A Superlevel Method for Molecular NLTE in Cool Atmospheres

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Abstract. Due to the low electron temperatures in the atmospheres of M and Brown Dwarfs the common assumption of LTE could be invalid because collisional rates might be much smaller than the radiative rates. It has been shown that NLTE effects of atomic lines are small but noticeable in the spectra of M Dwarfs. However, NLTE effects of molecules in cool and sub-stellar objects are potentially much larger and can have significant observational impact, since their atmospheres as well as their spectra are dominated by molecular lines. The large number of molecular levels and lines requires special computational methods for molecular NLTE because of the enormous computing requirements involved.

We present a method (based on the Superlevel formalism) to treat huge numbers of molecular NLTE levels with good accuracy. Our method treats each line individually. However, in order to solve the rate equations, we make the Superlevel approximation and group energetically similar levels together to reduce the size of the system by a factor of \( \approx 100 \), resulting in substantial savings in computer time and memory. This method allows us to calculate NLTE “model molecules” with a large number of actual levels with the existing operator splitting and rate operator techniques implemented in the stellar atmosphere code PHOENIX (e.g. Hauschildt et al. 1995, 1996b; Hauschildt, Baron & Allard, 1997, in press).

1. Introduction

The population densities in an atmosphere can be described by the LTE Boltzmann distribution only if the collisional rates are large enough to fully compensate for the deviations of the radiative rates from their Planckian thermodynamic equilibrium values. In extreme cool atmospheres, however, there are two properties which could lead to deviations from LTE. The first are the extremely low electron densities and consequently low collisional rates which might not be suffi-
cient to restore LTE. Collisions with other particles might be much less effective because of their much smaller relative velocities and their smaller cross sections. However, approximate values for collisional cross sections are only known very roughly by the formulae of Darwin (1961), Van Regemorter (1962) or as given in Allen (1973). Secondly, with decreasing effective temperature the maximum of the energy distribution stays at roughly 1.2 $\mu$m (Allard & Hauschildt, 1995). This means that not only the spectrum is far from a black body for $T = T_{\text{eff}}$, but also the maximum deviates strongly from the maximum of a black body and the radiative rates could "see" a much hotter temperature compared to the kinetic temperature. NLTE effects for atomic species like Ti have already been presented by Hauschildt et al. (1997, submitted; 1996b). Since molecules are the dominating opacities in cool objects, deviations form LTE can have a significant impact on the atmospheric structure and the spectra.

Modern techniques for solving simultaneously the rate equations and the radiative transfer equation use rate operators and operator splitting techniques (e.g. Hauschildt, 1993; Hauschildt, Störzer & Baron, 1994). The size of the rate operator matrix is determined by the number of levels to be calculated and reaches the computational limits even of modern computers for huge model molecules with thousands of levels.

We adopt the idea of superlevels which groups similar levels together and assumes LTE populations within each superlevel (first introduced by Anderson, 1989; also Hubeny & Lanz, 1995 and Dreizler & Werner, 1993). This reduces the size of the system to be solved enormously. Anderson's original criteria of levels being "similar" was their energy and abundance. However, we only want to require a certain "LTE-behaviour" within each superlevel. The exact specifications have to be done from case to case and we will discuss our example of CO below.

2. The superlevels

We will not follow Anderson's original approach in detail but use only a minimal number of definitions and approximations needed for solving the rate equations.

We construct a superlevel $I$ out of a number of actual levels $i$ and define the number density naturally by

$$n_I = \sum_{i \in I} n_i.$$

For the population densities of the actual levels within one superlevel we assume LTE and can use the Boltzmann equation:

$$n_i = n_I \frac{g_i e^{-E_i/kT}}{Z_I},$$

where

$$Z_I = \sum_{i \in I} g_i e^{-E_i/kT}$$

is the finite partition sum over the superlevel considered.
Figure 1. **Left panel**: Energy level diagram of the electronic ground state $X^1\Sigma^+$ of $^{12}C^{16}O$. The transitions have been omitted to keep the diagram readable. The horizontal lines mark the boundaries of the Superlevels. **Right panel**: Energy level diagram for two superlevels defined by the ground states of the vibrational states $\nu=12$ and $\nu=14$. Only the transitions between the superlevels have been plotted.

With these definitions we can express the rates between two levels by substituting $n_i \alpha_{ij} \lambda_{ij}$ by $n_i \alpha_{IJ}$. The absorption rate is then

$$n_I R_{IJ} = \sum_{i \in I} \sum_{j \in J} n_i R_{ij} = \frac{4\pi}{\hbar c} n_I \int \alpha_{IJ} J_\lambda d\lambda$$

and, when specifying upper and lower levels, the modified cross section $\alpha_{IJ}$ is

$$\alpha_{UL} = \alpha_{LU} = \sum_{i \in L} \sum_{u \in U} \lambda_{iu} \alpha_{iu} \frac{g_i}{Z_L} e^{-E_i/kT}$$

The emission rate and the collisional rates are constructed in a similar fashion.

The only purpose of the superlevels is to keep the system of the rate equations small. There is no need to keep the number of transitions small. PHOENIX is already using a line by line (LBL) treatment instead of opacity distribution techniques (Hauschildt et al., 1996b, 1994). Therefore, every absorption or emission coefficient is calculated between actual levels (because they are needed to solve the radiative transfer equation) and the cross sections $\alpha_{iu}$ are available for every actual transition at every wavelength point. This allows us to calculate “exact” cross sections $\alpha_{LU}$ with complicated “super line profile” without the use of ODF’s and the rates $R_{IJ}$ can be calculated directly with only little overhead of CPU time.

3. **Example: CO**

CO is a simple and well known molecule. For M dwarfs and substellar objects only the ro-vibrational levels of the electronic ground state $X^1\Sigma^+$ are important. This makes the level structure and the involved transitions very simple.

We used the detailed line data of Goorvitch (1994) to construct the CO model molecule. The original data contained 3623 levels and 19203 lines for
$^{12}C^{16}O$. We separated the levels into superlevels by using their energy. As energy boundaries we used the rotational ground states of the vibrational states since the levels close to the ground states are the most important ones. This method groups all the levels close to the ground state of one vibrational state and all the levels with similar energies of different vibrational states together. The vibrational level with the highest quantum number and the energetically corresponding other levels would produce a huge and wide spread superlevel. We divided this level in such a way that the resulting superlevels contain roughly the same number of levels per superlevel as the average superlevel does.

In Fig. 1 we show an energy level diagram of $^{12}C^{16}O$ with the divisions into superlevels. The right panel shows an example of two superlevels and all the transitions between them.

4. Summary

The purpose of this poster was to present a method to calculate molecular NLTE. We demonstrated how superlevels can be used to accomplish this task and how CO can be divided into such superlevels. However, actual calculations could not be completed up to this point but will be presented in the near future.

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References

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