NLTE effects on oxygen lines

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Abstract

The NLTE effects affecting oxygen-abundance determinations of solar-type stars are discussed. LTE is perfectly safe for the forbidden lines. The permitted triplet at 777 nm is expected to show NLTE effects on the order of a few tenths of a dex (always in the sense that LTE overestimates the abundance), but the magnitude of the effects is dependent on the still very uncertain cross sections of collisional excitation by collisions with neutral hydrogen atoms. Little is known about the NLTE effects on molecular line formation.

Key words: line: formation ; Sun: abundances ; stars: abundances

1 Introduction

The approximation of local thermodynamic equilibrium (LTE) is commonly used in the analysis of stellar spectra. It simplifies the computation of atomic and molecular level populations immensely by postulating Saha-Boltzmann equilibria, thus defining the state of the gas as a function of only temperature, pressure, and chemical composition. The solution of the equation of radiative transfer for the frequencies of interest is then straightforward. The implied assumption that the radiation field does not influence the properties of the gas is, however, not realistic. Thus we must question the validity of LTE and investigate the NLTE problem of spectral-line formation. This will here for most of the time be taken to mean the solution of the coupled equations of statistical equilibrium and radiative transfer for a trace species in a stellar photosphere. NLTE effects are then simply errors caused by the LTE approximation.

When discussing the NLTE effects on a spectral line, it is often clarifying to separate between effects on the line opacity and on the line source function. The line-opacity effect is described with the NLTE departure coefficient of the atomic population of the lower energy level involved in the transition:
\[ b_i = n_i / n_i^{LTE} \]. The departures from LTE of the line source function is described by its ratio to the local Planckian, \( S_L / B_\nu(T) \).

In the following, NLTE effects on lines used for oxygen-abundance determinations in unevolved or moderately evolved stars of approximately solar effective temperatures will be discussed. The discussion focuses only on departures from LTE, thus disregarding for a moment all other relevant uncertainties like missing background opacities, observational errors, stellar parameters, effects of granulation, line-damping treatment, etc.

2 \([\text{O I}] \) lines

The forbidden lines of oxygen, at 630 nm and 636 nm have not been claimed to be subject to any NLTE effects in cool stars. A typical NLTE calculation shows them to be exceedingly close to LTE both in line opacity and line source function.

The LTE value of the line opacity is due to the fact that the lower levels of these transitions belong to the ground term of neutral oxygen. Virtually all free oxygen atoms will be in that state because of the lack of excited levels of low energy and the high ionisation potential. (The amount of oxygen tied up in molecules is not enough to allow any departures from LTE in the molecular equilibrium to have an impact.) Thus, exceedingly large departures from LTE would have to be present to influence the line opacities significantly. Note that the ionisation equilibrium of oxygen is coupled to that of hydrogen via charge-exchange collisions due to the close correspondence of the ionisation potentials of these two atoms. This means that if NLTE effects would be significant, the problem would be a hydrogen problem rather than an oxygen one.

No departure of the line source function from the local Planckian is expected or seen in any computational results. This is because the lines are forbidden and weak with collisional rates dominating very much over radiative rates, and the upper level involved is collisionally excited.

3 \([\text{O I}] \) lines

The neutral oxygen triplet lines at 777 nm – called just the triplet hereafter for brevity – are well-known for being affected by NLTE effects, especially in early stars. For solar-type stars, the picture is a bit more unclear since the quantitative predictions have had problems when confronted with solar observations. There are of course other permitted optical lines that have been
Fig. 1. Departure coefficients related to the strongest triplet line in a model of the solar photosphere shown for $\varepsilon_O$ ranging from 6.80 to 9.10.

Fig. 2. NLTE abundance corrections computed from the same results as in Fig. 1 and plotted as a function of “LTE oxygen abundance”. They are, however, mostly weaker and thus less useful than the triplet at lower abundances. The NLTE effects on those lines are similar in mechanism though lesser in magnitude than those affecting the triplet.
3.1 Expected behaviour of the triplet

Figure 1 shows the theoretical behaviour of the strongest triplet line in a solar photospheric model. (Computed without any contribution of inelastic collisions with neutral hydrogen atoms – a problematic process discussed below.) We see that the line opacity stays close to its LTE value because the departure coefficient for the line’s lower level \( n_l/n_{LTE}^l \sim 1 \). The line source function \( S_L \) shows a significant departure from LTE as it dips below the Planckian, thus producing a line that is stronger than it would be in LTE.

The line source function behaves like that of the textbook two-level atom without continuum (e.g. Mihalas, 1978, Chap. 11),

\[
S_L = (1 - \varepsilon)\bar{J}_\nu + \varepsilon B_\nu(T),
\]

where \( \varepsilon \) measures the destruction probability of line photons by collisional deexcitation. It is the photon losses that cause \( S_L \) to fall below Planckian and scattering in the line makes this effect go further inwards than the monochromatic optical depth in the line would imply. The effect grows stronger with increased abundance as the line strength increases. But it does not generally go to zero as the abundance decreases since \( J_\nu < B_\nu(T) \) in the infrared continuum.

By constructing curves of growth from the LTE and the NLTE equivalent widths, one can compute NLTE abundance corrections, \( \Delta \varepsilon_{O}^{NLTE} = \varepsilon_{O}^{NLTE} - \varepsilon_{O}^{LTE} \), that can be added to abundances derived under the LTE assumption. These will always be negative, meaning that an LTE analysis will always overestimate the oxygen abundance. Figure 2 shows these corrections computed from the results of Fig. 1. For solar-type stars, \( \Delta \varepsilon_{O}^{NLTE} \) varies from 0 up to \(-0.5\) dex (e.g., Kiselman, 1991; Takeda, 1994), getting more significant with increased effective temperature and decreased surface gravity. No strong monotonous dependence on metallicity has been predicted that would be able to seriously change the slopes in [O/Fe] plots or remove the discrepancies between the trends from different oxygen-abundance indicators.

The two-level-atom behaviour is good for us because it makes it easier to analyse and understand the results physically. It also assures us that it is the processes in the line transition itself that are important – high-lying levels, photoionising radiation fields, and other things problematic to model do not matter. This also allows simplification in, for example, work on 3D radiative transfer (Kiselman & Nordlund, 1995). Note that the effect has nothing to do with the lines being of high excitation energy or that their lower level is metastable. This is just the natural behaviour of reasonably strong lines in the infrared with two-level-atom like behaviour and LTE-like opacity.
There is a limit to this two-level regime, however. Note that the departure coefficient of the lower level in Fig. 1 is not exactly equal to one. If the effective temperature is increased, we will eventually get a significant departure from LTE of the line opacity. The result will then depend on the rest of the atomic model and the interpretation of the results will be less straightforward. An important ingredient is probably the recombination flow from higher levels (Eriksson & Toft, 1979), but this transition to more complicated behaviour has not been analysed well yet.

3.2 Confrontation of theory with solar observations

Altrock (1968) investigated the centre-to-limb behaviour of the triplet in the sun and found that this was not consistent with the triplet being formed in LTE in that the line strengths do not fall off as quickly close to the limb. Sedlmayr (1974) could reproduce the solar observations well with an NLTE analysis. But then the accepted oxygen abundance from other spectral features increased and a discrepancy was noted (Sneden et al., 1979) and persisted (Kiselman, 1991). Kiselman (1993) found it impossible to reconcile observations with any reasonable one-dimensional photospheric model and an oxygen abundance $\varepsilon_O = \lg \frac{N_O}{N_H} + 12 \approx 8.9$, leaving granulation effects as the only possibility. However Kiselman & Nordlund (1995) found from 3D NLTE modelling in hydrodynamic granulation simulations that the effects on line strength and $\mu$ dependence could not significantly alleviate the situation.

This solar discrepancy may not be the most dramatic problem we have in astronomy – it is probably, after all, solved by allowing an abundance below 8.9 (e.g. Reetz, 1998) – but it illustrates the uncertainties surrounding spectral-line formation and their coupling to solar abundances. Indeed, the oxygen triplet lines should be among the easiest to model among solar lines affected by departures from LTE.

3.3 The problem of hydrogen collisions

Given the two-level nature of the triplet in solar-type stars, the most problematic atomic quantity is, as usual in NLTE work, collisional cross sections. While electron collisions are always uncertain, this is even more so for collisions involving neutral hydrogen atoms – the case of the oxygen triplet illustrates the effect of this uncertainty clearly.

Collisional excitation by atoms in cool-star NLTE work were introduced by Steenbock & Holweger (1984). They generalised the estimates of Drawin (1968, 1969), which related to collision between like atoms, to inelastic collisions
between hydrogen atoms and other species. These results have been used by many authors. Lambert (1993) reviewed these formalisms and suggested a reasonable improvement to them which, however, does not seem to have taken on.

The formulæ based on Drawin’s work can only be regarded as order of magnitude estimates, and perhaps not even that. Many authors have tried to get better estimates by multiplying the rates of Steenbock & Holweger (1984) with a factor \( x \) determined by some empirical fitting. Tomkin et al. (1992) fitted the triplet lines to the solar spectrum assuming \( \varepsilon_O = 8.92 \). This resulted in large collisional rates almost producing LTE. Takeda (1995) made a multiparameter fit of solar line profiles resulting in a scaling factor of \( x = 1.0 \), thus confirming the Steenbock & Holweger (1984) formulæ. King & Boesgaard (1995) confirmed that the solar centre-to-limb behaviour of the triplet was not consistent with LTE. Reetz (1998, 1999) used the \( \mu \) dependence and profiles of solar lines to find that the hydrogen collisions were negligible \( (x = 0.0) \). The same result came from his effort to minimise the difference between the abundances derived from the individual triplet lines for a set of stars of different effective temperatures. Gratton et al. (1999) found that \( x = 3.2 \) gave consistent abundances for different oxygen lines in RR Lyrae stars. Among other recent work that can be mentioned, Mishenina et al. (2000) chose \( x = 1/3 \) – probably because the use of that factor in the work on Fe in Pollux by Steenbock (1985).

Apparently the attempts to determine empirical cross sections are very model dependent, and it seems hard to avoid all other uncertainties related to stellar modelling and parameters – notably effective temperatures – to bias the procedure. If one therefore discards the extrasolar evidence and that depending on certain values of the solar oxygen abundance, it seems that the solar centre-to-limb behaviour is still a rather strong argument that hydrogen collisions are not very significant and that they definitely cannot induce LTE.

Circumstantial evidence comes from studies of other lines. There is now a detailed quantum mechanical calculation of the hydrogen excitation cross section of the Na D lines (Belyayev et al., 1999). This shows a cross section that is \( 10^{-2} \) – \( 10^{-4} \) of the Drawin-style prediction. See also Caccin et al. (1993).

In the time since the Kiel group pointed out inelastic collisions with hydrogen atoms as potentially very important in cool-star NLTE work, many large and expensive telescopes and spectrographs have gone from visionary ideas to first light. But our knowledge about these collisional rates – so important for interpreting some of the results of these technological wonders – has not advanced very much.
4 Molecular lines

We do not know much about the NLTE formation of molecular lines. Hinkle & Lambert (1975) estimated that the vib-rot levels among the electronic ground state of diatomic molecules in the solar photosphere should be in Boltzmann equilibrium but that departures from LTE could be expected in the line source functions of electronic transitions. For weak ultraviolet lines (think OH in metal-poor stars here) this could mean that the lines get weaker for a given abundance than LTE predicts and thus LTE abundances are underestimates. When the lines are strong, the effect could go the other way.

Another matter is the chemical equilibrium itself, where photodissociation could play a role in causing departures from LTE. It could even be that statistical equilibrium is not reached in the few minutes that the upwelling gas in a granule spends in and above the photosphere before falling back beneath the visible surface again. Uitenbroek (2000) has compared observed CO lines with simulations and suggests that this effect is really seen. If so, all modelling assuming statistical equilibrium will derive too low abundances.

There could thus be NLTE effects in the line radiative transfer which require collisional cross sections for modelling, NLTE effects in the statistical equilibrium of molecular abundances which require modelling of photodissociation, and maybe even dynamic modelling of molecular formation is required to properly model the formation of CO and OH lines.

5 Conclusions

For those in quest of accurate oxygen abundances of solar-type stars, it should be noted that:

- NLTE effects are utterly unimportant for the forbidden oxygen lines.
- The 777 nm triplet lines are not formed in LTE. NLTE effects will not change the slopes in the [O/Fe]–[Fe/H] diagrams very much, but they will surely influence the error bars because of the uncertainties in the collisional cross sections.
- The NLTE effects on the triplet are always expected to be negative. Thus LTE results define an extreme on the possible range of abundances, not a conservative mean hypothesis.
- NLTE effects on molecular lines should be investigated.
Acknowledgements

Martin Asplund is thanked for stimulating discussions as well as for comments on the manuscript.

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