Statistical equilibrium and the 670.776 and 670.791 nm Li I absorption lines in the spectrum of red giants. Procedure

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The procedure for a non-LTE calculation of statistical equilibrium for lithium in the atmosphere of a red giant is analyzed. The method of calculating the opacity of matter in the atmosphere of a cool star (averaged over absorption) with allowance for absorption in atomic lines is investigated in detail.

In determining the evolutionary status of late-type giants, the abundance of light elements ($Z < 9$) in their atmosphere is the most important criterion. Of the light elements, only lithium and hydrogen have absorption lines in the visible that are suitable for quantitative analysis in terms of the classical assumptions of the method of model atmospheres. The fact that the lithium abundance in a stellar atmosphere depends essentially on physical processes inside the star and at its surface enables one to use information about the lithium abundance in a stellar atmosphere to test many propositions of modern astrophysics.

An absolute majority of lithium abundance determinations in stellar atmospheres have been obtained by analyzing resonant absorption lines of the Li I 670.776, 670.791 nm doublet in the approximation of local thermodynamic equilibrium (LTE). The oscillator strengths of the components of this doublet are in a 2 : 1 ratio. It should be noted that in the vicinity of 670.78 nm there are lines of two lithium isotopes, $^6$Li and $^7$Li, separated by 15 pm, which can be separated into two individual absorption lines only in the solar spectrum. $^1$ We shall assume below that our presentation pertains to lines of $^7$Li, being the more abundant in nature. $^2$

Effects of departure from LTE can be considerable for lithium lines, since the optical depth of stellar atmospheres is small at the frequencies of these lines, and because of the low ionization potential ($E_{\text{ion}} = 5.39$ eV), radiative processes play an important role in establishing Li I/Li II ionization equilibrium. Changes in ionization equilibrium (in comparison with LTE) have the greatest effect on the profiles of Li I absorption lines. On the other hand, bound–bound radiative transitions can play an important role in establishing the balance of bound–free transitions, which, strictly speaking, determine the degree of lithium ionization (see Refs. 3 and 4).

We have calculated the non-LTE ionization balance of lithium in the atmospheres of a number of K and M giants. The characteristics of the model atmospheres of red giants with $\log g = 1.7$, $V_t = 1.7$ km/sec, and chemical composition $[\xi(\text{H}) = 12$ dex$]$, $[\xi(\text{C}) = 8.35$, $[\xi(\text{N}) = 8.20$, $[\xi(\text{O}) = 8.85$, and $[\xi(\text{Fe}) = 7.65$ are given below:

<table>
<thead>
<tr>
<th>$T_{\text{eff}}$</th>
<th>$\text{Spectral type}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3600</td>
<td>M3 III T3III</td>
</tr>
<tr>
<td>3800</td>
<td>M4 III T3III</td>
</tr>
<tr>
<td>4000</td>
<td>K0 III T3III</td>
</tr>
<tr>
<td>4400</td>
<td>K3 III T3III</td>
</tr>
<tr>
<td>4800</td>
<td>K7 III T3III</td>
</tr>
</tbody>
</table>

An analysis of our results enabled us to reveal the nature of the changes in effects of departure from LTE for lithium in the atmospheres of red giants over a large range of effective temperature. The model atmospheres were calculated in classical approximations using the SAM1 program. $^5$ In the calculations we allowed for sources of continuous absorption, typical of late-type stars, and absorption in bands of CO, H$_2$O, CN, TiO, and CN (see Ref. 6). Ionization–disassociation equilibrium was calculated in LTE with allowance for the most abundant molecules.

The combined system of steady-state equations and the radiative transfer equation (the non-LTE problem) was solved by partial linearization. $^7$ The populations of lithium levels obtained from the solution of the non-LTE problem were used to calculate theoretical profiles and equivalent widths of lines of the resonant Li I 670.776, 670.791 nm doublet, which were compared with the results of LTE calculations. Such a procedure has been used earlier in the solution of non-LTE problems for lithium in the atmospheres of the sun and red giants and has been described in more detail in Ref. 4. The results of that paper showed that effects of a departure from LTE are more pronounced in our calculations than in those of Steenbock and Holweger. $^3$ That fact was the reason for this paper, in which we investigate individual details of the procedure of a fundamental nature but that have not been discussed earlier. In Ref. 8 we describe the results of a solution of the non-LTE problem for lithium in the atmospheres of red giants with the parameters given above.

The model of the lithium atom used in the non-LTE solution of the problem is shown in Fig. 1. The sixth level of the model atom is the ground state of the Li II ion ($1S_0$) with statistical weight $g_k = 1.0$. In solving the non-LTE problem, Li I terms with $L > 0$ were represented as individual levels. Transitions due to inelastic collisions with free electrons and hydrogen atoms were taken into account (see Ref. 4). The

![FIG. 1. Model of the lithium atom. The radiative transitions taken into account are given. The wavelengths and oscillator strengths are indicated for bound–bound transitions.](image-url)
linearization procedure was applied only to lines of the resonant Li I doublet. The profile of the absorption coefficient for lithium atoms at frequencies of the doublet was determined by a sum of Voigt functions with appropriate weights. The radiation field at the frequencies of other radiative (bound—bound and bound—free) transitions hardly depends on absorption by lithium atoms. The radiative rates of these transitions remained fixed for the non-LTE solution of the problem.

The main difficulty in non-LTE calculations of the ionization balance of metals consists in allowing for opacity at the frequencies of their bound—free transitions due to absorption in atomic and molecular lines (see Refs. 3 and 4). A characteristic feature in the solution of the non-LTE problem for lithium is that photoionization from its lower levels occurs due to absorption of longer-wavelength photons than in the case of other metals. The limiting wavelengths of photoionization from the first and second levels of neutral lithium lie at 229.96 and 349.84 nm, respectively. The averaged radiation intensity $J_\nu$ was used to calculate the rates of these transitions. We calculated $J_\nu$ from the solution of the radiative transfer equation with coefficients of absorption $\chi_\nu$, emission $\eta_\nu$, and scattering $\chi_\nu'$ preliminarily averaged over spectral bandwidths $\Delta \lambda = c(\nu_2^{-1} - \nu_1^{-1}) = 0.4$ nm:

$$
\chi_\nu = \int \chi_\nu' dv / \int dv; \quad \eta_\nu = \int \eta_\nu' dv / \int dv;
$$

The average radiation intensity and absorption, emission, and scattering coefficients were calculated over the entire thickness of the atmosphere. To the sources of opacity taken into account in calculating the model atmospheres, we added absorption in atomic lines. The data on lines were taken from Kurucz’s list. In Fig. 2 we show the variation of $J_\nu/J_\nu'$ with depth in the 4400/1.7 model atmosphere of a red giant at the limiting frequencies of photoionization from five lithium levels, where

$$
J_\nu = \int J_\nu dv / \int dv.
$$

The calculated values of $J_\nu$, $J_\nu'$, and $J_\nu$ at the outer boundary of the atmosphere of a red giant in the vicinity of 349.8 nm (the limit of photoionization from the second level of lithium) are given in Fig. 3. The blanketing effect is significant in the blue and ultraviolet, but they also contain narrow-band, weakly blended sections. Absorption at these frequencies makes the main contribution to the photoionization rate. In the outermost layers of the atmosphere, the difference between $J_\nu$ and $J_\nu'$ increases rapidly (Fig. 2) and evidently indicates differences between the boundary conditions for the strongly and weakly blended sections of the spectrum. On the whole, Fig. 2 confirms the conclusion of Ref. 10 that for pronounced blending, the agreement between $J_\nu$ and $J_\nu'$ is good over a large range of depths in the atmosphere. In the long-wavelength range, there are only individual absorption lines in a 0.4-nm band, as a rule. In this case, $J_\nu$ and $J_\nu'$ may differ up to several fold in the outer part of a stellar atmosphere (Fig. 2). First, in the region of the atmosphere in which the line spectrum proper is formed ($\tau_{\text{Ross}} > 0.001$), the differences between these quantities decrease considerably, and second, $J_\nu$ exceeds $J_\nu'$ in the region $\tau_{\text{Ross}} > 0.01$. The use of $J_\nu$ to calculate the rates of radiative bound—free transitions should thus not result in significant errors in calculations of lithium level populations. The results of the solution of the non-LTE problem showed that the equivalent widths of the resonant Li I 670.8 nm doublet obtained from such a solution with $J_\nu$ and $J_\nu'$ at the frequencies of bound—free lithium transitions differ by 5%, which is far less than the relative change in $W_\lambda$ due to non-LTE effects (150-200% ; see Ref. 8). In Fig. 4 we show the variation of the ratio $J_\nu/B_\nu$ with depth in the atmosphere of a 4400/1.7 star, where $B_\nu$ is the Planck function. Three aspects seem important:

1. In the case of strong blending, which occurs in the range $\lambda < 230$ nm, the radiation field is “blocked” within the atmosphere, in which case we have $J_\nu \equiv J_\nu' \equiv B_\nu$. Here bound—free absorption of photons by metals makes an important contribution to the opacity.

2. In the blue, the differences between $J_\nu$ and $B_\nu$ in the outer part of the model atmosphere are considerable, despite the presence of numerous atomic lines in the spectrum: the steep gradient $dB_\nu/d\tau$ of the Planck function is more important here.

3. The gradient $dB_\nu/d\tau$ is not so pronounced in the long-wavelength range; as a consequence, $J_\nu$ exceeds $B_\nu$ by only a factor of five or six at the outer boundary of the atmosphere.

The above analysis highlights the role of free—bound transitions from different levels in establishing ionization balance of lithium in the atmospheres of late-type stars. The efficiency of photoionization from a specific level (in the sense of its domination over photorecombination) is determined by how much $J_\nu$ exceeds $B_\nu$ at the respective frequencies. The solution of the non-LTE problem thus depends to a large extent on the balance of free—bound transitions from the second level. In our case, the non-LTE problem was solved in two steps: the level populations were first determined by solving a system of steady-state equations, constructed from the rates of collisional transitions and the fixed rates of radiative (bound—bound and bound—free) transitions. Linearization for lines of the resonant lithium doublet was incorporated into the second step. A comparison of the characteristics of lithium absorption lines calculated in the first and second steps of the solution of the non-LTE problem made it possible to analyze interrelationships among radiative

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transitions between lithium levels. For moderately strong absorption lines ($W_\lambda \approx 5$ pm), the incorporation of the fairly strong radiative transition $2s^2S - 2p^2P^0$ ($\Sigma gf = 1.5$) into the calculation scheme ultimately leads to an increase in lithium reionization, and hence to weakening of the doublet lines: the central intensity of the stronger component (670.776 nm) increases by several percent (up to 5%). For more intense absorption lines ($W_\lambda \approx 30$ pm), absorption at line frequencies is more important: the equivalent widths of absorption lines in the second stage of the solution of the non-LTE problem increase up to 15%.

Reionization is similar, in a certain sense, to a decrease in lithium abundance. An interesting question is how much the profiles of lithium absorption lines in LTE and non-LTE calculations differ if their equivalent widths are equal. These calculations were carried out within the framework of this paper; their results are given in Fig. 5. The profile of the stronger line ($W_\lambda = 24.52$ pm) was calculated for a lithium abundance in the atmosphere of a 4400/1.7/1.7 K giant $\epsilon$(Li I) = 2.0 dex (LTE) and $\epsilon$(Li I) = 1.6 dex (non-LTE), and that of the weaker line ($W_\lambda = 7.46$ pm) was calculated for $\epsilon$(Li I) = 0.68 dex (LTE) and $\epsilon$(Li I) = 1.15 dex (non-LTE). The line cores are deeper and the emission intensity in their wings is lower in LTE calculations than in non-LTE profiles. The maximum differences (up to 3%) are obtained for the stronger line at its center. At the same time, even for the far less intense absorption line, the difference between the central intensities in LTE and non-LTE calculations is ~2%. These differences were obtained from theoretical calculations, however. It is scarcely possible to detect them in an observed spectrum, since the combined action of macroturbulence and instrumental broadening result in more pronounced changes in stellar absorption line profiles.

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