FORMATION OF \( \text{Li} \, i \) LINES IN PHOTOSPHERIC GRANULATION

DAN KISELMAN
The Royal Swedish Academy of Sciences, Stockholm Observatory, SE-133 36 Saltsjöbaden, Sweden; dan@astro.su.se

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ABSTRACT
The possibility of significant systematic errors due to the use of one-dimensional homogeneous atmospheres in lithium-abundance determinations of cool stars motivates a study of non–local thermodynamic equilibrium (NLTE) effects on \( \text{Li} \, i \) line formation in a three-dimensional solar granulation simulation snapshot. The NLTE effect on the equivalent width of the 671 nm resonance line is small in one-dimensional models or in integrated light from the granulation model. The line-strength variations over the granulation pattern are, however, markedly different in NLTE compared with LTE—observations of this may provide diagnostics to NLTE effects. The effects of horizontal photon exchange found in the granulation model are moderate and due entirely to bound-bound processes; ultraviolet overionization is unimportant.

Subject headings: line: formation — stars: abundances — stars: atmospheres — Sun: abundances — Sun: granulation

1. INTRODUCTION
Stellar lithium abundances are potentially very useful for testing astrophysical theories. The abundances derived from observed spectra have spawned a number of scientific debates; for a recent review, see Thorburn (1996) and the conference proceedings of Crane (1995) and Spite & Pallavicini (1995) and the introduction to Carlsson et al. (1994). It is important in this context that we can be confident in the derived abundances—which so far mostly have been derived using the questionable assumptions of line formation in local thermodynamic equilibrium (LTE) and plane-parallel homogeneous LTE photospheres.

Efficient computer codes and extensive atomic data sets have made possible realistic non-LTE (NLTE) spectral line modeling for light atoms in plane-parallel cool-star photospheres that can provide NLTE abundance corrections for the convenience of the stellar abundance community (e.g., Carlsson et al. 1994; Kiselman & Carlsson 1996).

A notable departure from plane-parallel homogeneity in the quiet solar photosphere is the granulation, now understood as a visible manifestation of convection below the photosphere (see, e.g., Spruit, Nordlund, & Title 1990). We also have some knowledge of granulation on stars adjacent to the Sun in the H-R diagram (Gray & Nagel 1989; Nordlund & Dravins 1990; Dravins & Nordlund 1990a, 1990b). How does granulation influence line strengths and abundance determinations? Holweger, Heise, & Kock (1990) argued that solar abundance ratios should not be seriously in error since they are based on line-strength ratios, which are approximately constant over the solar granulation pattern in the simulations of Steffen (1989). This notion was confirmed observationally by Kiselman (1994a), who found that lines of both neutral and singly ionized species of several elements behaved similarly by being stronger in bright granular regions and weaker in dark intergranular lanes. For other work on lines in realistic granulation simulations that is relevant for abundance analysis, see Nordlund (1984), Bruls & Rutten (1992), Atroschenko & Gadun (1994), and Kiselman & Nordlund (1995).

Of special interest is the question of NLTE effects on line formation in granulation. Nordlund (1984) found that three-dimensional NLTE effects could be of some importance for \( \text{Fe} \, i \) lines in solar granulation, while Kiselman & Nordlund (1995) found such effects for \( \text{O} \, i \) to be rather small. Note also that Mihalas, Auer, & Mihalas (1978) did not find any important two-dimensional effects in their investigation of artificial but solar-like atmospheric structures. Kurucz (1995) claimed that NLTE effects in extremely metal-poor solar-type stars can cause standard analyses to underestimate lithium abundances with a factor of 10. In this scenario, \( \text{Li} \, i \) lines will be weak in hot photospheric regions where \( \text{Li} \) is largely ionized. The cooler regions would show strong \( \text{Li} \, i \) lines if LTE was valid, but the ultraviolet radiation from adjacent hot regions will keep lithium largely ionized also there. The \( \text{Li} \, i \) resonance line in integrated light would thus be very much weaker than the result from a one-dimensional model representing a spatial and temporal average of the photospheric structure. Thus, the abundance would be underestimated when an analysis is performed with standard plane-parallel models. So far, there is no quantitative model to verify this effect, which would certainly have important impact on the debates related to stellar lithium abundances.

This Letter reports on NLTE aspects of \( \text{Li} \, i \) line formation as found with experiments on a three-dimensional solar granulation model. The results are thus directly applicable only for Sun-like stars, but they should give some indication of what we can expect for other stars as well.

2. SIMULATIONS
2.1. Methods
The \( \text{Li} \, i \) resonance doublet at 671 nm is very weak in the solar spectrum since the solar lithium abundance is so low—the standard value used here is \( A_{\text{Li}} = \log [N(\text{Li})/N(\text{H})] + 12 = 1.16 \) (Grevesse, Noels, & Sauval 1996; Müller, Peytremann, & de la Reza 1975). The feature is blended with several other weaker lines, the stronger (shorter wavelength) doublet component being less affected. The doublet splitting, together with hyperfine and isotopic splitting, is neglected here since the weakness of the line makes its equivalent width insensitive to line-broadening details. Thus, the lithium atomic model of Carlsson et al. (1994) is employed with the change that the 671 nm resonance doublet is treated as a single line. In principle, this treatment leads to a change in line formation height and some modification of the NLTE behavior. This is, however, not a problem here—the robustness of the results is indicated...
Fig. 1.—Li i 671 nm behavior in a three-dimensional hydrodynamic granulation snapshot. Upper row: LTE results. Lower row: 1.5-dimensional NLTE results. Left-hand side: Equivalent width as function of continuum intensity. Middle and right-hand side: Line source functions and total line-center opacities for six selected columns (A–F). Continuum intensities and source functions are normalized on the mean continuum intensity for the whole snapshot. Line-center opacities are normalized with the local continuum opacity.

by the qualitative behavior of the line being unchanged even when the abundance is increased by a factor of 10.

The three-dimensional photospheric model is a single snapshot from the hydrodynamic granulation simulations of Stein & Nordlund (1989) that was also used by Kiselman & Nordlund (1995)—see that paper for illustrations. It has been contracted to a $64 \times 64 \times 55$ grid of thermodynamic quantities corresponding to $6 \times 6 \times 1$ Mm on the solar surface and showing more than 10 granules. (The figures of this Letter display only $32 \times 32$ surface points.) This single snapshot may not be adequate for statistically reliable results, but it should show a representative sample of different kinds of photospheric behavior.

Line profiles are calculated with a hybrid technique using version 2.2 of the one-dimensional NLTE code MULTI (Carlsson 1986), which uses the operator perturbation techniques of Scharmer & Carlsson (1985). The radiative bound-free transitions, and some bound-bound transitions in the experiments below, are treated as fixed rates using a background three-dimensional radiation field computed in (strong) LTE with the methods of Kiselman & Nordlund (1995). The equation of transfer was solved along a set of rays—five inclination angles ($\cos \theta = \mu$) and eight azimuthal angles ($\phi$)—and the resulting intensities along each ray were used to calculate a mean intensity $I_x$ in each $(x, y, z)$ point. The treatment can thus not really be called “three-dimensional NLTE,” but it does include three-dimensional effects and NLTE effects.

All line results presented here are for disk center, i.e., for vertical rays with $\mu = 1.0$.

2.2. LTE and the 1.5-dimensional Case

The general diagnostic to be discussed here is the dependence of line strength on continuum intensity. The upper left-hand panel of Figure 1 shows the equivalent width of the 671 nm line plotted as a function of continuum intensity when the line is computed in LTE. Each point represents the vertically emergent spectrum from one $(x, y)$ column of the simulation snapshot. Six points marked with letters have been chosen as examples of different kinds of regions. The neighboring plots show the local Planck function (normalized with the emergent mean continuum intensity from the snapshot) and the total opacity at line center (normalized on the continuum opacity) at these selected locations. The Planck function plot naturally also illustrates the temperature structure. Note the typical crossing over of temperatures, with the hot bright regions (i.e., granules) like A and B having much steeper temperature gradients than a typical intergranular region like F. C is an intermediate point, and D and E represent dark intergranular regions covered with cooler gas.

The overall appearance of the LTE $I_c$–$W$ diagram is typical of most lines studied so far (Kiselman 1994a). The strength of the Li i line generally increases with continuum brightness, but there is a significant scatter, especially in the darker regions. It is possible to understand this behavior in a simple qualitative way. The line is strong where the temperature gradient is steep and/or if the temperature in the line-forming layers is low. These very weak lines are formed in a fairly extended region around $\log \tau_c \approx -1.5$, as evidenced from inspection of the contribution function due to Magain (1986).

The large scatter in the LTE $I_c$–$W$ diagram is due to the high temperature sensitivity of the line opacity and reflects the variation in temperature in the upper layers of the granulation model. Note how the dark examples (D, E, and F) have similar low temperatures where the continuum is formed—the respective curves meet in the upper right-hand panel around $\log \tau_c = 0$—and thus similar continuum brightness. Higher up in the line-forming layers, the curves diverge, causing the line opacity to differ via the Saha ionization equilibrium. Thus, the difference in equivalent width [$W(E) > W(D) > W(F)$] is a direct reflection of the temperatures there, with higher temperatures meaning less Li i and weaker lines.

The plots in Figure 2 show results for an effective temperature range of plane-parallel photospheric models computed with the OSMARCS code of Edvardsson et al. (1993). The LTE line behavior is much simpler in these models than in the granulation snapshot.

Let us then consider the results when the lines are calculated in NLTE and 1.5-dimensional geometry. This term is used here...
to signify that each vertical column in the granulation snapshot is treated as a plane-parallel photosphere, thus neglecting any horizontal photon exchange in the model. The lower left-hand panel of Figure 1 shows the resulting $I_c - W$ plot, which differs from the LTE plot in three important respects. First, the line is on the average weaker in NLTE. Second, the LTE case shows increasing line strength in brighter regions, while the opposite is true in the NLTE. Also striking is the narrow brightness dependence in the NLTE plot, which contrasts to the big scatter among the points in the LTE plot.

The NLTE-LTE difference in integrated-light equivalent widths is about 30%, which is more than the 10% found in the one-dimensional results of Figure 2. Considering, however, uncertainties in abundances, $f$-values, fundamental stellar parameters, and the like, such effects are barely significant in typical stellar work. It is thus hardly possible to test either the NLTE or the granulation results in integrated light alone. The different appearance of the LTE and the NLTE plots shows, however, that even if effects of departures from LTE look insignificant in integrated light or in one-dimensional models, they can cause a definite qualitative difference in the spatially resolved $I_c - W$ behavior. This supports the idea (Kiselman 1996) that NLTE effects can be discovered and diagnosed in this way.

The 1.5-dimensional NLTE plot is in fact easily understood. When we leave the LTE approximation, the atomic-level populations will be more or less decoupled from the local kinetic temperature, and the radiation field will govern them instead. Thus, the relevant quantities for the line, its line source function and the line opacity, will be set by the radiation field. This is exactly what the plot shows: for each value of the background continuum intensity, the line equivalent width is the same. The low lithium abundance will make all Li i lines and ionization edges very weak, having virtually no impact on the radiation field—thus, we only have to consider the continuum background radiation fields. The weakness of the Li i 671 nm line, together with the fact that the line-photon-destruction probability is rather small ($\epsilon < 0.1$), makes the line source function $S'$ follow the continuum angular mean intensity, $J_c$, rather closely. A greater $J_c$ will thus lead to a greater $S'$ and a weaker line. Furthermore, the line opacity is set by the population of the Li i ground state, and so it is the ionization balance between Li i and Li ii that sets the line opacity. In the NLTE case, the radiation field (in the ionization edges themselves or at other wavelengths) is obviously important for the ionization balance.

This explains why the range of one-dimensional models in Figure 2 seems a much better approximation of the granulation simulation results in NLTE than in LTE. The radiation temperature is set in the deeper layers, where the granulation structure is much more like the one-dimensional models than is the case higher up.

2.3. Diagnostic Experiments

The interest here is in finding the processes important for the overall picture, not to explain NLTE mechanisms operating in individual columns of the granulation snapshot. The $I_c - W$ plots in Figure 3 illustrate what happens when the 1.5-dimensional results already discussed are perturbed. These experiments will be referenced to according to the figure’s panel designations.

The importance of overionization caused by $J_c > B_c$ in bound-free edges is assessed by computing the photoionization rates with $J_c = B_c$ (panel bf B). The small change shows that ultraviolet overionization is unimportant.

A large majority of all Li i is in the ground state that sets the 671 nm line opacity. It will depart from its LTE value in a way dependent on the excitation balance among the Li i levels, since departures from Boltzmann equilibrium have an impact on the ionization equilibrium. The general rule is that there will be overionization if the excitation balance is shifted upward, since the bound-free cross section of the ground state is small and since there simply are more photons at the longer wavelengths of the excited levels’ ionization edges. This effect was found for B i by Kiselman (1994b), and it can be thought of as the opposite of the photon suction discussed by Bruls, Rutten, & Shchukina (1992) for Na i and K i. Quenching the pumping effect of the ultraviolet resonance line at 323 nm by treating it as a fixed rate given by $J_c = B_c$ has a very small impact (panel 323 nm B). This specific pumping is unimportant for the formation of the 671 nm line. When all radiative transitions except the 671 nm line are treated in the same way (panel bf &bbb B), about half of the NLTE effect remains. The remaining departures from LTE are due to the resonance line itself.

The importance of three-dimensional effects is assessed by...
treating radiative transitions as fixed using the precomputed three-dimensional radiation field. Doing this to the photoionizations causes insignificant changes (panel bf 3D). Treating all radiative transitions, except the 671 nm line, in three dimensions (panel bf&kbb 3D) gives an anticipated spread in the $I_1 - W$ diagram since the local $I_1$ is influenced by neighboring points in the snapshot.

Finally (panel all 3D), all radiative transitions, including the 671 nm resonance lines, are treated as fixed in three dimensions, now also with the application of a correction for line blanketing in the background radiation fields. This is the most sophisticated simulation presented here, but its shortcomings must be remembered—the three-dimensional radiation fields have been calculated in LTE in a somewhat schematic way, all radiative transitions have been treated as fixed, and the correction for line blanketing is schematic. The $I_1 - W$ plot shows a rather flat slope and a significantly larger spread than in the 1.5-dimensional case. Apparently, effects of horizontal photon transfer are of some importance through the line transitions. However, the difference in intensity-weighted mean equivalent width between the 1.5- and the three-dimensional cases is only 3%.

Experiments with higher abundances show that the line behavior described here is qualitatively the same at an abundance 10 times higher (2.1), but at an abundance of 3.1 we leave the regime of weak-line behavior, and the typical effects of strong resonance lines (Carlsson et al. 1994) set in.

3. CONCLUSIONS

Line formation in granulation is not well approximated with simple “cold” and “hot” regions or streams. The strongly varying photospheric temperature gradient, the typical inversion of the temperature pattern above a certain height, and the presence of inclined thermal inhomogeneities complicate the situation to the extent that conclusions regarding spectral lines must be based on realistic granulation simulations. A case has been made that such simulations and spatially resolved solar spectroscopy can be used as diagnostics of NLTE effects. Another paper (Kiselman 1997) will follow up on this and compare simulations with solar observations of Li i.

The current calculations do not show evidence for any large NLTE effects in quiet granulation that would seriously affect lithium abundance determinations for solar-like stars. This is not to say that effects of granulation are altogether unimportant—more comprehensive studies are needed to quantify granulation abundance corrections corresponding to the commonly used NLTE abundance corrections. One may also speculate that three-dimensional NLTE effects could be important in regions of enhanced magnetic activity and thus be relevant to problems such as the apparent lithium abundance spread in the Pleiades (cf. Stuik, Bruls, & Rutten 1997).

To draw conclusions about very metal-poor solar-type stars and the NLTE effect proposed by Kurucz (1995) would be to extrapolate—the nature of these stars’ surface inhomogeneities is unknown but probably different from the solar (Allende Prieto et al. 1995). One can note, however, that bound-bound processes may be important for the statistical equilibrium of Li there as well as in the solar case studied here. Wherever line transitions are the dominating drivers of departures from LTE, any three-dimensional effects are likely to be milder than if bound-free processes govern the NLTE behavior, because the contrast of granulation or other thermal inhomogeneity is lower at the longer wavelengths of the Li i spectral lines than in the blue and ultraviolet continua.

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