3D non-LTE corrections for Li abundance and $^6\text{Li}/^7\text{Li}$ isotopic ratio in solar-type stars

I. Application to HD 207129 and HD 95456


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ABSTRACT

Context. Convective motions in solar-type stellar atmospheres induce Doppler shifts that affect the strengths and shapes of spectral absorption lines and create slightly asymmetric line profiles. One-dimensional (1D) local thermodynamic equilibrium (LTE) studies of elemental abundances are not able to reproduce this phenomenon, which becomes particularly important when modeling the impact of isotopic fine structure, like the subtle depression created by the $^6\text{Li}$ isotope on the red wing of the Li resonance doublet line.

Aims. The purpose of this work is to provide corrections for the lithium abundance, $A(\text{Li})$, and the $^6\text{Li}/^7\text{Li}$ isotopic ratio that can easily be applied to correct 1D LTE lithium abundances in G and F dwarf stars of approximately solar mass and metallicity for three-dimensional (3D) and non-LTE (NLTE) effects.

Methods. The corrections for $A(\text{Li})$ and $^6\text{Li}/^7\text{Li}$ are computed using grids of 3D NLTE and 1D LTE synthetic lithium line profiles, generated from 3D hydro-dynamical CO5BOLD and 1D hydrostatic model atmospheres, respectively. For comparative purposes, all calculations are performed for three different line lists representing the Li I $\lambda670.8$ nm spectral region. The 3D NLTE corrections are then approximated by analytical expressions as a function of the stellar parameters ($T_\text{eff}$, $\log g$, [Fe/H], $v\sin i$, $A(\text{Li})$, $^6\text{Li}/^7\text{Li}$). These are applied to adjust the 1D LTE isotopic lithium abundances in two solar-type stars, HD 207129 and HD 95456, for which high-quality HARPS observations are available.

Results. The derived 3D NLTE corrections range between $-0.01$ and $+0.11$ dex for $A(\text{Li})$, and between $-4.9$ and $-0.4\%$ for $^6\text{Li}/^7\text{Li}$, depending on the adopted stellar parameters. We confirm that the inferred $^6\text{Li}$ abundance depends critically on the strength of the Si I $670.8025$ nm line. Our findings show a general consistency with recent works on lithium abundance corrections. After the application of such corrections, we do not find a significant amount of $^6\text{Li}$ in any of the two target stars.

Conclusions. In the case of $^6\text{Li}/^7\text{Li}$, our corrections are always negative, showing that 1D LTE analysis can significantly overestimate the presence of $^6\text{Li}$ (up to 4.9% points) in the atmospheres of solar-like dwarf stars. These results emphasize the importance of reliable 3D model atmospheres combined with NLTE line formation for deriving precise isotopic lithium abundances. Although 3D NLTE spectral synthesis implies an extensive computational effort, the results can be made accessible with parametric tools like the ones presented in this work.

Key words. stars: abundances – stars: atmospheres – radiative transfer – line: formation – line: profiles

1. Introduction

The lithium abundance, $A(\text{Li})$, and the $^6\text{Li}/^7\text{Li}$ isotopic ratio measured in stellar atmospheres can provide valuable information contributing to understanding different problems in astrophysics such as stellar structure and evolution, stellar activity, exoplanetary system evolution and even cosmology. A reliable determination of the lithium content in stellar atmospheres is important, and apart from requiring high-resolution stellar spectra with high signal-to-noise ratios ($S/N$), it also requires realistic stellar atmosphere models allowing a sound theoretical interpretation of both the strength and the shape of the Li lines.

The stable isotope $^7\text{Li}$ is among the few light elements that have been produced in the Big Bang. In contrast, the other stable isotope, $^6\text{Li}$, is not produced in significant amounts in standard Big Bang nucleosynthesis (e.g., Thomas et al. 1993), but mainly through spallation and $\alpha+\alpha$ fusion reactions triggered by high-energy collisions between Galactic cosmic rays and He, C, N, O nuclei in the interstellar medium (e.g., Meneguzzi et al. 1971; Prantzos et al. 1993; Prantzos 2012). Additional $^7\text{Li}$ is produced by the same mechanism, and partly by stellar nucleosynthesis as well. The current $^6\text{Li}/^7\text{Li}$ in the local interstellar medium (ISM) is measured to be $\sim 13\%$ (Kawanomoto et al. 2009, see also Howk et al. 2012), while the solar system (meteoritic) $^6\text{Li}/^7\text{Li}$ is 8.2% (Lodders 2003).

Both $^6\text{Li}$ and $^7\text{Li}$ are very fragile with respect to nuclear reactions with protons and are destroyed in stellar interiors at temperatures above $\sim 2.0 \times 10^8$ K and $\sim 2.5 \times 10^8$ K, respectively (e.g., Pinsoneault 1997). According to standard stellar

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* The table with the 3D NLTE corrections is only available at the CDIS via anonymous ftp to cdsarc.u-strasbg.fr (130.79.128.5) or via http://cdsarc.u-strasbg.fr/viz-bin/qcat?J/A+A/618/A16

$A(\text{X}) = \log(N(\text{X})/N(\text{H})) + 12$, where $X$ is the chemical element.
evolution models, $^6$Li, being the more fragile of the two isotopes, undergoes an intense destruction during pre-main sequence evolution (e.g., Forestini 1994; Proffitt & Michaud 1989; Montalbán & Rebolo 2002). The standard models predict that by the time a solar-type solar-metallicity star reaches the main sequence its $^6$Li has already been destroyed by nuclear reactions at the base of the extended, completely mixed convective envelope. In non-standard stellar evolution, where additional processes such as rotational mixing, atomic diffusion, internal gravity waves, and the effect of magnetic fields are included in order to explain the observed lithium abundances in stellar atmospheres (see Talon & Charbonnel 2005 and references therein), lithium destruction is generally even enhanced compared to the standard models.

This suggests that any significant detection of the fragile $^6$Li isotope in the atmosphere of a solar-type star would most probably indicate an external pollution process, for example by plane

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currently in the literature. For example, Pfalzner et al. (2012) found evidence for the presence of $^6$Li in the active solar system HD 123351, both in 1D LTE and in a full 3D NLTE analysis of very-high-quality spectra. Since the latter investigations use dedicated 3D model atmospheres to analyze individual stars, they do not provide a systematic grid of isotopic abundance corrections.

In this work, we use a grid of synthetic spectra computed from 3D hydrodynamical CO$^2$BOLD models and 1D hydrostatic LHD model atmospheres for a typical range of stellar parameters for solar-type stars. The intention is to provide a set of 3D NLTE corrections for the lithium abundance, A(Li), and in particular for $^6$Li/$^7$Li that can be directly used to correct the results of a 1D LTE analyses.

The ultimate purpose of this work is to facilitate the analysis of high-resolution and high-S/N spectra of a large sample of solar-type stars with and without known giants. In case of any positive detection of the fragile $^6$Li isotope in the atmosphere of our target stars, we aim to investigate its possible source (e.g., planetary material accretion, flare production, etc.) by looking for correlations between the derived lithium content and the presence of a giant planet or planetary system.

This manuscript consists of two major parts. In Sect. 2, the methods and the results of the computations of 3D NLTE corrections for A(Li) and $^6$Li/$^7$Li are presented, and the analytical expressions for their quick evaluation are provided. Section 3 explains the analysis and gives the results for A(Li) and $^6$Li/$^7$Li measurements in two solar-type stars, HD 95456 and HD 207129, using their HARPS spectra. A summary and our conclusions are presented in Sect. 4.

### 2.1. Model atmospheres

For deriving our 3D NLTE corrections, we adopted a subset of the CIFIST 3D hydrodynamical model atmospheres grid (Ludwig et al. 2009), computed with the CO$^2$BOLD code (Freytag et al. 2002, 2012). In total, 24 3D model atmospheres were used, covering three different effective temperatures ($T_{\text{eff}}$), two surface gravities (log g) and four metallicities ([Fe/H]). Table 1 lists the assigned number of each model (Model N) and its effective temperature, surface gravity, metallicity, number of the representative snapshots ($N_{\text{snap}}$), and the number of opacity bins ($N_{\text{bins}}$) for treating the radiative energy transport in the 3D simulations. The final $T_{\text{eff}}$ of each CO$^2$BOLD hydrodynamical model atmosphere is determined after the selection of a number

<table>
<thead>
<tr>
<th>Model</th>
<th>$T_{\text{eff}}$ (K)</th>
<th>log g</th>
<th>[Fe/H]</th>
<th>$N_{\text{snap}}$</th>
<th>$N_{\text{bins}}$</th>
</tr>
</thead>
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<tr>
<td>A</td>
<td>5500</td>
<td>3.8</td>
<td>-1</td>
<td>4</td>
<td>500</td>
</tr>
<tr>
<td>B</td>
<td>6200</td>
<td>3.5</td>
<td>-0.3</td>
<td>6</td>
<td>300</td>
</tr>
<tr>
<td>C</td>
<td>6900</td>
<td>3.2</td>
<td>0.0</td>
<td>8</td>
<td>200</td>
</tr>
<tr>
<td>D</td>
<td>7600</td>
<td>3.0</td>
<td>0.3</td>
<td>10</td>
<td>100</td>
</tr>
</tbody>
</table>

A similar approach was followed by Sbordone et al. (2010) for the lithium abundance. They derived analytical approximations to convert the equivalent widths (EW) of the lithium 670.8 nm line into A(Li) (and vice versa) in 1D LTE, 1D NLTE and 3D NLTE, which, in principle, can be used to infer the 3D NLTE abundance correction by comparing the 1D LTE and 3D NLTE A(Li) for a given EW, $T_{\text{eff}}$, log g and [Fe/H].

Several authors have previously performed 1D NLTE analyses of A(Li), covering a large range of stellar parameters (e.g., Carlsson et al. 1994, Pavlenko & Maguzzu 1996, Takeda & Kawanomoto 2005, Lind et al. 2009). We compare our 3D NLTE and 1D NLTE results with some of the previous works in Sect. 2.6. In the context of very metal-poor stars, where no blend lines interfere, the most advanced full 3D NLTE analyses of $^6$Li/$^7$Li have been performed by Lind et al. (2013), who showed that previous detections of $^6$Li based on 1D and 3D LTE modeling could not be confirmed when reanalyzed with refined 3D NLTE methods. On the other hand, Mott et al. (2017) found clear evidence for the presence of $^6$Li in the active giant HD 123351, both in 1D LTE and in a full 3D non-LTE analysis of very-high-quality spectra. Since the latter investigations use dedicated 3D model atmospheres to analyze individual stars, they do not provide a systematic grid of isotopic abundance corrections.
of snapshots from their averaged radiative surface flux (this $T_{\text{eff}}$ is given in Table 1) and usually differs slightly from the intended $T_{\text{eff}}$ value. Therefore, the model atmospheres in our grid do not have exactly the same effective temperatures for each nominal temperature point of the grid.

To each CO$^3$BOLD model atmosphere (Caffau et al. 2008) is associated, having the same effective temperature, metallicity, and surface gravity. Using these particular 1D model atmospheres for comparison with the 3D models is advantageous since they employ the same opacity tables and equation of state as the CO$^3$BOLD models. Such a differential analysis minimizes unphysical (numerical) intrinsic differences between 1D and 3D models and isolates the true 3D effects. The 1D LHD model atmospheres employ the mixing-length theory to describe convection, and a typical mixing length parameter $\alpha_{\text{MLT}} = 1.0$ is used in this work. Several authors (e.g., Klevas et al. 2016; Mott et al. 2017) have shown (as verified in Sect. 2.4.2 below) that the choice of this parameter is not critical for our A(Li) and $^6$Li/$^7$Li studies. This is because, in the framework of the mixing-length theory, the line-forming layers of the considered stellar atmospheres are not strongly affected by convection.

### 2.2. Spectral synthesis

For each 3D CO$^3$BOLD and 1D LHD model atmosphere, a corresponding grid of synthetic spectra for the Li I $\lambda$670.8 nm region has been computed using the spectral synthesis code Linfor3D (Steffen et al. 2015). The NLTE lithium line profiles for the 3D case were computed for combinations of three different Li abundances ($A(\text{Li})_{\text{3DNLTE}} = 1.5$, 2.0, 2.5) and three different $^6$Li/$^7$Li isotopic ratios ($q(\text{Li})_{\text{3DNLTE}} = 0\%$, 5\%, 10\%); hereafter $q(\text{Li}) = n(^6\text{Li})/n(^7\text{Li})$.

A 17-level lithium model atom including 34 bound-bound transitions was adopted for the computation of the NLTE departure coefficients. This model atom was initially developed by Cayrel et al. (2007) and further updated and used by several authors (e.g., Sbordone et al. 2010; Steffen et al. 2012; Klevas et al. 2016; Mott et al. 2017). Individually for each of the three assumed lithium abundances, NLTE departure coefficients were computed with the code NLTE3D (Steffen et al. 2015).

In the 1D case, a series of LTE synthetic line profiles were computed for combinations of nine Li abundance values (from 1.00 to 3.00 with a step of 0.25), nine different $^6$Li/$^7$Li isotopic ratios (from 0\% to 16\% with a step of 2\%), and three different microturbulence velocities ($V_{\text{micro}}$), centered on the value obtained from the analytic expression derived from a set of 3D model atmospheres by Dutra-Ferreira et al. (2016), with an offset of 0.5 km s$^{-1}$.

To examine the dependence of our results on the list of blend lines used in the spectral synthesis, we replicated the computation of the full grids of 3D NLTE and 1D LTE line profiles using three different line lists. The first line list includes only the Li I atomic lines adapted from Kurucz (1995). The original hyperfine structure was simplified to include six $^6$Li and six $^7$Li components (hereafter, K95; as given in Mott et al. 2017). The second line list was constructed by Ghezzi et al. (2009; hereafter, G09), including 31 blend lines in addition to Li, whereas the third line list with 36 additional blend lines has been taken from Meléndez et al. (2012; hereafter, M12). In the case of G09 and M12, we have replaced the Li I hyperfine structure by the same data as in K95.

Moreover, to be able to distinguish between the contributions of 3D and NLTE effects in the combined 3D NLTE corrections, we computed 1D NLTE spectra with the same methods and for the same grid as the 3D NLTE spectra but only for $A(\text{Li})_{\text{3DNLTE}} = 2.0$ and $^6$Li/$^7$Li$_{\text{3DNLTE}} = 5\%$, adopting the line list K95. The 1D NLTE spectra were computed using the 1D LHD model atmospheres together with NLTE departure coefficients computed with NLTE3D.

All the synthetic spectra are computed in the wavelength range between 670.69 and 670.87 nm for the K95 line list, and between 670.67 and 670.88 nm in case of line lists G09 and M12, to be able to include in the synthesized spectral region the blends other than lithium that are present in the line lists.

#### 2.3. 3D–1D fitting procedure

At first we derived the 1D LTE lithium abundance and the $^6$Li/$^7$Li isotopic ratio by fitting each 3D NLTE line profile with the grid of pre-computed 1D LTE spectra. This is done for each value of $A(\text{Li})_{\text{3DNLTE}}$ and $q(\text{Li})_{\text{3DNLTE}}$ of the 3D NLTE grid. All 3D spectra were broadened with a Gaussian instrumental profile of $FWHM = 3.0$ km s$^{-1}$, a value close to the resolution of the HARPS spectrograph. The fitting was performed through interpolation within the 1D LTE grid, driven by the least-squares fitting algorithm MPFIT (Markwardt 2009). Four free parameters were varied to achieve the best fit ($\chi^2$ minimization): $A(\text{Li})$, $q(\text{Li})$, the FWHM of the Gaussian line broadening, and a global wavelength shift ($\Delta\lambda$). The Gaussian broadening accounts for instrumental broadening and macroturbulence velocity ($V_{\text{macro}}$) in the 1D case.

In addition, to investigate the possible dependence of our results on the rotational broadening, we applied identical
rotational broadening to the 3D and 1D spectra, ranging from \( v \sin i = 0 \) to 6 km s\(^{-1}\) with a step of 2 km s\(^{-1}\). The rotational broadening is applied using the flux convolution approximation, assuming a typical limb darkening coefficient of \( \varepsilon = 0.6 \) (e.g., Gray 2005).

2.4. 3D NLTE corrections for \( A(\text{Li}) \) and \( ^6\text{Li}/^7\text{Li} \)

We define the 3D NLTE correction of the lithium abundance, \( \Delta A_{\text{NLTE}} \), as the difference between the \( A(\text{Li})_{\text{3DNLTE}} \) value assumed in the 3D NLTE synthesis and the \( A(\text{Li})_{\text{1DLTE}} \) value obtained from the best 1D LTE fit to the 3D NLTE spectrum. Similarly, the 3D NLTE correction for the lithium isotopic ratio, \( \Delta q_{\text{NLTE}} \), is defined as the difference between the assumed \( ^6\text{Li}/^7\text{Li}_{\text{3DNLTE}} \) of the 3D NLTE spectrum and the best-fitting 1D LTE \( ^6\text{Li}/^7\text{Li} \) value. The asterisk indicates that the corrections are computed on a grid of given 3D NLTE Li abundances.

2.4.1. Fitting the pure lithium feature

As an example, we show in Fig. 1 (top panel) the best fit to the pure lithium 3D NLTE spectrum achieved for \( T_{\text{eff}} = 5870 \) K, \( \log g = 4.5 \), \( [\text{Fe}/\text{H}] = 0 \), \( A(\text{Li})_{\text{3DNLTE}} = 2.0 \) and \( q(\text{Li})_{\text{3DNLTE}} = 5 \% \), computed adopting the Li hyperfine components from the line list K95. The \( ^6\text{Li}/^7\text{Li} \) isotopic ratio obtained by the best 1D LTE fit is \( q(\text{Li}) = 6.1 \% \), thus overestimating the true 3D NLTE \( ^6\text{Li}/^7\text{Li} \) of 5% by 1.1% points, and underestimating the lithium abundance by \( \sim 0.08 \) dex.

The 3D NLTE corrections (\( \Delta A_{\text{3DNLTE}-\text{1DLTE}} \) and \( \Delta q_{\text{3DNLTE}-\text{1DLTE}} \)) are computed for a grid of three \( A(\text{Li})_{\text{3DNLTE}} \) and three \( q(\text{Li})_{\text{3DNLTE}} \) values for each 3D model atmosphere given in Table 1. These corrections are meant for correcting the 1D LTE results without knowing the 3D NLTE \( A(\text{Li})_{\text{3DNLTE}} \) and \( ^6\text{Li}/^7\text{Li}_{\text{3DNLTE}} \) of the observed spectrum, and therefore, they should not depend on the 3D NLTE values of \( A(\text{Li})_{\text{3DNLTE}} \) and \( q(\text{Li})_{\text{3DNLTE}} \) but on the measured 1D LTE values. Therefore, we converted our 3D NLTE corrections such that they depend on the 1D LTE lithium abundance, \( A(\text{Li})_{\text{1DLTE}} \), and 1D LTE isotopic ratio, \( q(\text{Li})_{\text{1DLTE}} \), instead of depending on the true (3D NLTE) values \( A(\text{Li})_{\text{3DNLTE}} \) and \( q(\text{Li})_{\text{3DNLTE}} \). To do this, we used the best-fitting 1D LTE values of the lithium abundance and the \( ^6\text{Li}/^7\text{Li} \) isotopic ratio for each \( A(\text{Li})_{\text{1DLTE}} \) and \( q(\text{Li})_{\text{1DLTE}} \) point of our 3D LTE grid and interpolated the 3D NLTE corrections to the 1D LTE values \( A(\text{Li})_{\text{1DLTE}} = 1.5, 2.0, 2.5 \) and \( q(\text{Li})_{\text{1DLTE}} = 5 \% \), and 10%. All the subsequent plots and tables presented in this work will be using these 3D NLTE corrections as a function of \( A(\text{Li})_{\text{1DLTE}} \) and \( q(\text{Li})_{\text{1DLTE}} \), denoted as \( \Delta A_{\text{3DNLTE}-\text{1DLTE}} \) and \( \Delta q_{\text{3DNLTE}-\text{1DLTE}} \)-respectively.

Figure 2 shows the 3D NLTE corrections plotted vs. \( T_{\text{eff}} \) for \( ^6\text{Li}/^7\text{Li} \) (upper left panel) and \( A(\text{Li})_{\text{1DLTE}} \) (lower left panel) for \( [\text{Fe}/\text{H}] = 0 \), \( A(\text{Li})_{\text{1DLTE}} = 2.0 \) and \( q(\text{Li})_{\text{1DLTE}} = 5 \% \). The corrections for surface gravities 4.0 and 4.5 are plotted as blue circles and red triangles, respectively, and are connected with lines of different style for different \( v \sin i \) values. For a given \( \log g \), the 3D NLTE corrections of \( ^6\text{Li}/^7\text{Li} \) (\( \Delta q_{\text{3DNLTE}-\text{1DLTE}} \)) become larger (more negative) for higher temperatures, and they are larger for the lower \( \log g \). We note that \( \Delta q_{\text{3DNLTE}-\text{1DLTE}} \) depends also on \( \sin i \), \( A(\text{Li})_{\text{1DLTE}} \), and \( q(\text{Li})_{\text{1DLTE}} \): for a given \( \log g \) and \( T_{\text{eff}} \), they become smaller (more positive) for higher \( \sin i \), and for a given stellar parameters they will be higher for stars with higher lithium abundance and isotopic ratio. The dependence of \( \Delta q_{\text{3DNLTE}-\text{1DLTE}} \) on the \( V_{\text{micro}} \) used for 1D LTE spectral synthesis is negligible, and we take the central value of \( V_{\text{micro}} \) as representative for this work.

Fig. 1. The impact of the blending lines in the Li i \( 6707.8 \) nm region on the resulting 3D NLTE corrections. The best fitting 1D LTE spectrum (black continuous line) is superimposed on the 3D NLTE spectrum (black dotted line) computed for \( T_{\text{eff}} = 5870 \) K, \( \log g = 4.5 \), \( [\text{Fe}/\text{H}] = 0 \), \( A(\text{Li})_{\text{3DNLTE}} = 2.0 \), \( ^6\text{Li}/^7\text{Li}_{\text{3DNLTE}} = 5 \% \) and representing the “observation”. The synthetic spectra are computed adopting only the Li i doublet including hyperfine structure (line list K95, upper panel), and the line list G09 (lower panel), which includes also other atomic blends. The right y-axis gives the scale of the residuals (blue dashed line). We measure \( A(\text{Li})_{\text{1DLTE}} = 1.92 \) and \( ^6\text{Li}/^7\text{Li} = 6.1 \% \) for line list K95, and \( A(\text{Li})_{\text{1DLTE}} = 1.92 \) and \( ^6\text{Li}/^7\text{Li} = 5.4 \% \) in case of line list G09.

On the other hand, the 3D NLTE corrections for the lithium abundance, \( \Delta A_{\text{3DNLTE}-\text{1DLTE}} \), become larger for lower effective temperatures. There is only a slight dependence on the surface gravity, and their dependence on the \( v \sin i \) can be neglected (see Fig. 2, lower left panel). The \( \Delta A_{\text{3DNLTE}-\text{1DLTE}} \) corrections do not show variations for different \( V_{\text{micro}} \) and \( q(\text{Li})_{\text{1DLTE}} \) values, whereas they are decreasing slightly with larger \( A(\text{Li})_{\text{1DLTE}} \) values.

Similar plots for the other three metallicities of our grid are given in Appendix A. For full details, we provide electronically a table of the corrections for \( T_{\text{eff}} = 5900, 6300, 6500 \) K, \( \log g = 4.0 \) and 4.5, \( [\text{Fe}/\text{H}] = -0.5, 0.0, 0.5 \), \( A(\text{Li})_{\text{1DLTE}} = 1.5, 2.0, 2.5 \), \( q(\text{Li})_{\text{1DLTE}} = 5 \% \), and \( v \sin i = 0.0, 2.0, 4.0, 6.0 \) km s\(^{-1}\), based on the pure lithium line list K95.

2.4.2. The impact of the mixing-length parameter

To investigate the dependence of our results on the choice of the mixing length parameter for 1D LHD models, we computed \( \Delta A_{\text{3DNLTE}-\text{1DLTE}} \) and \( \Delta A_{\text{3DNLTE}-\text{1DLTE}} \) using the models N 1–6 and N 13–18 with \( \alpha_{\text{MLT}} = 0.5 \) and 1.5 (N 3, 15 and 17 only with \( \alpha_{\text{MLT}} = 0.5 \)). As expected, the choice of this parameter did not
effect the $\Delta q_{\text{3DNLTE-1DLTE}}$ results, while $\Delta A_{\text{3DNLTE-1DLTE}}$ varied slightly by $\pm 0.01$ dex over the considered range of $\alpha_{\text{MLT}}$.

### 2.4.3. The impact of blend lines

The bottom panel of Fig. 1 shows the best fit to the 3D NLTE spectrum computed for the same parameters as in Sect. 2.4.1, but now adopting line list G09 that includes atomic and molecular blends partly overlapping with the Li feature. In this case, the 3D NLTE correction of the $^6\text{Li}/^7\text{Li}$ isotopic ratio is somewhat smaller ($-0.45\%$ points), while the 3D NLTE correction for $A$(Li) is similar to the K95 case ($+0.08$ dex).

Initially, we were expecting that the fitting results would depend only weakly on the adopted line list. Comparison of the lower panels of Fig. 2 shows that this is basically the case for the $A$(Li) correction. However, while the $^6\text{Li}/^7\text{Li}$ corrections derived with line list G09 are qualitatively similar to those obtained from fitting the pure lithium spectrum, there are quantitative differences that depend on a variety of factors.

As shown in Fig. 1 (bottom), the blends in this spectral region may be quite strong (e.g., the Fe I line at $\sim 670.74$ nm and can play an even greater role in the fitting procedure than the Li I line itself. We recall that the main fitting parameters are $A$(Li) and $q$(Li), both only influencing the Li line, while the two remaining fitting parameters, global Gaussian line broadening and line shift, act on all spectral lines. However, to keep the dimensionality of the problem manageable, the strength and wavelength shift of the individual blend lines is not adjusted in the fitting procedure. This deficiency of our method can lead to meaningless fitting results, because poorly reproduced stronger blend lines determine the global line broadening and shift of the best fit, and therefore indirectly dictate an ill-defined solution for $^6\text{Li}/^7\text{Li}$. This is especially true for the case of high metallicity ([Fe/H] = +0.5) and low lithium abundance ($A$(Li) = 1.5), where the $^6\text{Li}/^7\text{Li}$ corrections obtained with line list G09 are essentially useless.

It is therefore hardly surprising that line lists G09 and M12 produce somewhat different fitting results (compare Figs. 2 and A.4), which moreover depend strongly on the wavelength range selected for fitting the Li I 670.8 nm spectral region, as well as on whether the continuum placement is free or a fixed parameter.

The above-mentioned difficulties do not exist if we derive the 3D NLTE corrections using the line list K95 which includes only the Li I components. We also notice that the results obtained with this line list are much less sensitive to the value of $v\sin i$ than in the case of line lists G09 and M12. We argue that the fitting results obtained by considering only Li I lines must be very similar to those one would derive if all blend lines were fitted individually in the line lists G09, M12, or any other line list representative of the Li region. This argument is illustrated and supported by the investigations presented in Appendices B...
and $C$, where we show that a line list adjusted to fit a given spectrum in 1D generally produces a less satisfactory fit when used for 3D modeling. An equally good fit in 3D can only be achieved by readjusting the line list to account for 3D abundance corrections and differential wavelength shifts of the blends. When using the 1D and 3D fine-tuned line lists, respectively, the differential 1D-3D lithium isotopic abundances become largely independent of the blend lines and are well approximated by the corrections obtained with line list K95 (only $Li$).

### 2.5. Analytical expressions

We derived analytical expressions for the corrections derived from the "only Li" line list K95 to be able to numerically evaluate $\Delta A_{3DNLTE-1DLTE}$ and $\Delta q_{3DNLTE-1DLTE}$ as a function of the stellar parameters for any target star within the range of our grid.

As mentioned above, the $A(Li)$ abundance corrections for all the models in our grid show only a weak dependency on the surface gravity. Assuming a log $g$ of 4.0 or 4.5, the resulting $A(Li)$ corrections are very similar, as shown in the lower panels of Fig. 2. Within the modeling uncertainties (see below), the log $g$ dependence may be neglected. For this reason, we assumed $\Delta A_{3DNLTE-1DLTE}$ to be independent of log $g$ while deriving the analytic approximation.

Somewhat unexpectedly, model atmosphere N2, with $T_{\text{eff}} = 5920$ K, log $g = 4.5$, [Fe/H] = −1, results in a smaller $\Delta A(Li)$ than expected from the trends of the corrections derived using other models in our grid (see Figs. A.1–A.3). A possible explanation for this discrepancy is that this model was computed for a smaller number of snapshots (8) in comparison to the other models (20). We decided not to use this result and instead consider it to be equal to the correction computed for the model N1 (with the same $T_{\text{eff}}$ but log $g = 4.0$) in deriving the numerical fitting function for $\Delta A_{3DNLTE-1DLTE}$.

We provide a link to a web page\(^2\) that uses the analytical expressions developed in this work and allows the user to compute the $\Delta q_{3DNLTE-1DLTE}$ corrections as a function of $T_{\text{eff}}$, [Fe/H], log $g$, $v \sin i$, $A(Li)$ and $\delta Li/\delta Li$, and the $\Delta A_{3DNLTE-1DLTE}$ corrections as a function of $T_{\text{eff}}$, [Fe/H] and $A(Li)$. However, below we also provide simplified analytical expressions for a quicker evaluation of the 3D NLTE corrections.

The simplified expressions for $\Delta A_{3DNLTE-1DLTE}$ and $\Delta q_{3DNLTE-1DLTE}$ provided in this section are based on all available data points for $v \sin i = 2.0$ km s\(^{-1}\), $A(Li) = 2.0$, $q(Li) = 5\%$, and are functions of $T_{\text{eff}}$, (log $g$), and [Fe/H]. The two fitting functions are described by the following equations:

\begin{align}
\Delta A_{3DNLTE-1DLTE} &= C_0 + C_1 x + C_2 x^2 + C_3 z + C_4 x^2 z + C_5 x z^2, \quad (1) \\
\Delta q_{3DNLTE-1DLTE} &= \sum_{i=0}^{2} \sum_{j=0}^{2} C_{i,j} x^i y^j z^j, \quad (2)
\end{align}

where $x \equiv (T_{\text{eff}} - T_{\text{eff}}^*)/T_{\text{eff}}^*$, $y \equiv \log g - \log g^*$, and $z \equiv [Fe/H]/[Fe/H]^*$, with $T_{\text{eff}}^* = 5900$ K and log $g^* = 4.0$. The valid parameter ranges are $0 \leq x \leq 0.1$, $0 \leq y \leq 0.5$; $-1.0 \leq z \leq 0.5$. The formulae consist of six ($C_{0,5}$) and 18 ($C_{i,j}$) numerical coefficients for $\Delta A$ and $\Delta q$, respectively (explicitly given in Table 2).

To visualize the resulting 3D NLTE corrections generated with this tool, we present in Fig. 3 the contours of $\Delta A_{3DNLTE-1DLTE}$ in the $T_{\text{eff}} - [Fe/H]$ plane (upper panel), and contour plots of $\Delta q_{3DNLTE-1DLTE}$ in the $T_{\text{eff}} - [Fe/H]$ and $T_{\text{eff}} - \log g$ plane (middle and lower panel, respectively).

### Table 2. Numerical coefficients in Eqs. (1) and (2) derived for the line list K95 with representative 1D LTE values of $A(Li) = 2.0$, $q(Li) = 5\%$, and $v \sin i = 2.0$ km s\(^{-1}\).

<table>
<thead>
<tr>
<th>Coeff.</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_0$</td>
<td>0.074205</td>
</tr>
<tr>
<td>$C_1$</td>
<td>0.0607931</td>
</tr>
<tr>
<td>$C_2$</td>
<td>1.518850</td>
</tr>
<tr>
<td>$C_3$</td>
<td>0.053601</td>
</tr>
<tr>
<td>$C_4$</td>
<td>0.023510</td>
</tr>
<tr>
<td>$C_5$</td>
<td>-0.159625</td>
</tr>
<tr>
<td>$c_{00}$</td>
<td>-1.5994</td>
</tr>
<tr>
<td>$c_{01}$</td>
<td>1.0167</td>
</tr>
<tr>
<td>$c_{02}$</td>
<td>-0.4877</td>
</tr>
<tr>
<td>$c_{11}$</td>
<td>0.2553</td>
</tr>
<tr>
<td>$c_{02}$</td>
<td>-0.1548</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>0.3447</td>
</tr>
<tr>
<td>$c_{03}$</td>
<td>-7.7112</td>
</tr>
<tr>
<td>$c_{10}$</td>
<td>6.0203</td>
</tr>
<tr>
<td>$c_{11}$</td>
<td>4.6808</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>1.0406</td>
</tr>
<tr>
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<td>-12.9981</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>-96.3931</td>
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<tr>
<td>$c_{12}$</td>
<td>191.2326</td>
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<tr>
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</tr>
<tr>
<td>$c_{12}$</td>
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</tr>
<tr>
<td>$c_{12}$</td>
<td>-68.1011</td>
</tr>
<tr>
<td>$c_{12}$</td>
<td>223.1616</td>
</tr>
</tbody>
</table>

The functional forms provided in this work allow a quick estimate of 3D NLTE corrections for a limited range of stellar parameters. For a complete overview and more precise 3D NLTE corrections, we refer to the table at the CDS, and to the above-mentioned web page.\(^2\) To give an example, our full analytical expressions give the following corrections for HD 82943 ($T_{\text{eff}} = 6025$ K, log $g = 4.53$, [Fe/H] = +0.30): $\Delta A_{3DNLTE-1DLTE} = +0.08$ dex and $\Delta q_{3DNLTE-1DLTE} = -1.7\%$ points.

The root mean square (rms) difference between the global fitting function used by the above-mentioned web page and the input data points of the regular grid is 0.007 dex for $\Delta A_{3DNLTE-1DLTE}$ and 0.07\% points for $\Delta q_{3DNLTE-1DLTE}$. These numbers represent the mean fitting function errors of the two quantities for stellar parameters that lie close to our grid points.

In order to evaluate the interpolation errors of our analytical expressions outside of the grid points, we computed $\Delta A_{3DNLTE-1DLTE}$ and $\Delta q_{3DNLTE-1DLTE}$ for intermediate $T_{\text{eff}}$, log $g$ and $A(Li)$ values by using two additional 3D model atmospheres with [Fe/H] = 0.0, log $g = 4.3$ and $T_{\text{eff}} = 6110$ and 6430 K. The 3D NLTE spectra have been computed for $A(Li)_{3DNLTE} = 1.5, 1.75, 2.0, 2.25, 2.5$ and for the same $\delta Li/\delta Li$ and $v \sin i$ values as in case of the original grid. The rms difference between the global fitting function and these new intermediate data points is again 0.007 dex for $\Delta A_{3DNLTE-1DLTE}$ and 0.10\% points for $\Delta q_{3DNLTE-1DLTE}$. Even if we do not have the possibility to compute 3D NLTE corrections for intermediate points in [Fe/H], due to the lack of 3D hydrodynamical model atmospheres, we assume that the mean interpolation errors of 0.01 dex for $\Delta A$ and 0.10\% points for $\Delta q$ are valid for the whole parameter space covered by our grid. The largest errors in $\Delta A$ of ±0.015 dex are encountered at low temperatures ($T_{\text{eff}} \approx 5900$ K), while the largest errors in $\Delta q$ of ±0.2\% points are mainly incurred at high temperatures ($T_{\text{eff}} \approx 6500$ K).

### 2.6. 1D NLTE corrections and comparison with other works

In order to distinguish between the contributions of 3D and NLTE effects in the combined 3D NLTE correction, we repeated
with a standard deviation of 0.08%. This is expected as both LTE and NLTE line profiles are intrinsically symmetric. On the other hand, the 1D NLTE corrections for \( A(\text{Li}) \) show a similar trend as the 3D NLTE corrections, although with an offset to slightly smaller values (see Fig. 4). We have derived an equation similar to the Eq. (1) for the 1D NLTE case to facilitate the comparison with our 3D corrections and with the results from the literature (see below).

Figure 4 shows the functions for estimating the 3D NLTE and 1D NLTE \( A(\text{Li}) \) corrections derived in this work for metallicities \([\text{Fe}/\text{H}] = -1.0, -0.5, 0.0, \) and +0.5, together with the results obtained by Takeda & Kawanomoto (2005) and Lind et al. (2009). Our 3D and 1D NLTE corrections follow similar trends but with small offset towards lower values (ranging between 0.01 and 0.03 dex, depending on \([\text{Fe}/\text{H}] \) and \( T_{\text{eff}} \)). This only small difference indicates that the 3D effects slightly enhance the non-LTE effects, while the latter generally dominate over the 3D effects in the combined 3D NLTE corrections.

The overall trends of our 1D NLTE corrections are similar to the trends obtained by Lind et al. (2009), with an offset ranging between 0.02 and 0.06 dex, depending mainly on the metallicity, while the curves of Takeda & Kawanomoto (2005) have a slightly different slope. Such differences in the 1D NLTE lithium abundance corrections, being −0.06 dex at most, are not unexpected due to the differences in the methods (model atmospheres, model atom, numerical procedure for computing departure coefficients, etc.) used by different authors. Nevertheless, we performed a test to check if the difference in the 1D NLTE \( A(\text{Li}) \) corrections could be explained by the different model atmospheres used in the spectral synthesis in this work (1D LHD models) and in Lind et al. (2009; MARCS models), respectively. The test was performed using a 1D NLTE spectrum computed from a MARCS model with \( T_{\text{eff}} = 6500 \) K, \([\text{Fe}/\text{H}] = -1.0, \log g = 4.0, \) assuming \( A(\text{Li})_{\text{IDLTE}} = 2.0 \) and \( ^6\text{Li}/^7\text{Li}_{\text{IDLTE}} = 5 \% \), and a corresponding grid of 1D LTE spectra computed for combinations of nine \( A(\text{Li}) \) and nine \( ^6\text{Li}/^7\text{Li} \) values, using the same MARCS model atmospheres (Gustafsson et al. 2008) as in Lind et al. (2009). The MARCS NLTE spectrum was fitted by the grid of MARCS LTE line profiles following the same fitting procedure as described in Sect. 2.3. The resulting 1D LTE \( A(\text{Li}) \) correction is −0.055 dex, in very good agreement with the correction of −0.053 dex obtained for those stellar parameters by Lind et al. (2009). This result confirms that the shift of −0.05 dex between our 1D NLTE lithium abundance corrections and the ones by Lind et al. (2009; see Fig. 4, top left panel) are likely due to the different model atmospheres adopted in the spectral synthesis.

The analytical expressions given in Sbordone et al. (2010) for \( A(\text{Li}) \) were derived using 3D model atmospheres with metallicities −2 and −3 that do not overlap with our grid. Since we do not observe a linear dependence of the \( A(\text{Li}) \) 3D NLTE corrections on the metallicity, the extrapolated corrections from Sbordone et al. (2010) would be too uncertain for a useful comparison with our results. Therefore, we do not present such a comparison.

We compared the 3D NLTE corrections for \(^6\text{Li}/^7\text{Li} \) derived in this work with the corrections presented by Steffen et al. (2012) and found very good agreement. This was expected, since the model atmospheres and methods used in these two works are similar. The present study extends the work of Steffen et al. (2012), using a 3D NLTE grid with more metallicity points around the solar value, and also investigating the dependence of the 3D NLTE corrections on \( A(\text{Li}), ^6\text{Li}/^7\text{Li}, \log g \), and \( \sin i \), and the list of blend lines.
3. Li abundance and $^{6}\text{Li}/^{7}\text{Li}$ isotopic ratio in HD 207129 and HD 95456

In this section, we analyze two solar-type stars, HD 207129 and HD 95456, in order to determine $A(\text{Li})$ and the $^{6}\text{Li}/^{7}\text{Li}$ isotopic ratios, at first with a 1D LTE approach, and afterwards applying our already pre-computed 3D NLTE corrections. These stars have been selected for this study because the difference in their effective temperatures places them at two extreme positions in our correction grid. They are part of a larger sample of stars with high lithium content and low activity levels, for which high-resolution and very-high-S/N spectra are available that allow a sensitive analysis of $^{6}\text{Li}/^{7}\text{Li}$. We point out that Gomes da Silva et al. (2014) performed long-term activity studies of HD 207129 and HD 95456 using CaTi II H & K and Hα lines in their HARPS spectra (Mayor et al. 2003), and found both stars to show very low activity levels with no significant long-term variability.

3.1. Observations and stellar parameters

The observed spectra used in this work have been obtained with the HARPS spectrograph at La Silla observatory (ESO, Chile) within the framework of the HARPS GTO planet search program (subsample HARPS-I, Mayor et al. 2003). The spectral resolution of $R \sim 115000$ and the high S/N of $\sim 2000$ of the combined spectrum of each star provide the quality that is needed for analysis of the Li I $\lambda 6707.8$ nm region in the context of the $^{6}\text{Li}/^{7}\text{Li}$ measurements.

The stellar atmospheric parameters ($T_{\text{eff}}$, log $g$, [Fe/H] and $V_{\text{micro}}$) of both stars were derived by Sousa et al. (2008) and are summarized in Table 3. The abundances of several elements with blending lines present in the line lists (Si, Ca, Ti, V) were adopted from Adibekyan et al. (2012), whereas the carbon and oxygen abundances were taken from Suárez-Andrés et al. (2017) and Bertran de Lis et al. (2015), respectively, and the nitrogen abundance was chosen to be equal to the carbon abundance. The elemental abundances adopted for the Sun, HD 207129, and HD 95456 are given in Table 4.

3.2. Rotational broadening and iron abundance

A list of atomic line data has been constructed for a number of isolated, unblended Fe I lines taken from Doyle et al. (2014), Tsantaki et al. (2013) and from the VALD-v3 database (Kupka et al. 2011) to estimate the projected rotational velocity ($v \sin i$) and the possible small iron abundance correction for the stars studied in this work. For each line of each star, a grid of nine 1D LTE Kurucz Atlas spectra was computed assuming an iron abundance range of $\pm 0.2$ dex around the adopted iron abundance (metallicity) value, with a step of 0.05 dex. The spectra
were computed using the 2014 version of the spectral synthesis code MOOG (Sneden 1973).

The fitting procedure was performed for the solar flux atlas from Kurucz (2005), and for the HARPS spectra of HD 207129 and HD 95456. The HARPS spectra have been locally normalized for each Fe line. We investigated the quality of the fits by means of a \( \chi^2 \) analysis. All the lines that seemed to be blended with other spectral features (at least in one of the two stars or the Sun), or provided a non-satisfactory fit to the observations, were excluded from the sample. Eventually, we were left with 10 “clean” Fe I lines which are well isolated and can be fitted well in the solar spectrum and the HARPS spectra of the two stars. Table 5 lists the atomic data of the selected Fe I lines: wavelength, excitation potential (EP), oscillator strength (\( \log gf \)), and the reference to the source they were taken from for each individual Fe I line.

Four parameters were varied to achieve the best fit: [Fe/H], \( v \sin i \), the global wavelength shift (\( \Delta \lambda \)), and the continuum level. Since it was difficult to obtain both \( V_{\text{macro}} \) and \( v \sin i \) individually from the fitting procedure due to a “degeneracy” of the solution, a fixed Gaussian macroturbulence velocity (\( V_{\text{macro}} \)) was assumed for the fitting. \( V_{\text{macro}} \) was adopted from Doyle et al. (2014) and used after the application of a factor to convert the radial-tangential (RT) macroturbulence parameter (\( V_{\text{RT}} \)) provided by these authors to the Gaussian macroturbulence parameter \( V_{\text{macro}} \) that we use. This conversion factor was determined for the solar case using the same solar \( v \sin i \) and atmospheric parameters (including \( V_{\text{macro}} = 1.0 \text{ km s}^{-1} \)) as assumed in Doyle et al. (2014). We derive a solar [Fe/H] = −0.02 ± 0.06 and \( V_{\text{macro}} = 2.12 ± 0.10 \text{ km s}^{-1} \) resulting in the conversion formula \( V_{\text{macro}} \sim 0.66 V_{\text{RT}} \). The relation between the different macroturbulence velocity models has been discussed in a recent work by Takeda & Ueno (2017), and the conversion factor of 0.66 that we derive is in agreement with their results. For a given \( V_{\text{macro}} \), each line profile has been broadened by nine different \( v \sin i \) values with the flux convolution approximation, assuming a limb darkening coefficient of \( e = 0.6 \) (Gray 2005). The least-squares fitting method that we apply (MPFIT; Markwardt 2009) relies on interpolation in the grid of the precomputed synthetic spectra with different [Fe/H] and \( v \sin i \). For each star, the best fit values of [Fe/H] and \( v \sin i \) were averaged over the ten different Fe I lines and the uncertainties were derived from the standard deviations (cf. Table 5).

For HD 207129, we obtain \( v \sin i = 2.21 ± 0.24 \text{ km s}^{-1} \) and an iron abundance correction of \( \Delta[\text{Fe/H}] = 0.025 ± 0.063 \text{ dex} \). For HD 95456, the radial-tangential macroturbulence is \( V_{\text{RT}} = 5.05 \text{ km s}^{-1} \) according to Doyle et al. (2014), which is large enough to broaden the synthetic line profiles to such an extent that the fits were not very different for \( v \sin i \) between 0 and 3 \text{ km s}^{-1}. For instance, when we use the \( V_{\text{macro}} \) value from Doyle et al. (2014), we obtain a formal \( v \sin i \) of 0.88 \text{ km s}^{-1}. As we discuss in Sect. 3.5, the measured \( \Delta[\text{Li}] \) and \( ^6\text{Li}/^7\text{Li} \) for HD 95456 essentially do not change with different \( v \sin i \) assumptions. We therefore prefer the \( v \sin i \) value of 3.28 \text{ km s}^{-1} determined by Delgado Mena et al. (2015), based on a combination of Fourier transform and goodness-of-fit methods. We derive a small Fe abundance correction of \( \Delta[\text{Fe/H}] = −0.068 ± 0.067 \text{ dex} \) (relative to the literature value of [Fe/H]) for HD 95456.

### 3.3. Blend lines in the lithium \( \lambda 670.8 \text{ nm} \) region

One of the challenges in \( ^6\text{Li}/^7\text{Li} \) measurements is the presence of several other atomic and molecular lines overlapping with the resonance doublet. While the contribution of these blends may be very small in metal poor stars, they become more significant at higher metallicities and must be treated carefully for stars having metallicities close to solar or higher. There are several lists of atomic and molecular lines currently available in the literature which have been carefully constructed to reproduce the Li \( \lambda 670.8 \text{ nm} \) region (e.g., Mandell et al. 2004, Ghezzi et al. 2009, Meléndez et al. 2012, Israeli 2014; priv. comm.) and are fitted for very sensitive measurements of the \( ^6\text{Li}/^7\text{Li} \) isotopic ratio in solar-type stars. It has already been demonstrated that the use of different lists of atomic and molecular lines interfering with the \( \lambda 1 \) \( \lambda 670.8 \text{ nm} \) doublet can lead to noticeable differences in the measured values of \( ^6\text{Li}/^7\text{Li} \) (e.g., Israeli et al. 2003; Mott et al. 2017). We therefore perform our analysis using different line lists provided in the literature and compare the results.

Specifically, we used three different line lists for the analysis of \( \Delta[\text{Li}] \) and \( ^6\text{Li}/^7\text{Li} \) in the atmospheres of HD 207129 and HD 95456. In addition to G09 and M12, we used the line lists constructed by Israeli (2014; priv. comm.), as given by Mott et al. (2017; hereafter, I14). The line lists were adjusted by computing 1D LTE synthetic spectra and fitting the 670.8 nm region in the solar spectrum (G09) or in spectra of other stars (I14). The above authors assumed different elemental abundances from what we assume for the Sun (Table 4, Col. 2). Specifically, we adopted the solar abundance values for 12 elements (Li, C, N, O, P, S, K, Fe, Eu, Hf, Os, Th) from Caffau et al. (2011; their Table 5), and for other elements we used the internal solar elemental abundances
Table 5. Fe I lines used for deriving \( \mathbf{v} \sin \mathbf{i} \) and the iron abundance correction \( \Delta [\text{Fe}/H] \).

<table>
<thead>
<tr>
<th>Chemical Species</th>
<th>Wavelength ( \lambda ) (Å)</th>
<th>EP (eV)</th>
<th>( \log gf ) (dex)</th>
<th>Source</th>
<th>( V_{\text{macro}} ) (km s(^{-1}))</th>
<th>( \Delta [\text{Fe}/H] ) (dex)</th>
<th>( \mathbf{v} \sin \mathbf{i} ) (km s(^{-1}))</th>
<th>( \Delta [\text{Fe}/H] ) (dex)</th>
<th>( \mathbf{v} \sin \mathbf{i} ) (km s(^{-1}))</th>
<th>( \Delta [\text{Fe}/H] ) (dex)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fe I</td>
<td>6094.3800</td>
<td>4.650</td>
<td>−1.566</td>
<td>T13</td>
<td>2.14</td>
<td>−0.088</td>
<td>2.53</td>
<td>−0.088</td>
<td>1.58</td>
<td>−0.118</td>
</tr>
<tr>
<td>Fe I</td>
<td>6200.3190</td>
<td>2.609</td>
<td>−2.437</td>
<td>Do14</td>
<td>2.06</td>
<td>−0.019</td>
<td>1.97</td>
<td>−0.022</td>
<td>0.00</td>
<td>−0.091</td>
</tr>
<tr>
<td>Fe I</td>
<td>6481.8800</td>
<td>2.280</td>
<td>−2.929</td>
<td>T13</td>
<td>1.94</td>
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<td>1.95</td>
<td>−0.074</td>
<td>0.00</td>
<td>−0.130</td>
</tr>
<tr>
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<td>−2.384</td>
<td>T13</td>
<td>2.05</td>
<td>−0.049</td>
<td>1.94</td>
<td>−0.055</td>
<td>0.00</td>
<td>−0.134</td>
</tr>
<tr>
<td>Fe I</td>
<td>6699.1408</td>
<td>4.593</td>
<td>−2.101</td>
<td>Vald3</td>
<td>2.23</td>
<td>−0.078</td>
<td>2.14</td>
<td>−0.119</td>
<td>1.59</td>
<td>−0.112</td>
</tr>
<tr>
<td>Fe I</td>
<td>6703.5655</td>
<td>2.759</td>
<td>−3.160</td>
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<td>0.069</td>
<td>0.61</td>
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</tr>
<tr>
<td>Fe I</td>
<td>6725.3553</td>
<td>4.103</td>
<td>−2.303</td>
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<td>2.23</td>
<td>0.051</td>
<td>2.41</td>
<td>0.052</td>
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<td>0.0288</td>
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<tr>
<td>Fe I</td>
<td>6726.6658</td>
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<td>−1.094</td>
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<td>2.19</td>
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<td>0.010</td>
<td>2.53</td>
<td>0.019</td>
<td>1.51</td>
<td>−0.015</td>
</tr>
</tbody>
</table>

Average

\[ \begin{align*}
\mathbf{v} \sin \mathbf{i} & = 2.12 \pm 0.021 \\
\Delta [\text{Fe}/H] & = 0.10 \pm 0.056 \\
\end{align*} \]

Table Notes:

- The lines and their parameters are adopted from the VALD-v3 database Kupka et al. (2011; Vald3), Tsantaki et al. (2013; T13) or Doyle et al. (2014; Do14), as indicated in the fifth column. For the Sun, we used a fixed \( \mathbf{v} \sin \mathbf{i} \) of 1.9 km s\(^{-1}\) in order to derive its \( V_{\text{macro}} \) whereas for HD 207129 and HD 95456 we proceeded the other way round, fixing the \( V_{\text{macro}} \) values at 2.33 and 3.33 km s\(^{-1}\), respectively, in finding their \( \mathbf{v} \sin \mathbf{i} \) (see Sect. 3.2).

- A molecule that is present in all line lists representing the Li 670.8 nm region is CN. The presence of several lines of this molecule is important in the \(^{6}\text{Li}\) determination, and assuming the correct C, N, and O abundances (because O can influence the equilibrium of the molecular reaction network) can be crucial. Particularly, the assumptions for solar abundances of O and N were significantly different between the authors of the line lists and our work. Therefore, we made some calibrations to eliminate the differences arising from different assumptions of solar abundances while constructing the line lists for performing our analysis. For elements other than C, N, and O abundances were lower by up to 0.17 and 0.19 dex, respectively, and by 0.06 dex for Fe. In this case, we have scaled the \( \log gf \) values of all the CN lines in this region by a constant factor. This factor was derived by fitting the solar flux atlas with a pre-computed grid of 1D LTE synthetic spectra for the Sun. For each line list, a grid of 1D LTE spectra was computed applying different factors (within the range of ±0.3 dex with a step of 0.01 dex) to the \( \log gf \) values of all the CN lines. Then, for a given line list, we adopted the \( \log gf \) factor resulting in the best fit (\( \chi^2 \) minimization) to the solar flux atlas. This factor was ±0.20 dex in case of the G09 and M12 line lists, and ±0.19 dex in case of the I14 line list. For elements other than C, N, and O present in the line lists, the small solar abundance differences were taken into account by applying corresponding corrections to the \( \log gf \) values of the individual lines of each element. After this adjustment, all line lists are “normalized” to our adopted solar abundances.

- In addition, the wavelength and the \( \log gf \) value of the V I line at 670.81096 nm have been updated according to the recently published values by Lawler et al. (2014). This blend is positioned close to one of the \(^{6}\text{Li}\) components and may affect the result of the \(^{6}\text{Li}/^{7}\text{Li}\) determination if incorrect line parameters are assumed (see Sect. 3.7).

3.4. Spectral synthesis for \(^{6}\text{Li}/^{7}\text{Li}\) studies of HD 207129 and HD 95456

In order to derive \(^{6}\text{Li}\) and \(^{6}\text{Li}^{7}\) in the two solar-type stars, we perform a standard 1D LTE analysis using the 2014 version of the spectral synthesis code MOOG (Sneden 1973) together with Kurucz ATLAS9 1D model atmospheres (Kurucz 1993).

3.5. Fitting procedure for the HARPS spectra

To fit the observed spectra of the two target stars, we followed a procedure similar to the one already described in Sect. 2.3. The HARPS spectra of HD 207129 and HD 95456 were fitted through interpolation across a grid of 1D LTE line profiles computed with MOOG for line lists G09, M12 and I14.
To achieve the best fit evaluated by means of a $\chi^2_{\text{red}}$ minimization method, four free parameters were varied: $\Delta(\text{Li})$, $q(\text{Li})$, the global wavelength shift ($\Delta v$) and the FWHM of the Gaussian line broadening, which accounts also for $V_{\text{macro}}$, while $v \sin i$ and $V_{\text{micro}}$ are fixed at the values given in Table 3. Additionally, for each combination of stellar parameters and line list, we used the 1D LTE spectra assuming different Fe and CNO abundances. This allowed us to achieve an even better fit, allowing for possible small abundance deviations from the adopted values. We applied a similar fitting procedure to derive the lithium abundance and $^6\text{Li}/^7\text{Li}$ isotopic ratio in the Sun (Sect. 3.8).

### 3.6. Fitting results for HD 207129 and HD 95456

Figure 5 shows the best 1D LTE fit to the HD 207129 (left panels) and HD 95456 (right panels) HARPS spectra, obtained with line lists G09, M12, and I14 (from top to bottom), with modifications described in Sect. 3.3. The right $y$-axis defines the scale of the residuals (dashed line).
For reference, we also show the fitting result for the Sun obtained with line list G09. The 3D NLTE values are obtained by applying the optimal choice of [Fe/H] and CNO. We note that the best fits shown in Fig. 5 are based on the values of [Fe/H] and CNO derived from Fig. 6. The uncertainties related to the different lists of blend lines (see Sect. 3.6). For the Sun, the error in A(Li) corresponds to a continuum placement uncertainty of ±0.05%, while the error in $^{6}\text{Li}/^{7}\text{Li}$ is the formal 1σ fitting error.

HD 207129, this V$_{\text{macro}}$ is in good agreement with the V$_{\text{macro}}$ used for fitting the Fe i lines given in Table 5 (Sect. 3.2). For HD 95456, the V$_{\text{macro}}$ derived with this procedure is lower, since we adopted a larger v sin i (Table 3) than its resulting value from the fitting of the Fe i lines (Sect. 3.2). The errors given in Fig. 5 are the 1σ formal fitting errors. The 1D LTE best-fit values for A(Li) and $^{6}\text{Li}/^{7}\text{Li}$ for all three line lists are collected in Table 6. The different line lists result in somewhat different $^{6}\text{Li}/^{7}\text{Li}$ for the same star. We adopt the results obtained using line list G09 as the representative result of our analysis since $^{6}\text{Li}/^{7}\text{Li}$ obtained with this set of blends falls between the values from the analysis with line lists M12 and I14. The uncertainty due to the different line lists is included as one contribution to the total error (see below).

Figure 6 shows the best fitting $\chi^2_{\text{red}}$ values obtained by fitting the HARPS spectra of HD 207129 (upper panel) and HD 95456 (lower panel) with synthetic 1D LTE spectra computed for all the combinations of Fe and CNO abundances based on the preferred line list G09. From this figure, it is clear that the lowest $\chi^2_{\text{red}}$ values are obtained around the adopted abundances of Fe and CNO. We note that the best fits shown in Fig. 5 are based on the optimal choice of [Fe/H] and CNO derived from Fig. 6.

The 3D NLTE corrections for the lithium abundance and $^{6}\text{Li}/^{7}\text{Li}$ for HD 207129 and HD 95456 were obtained using the analytical approximations developed in this work. The 3D NLTE corrections of A(Li) were computed as a function of T$_{\text{eff}}$, [Fe/H], and A(Li), the 3D NLTE corrections of $^{6}\text{Li}/^{7}\text{Li}$ as a function of T$_{\text{eff}}$, log g, [Fe/H], v sin i, A(Li) and $^{6}\text{Li}/^{7}\text{Li}$. We derive 3D NLTE A(Li) corrections of +0.07 dex and +0.05 dex, and $^{6}\text{Li}/^{7}\text{Li}$ corrections of −1.1 and −1.9% points for HD 207129 and HD 95456, respectively. Afterwards, we applied these corrections to the measured 1D LTE best-fitting values of A(Li) and $^{6}\text{Li}/^{7}\text{Li}$. The derived values after such corrections are also presented in Table 6.

We compute the errors of the 1D LTE lithium abundance and $^{6}\text{Li}/^{7}\text{Li}$ by considering seven sources of uncertainty: uncertainties related to the choice of the effective temperature ($\Delta T_{\text{eff}} = \pm 50$ [K]) and surface gravity ($\Delta \log g = \pm 0.1$) as well as the continuum placement (1.0 ± 0.05%), the internal fitting error, the fitting errors related to different Fe ($\Delta$[Fe/H]) is ±0.1 for HD 207129 and ±0.05 for HD 95456) and CNO abundance factors ($\Delta$[CNO] = ±0.05%). These six errors are computed for the line list G09. The seventh error is related to the different lists of atomic and molecular blends used in this work, and for both lithium abundance and isotopic ratio is computed as the standard deviation of measured A(Li) and $^{6}\text{Li}/^{7}\text{Li}$, respectively, adopting line lists G09, M12, and I14. These seven different error contributions are combined in quadrature and are given as the total error in Table 6.

Finally, to test the dependence of our results on the used v sin i value, we applied a v sin i of 0.85 km s$^{-1}$ to the synthetic spectra of HD 95456, as measured in Sect. 3.2 using Fe i lines, and repeated the fitting procedure for the best fitting values of Fe and CNO abundance for the line list G09. The resulting LTE values of A(Li) = 2.65 and g(Li) = 2.7% are in very good agreement with the values derived assuming v sin i = 3.28 km s$^{-1}$, demonstrating that an accurate determination of the rotational broadening is not critical.

3.7. Tests with the Si i and V i lines

As mentioned in Sect. 3.3, the measurement of the $^{6}\text{Li}/^{7}\text{Li}$ isotopic ratio is sensitive to the list of atomic and molecular lines adopted for the spectral synthesis. In the case of HD 95456, we find a difference as high as ~2.2%, where the lowest $^{6}\text{Li}/^{7}\text{Li}$ is 0.8% when the M12 line list is adopted, and the highest $^{6}\text{Li}/^{7}\text{Li}$ is 3.0% when I14 is used (see Table 6). The differences among the line lists arise not only from the adopted atomic data of specific lines (wavelength, log gf, excitation potential), but also from the different chemical elements present in each particular list of blends.

The Si i 670.8025 nm line is of particular interest since it lies very close to the $^{6}\text{Li}$ feature and has been shown to have an impact on the $^{6}\text{Li}/^{7}\text{Li}$ measurements (e.g., Israeliian et al. 2001, 2003). This line was first introduced by Müller et al. (1975) in their analysis of the solar spectrum and later investigated in detail by Israeliian et al. (2003) in a number of solar-type metal-rich stars. The latter authors have shown that the Si i line at 670.8025 nm is the best candidate for this unidentified feature severely blended with the $^{6}\text{Li}$ line. We also note that this line has
Figure 6 shows the $\chi^2_{red}$ (upper panel) of the best fit and the resulting $^6\text{Li}/^7\text{Li}$ (middle panel) plotted vs. the deviation (in dex) from the adopted silicon abundance for line lists G09 (red circles), M12 (green triangles), and I14 (blue stars). It is worth noting that, when the silicon abundance is reduced, the measured $^6\text{Li}/^7\text{Li}$ increases, showing that changing the silicon abundance by just 0.1 dex can alter the measured $^6\text{Li}/^7\text{Li}$ by more than 1% point for this star, while the reduced $\chi^2_{red}$ value changes only marginally. Furthermore, after increasing the Si abundance by a certain amount, depending on the line list (+0.3, +0.2, and +0.4 dex for G09, M12 and I14, respectively), the measured $^6\text{Li}/^7\text{Li}$ reaches 0%, indicating that the potential $^6\text{Li}$ feature is fully (over-)compensated by the SiI line.

This test shows that the atomic data of this particular blend line are very important for the measurements of $^7\text{Li}/^7\text{Li}$ in solar-type stars, as suggested by Israelian et al. (2003), and might be the main factor responsible for the differences in the results achieved with the different line lists. It is worth noting that the log gf of this line was calibrated by Israelian et al. (2003) in high-S/N spectra of several solar-type stars (as well as the Sun) with different effective temperatures and metallicities. In the alternative case of G09 and M12 line lists, the log gf of this line and of other blend features have been adjusted in order to better reproduce the solar spectrum.

In fact, if we assume the same log gf for the Si line in all the line lists, the results appear to be in very good agreement despite differences in the other adopted blends. This shows that differences in log gf of the Si line are indeed the reason for the differences in the $^6\text{Li}/^7\text{Li}$ isotopic ratio. We can assume that this is generally the case, at least for stars with atmospheric parameters similar to HD 95456.

Because of the recently revised log gf of the V I blend, we repeat the same test as above also for the V I line. Lawler et al. (2014) gave a log gf higher by 0.3–0.5 dex, dependent on the line list considered. The resulting plot (Fig. 7, lower panel) indicates that this line does not considerably affect the $^7\text{Li}/^7\text{Li}$ measurement, giving differences of $\Delta g \sim 1\%$ point for a 1-dex change in the vanadium abundance. Therefore, this line is not expected to change the $^7\text{Li}/^7\text{Li}$ result significantly, at least for stars with stellar parameters similar to HD 95456.

3.8. Fitting results for the Sun

We applied a similar fitting procedure to derive the lithium abundance and the $^6\text{Li}/^7\text{Li}$ isotopic ratio in the Sun by fitting the solar flux atlas of Kurucz (2005). The 1D LTE synthetic line profiles were computed from a solar ATLAS9 model ($T_{\text{eff}} = 5770\text{K}$, log $g = 4.44$, $V_{\text{micro}} = 1.24\text{ km s}^{-1}$, $\sigma_{\text{MEK}} = 1.25$; see Kurucz 1993) with MOOG for combinations of 21 A(Li) and 21 $^6\text{Li}/^7\text{Li}$ values, assuming a rotational broadening of $v$ sin $i = 1.9\text{ km s}^{-1}$.

Using line list G09 (with modifications described in Sect. 3.3) and fixing the continuum level at $c_1 = 0.9975$ (relative to the continuum placement of the solar flux atlas) as in Ghezzi et al. (2009), the best fit was obtained for $\text{A}(\text{Li}) = 0.99 \pm 0.01\text{ dex}$ and $^6\text{Li}/^7\text{Li} = 0.12 \pm 0.02\%$ (Case A, Table 6), where the errors are the 1 $\sigma$ formal fitting errors. The derived isotopic ratio close to zero reflects the fact that Ghezzi et al. (2009) constructed their line list under the assumption that $^6\text{Li}/^7\text{Li} = 0$. An even better fit of the solar Li region can be achieved by allowing small adjustments in the continuum level and in the abundances of Fe and CNO, as described above for the stellar fits. In this case, the best fit was obtained for $c_1 = 0.9977$, $\text{A}(\text{Li}) = 0.98 \pm 0.015\text{ dex}$ and $^6\text{Li}/^7\text{Li} = 1.71 \pm 2.9\%$ (Case B, Table 6). Allowing in addition slight adjustments of the Si and V
abundances leads to a marginal improvement of the fit, but with even larger formal fitting errors: $c_1 = 0.9977$, $A(\text{Li}) = 0.98 \pm 0.02$ dex, $^6\text{Li}/^7\text{Li} = 0.71 \pm 4.1\%$ (Case C, Fig. 8).

For the Sun, our grid of 3D NLTE corrections suggests (after slight extrapolation) $\Delta A_{\text{3DNLTE-1DLTE}} \sim +0.1$ dex and $\Delta q_{\text{3DNLTE-1DLTE}} \sim -0.73\%$, while the direct calculation of the corrections from 3D NLTE and 1D LHD synthetic solar Li line profiles by the method described in Sect. 2.3 yields $\Delta A_{\text{3DNLTE-1DLTE}} \sim +0.1$ dex and $\Delta q_{\text{3DNLTE-1DLTE}} \sim -0.83\%$.

After applying the 3D NLTE correction for $A(\text{Li})$ to our 1D LTE best fit result (Case C), we obtain $A(\text{Li}) = 1.08 \pm 0.03$, where the error is estimated from measurements with different continuum locations (best fit location $\pm 0.05\%$). The $^6\text{Li}/^7\text{Li}$ isotopic ratio obtained from the best 1D LTE fit (Fig. 8) is $-0.1\%$ after application of the 3D NLTE correction of $-0.83\%$, with a large formal fitting error of $\pm 4\%$.

The lithium abundance obtained in this way is in very good agreement with a recent 3D NLTE analysis of a very-high-resolution PEPSI spectrum of the Li i $\lambda 670.8$ nm region of the Sun by Strassmeier et al. (2018) who measured $A(\text{Li}) = 1.09 \pm 0.04$. Their estimate of $^6\text{Li}/^7\text{Li} = 1.4 \pm 1.6\%$ agrees with our above $^6\text{Li}/^7\text{Li}$ value within the large error bars.

We point out that Strassmeier et al. (2018) also employed line list G09, which is custom-made for 1D modeling and therefore leads to an inferior fit when used unaltered for 3D spectrum synthesis. This is very likely the reason why the derived $^6\text{Li}/^7\text{Li}$ is not fully consistent with our corrected 1D result. $^6\text{Li}/^7\text{Li} \sim 0$

A more consistent fit in 3D can only be achieved if the line list is adapted to account for 3D effects, in particular adjusting the strength and wavelength of the silicon line (see Appendix B). We present a detailed comparison of fine-tuned 3D and 1D fits to the solar Li i $\lambda 670.8$ nm spectral region in Appendix C.

4. Summary and conclusions

We presented 3D NLTE corrections for lithium abundance, $A(\text{Li})$, and the $^6\text{Li}/^7\text{Li}$ isotopic ratio, $q(\text{Li})$, based on a six-dimensional grid of 3D NLTE spectra. The stellar parameters defining the grid are effective temperatures, $T_{\text{eff}}$ (3 different values), gravity, $\log g$ (2), microturbulence velocity, $V_{\text{micro}}$ (3), metallicity, $[\text{Fe/H}]$ (4), lithium abundance, $A(\text{Li})$ (3), and isotopic ratio, $q(\text{Li})$ (3; see Sect. 2 for details). In addition, four different $v \sin i$ values of rotational broadening were applied to the 3D NLTE and 1D LTE spectra. For each list of atomic and molecular blend lines (K95, G09, and M12), this results in a total of 2592 3D NLTE corrections for both $A(\text{Li})$ and $q(\text{Li})$. The results obtained using the line lists G09 and M12 depend strongly on the wavelength range selected for fitting the Li i...
670.8 nm spectral region, as well as on whether the continuum placement is a free or a fixed parameter. As a consequence, the 3D NLTE $^6\text{Li}/^7\text{Li}$ corrections depend on the atomic and molecular blends used for the spectral line synthesis. Eventually, we rely only on the 3D NLTE corrections based on line list K95 (Li only). This definition is supported by detailed fits of the solar Li spectral region with both 1D- and 3D-based synthetic spectra computed with fine-tuned line lists (Appendix C).

$^6\text{Li}/^7\text{Li}$ derived by fitting a given 3D NLTE spectrum with the grid of 1D LTE line profiles is found to be always larger than the input 3D NLTE values by 0.4–4.9% for the range of stellar parameters studied in this work. This implies that a 1D LTE spectral analysis leads to an overestimation of the $^7\text{Li}/^6\text{Li}$ isotopic ratio by up to 4.9% points in solar-type stars covered by our grid. The 3D NLTE corrections, $\Delta q_{\text{3DNLTE} - \text{1DLTE}}$, are therefore always negative.

The corrections show a systematic dependence on the stellar parameters. For a given metallicity, generally $\Delta q_{\text{3DNLTE} - \text{1DLTE}}$ becomes larger with higher $T_{\text{eff}}$ and lower $\log g$. For given $T_{\text{eff}}$ and $\log g$, they become larger with higher metallicity, $A(\text{Li})$, and isotopic ratio $q_{\text{Li}}$. Moreover, we observe a dependence of $\Delta q_{\text{3DNLTE} - \text{1DLTE}}$ on the applied rotational broadening: the higher the $\sin i$, the smaller the corrections. Furthermore, the quality of the fit improves assuming higher $\sin i$ values applied simultaneously to the 3D NLTE and 1D LTE spectra, leading to lower values of $\chi^2_{\text{red}}$ (but also implying larger fitting errors). On the other hand, we observe only a very weak variation of $\Delta q_{\text{3DNLTE} - \text{1DLTE}}$ with the small changes ($\pm0.5\text{ km s}^{-1}$) of the microturbulence parameter, and therefore adopt the results obtained assuming the central $v_{\text{micro}}$ values as representative corrections.

Similarly, the abundance corrections, $\Delta A_{\text{3DNLTE} - \text{1DLTE}}$, show a systematic dependence on the stellar parameters. For a given $[\text{Fe/H}]$, they generally become larger towards lower $T_{\text{eff}}$. We observe small variations of $\Delta A_{\text{3DNLTE} - \text{1DLTE}}$ for different $\log g$ values (4.0 or 4.5) and $A(\text{Li})$, whereas the dependence on $^6\text{Li}/^7\text{Li}$, $v_{\text{micro}}$, and $\sin i$ is negligible. The 3D NLTE correction for $A(\text{Li})$ turned out to be very similar for different lists of the atomic and molecular data used for the spectral line synthesis. They are found to range between $-0.01$ and $+0.11$ dex.

We provide analytical expressions (Eqs. (1) and (2))) which allow to estimate the 3D NLTE correction for $A(\text{Li})$ and $^6\text{Li}/^7\text{Li}$ as a function of $T_{\text{eff}}$, $\log g$, and $[\text{Fe/H}]$ (see Sect. 2.5). These mathematical functions are valid for the representative values $A(\text{Li}) = 2.0$, $q(\text{Li}) = 5\%$, and $\sin i = 2\text{ km s}^{-1}$ for a quick evaluation of the 3D NLTE corrections in the investigated range of stellar parameters. For full details, we provide a (electronic) table with the complete grid of the 3D NLTE corrections, and a link to a web page that allows the user to compute the 3D NLTE corrections of $A(\text{Li})$ as a function of $T_{\text{eff}}$, $\log g$, $[\text{Fe/H}]$, $\sin i$, $A(\text{Li})$, and $^6\text{Li}/^7\text{Li}$.

Our analytical expressions, valid for solar-type stars, allow to account for 3D plus NLTE effects without the need of direct access to complex 3D NLTE computations. This is particularly important when a large sample of stars needs to be analyzed in terms of lithium abundance and isotopic ratio, since 3D NLTE analysis for even a single target is computationally demanding and time consuming. The analysis of the observed spectra can be carried out at first by using standard 1D LTE spectrum synthesis techniques. Afterwards, the 1D results can be corrected for the 3D NLTE effects by applying the precomputed 3D NLTE corrections interpolated to the desired set of stellar parameters.

In the second part of this work, we use high-quality HARPS spectra of two solar-type stars in order to derive the $A(\text{Li})$ and $^6\text{Li}/^7\text{Li}$ in their atmospheres. The stars were selected because they are located at opposite sides of the investigated $T_{\text{eff}}$ range where the corrections show the largest differences. The lithium doublet in these two stars was first analyzed with a standard 1D LTE approach, and subsequently corrected for 3D NLTE effects using the pre-computed 3D NLTE corrections. After applying the 3D NLTE corrections, we obtain $A(\text{Li}) = 2.37 \pm 0.04$ and $^6\text{Li}/^7\text{Li} = -0.9\% \pm 0.7\%$ for HD 207129, whereas we derive $A(\text{Li}) = 2.70 \pm 0.04$ and $^6\text{Li}/^7\text{Li} = 0.9\% \pm 1.4\%$ for HD 95456. The correction for $^6\text{Li}/^7\text{Li}$ is estimated to be $\Delta q_{\text{3DNLTE} - \text{1DLTE}} = -1.1\%$ for HD 207129 and $\Delta q_{\text{3DNLTE} - \text{1DLTE}} = -1.9\%$ for HD 95456.

In the case of HD 95456, the $2\sigma$ detection of $^6\text{Li}$ in the 1D LTE analysis is turned into a clear non-detection after applying the 3D NLTE correction. In conclusion, we do not find significant amounts of $^6\text{Li}$ in either of the two stars.

Additionally, we studied the impact of two weak absorption lines (Si I, V I) on our $^6\text{Li}/^7\text{Li}$ measurements in HD 95456, and concluded that the Si I 670.8025 nm feature is the most critical blend for this analysis, confirming the result of Israelian et al. (2003).

Finally, we have demonstrated that a list of blend lines that are adjusted (like G09) by fine-tuning $\log gf$-values and wavelength positions to yield a perfect fit to the solar Li spectral region with a particular 1D model atmosphere cannot be expected to produce an equally good fit when employed unaltered for 3D modeling. For this reason, fitting 3D model spectra directly to observations may not always be the most desirable approach.

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References


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Appendix A: 3D NLTE corrections for \( A(\text{Li}) \) and \( ^{6}\text{Li}/^{7}\text{Li} \)

Figures A.1–A.3 present the plots of 3D NLTE corrections \( \Delta q(3D\text{NLTE})-1\text{DLTE} \) (left panels) and \( \Delta A(3D\text{NLTE})-1\text{DLTE} \) (right panels) derived with line list K95 vs. the effective temperature for three metallicities of our 3D NLTE spectral grid (\([\text{Fe/H}]= -1.0, -0.5 \) and 0.5, respectively). Figure A.4 shows the same 3D NLTE corrections derived with line list M12 for metallicity \([\text{Fe/H}]= 0.0 \).

![Fig. A.1.](image1)

**Fig. A.1.** 3D NLTE corrections for \( ^{6}\text{Li}/^{7}\text{Li} \) (left panel) and \( A(\text{Li}) \) (right panel) vs. \( T_{\text{eff}} \) for \([\text{Fe/H}]= -1.0, A(\text{Li})= 2.0, q(\text{Li})= 5\% \), derived with line list K95. The blue circles and the red triangles correspond to \( \log g = 4.0 \) and \( \log g = 4.5 \), respectively. The corrections for different \( v \sin i \) values are connected with lines of different styles.

![Fig. A.2.](image2)

**Fig. A.2.** As Fig. A.1 but for \([\text{Fe/H}]= -0.5 \).

![Fig. A.3.](image3)

**Fig. A.3.** As Fig. A.1 but for \([\text{Fe/H}]= +0.5 \).
Fig. A.4. Same corrections as shown in Figs. A.1–A.3, but derived with line list M12 for [Fe/H] = 0.0.

Table B.1. Summary of 3D–1D fitting results.

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<th>Fit ID</th>
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<th>A(Li) (dex)</th>
<th>g(Li) (%)</th>
<th>A(Si) (dex)</th>
<th>∆ν (Si) (km s⁻¹)</th>
<th>FWHM (km s⁻¹)</th>
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<td>LTE</td>
<td>⁶Li+⁷Li+Si</td>
<td>1.0001</td>
<td>0.80</td>
<td>7.5081*</td>
<td>0.500</td>
<td>−0.211*</td>
<td>4.058</td>
<td></td>
</tr>
</tbody>
</table>

Notes. Rows for 3D model specify the input parameters for the 3D spectrum synthesis; rows for 1D model give the results of the best fit (right part of the table), except numbers marked by an asterisk which are fixed input parameters. ∆ν(Si) (Col. 8) gives the artificial wavelength shift (converted to velocity) of the Si I line introduced in the line list for the 1D LTE spectrum synthesis. The relative quality of the fits can be judged by comparing their χ² (given on an arbitrary absolute scale).

Appendix B: Test case solar Li I + Si I blend

This numerical experiment is to demonstrate that the corrections ∆A³DNLTE–1DLTE and ∆ν³DNLTE–1DLTE derived from fitting a 3D NLTE Li line profile with overlapping blend lines by a grid of corresponding 1D LTE spectra are very similar to the corrections obtained from fitting the pure Li 3D NLTE line profile with a grid of 1D LTE pure Li spectra, provided that the blend lines in the 1D spectrum synthesis are adjusted to correct for 3D effects.

We model the Li doublet in its full complexity, including all hyperfine structure levels of both ⁶Li and ⁷Li. The blends are represented by a single silicon line (Si I 670.8025 nm) which is known to have a critical influence on the derived ⁶Li/⁷Li (see Sect. 3.7). The Sun is a good test case since the solar Li abundance (A(Li) = 1.1) is at least ten times lower than in our target stars (A(Li) ≥ 2.3) and hence the Si I line has an even larger impact on the Li profile.

As a first step, we fit the pure ⁷Li 3D NLTE line profile computed with NLTE3D + Linfor3D from a 3D solar CO-BOLD model with a grid of 1D LTE pure ⁶Li+⁷Li spectra based on a solar LHD model. The fitting parameters are (i) the Li abundance A(Li), (ii) the ⁶Li/⁷Li isotopic ratio g(Li), (iii) the width of a global Gaussian line broadening kernel FWHM, and (iv) a global Doppler shift ∆v. The same procedure is repeated with the single Si I line, which is modeled in LTE both in 3D and in 1D, assuming the same atomic line parameters as in line list G09. Here the fitting parameters are A(Si), FWHM, and ∆v. The best fit results are summarized in Table B.1 (Fit 0 and Fit 1). We notice that the 3D LTE abundance correction for the Si line is ∆A(Si) = +0.0419 dex, the absolute convective blue shift is ∆v = −0.399 km s⁻¹, and the shift relative to Li is ∆v = −0.399 + 0.188 = −0.211 km s⁻¹.

In a second step, we fit the 3D composite spectrum of Li (NLTE) plus Si (LTE) with a grid of 1D LTE composite spectra covering a range in A(Li) and ⁶Li/⁷Li, but assuming the same fixed silicon abundance as in the 3D spectrum synthesis (A(Si) = 7.55). Under these constraints, the best fit is found for an isotopic ratio of ⁶Li/⁷Li = −1.9%. However, this fit (Fit 2a) is rather poor (see top panel of Fig. B.1 and Table B.1).

The fit can be improved if we reduce the silicon abundance by ∆A(Si) = −0.0419 dex, thus accounting for the 3D abundance corrections indicated by Fit 1. The resulting fit (Fit 2b) is significantly better and indicates ⁶Li/⁷Li = +1.9%. Still, the fit is clearly unsatisfactory (see middle panel of Fig. B.1).
Appendix C: Fitting the solar Li $\lambda$ 670.8 nm region with 1D LHD and 3D CO$^3$BOLD synthetic spectra

In this Appendix, we derive the solar lithium abundance and $^6$Li/$^7$Li by fitting the Li $\lambda$ 670.8 nm spectral region of solar flux spectrum (Kurucz 2005) with synthetic spectra computed from a solar 1D LHD model ($T_{\text{eff}} = 5780$ K, $\log g = 4.44$, $V_{\text{micro}} = 1.0$ km s$^{-1}$, $\alpha_{\text{MLT}} = 1.0$) and a 3D CO$^3$BOLD model atmosphere, respectively. The purpose of this investigation is to test the expected relation between the 1D and the 3D results.

In both cases, the spectrum synthesis is performed with Linfor3D, applying a fixed rotational broadening of $\nu \sin i = 1.85$ km s$^{-1}$ in the flux computation. As before, the Li doublet includes all hyperfine structure levels of both $^6$Li and $^7$Li and is treated in NLTE (LTE) when computing the grid of spectra from the 3D (1D LHD) models.

The grid of 1D LHD spectra is computed with line list G09. The fitting of the solar flux spectrum with this grid follows the same methodology as the fitting with the ATLAS/MOOG spectra described in Sect. 3.8. For a fixed continuum level, the basic fitting parameters are (i) the Li abundance $A(\text{Li})$, (ii) the $^6$Li/$^7$Li isotopic ratio $q(\text{Li})$, (iii) the width of a global Gaussian line broadening kernel FWHM, and (iv) a global Doppler shift $\Delta v$. In addition, we allow for small adjustments of the strengths (abundances or $\log gf$ values) of the CN, FeI, SiI, and V I lines to further optimize the fit.

In Case I, we fix the continuum at the same level as for the best fit with the ATLAS/MOOG spectra (Case C, Fig. 8), $c_1 = 0.9977$ (relative to the continuum placement of the solar flux atlas). The best fit with our grid of 1D LHD synthetic spectra if found for $A(\text{Li}) = 0.94$ and $q(\text{Li}) = 0.69$% (see Fig. C.1). These results can be compared to those of Case C, $A(\text{Li}) = 0.98$ and $q(\text{Li}) = 0.71%$. While the derived $^6$Li/$^7$Li is practically identical, the lithium abundance indicated by the LHD fit is slightly lower. This must be related to slight differences in the temperature stratification of the solar LHD model relative to the ATLAS9 model.

Next we fit the observed spectrum with a grid of synthetic spectra derived from the CO$^3$BOLD 3D solar atmosphere, now treating the Li doublet in NLTE. Adopting the same continuum level as for the 1D fitting, we try out different assumptions about the chemical abundances and the wavelengths of the blend lines.

In Case Ia, we use the same line list ($G09$) as in Case I together with the same 1D-optimized individual abundances obtained from the best fit with the 1D LHD spectra. Under these constraints, the best fit requires $A(\text{Li}) = 1.05$ and $q(\text{Li}) = 1.86%$. As expected, the fit is rather poor (see Fig. C.2, top panel).

At the next stage (Case Ib), we adjust the strengths of the CN, Fe, Si, and V blend lines according to the 3D–1D abundance corrections inferred from fitting the 3D synthetic line profiles of the individual blend lines by a grid of corresponding 1D spectra of different abundance, as described for the Li and Si lines in Appendix B. The fit with these adjusted abundances is shown in Fig. C.2 (middle panel), indicating $A(\text{Li}) = 1.04$ and a strongly negative $^6$Li/$^7$Li of less than $-2%$. While the fit is generally improved with respect to Case Ia, the Fe+CN blend at $\lambda$ 670.74 nm is by far not reproduced to the level of precision achieved with the 1D LHD fit (cf. Fig. C.1).
A 3D fit of comparable quality can be accomplished by readjusting the rest wavelengths of the main blend components according to their differential convective Doppler shifts. The latter are again deduced from fitting the synthetic 3D line profiles by their 1D counterparts, as described for the Li and Si lines in Appendix B. In Case Ic, we applied both these “theoretical” convective wavelength shifts and related abundance corrections to the CN, Fe, Si, and V blend lines. Indeed, the applied wavelength shifts lead to a dramatic improvement of the fit (see Fig. C.2, bottom panel). Now the best solution is found for \( A(\text{Li}) = 1.05 \) and \( q(\text{Li}) = -0.18\% \). We notice that the \(^6\text{Li}/^7\text{Li}\) found from this fine-tuned 3D fit is now in very good agreement with the result from the LHD fit after application of the \( \Delta q_{\text{3DNLTE}}-\Delta q_{\text{1DLTE}} \) correction \((0.69 - 0.83 = -0.14\%)\).

We performed the same exercise for a different continuum level, \( c_1 = 0.9980 \) (Case II), which corresponds closely to the continuum placement adopted for the analysis of the PEPSI spectrum in Strassmeier et al. (2018). We verified (Case Ix) that we obtain very similar results when adopting their set of abundances: \( A(\text{Li}) = 1.09 \) and \( q(\text{Li}) = 1.77 \pm 2.2\% \), compared to \( A(\text{Li}) = 1.09 \) and \( q(\text{Li}) = 1.44 \pm 1.6\% \) in Strassmeier et al. (2018). Quantitatively, the two series of fits at slightly different continuum levels show a systematic offset in the absolute values of \( A(\text{Li}) \) and \( q(\text{Li}) \), but otherwise follow the same qualitative trends and lead to the same conclusions. Details of all fits discussed above can be found in Table C.1.

In summary, the fits of the solar spectrum by grids of 1D LHD and 3D CO\(^3\)BOLD synthetic spectra computed with the full G09 line list justify our definition of the 3D NLTE corrections for \( A(\text{Li}) \) and \( q(\text{Li}) \) based on the comparison of 3D NLTE and 1D LTE Li-only line profiles. This conclusion is not limited to the solar case but should apply even more to the target stars of this paper, where a strong lithium feature dominates over relatively weak blend lines.

We chose the Sun for demonstration because all involved spectral lines are weak and therefore the combined spectrum may be constructed by linear superposition of the individual components. The presence of stronger lines would require a full spectrum synthesis of the complete spectrum for each individual configuration. Under these conditions, a fine-tuned 3D (NLTE) fit to the observed spectra of our target stars would be next to impossible. However, the exercise presented in this Appendix also strongly suggests that using 3D model spectra directly for the fitting is not really the most desirable approach since it requires non-trivial adjustments in the line lists that are fine-tuned by 1D methods.

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\(^3\) The asymmetric 3D profile of the Fe line at 1670.74 nm is represented by two components in 1D.
Table C.1. Summary of the results of fitting the Li region of the solar flux spectrum (Kurucz 2005) with 1D LHD and 3D CO\textsuperscript{5}BOLD synthetic spectra.

<table>
<thead>
<tr>
<th>Fit ID</th>
<th>Model</th>
<th>Continuum level</th>
<th>Abundances</th>
<th>Wavelengths</th>
<th>( A(\text{Li}) ) (dex)</th>
<th>( q(\text{Li}) ) (%)</th>
<th>( \chi^2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>I</td>
<td>1D LHD</td>
<td>0.9977</td>
<td>adjusted</td>
<td>G09</td>
<td>0.94</td>
<td>0.69</td>
<td>8.2</td>
</tr>
<tr>
<td>Ia</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9977</td>
<td>as Fit I</td>
<td>G09</td>
<td>1.05</td>
<td>1.86</td>
<td>251.3</td>
</tr>
<tr>
<td>Ib</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9977</td>
<td>Fit I +( \Delta A )</td>
<td>G09</td>
<td>1.04</td>
<td>&lt;(-2.0)</td>
<td>53.6</td>
</tr>
<tr>
<td>Ic</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9977</td>
<td>Fit I +( \Delta A )</td>
<td>G09 +( \Delta \lambda )</td>
<td>1.05</td>
<td>(-0.18)</td>
<td>7.3</td>
</tr>
<tr>
<td>II</td>
<td>1D LHD</td>
<td>0.9980</td>
<td>adjusted</td>
<td>G09</td>
<td>0.96</td>
<td>1.67</td>
<td>7.9</td>
</tr>
<tr>
<td>IIa</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9980</td>
<td>as Fit II</td>
<td>G09</td>
<td>1.06</td>
<td>2.88</td>
<td>247.3</td>
</tr>
<tr>
<td>IIb</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9980</td>
<td>Fit II +( \Delta A )</td>
<td>G09</td>
<td>1.06</td>
<td>(-0.89)</td>
<td>54.0</td>
</tr>
<tr>
<td>IIc</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9980</td>
<td>Fit II +( \Delta A )</td>
<td>G09 +( \Delta \lambda )</td>
<td>1.06</td>
<td>0.88</td>
<td>6.1</td>
</tr>
<tr>
<td>IIx</td>
<td>3D CO\textsuperscript{5}BOLD</td>
<td>0.9980</td>
<td>SIS18</td>
<td>G09</td>
<td>1.09</td>
<td>1.77</td>
<td>29.5</td>
</tr>
</tbody>
</table>

Notes. Column (4): \( \Delta A \) symbolizes the individual 3D abundance corrections; “SIS18” indicates the same abundances as used in Strassmeier et al. (2018). Column (5): G09 denotes the line list of Ghezzi et al. (2009), \( \Delta \lambda \) symbolizes the individual convective line shifts. The relative quality of the fits can be judged by comparing their \( \chi^2 \) (given on a common absolute scale).