0.4$ dex at [Fe/H] $\sim -3.5$. It is also interesting that the NLTE corrections for the dwarf models critically depend on $T_{\text{eff}}$. Figure 3 (right-hand panel) shows that for the coolest models, $T_{\text{eff}} \sim 5000$ K, one may safely adopt the LTE approximation down to the lowest metallicities. However, LTE leads to severe errors in surface gravity estimates for warm turn-off stars of $T > 6000$ K.

On the other side, the non-negligible errorbars indicate that there are line-to-line variations of the NLTE abundance corrections for the same model atmosphere. The spread of $\Delta_{\text{NLTE}}$ among Fe i lines with different equivalent widths $W_\lambda$ and excitation potentials $E_{\text{low}}$ strongly increases with decreasing metallicity for giants, and less so for dwarfs. Furthermore, this scatter is not random, but corresponds to a trend of $\Delta_{\text{NLTE}}$ with $E_{\text{low}}$, as we show in Fig. 4. The figure demonstrates the variation of NLTE corrections with the lower level excitation potential for models with parameters: $T_{\text{eff}} = 5000$, log $g = 2.2$, [Fe/H] $\sim -2.4$ (left-hand panel) and $T_{\text{eff}} = 5800$, log $g = 4.6$, [Fe/H] $\sim -2.4$ (right-hand panel). The stronger lines, $W_\lambda > 60$ mA, tend to exhibit smaller departures from LTE compared to the weaker lines, but they also demonstrate systematically increasing $\Delta_{\text{NLTE}}$-values with increasing $E_{\text{low}}$. No such effect is observed for the weak lines of $W_\lambda \leq 60$ mA, which, with some exceptions, have very similar NLTE corrections independent of their excitation potential.

Thus, our results suggest that LTE $T_{\text{eff}}$ determinations become very inaccurate at [Fe/H] $< -2$ and there are systematic effects in the $T_{\text{eff}}$-scale of dwarfs and giants.

![Figure 4](image.png)

**Figure 4.** NLTE abundance corrections for the Fe i lines as a function of the lower level excitation potential. Red and blue colors separate the spectral lines with $W_\lambda$ greater and less than 60 mA, respectively. Stellar parameters are indicated in the plots.

### 4. Conclusions

We have constructed a new NLTE Fe model atom using the most up-to-date theoretical and experimental atomic data. The model has been tested on a number of well-studied late-type stars with the parameters determined by other independent methods (Bergemann et al., in preparation).

Our preliminary results for the NLTE effects on Fe i and Fe ii in the atmospheres of late-type stars are qualitatively consistent with other studies. Kinetic equilibrium of Fe, which is a minority ion at the typical conditions of these cool and dense atmospheres, favors lower number densities of Fe i compared to LTE. The number densities of Fe ii are hardly affected by NLTE. In general, this leads to a weakening of Fe i lines compared to LTE, which, in turn, requires a larger Fe abundance to fit a given observed spectral line. The magnitude of the departures and the NLTE corrections critically depend on the stellar parameters. Whereas NLTE abundance
corrections for the Fe I lines do not exceed $\sim 0.05$ dex for solar metallicity dwarfs, they can be as large as 0.6 dex for metal-poor giants.

We find that both the excitation and ionization balance are affected by NLTE effects on Fe I. The NLTE corrections to the Fe I lines increase with decreasing [Fe/H] and log $g$, thus the ionization balance achieved assuming LTE leads to progressively underestimated surface gravities and metallicities. On the other side, Fe I levels are neither in thermal equilibrium with respect to each other, and for the stronger lines the NLTE abundance corrections show trends with the line excitation potential. In particular, we find that LTE $T_{\text{eff}}$ determinations become very inaccurate at low metallicities and significant systematic effects in the $T_{\text{eff}}$-scale of dwarfs and giants can be expected.

The NLTE abundance corrections will become publicly available through an interactive online database, which is currently under construction. Users will be able to retrieve NLTE abundances and/or NLTE abundance corrections for the input, e.g., observed, equivalent line widths. We also consider an option to provide a functional dependency of the NLTE corrections on spectral line parameters for a grid of stellar parameters ($T_{\text{eff}}$, log $g$, [Fe/H]). This is a more convenient solution for the implementation in automated codes used in large-scale spectroscopic studies, such as follow-up spectroscopy of Gaia targets.

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