3D Multi-Level Non-LTE Radiative Transfer for the CO Molecule

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Abstract. The photospheres of cool stars are both rich in molecules and an environment where the assumption of LTE can not be upheld under all circumstances. Unfortunately, detailed 3D non-LTE calculations involving molecules are hardly feasible with current computers. For this reason, we present our implementation of the super level technique, in which molecular levels are combined into super levels, to reduce the number of unknowns in the rate equations and, thus, the computational effort and memory requirements involved, and show the results of our first tests against the 1D implementation of the same method.

1. Introduction

To solve the multi-level non-LTE problem in 3D radiative transfer for molecules, we have implemented the super level method for the PHOENIX/3D atmosphere code (Hauschildt & Baron 2006; Baron & Hauschildt 2007; Hauschildt & Baron 2010). his method was originally devised for the same problem for both atoms and molecules in spherically symmetric RT, as described by Anderson (1989) and Schweitzer et al. (2000).

In this method, the real molecular levels i of the molecule are sorted into a smaller number of super levels I with total occupation number

$$n_I = \sum_I n_i \tag{1}$$

where the occupation numbers of the individual levels within every super level are treated as being in LTE:

$$n_i = \frac{g_i}{Z_I} n_I \tag{2}$$

This reduces the complexity of the problem by reducing the number of unknowns in the rate equation system and, therefore, the size of the rate matrix, which needs to be solved for

a large number of points in any 3D calculation. The super levels are connected by a number of super transitions, which are the sum of all transitions between each individual level within the connected levels. These super level transitions have fairly complex line profiles, but can be easily calculated using the individual lines of the molecule.

The solution of the non-LTE problem can be done in the same way, as would be the case for regular levels, which is described for PHOENIX by Hauschildt (1993); Hauschildt & Baron (2014).

In the case of CO, with 3500 known levels and roughly 19000 transitions, we have set up three super level models using different physical properties to determine, which levels are combined to a super level:

- the vibrational quantum number ν (24 super levels)
- the energy E_i of the level (27 super levels)
- a combination of both (350 super levels)

the individual models are described in more detail by Schweitzer et al. (2000).

2. Implementation Tests

The new 3D implementation of the method has been tested extensively against standard test cases, and the existing 1D implementation, using spherical symmetric models with $T_{\rm eff} = 2700\ K$ and $\log g = 5.0$ in both cases, while only CO lines were considered.

The standard tests are calculating a case of pure collisions without including radiative rates, as well as calculating a case where the mean intensity $J(\lambda)$ is given by plancks law with $J(\lambda) = B(\lambda)$ througout the atmosphere. In both cases, LTE was restored as expected.

Figure .1 shows the resulting departure coefficients $b_I = \frac{n_I}{n_I^*}$, where n_I^* are the LTE occupation numbers, for all three super level models compared to a 1D solution using full non-LTE for all known CO levels. As far as it is possible to compare results using different super level definitions, the models using energy as a sorting condition show non-LTE effects in the same temperature range, as the full non-LTE calculation, while the model using only the vibrational quantum number results in non-LTE effects beginning at a lower temperature threshold. At the upper boundary of the atmosphere, all models show non-LTE effects of similar magnitude.

The results of both energy sorted models as well as the full non-LTE results in figure .1 have been color coded by level energy, marking all levels with the color of the level, which they were sorted into for the purely energy sorted model. Comparing the models in this way suggests that levels of similar energy show non-LTE effects of similar magnitude, though the super level models seem to underestimate especially levels of high level energy E_i.

All calculations were repeated with PHOENIX/1D using the same atmospheric structure and super level definitions - the resulting departure coefficients matched the results shown in figure .1, thus, verifying the new implementation.

Figure .2 shows the resulting spectra for a section of the $\Delta\nu = 1$ band around 44 micron. The black lines are the resulting outward fluxes F_r for all surface voxels, while the coloured points show the results of the 1D calculation for the same super level definition (red) and the

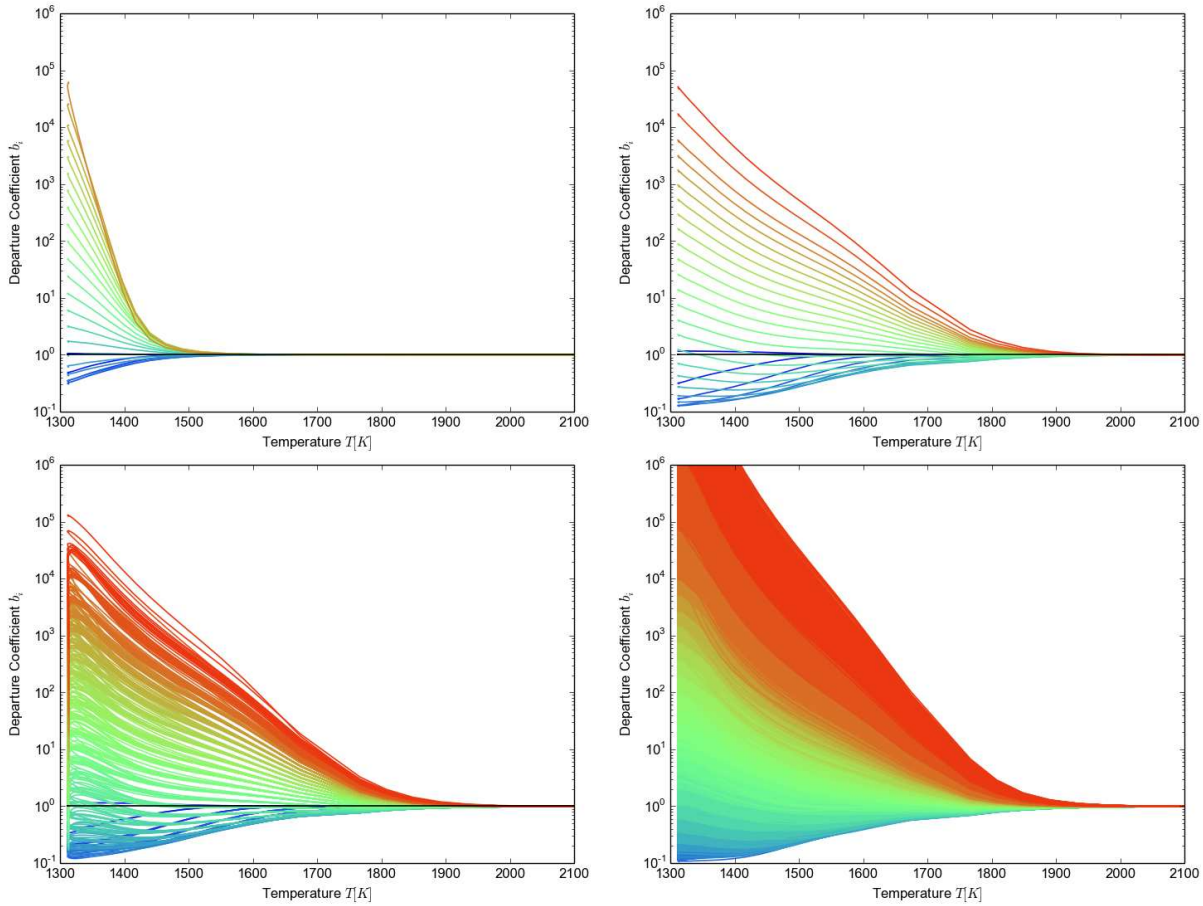

Figure .1: Departure coefficients b_I for different models. ν divied model (upper left), E_i divided model (upper right), $E_i\&\nu$ divided model (lower left), 1D full non-LTE (lower right).

full non-LTE calculation (green). Shown are only the first two models, since the differences between the energy divided model and the energy and quantum number divided model are extremely small.

3. Summary

The 3D implementation of the super level method has passed all standard tests. Furthermore, the results from the spherical symmetric tests agree with the existing and tested 1D implementation of the same method. We conclude that, within the limitations of the tests we have done, the new solver is working correctly.

Our test calculations have shown that the actual solution of the rate equation system now takes little time compared to the radiative rate integration, which requires the calculation of a wavelength integral with a sufficient, and, thus, very large number of wavelength points, which is now the more expensive part of the problem.

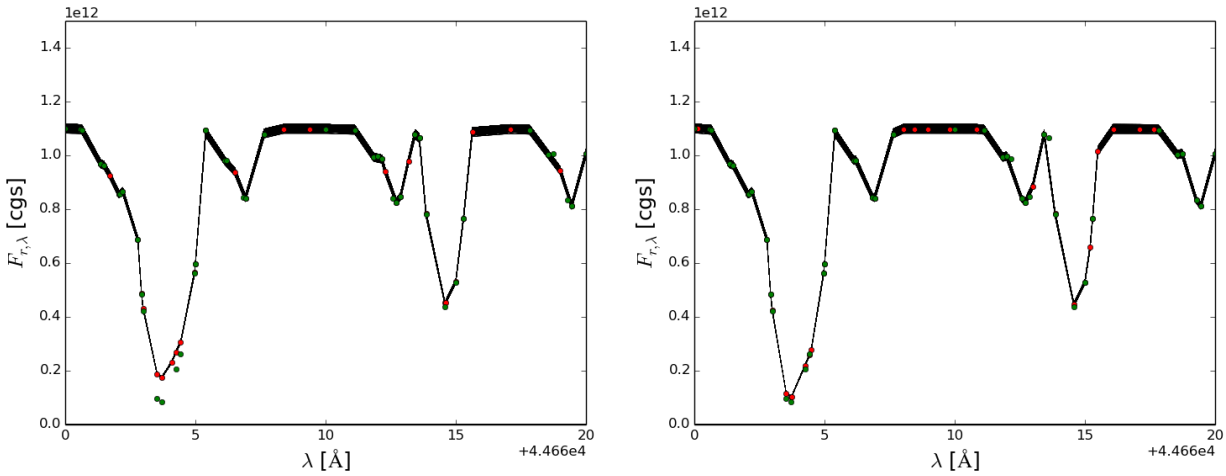

Figure .2: Resulting spectrum for outward Flux F_r for ν model (left), E_i model (right) compared to 1D models of same level (red) and full non-LTE (green).

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