

ATKIEL: a NLTE code fully consistent with ATLAS9 models

Fiorella Castelli

INAF-Osservatorio Astronomico di Trieste, Italy

1 Introduction

The ATKIEL code computes b factors and LTE and NLTE line profiles and equivalent widths for a given trace element. Most computations were derived both from the ATLAS11 code from Kurucz (1995) and from the NLTE Kiel code, which was made available at the Trieste Observatory by Inga Kamp in year 1994. The ATKIEL code uses ATLAS9 model atmospheres as input models.

The Kiel code (<http://www-inst.stsci.edu/~kamp/>) is a two steps program. The first step is formed by two codes which compute the input model atmosphere starting from a $T\text{-}\tau_{5000}$ tabulation. The second step solves the statistical and transfer equations and computes the b-factors. Because the depth scale of the ATLAS9 models is the mass RHOX, some preliminary computations have to be performed to transform the T-RHOX relation into a T- τ_{5000} relation. Furthermore, the model structure recomputed by the the Kiel code may be not exactly the same as that of the original ATLAS9 model.

The ATKIEL code makes the first step of the Kiel code unnecessary when the input model is an ATLAS9 model. The aim of the ATKIEL code is to provide ATLAS9 users with a friendly NLTE code. Here, we make the example of Li I whose model atom with 44 energy levels was taken from Kurucz (1995).

2 The Procedure

In the ATKIEL code, the simultaneous solution of the statistical equilibrium and transfer equations is performed either with a simple iteration procedure or with the complete linearization scheme. The first method is more time consuming than the second one but much more simple. The speed of the modern computers makes today the time difference almost negligible. Because the second method is the same of the NLTE Kiel code, we outline here only the simple iteration procedure.

Starting from a given ATLAS9 model and a given model atom, the LTE populations for all the elements are computed by solving the Saha-Boltzmann equations. LTE continuous and line opacities and LTE continuous and line source functions are used to solve the transfer equation at the frequencies of the big ODFs. The mean intensity J_ν is used to compute **photoionization rates R_{ik} and R_{ki}** for the trace element. Then, the b-f and the b-b **collisional rates by electrons C_{ik} , C_{ki} , C_{ij} , C_{ji}** are computed. Both photoionization rates and collisional rates are considered as fixed rates, i.e. they are not recomputed at each iteration.

To get a first estimate of the NLTE population of the trace element, the statistical equilibrium equations are solved assuming detailed radiative balance in the lines (i.e. $R_{ij}=R_{ji}=0$) so that the elements of the coefficient matrix A are obtained only from the fixed rates. The B vector of the known terms is zero for all the levels except the last one where it has the value of the LTE total number density of the trace element.

The approximate NLTE population is then used to solve the transfer equation and derive J_ν for each considered transition. The **radiative b-b rates R_{ij} and R_{ji}** are computed with the mean intensity J_ν . A new coefficient matrix A is formed with all the rate coefficients and the statistical equilibrium equations are solved. The whole process is iterated until the difference in the populations of two successive iterations is smaller than a fixed value of the order of 10^{-3} .

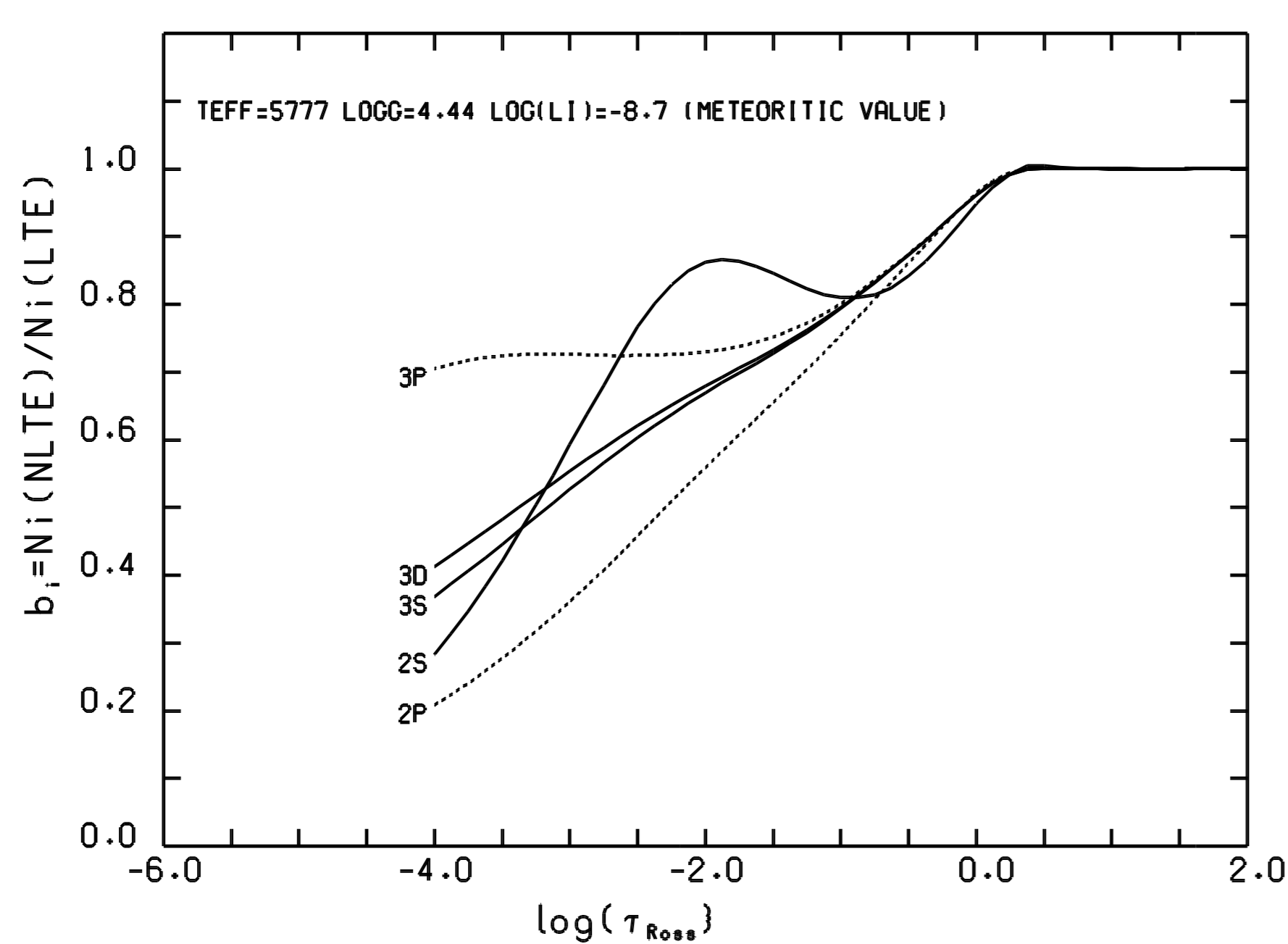


Figure 1: Departure coefficients $b_i=N_i(\text{NLTE})/N_i(\text{LTE})$ for a solar model and a lithium abundance equal to the meteoritic value. The behaviour of the $b_i\text{-}\log(\tau_{\text{Ross}})$ curves is similar to that in Carlsson et al. (1994), but the NLTE effects are larger here.

3 Example of command file

```
ln -s atomli1_44l.dat fort.11
ln -s ap00t5777g44377k1odfnew.dat fort.3
ln -s p00big1.bdf fort.9
ln -s kapp00.ros fort.1
ln -s moleculesli.dat fort.2
cat <<EOF >fort.25
3.00 0
EOF
./atkiel.exe<<EOF>atkiel.out
READ KAPPA
READ PUNCH
MOLECULES ON
READ MOLECULES
CORRECTION OFF
FREQUENCES 337 1 337 BIG
ITERATIONS 1 PRINT 1 PUNCH 0
VTURB 1.0E+05
ABUNDANCE CHANGE 3 -8.7
BEGIN
END
EOF
mv fort.38 bfp00t5777g44377k1odfnew_li.out
mv fort.39 profilesli.out
rm fort.*
```

Input Files:

- 1) atomli1_44l.dat→the model atom
- 2) ap00t5777g44377k1odfnew.dat→the ATLAS9 model atmosphere
- 3) p00big1.bdf→The big-ODF file consistent the ATLAS9 input model
- 4) kapp0.ros→Rosseland opacity table consistent with the ATLAS9 model
- 5) moleculesli.dat→The molecules.dat file including the trace element

Input data inside the command file:

- a) The code of the element (i.e. 3.00 for Li I) and the ICORR index. ICORR=0 the simple iterative method is used; ICORR=1 the complete linearization method is used.
- b) Some typical ATLAS9 cards. The ABUNDANCE CHANGE card allows to fix the abundance of the trace element.

Output files

- 1) bfp00t5777g44377k1odfnew_li.out →The b-factors for all the considered energy levels
- 2) profilesli.out→ Line profiles and equivalent widths both in LTE and NLTE.
- 3) atkiel.out→ File which controls the whole output.

4 Results

Results from the command file given in Sect. 3 are shown in Fig. 1 and Fig 2. They are relative to a solar model and a meteoritic Li abundance ($\log(N_{\text{Li}}/N_{\text{tot}})=-8.7$).

5 References

- Carlsson, M., Rutten, R.J., Bruls, J.H., Shchukina, N.G. 1994, A&A 288, 860
Kurucz, R.L., 1995, ApJ 452, 102

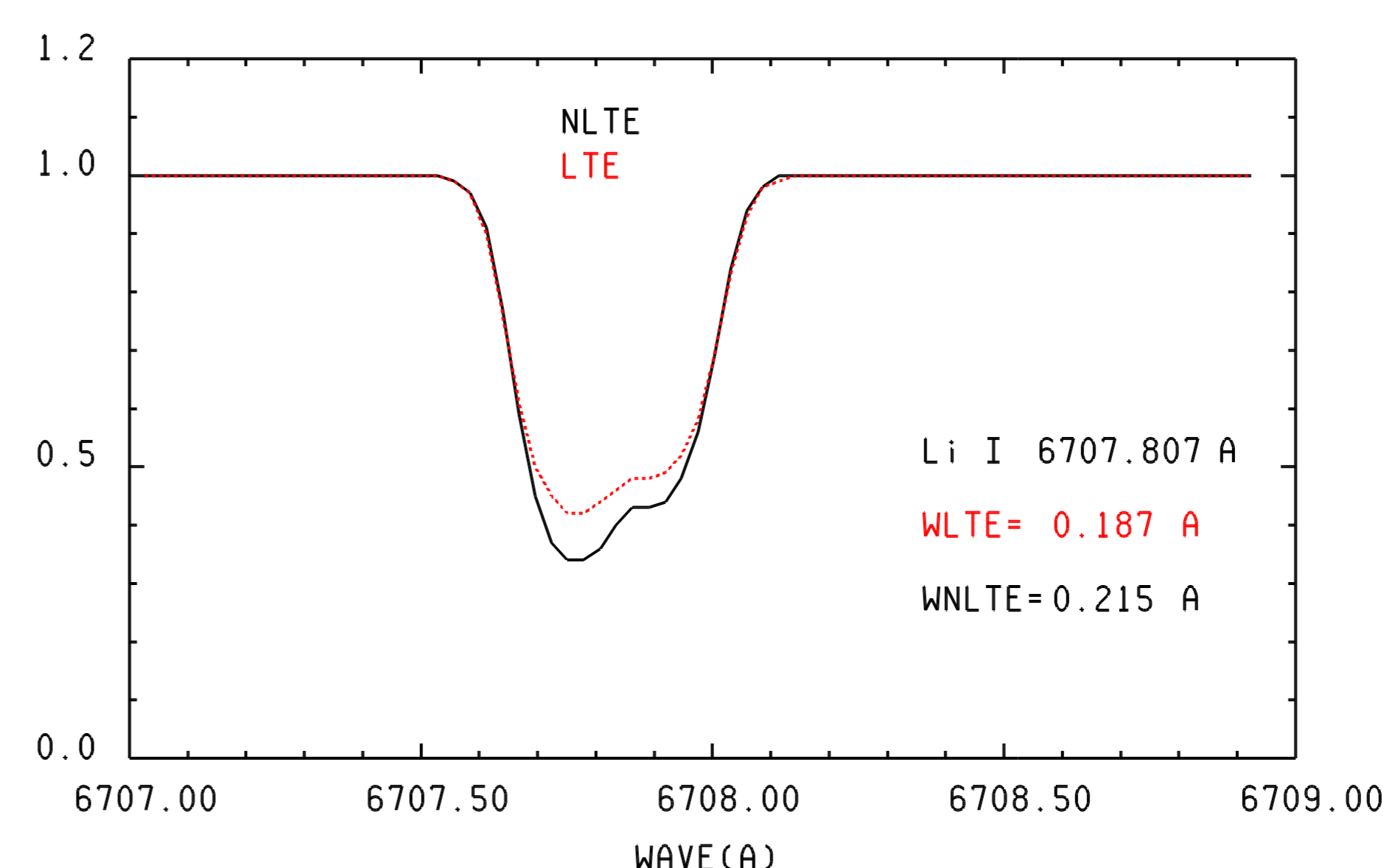


Figure 2: Comparison of LTE and NLTE line profiles for Li I 6707.7 Å relative to the populations of the 2s and 2p levels shown in Figure 1. The LTE and NLTE equivalent widths are 0.187 Å and 0.215 Å, respectively.