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NLTE line formation

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Abstract
I review some of the present achievements and future challenges of non-local thermodynamic equilibrium (NLTE) line-formation calculations for solar-type stars. It is concluded that the full potential of NLTE still remains to be tapped, in particular in view of the current transition from one-dimensional (1D) hydrostatic to 3D hydrodynamic model atmospheres.

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1. Introduction

The spectra of solar-type stars contain a wealth of information that we can use to study the Universe: stellar fluxes and spectral lines can be used to constrain the thermodynamic quantities (most often the kinetic temperature and gas pressure) of the photospheric plasma that govern the line formation process. Simultaneously, the lines contain information about the composition of the stellar atmosphere, which can be used to assign the star to a population and to study the chemical evolution of the Galaxy.

Undoubtedly, quantitative stellar spectroscopy is a mature discipline within astrophysics. Why is it then that most of the chemical abundance studies in the literature assume local thermodynamic equilibrium (LTE)? Are we not 'building palaces upon sand' when drawing conclusions on the chemical evolution of the cosmos based on LTE analyses (Gustafsson *et al* 2007)? Thanks to efficient spectrographs on 8 m-class telescopes, the observational material for galactic stars is of excellent quality (even for bulge giants; see Ryde, this volume). For certain elements, star-to-star scatter is practically absent down to [Fe/H] = −4 (Cayrel *et al* 2004, Arnone *et al* 2005). To correctly delineate abundance trends as a function of metallicity is thus no longer a question of resolving power and signal-to-noise ratio, but mainly a matter of how accurate the line formation process can be modelled over orders of magnitude in [Fe/H]. This is where departures from LTE (aka non-LTE or NLTE effects) come into play.

In the following, some aspects of NLTE line formation will be discussed. In this, the focus will lie on restricted steady-state statistical equilibrium (SSSE) in one-dimensional (1D) hydrostatic model atmospheres of FGK-type stars in LTE with a statistical representation of opacities (either via opacity sampling, OS, or opacity distribution functions, ODF) and mixing-length-type (MLT) treatment of convection (hereafter simply referred to as NLTE). The word restricted indicates that the T-τ-relation is assumed to be unaffected by departures from LTE, which can only be the case if the element we study is a trace element that does not contribute opacity or free electrons in appreciable amounts. This is by far the most widespread NLTE problem that is addressed (see, e.g. Bergemann, this volume). Others solve the restricted NLTE problem for dominant species (Barklem, this volume), many atoms (Kudritzki, this volume), in 1.5-dimensional (1.5D) (Collet, this volume) or in 3D (Carlsson, this volume). In 1D, even the full (yet time-independent) NLTE problem can be dealt with (Short and Hauschildt 2003).

In the paragraph above, numerous assumptions are listed. NLTE lifts the LTE approximation. Hydrodynamic model atmospheres do away with the hydrostatic approximation. It is, however, important to realize that our modelling rests on many assumptions (and choices!) which are tested together with the physics we hope to assess. In this sense, apparent shortcomings of NLTE may well turn out to be caused by one of the underlying assumptions. With these cautionary words, let us take a look at NLTE.

2. When LTE is good, and why

In cool-star research, LTE has been a widespread assumption for a variety of (good?) reasons: for many decades, the data one could obtain with moderate-sized telescopes with moderately efficient spectrographs were limited both in number and quality. Even with the much improved data we

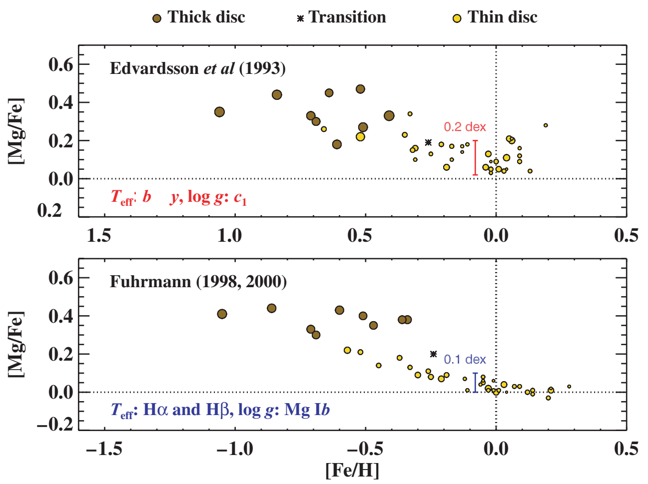

Figure 1. Comparison of Mg and Fe abundances of 44 stars in common between Edvardsson *et al* (1993, top panel) and Fuhrmann (1998, 2000, bottom panel). Without the colour coding taken from Fuhrmann, the thick-disc stars would appear as a thin-disc extension to lower metallicities in the Edvardsson *et al* study.

now have access to, NLTE effects are hardly ever directly visible (a notable exception being photospheric emission lines (Sundqvist *et al* 2008) and the cores of strong resonance lines). In addition, the input data necessary to fill rate equations are not as complete as one would hope. Who would want to trust NLTE when the uncertainties associated with the input data exceed the predicted NLTE abundance corrections?

And, admittedly, there are beautiful results based on LTE. In a series of papers, Klaus Fuhrmann (Fuhrmann (2008) and references therein) has studied the stellar inventory of F and G stars within 25 pc around the Sun. He uses spectra of good quality (typically, $R = 60\,000$ and $S/N = 200$ per pixel) to derive spectroscopic stellar parameters, photospheric abundances of magnesium and iron and isochrone ages. When the spectroscopic distances are compared with the Hipparcos astrometry (Perryman *et al* 1997), the offset turns out to be $0.5 \pm 5.1\%$ (rms). This offset corresponds to an accuracy in $T_{\rm eff}$ of 10 K or 0.005 dex in $\log g$! At 50 K and 0.05 dex, even the rms precision is astonishingly high. When studying chemical abundances, the thin-disc stars show hardly any star-to-star scatter ($\sigma < 0.03$ dex) at a given metallicity and the thick-disc stars can be separated from the thin disc on a star-by-star basis. This is a significant improvement over the seminal study of Edvardsson *et al* (1993) in which thick-disc stars were not identified chemically (see figure 1).

How can a simple LTE analysis be this accurate? The answer lies in the combination of homogeneous high-quality observational data, a strictly differential approach (line-by-line relative to the Sun) and, in spite of being interactive, a fully homogeneous data analysis performed by a single neural-network pattern-recognition software called KF's brain. NLTE effects between the Sun-like stars and the Sun effectively cancel. This works as long as the range in stellar parameters ($T_{\rm eff}$, $\log g$ and [Fe/H]) is sufficiently small. It will not work when studying stars across orders of magnitude in surface gravity or metallicity. In that case, one needs to take a more sophisticated approach.

3. Advanced armoury

At this symposium, I compared the situation with LTE and NLTE to the combat capabilities of orcs and elves in Tolkien's Middle-earth: whereas the former is a fierce fighter applying brute force in one-on-one (local!) combat, the latter takes on a refined approach, uses a bow and arrow (a non-local tool!) and fights in formation. In less mythological terms, LTE is a single-shot rifle, whereas NLTE is a machine gun with thousands of shots[1] (per iteration). Now, which one would you like to own in order to defend your territory? And what is the price you have to pay? While the former question is purely rhetorical, the latter deserves some explanation. You may have to pay in terms of the investment of research time to learn NLTE (yes, this can be toilsome or even painful). Relaxing LTE means also opening the door to additional degrees of freedom in the modelling. In the worst case, these extra degrees of freedom will turn out to host free parameters that one needs to deal with one way or another. But by using NLTE you will be equipped to master situations that LTE has no chance of tackling.

4. NLTE in a nutshell

Among others, nutshell reviews of NLTE have been made by Kiselman and Carlsson (1995) and Kiselman (1999); here I will attempt to be even nuttier.

In NLTE, a set of rate equations is solved together with the equation of radiative transfer. Every level is represented by one rate equation of the form

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

which states that in a steady-state situation ($d/dt = 0$) the processes depopulating level i are balanced by the processes that populate that level. The atomic processes separate into two main groups: radiative (R_{ij}) and collisional (C_{ij}) processes. Physically, the collisional processes are not problematic: they are strictly local (orcs!), as particles need to come close to one another to collide. As a rule of thumb, more efficient collisions will therefore drive a level's populations towards LTE (there are non-academic exceptions to this rule). In contrast, photons carry non-local information (elves!) if their mean free path is sufficiently long. If enough of them do, then the atoms and ions will react to the non-local radiation field, by occupying levels/ionization stages in a way that departs from the local Saha–Boltzmann statistics. Photo-ionization feeding on the UV flux is the main agent of NLTE effects.

These basic considerations already give us an idea of where to expect departures from LTE: a metal-poor early-type giant is more prone to NLTE effects than a metal-rich late-type dwarf star. Furthermore, it is easier to perturb the occupation densities of minority species such as Fe I. This is why the use of Fe II lines as metallicity indicators is advocated (but see section 5).

LTE is thus the limiting case of a continuum (an ocean, if you will) of physical excitation and ionization situations.

[1] I am a pacifist and approve of military violence only in the world of fiction.

Table 1. NLTE studies of Fe I and some of their input parameters.

No. of levels	Up to [eV]	Source	S_H
15	4.30	Athay and Lites (1972)	not included
256	6.48	Thévenin and Idiart (1999)	assumed to be 1
50 (+9)	6.88 (7.77)	Gratton *et al* (2001)	calibrated to 30
846	7.79	Korn *et al* (2003)	calibrated to 3
334	6.91	Collet *et al* (2005)	assumed to be 0.001

Because of that, LTE is not the 'safe harbour' it is sometimes perceived to be.

There are codes that take care of the numerical part of the problem: DETAIL (Butler and Giddings 1985) and MULTI (Carlsson 1986) are two examples. The model atoms, however, fall within the responsibility of the user.

So, how do I implement NLTE effects into my favourite line-formation code? NLTE effects are usually tabulated as departure coefficients $b_i = n_i/n_i^*$, where n_i is the true NLTE population of level i and n_i^* the one in LTE. The dimensionless b_i values (given as a function of a depth variable) are then used in any LTE line-formation code to modify the line source function (where the ratio of n_l (lower level) to n_u (upper level) enters) and the line opacity ($\propto n_l$) which in turn enters the optical depth scale.

5. The crown jewel: iron

Iron has a special place in stellar astrophysics. It is a relatively abundant and relatively heavy element that has many lines in the optical and near-UV part of the spectrum arising from both transitions within neutral and singly ionized iron. It is an important source of opacity and electrons for cool stars which is why one needs to determine its abundance to construct a model atmosphere for a specific star.

Due to the complexity of its term system (Bob Kurucz has computed of order 800 000 predicted lines), meaningful NLTE studies of iron have been difficult to perform. Table 1 lists some of the input parameters of selected NLTE studies of neutral iron. In column 1, the number of levels considered is listed. It is clear that one has to have a sufficiently large number of levels to realistically model how Fe I will behave under the prevailing processes such as photo-ionization and collisions. The highest level considered is another key parameter (column 2), as it decides how well the term system couples to the continuum. When levels are densely spaced (as is the case close to the ionization energy of Fe I), the consideration of levels with high-enough statistical weights is more important than a realistic treatment of how they are distributed. In other words, these levels can be grouped into superlevels, but they must not be left out. If an artificial gap larger than $\approx$ 0.5 eV (kT at 6000 K) is introduced below the ionization energy ($\chi_{\mathrm{Fe\,I}} = 7.78$ eV), then collisions with free electrons cannot keep the highest levels coupled to the continuum and the ground state of Fe II. This will tend to aggravate NLTE effects in Fe I.

It is usually the collisional side of the rate equations that is most uncertain. For electron collisions, many calculations exist, but they need to be complemented with the help of formulae (see Mashonkina *et al* (2007) for examples of this). Worse yet is the situation for collisions with neutral hydrogen. While the scarce experimental/theoretical data point towards their being rather inefficient for resonance transitions (Belyaev 1999) or simple atoms (Barklem *et al* 2003), they are needed for all transitions throughout the whole term system. To include them, one usually uses a simplistic formula (Drawin 1968, Steenbock and Holweger 1984, Lambert 1993) and scales it with an equally simplistic factor called S_H (column 4). Some schools (including the one that I have gone through) consider this factor to be the main free parameter of the NLTE modelling. To determine its value, one tries to find constraints from observations (see section 6).

Overall, the differences in the predicted NLTE abundance corrections are very large: some authors predict NLTE abundance corrections to be negligible for all metallicities (Gratton *et al* 2001), whereas others find corrections as large as 0.55 dex for the metal-poor subgiant HD 140283 (Collet *et al* 2005). Note that corrections to surface gravities based on the iron ionization equilibrium are typically a factor of two to three larger, thus exceeding 1 dex for the aforementioned star. The work that I have been involved in predicts small corrections for dwarfs and subgiants, but effects become significant for metal-poor giants (Korn *et al* 2003, reinvestigation underway). These differences can be traced to the different input assumptions (large energy gaps and low collisional efficiencies will aggravate NLTE effects). Some claim that Fe II lines are not immune to NLTE, either (Collet *et al* 2005). It is, however, clear that there can only be one realistic NLTE correction per line per star. How can we tell right from wrong?

6. Do like photometrists do: calibrate

Unknown atomic physics like the strength of collisions with neutral hydrogen in tenuous media such as stellar atmospheres is troublesome and there are three principle reactions: (1) head in the sand, (2) flight forward and (3) use of quantum-chemistry predictions. Until option 3 materializes, I prefer option 2 over option 1. If there is only one free parameter in the modelling, then one can determine it from adequate observations (but see the cautionary note at the end of the introduction). Nature supplies laboratories where we can put our modelling to the test. First and foremost, we have the Sun. It is advantageous to perform such calibrations on the Sun (see Kiselman, this volume) as more observables than usual can be utilized (centre-to-limb variation of lines and the continuum, intensity spectra of granules and sunspots). Generally speaking, NLTE effects of solar spectral lines are, however, relatively small. The next level of objects are those whose parameters are well constrained, ideally from fundamental measurements of absolute fluxes, angular radii and distances. Then come stars that we have grown fond of

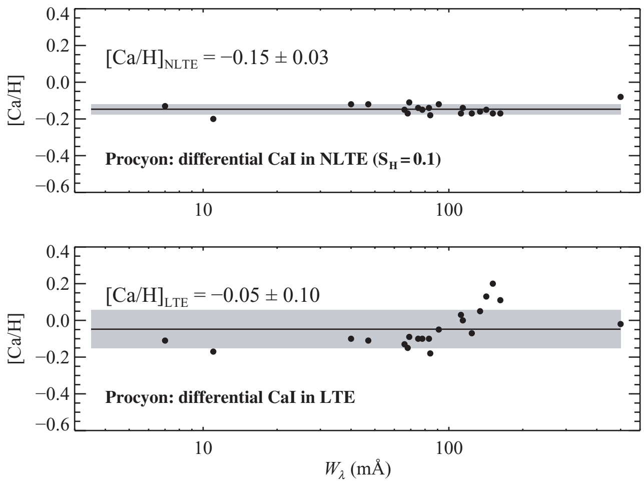

Figure 2. Procyon's calcium abundance as derived from Ca I lines as a function of line strength. While the LTE analysis (bottom panel) shows a very distinct abundance trend for strong lines, the NLTE analysis (top panel) produces a single calcium abundance with significantly reduced line-to-line scatter. Procyon turns out to be surprisingly calcium-poor.

over the years, in which we have considerable trust that they are well behaved. A list of such stars (biased by personal taste) could look like this: Sun, Procyon, Arkturus, HD 103095, HD 84937 and HD 122563.

Then there are stars that belong to stellar systems with numbers of stars ranging from two (aka binaries) to a few hundred thousands (aka globular clusters). Just the fact that all stars in a distant cluster are equally far from us can be of high diagnostic value.

There are several observables which can, in principle, be used to calibrate the unknown strength of hydrogen collisions. The observables vary from element to element, but generally one tries to achieve the highest possible consistency between different features minimizing trends and line-to-line scatter as a function of line strength (see figure 2), excitation and ionization, for atomic and molecular features alike.

A good example of this procedure is given by Mashonkina *et al* (2007). In this study of NLTE effects in neutral and singly ionized calcium, the ionization-equilibrium condition was used in conjunction with the known surface gravities of metal-poor stars with significant Hipparcos parallaxes to put constraints on the allowed range of S_H. For a small sample of stars, good overall agreement was found for an S_H value of 0.1 with clear indications that neglecting hydrogen collisions altogether will overestimate NLTE effects. The model atoms calibrated in this way have been successfully applied to the three most iron-poor stars known (HE 0107–5240, HE 1327–2326 and HE 0557–4840). LTE analyses of Ca I/II in the spectra of these stars indicate large systematic discrepancies, ranging from 0.37 dex (Norris *et al* 2007) to 0.57 dex (Aoki *et al* 2006). In HE 1327–2326, calcium remains the only element represented by two ionization stages. For this star, the ionization equilibrium in NLTE can be established at a surface gravity of 3.7 (Korn *et al*, in preparation). The NLTE abundance correction for the weak ($W_\lambda = 2.6$ mÅ) Ca I resonance line at 4226 Å is +0.31 dex.

Harmonizing the abundances of an elements between stars is a globular cluster has turned out to be dangerous or outright wrong, as there are evolutionary effects that all elements are subject to (Korn *et al* 2007). Bengt is currently leading an observational campaign on M 67 at the VLT, to test to what extent younger, more metal-rich stars are affected by diffusive processes.

Hydrodynamic models coupled with LTE line formation predict abundance corrections for the Ca I resonance line of roughly−0.5 dex in a star like HE 0107–5240 (Collet *et al* 2007). Corrections for Ca II lines have not been published, but are expected to be smaller. It thus remains to be seen whether a full 3D NLTE approach is capable of establishing the Ca I/II ionization equilibrium and at which value of the surface gravity. One can shift giants like HE 0107–5240 up and down the giant branch, but this is not possible in the case of the hot subgiant HE 1327–2326.

7. Where to go from here

The demands on stellar parameters and chemical abundances will continue to increase, as we collect larger and more diverse samples of stars in upcoming wide-angle surveys such as LAMOST (Christlieb, this volume) or Gaia (Thévenin, this volume). The more inhomogeneous these samples are, the more ambitious we have to be to control systematic effects. The same is true for the few spectral features visible in the spectra of the most iron-poor stars: we have to understand their line formation better to correctly read the chemical fingerprints of the first stars that enriched them with the first metals.

Surveys are treasure chests which one should use to identify stars with specific properties. For example, one can select stars that mainly differ in one of the stellar parameters, thereby testing certain parts of the NLTE modelling specifically: when α-elements supply most of the electrons, a sequence of stars with different [α/Fe] will serve to test electron collisions. Along similar lines, more such tests can be devised.

For homogeneous samples of stars, the situation is easier and we can be more ambitious in our science goals: at a given metallicity, we attempt to use small (0.1 dex) differences in abundances to chemically tag a star and to uniquely identify its origin and/or population membership. The same is true for the study of stellar evolutionary effects of all kinds.

As a hardliner, one should therefore demand: LTE line formation is acceptable only when shown to be valid by detailed NLTE calculations. This would require several groups to either change subject or to form alliances with groups capable of performing NLTE calculations. An alternative would be for the latter groups to make their results available to the community. There are ways that will make even the sceptics adopt NLTE: show them where NLTE is critical and supply NLTE results in a simple-to-use way. One can publish departure coefficients and tabulated abundance/flux corrections via web interfaces. For the 1D case, even automated on-demand calculations are computationally not prohibitive. As part of Uppsala's Gaia involvement, we are in the process of making high-resolution spectra of the RVS wavelength range with Ca IR triplet lines in NLTE available for the whole grid of MARCS model atmospheres.

Concerning the modelling, efforts should be made to do away with all these formulae which serve as a crutch for our ignorance. They cloud and lessen the predictive power of NLTE calculations.

Ultimately, one should relax additional assumptions. There is no principle obstacle that prevents one from iteratively solving the non-restricted NLTE problem, i.e., solving the restricted NLTE problem for one element, reiterating the atmospheric structure, solving the restricted NLTE problem for a second element and so on until self-consistency is achieved. A different line of attack will be to couple 3D and NLTE. This is already possible for simple atoms (see Barklem *et al* (2003) for lithium) and it will undoubtedly become a key technology for the analysis of cool stars in the not-so-distant future. Full-scale NLTE analyses in 1D (with hundreds of levels) can serve as a guideline on how to reduce model-atom complexity for 3D applications. Together with other refinements (see Caffau *et al* (2008) for news on oxygen), 3D plus NLTE may even hold the solution to the current conflict between solar photospheric abundances and helioseismology.

Acknowledgments

I thank Bengt for the enthusiasm, support and comradeship he has given to me over the years. He is one of the giants on whose shoulders I stand and this fact has allowed me to look further (into the stars!) than I thought was possible. I feel honoured and proud to be part of his scientific family.

Appendix. Discussion

Q: (Bengt Gustafsson) In spite of this wealth of interesting numerical results for particular atoms and stars, we still lack understanding of these complex systems. You mentioned this indirectly in stressing the complexity which makes it difficult to even foresee the qualitative result of a NLTE calculation for a new model atom. It would be very important to develop such a physical theory, not the least when designing working methods for 3D NLTE.

A: I agree in principle. I was more talking about detailed NLTE abundance corrections for specific lines, not the overall (mean) NLTE effect of a whole ionization stage of an element. In the case of a specific line, I'm afraid it will be more difficult to devise such a predictive theory, also in view of the accuracy that we have to aim for (0.1 dex).

Q: (Jeff Linsky) At the beginning of your presentation, you listed those properties of a stellar atmosphere that would likely lead to large NLTE effects. I would like to add to the list stellar youth. Young stars, in particular pre-MS stars, have strong chromospheric ultraviolet emission that will photo-ionize atoms in the upper photosphere leading to NLTE ionization equilibria.

A: The list I presented was biased by my personal interests, mainly galactic chemical evolution. From a modelling point of view it is clear that using young stars to constraint photospheric NLTE diagnostics will require model atmospheres with chromospheres.

Q: (Rolf Kudritzki) You suggested a number of tests for the accuracy of NLTE. I was surprised you did not mention binaries. With an uncertainty of 1 dex for $\log g$ from Fe I/II, binaries would be ideal to compare between $\log g$ from binarity and NLTE spectroscopy.

A: I agree, (eclipsing) binaries are wonderful laboratories. I am, however, not aware of a well-studied system with a metallicity below $[\mathrm{Fe/H}] < -2$ where effects become large (even though it is clear that such systems exist).

Q: (Carlos Allende Prieto) I have a comment and a question. The comment is that you did not mention the one result, perhaps the most extreme, for the Fe I abundance correction in NLTE: the work by Shchukina and Trujillo Bueno. The question concerns the data for clusters: I noticed you mentioned that one parameter is adjusted for the diffusion model and another for the NLTE calculations (S_H). Is that something to worry about?

A: Shchukina *et al* (2004) find very large NLTE corrections for both Fe I and Fe II, both in 1D and 3D. However, they do not use the Fe I photo-ionization cross-sections of Bautista (1997) which would result in even larger NLTE corrections for Fe I. In this sense, the situation for HD 140283, its surface gravity and metallicity remains inconclusive. Concerning our work on NGC 6397: free parameters are always worrisome and efforts should be made to replace them with physical concepts (ideally derived from first principles). In this particular case, I am not worried that these two free parameters conspire to produce the abundance signatures we have identified. With the exception of calcium, the abundance trends in LTE and NLTE are very similar.

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