Using Superlevels to Calculate Molecular NLTE Problems

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Abstract. We present the method we use in our atmosphere code to calculate molecular NLTE problems. It is based on the concept of superlevels. Superlevels consist of many levels having similar quantum properties, grouped together, and assumed to be populated relative to each other by a LTE distribution. This reduces the size of the system of rate equations tremendously. However, we modified the classical superlevel method, and combined it with our dynamical opacity sampling technique, which allows us to treat millions of lines. Therefore, we can calculate the transitions with maximum accuracy. We demonstrate the qualities of this method with the examples of CO and TiO.

1. Introduction

Solving a NLTE problem requires computations with a matrix of which the rank scales with the number of levels of the system. Such operations are both memory- and CPU-time consuming. To compute the matrix elements accurately it is necessary to calculate transition-rates for which the CPU-time requirements scale with the number of transitions of the system. For systems with many levels and lines this direct approach becomes computationally too costly. Superlevels are used to reduce such a system with a large number of levels and transitions to a system with only a few levels. By making plausible assumptions (see below for a detailed description) it is then possible to account for only a small number of levels and transitions.

Today, superlevels are widely used to calculate atomic systems with large numbers of levels, as can be seen in a number of contributions in these proceedings. The term "superlevels" was first introduced by Anderson (1989) and subsequently used by Dreizler & Werner (1993), and Hubeny & Lanz (1995). However, as a historical note, the concept of superlevels, in a sense, had been used even earlier without explicitly naming it. For example, Uitenbroek (2000), Ayres & Wiedemann (1989), Carbon et al. (1976), and Thompson (1973) (and references therein) used rotational LTE to calculate the NLTE excitation of CO.
in the solar transition region and late type stars, and Kutepov et al. (1991, 1997) also use a similar concept to calculate molecular NLTE in the Earth’s atmosphere. Both methods are conceptionally very similar to superlevels.

Molecules have many more levels and lines than atoms and ions. Typical molecules have about $10^5$-$10^6$ levels and $10^4$-$10^8$ lines. Therefore, we use superlevels to address the problem of the size of the rate matrix. As will be described later, we will not use superlevels to reduce the number of lines to be calculated. In that sense we distinguish our work from the original superlevel formalism by using our existing so-called “dynamical opacity sampling” method to account for the millions of lines.

2. Theory

The general idea of superlevels is to group “similar” levels together into one superlevel and solve the rate equation only for the many fewer superlevels. This strategy is an advantage if the populations for the individual levels can be expressed in a computationally-cheap way. Boltzmann statistics provides such a computationally-cheap description, and it is physically accurate if the relative populations within one superlevel thermalize easily and exhibit LTE behavior.

For molecular systems such superlevel groupings can be very good approximations if the selection criterion is constant vibrational quantum-number. The pure rotational transitions, having a given vibrational quantum number, have very long lifetimes compared to ro-vibrational transitions. Therefore, collisional thermalization of those transitions can occur very quickly. As the name implies, this is the basis for the rotational-LTE approximation mentioned earlier.

As described in detail in Schweitzer, Hauschildt, & Baron (2000) it means that for a given level $i$ which is part of a superlevel $I$, the number density $n_i$\textsuperscript{1} can be expressed as

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

where

$$n_I = \sum_{i \in I} n_i \quad \text{and} \quad Z_I = \sum_{i \in I} g_i e^{-E_i/kT},$$

are the population $n_I$ of the superlevel $I$, and the finite partition sum $Z_I$ over the superlevel $I$.

The emission rate between two superlevels is the sum of all emission rates $n_u R_{ul}$ between all relevant actual levels. Expressing $R_{ul}$ by the cross section

\textsuperscript{1}The indices have the following meanings: $l$ always stands for a lower level, $u$ always stands for an upper level and $i$ or $j$ are used where a distinction between upper and lower level is not possible or not necessary. Capital letters like $I$ or $U$ are used for superlevels, and lower case letters like $i$ or $l$ are used for actual levels.
\( \alpha_{ul}^{em} \) of individual lines allows us to define \( n_U R_{UL} = \sum_{u \in U} n_u R_{ul} \) which becomes

\[
n_U R_{UL} = n_U \left\{ \frac{4\pi}{\hbar c} \int_0^\infty \sum_{u \in U} \sum_{i \in U} \frac{g_i}{Z_L^2} \alpha_{ul}^{em} \left( \frac{2hc^2}{\lambda^5} + J_\lambda(\lambda) \right) e^{-E_i/kT} \lambda d\lambda \right\}.
\]

Similarly, the absorption rate \( n_L R_{LU} = \sum_{i \in U} n_i R_{iu} \) becomes

\[
n_L R_{LU} = n_L \left\{ \frac{4\pi}{\hbar c} \int_0^\infty \sum_{u \in U} \sum_{i \in U} \frac{g_i}{Z_L^2} \alpha_{iu}^{abs} J_\lambda(\lambda) \lambda d\lambda \right\}.
\]

These are the expressions we calculate to obtain the rates \( n_f R_{ij} \) required by the much smaller systems of rate equations to solve for \( n_f \). Although we now have only \( j_{\text{max}} \) levels instead of \( i_{\text{max}} \) levels, we still need to calculate all actual transitions to carry out the sums (3) and (4). However, PHOENIX (Hauschildt & Baron 1999), the code we use, successfully uses dynamical opacity-sampling (see e.g. Schweitzer et al. 2000; Hauschildt et al. 1994) to treat millions of lines and there is no need to reduce the number of calculated lines. We only need to assign each actual line to the supertransition to which it belongs. The advantage is that we have a small system of rate equations, yet we have accurate transition rates. The equivalent expressions for the collisional rates look very similar (see Schweitzer et al. 2000) except that it is not necessary to integrate over wavelength. Hence, to sum over all actual collisional transitions is computationally cheap because it is done only once. Finally, to solve the NLTE rate equations we use an operator-splitting technique (Hauschildt 1993, and references therein) which is also called “preconditioning” in these proceedings.

### 3. Examples

We implemented our variation of the superlevel method for CO and are currently implementing it for TiO. To illustrate the quality of our technique we will limit the following discussion to an artificial molecule based on CO. The only difference from real CO is that our artificial molecule is immune against collisions with H, He and H\(_2\). If those collisions are allowed, CO will stay in LTE under photospheric conditions. We refer to Schweitzer et al. (2000) for a detailed discussion of CO.

By using the quantum-number criterion we reduced the original 3623 levels of CO to 24 superlevels (Model A). For atomic systems, it is common practice to use energy as the selection criterion. When following that approach we created 27 superlevels (Model B). When we combined both criteria, i.e. we divided each superlevel created from the constant quantum-number criterion into “energy regions”, we got 350 superlevels (Model C). See also Fig. 1 for an illustration. To evaluate the accuracy of our method we also did a direct NLTE calculation with all 3623 levels (Model Z).
Figure 1. Energy level diagrams of the electronic ground state of CO (left, data from Goorvitch (1994)) and of TiO (right, data from Schwenke (1998)). The grey lines in the left panel indicate the superlevel boundaries. If one considers only the vertical boundaries, the criterion is the quantum number (Model A); if one considers only the horizontal boundaries the criterion is energy (Model B); if uses both criteria we call it Model C. In the right panel, each electronic state has 20 vibrational states and each dot corresponds to one level.

Fig. 2 shows the first overtone ($\Delta \nu = 1$) band of CO for a $T_{\text{eff}}=2700$ K, $\log(g)=5.0$ model. The model is fully converged and representative for a late M dwarf (see Allard et al. 2001, for details of the models). For all superlevel models we considered, including the direct NLTE calculation, we obtained identical spectra, all of which show stronger absorption than the LTE spectrum. The departure from LTE is similar for all superlevel models. Although it is impossible to compare the departure coefficients from different superlevel models, they show a consistent underpopulation in the outer layers of the atmosphere (see Schweitzer et al. 2000).

We are therefore confident that our method is accurate enough to treat systems like TiO which have many more levels. An energy level diagram of TiO is shown in Fig. 1. We grouped the 269300 levels by quantum number and by electronic state and reduced the system to 260 superlevels (13 electronic states, each with 20 vibrational states). Results, however, are not yet available.

4. Conclusions and Outlook

We have successfully implemented an accurate variation of the superlevel formalism. We will apply this method to more molecules which are important in cool stars. In future work we will also need to allow for dissociation.

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Figure 2. The $\Delta \nu=1$ band of CO between 4.3 and 6 $\mu$m. The right figure is an arbitrary region of this band. The LTE spectrum and the non–LTE spectra for the different models of the superlevel are indicated in the figure. All non–LTE spectra lie on top of each other.

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