Radiative Transfer in Molecular Lines

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Abstract. Molecular lines are generally very good tracers of the physical conditions in cold regions of the Universe (e.g. molecular clouds, cool stars, brown dwarfs, etc.), but molecular species are also found in not so cold environments (e.g. the magnetized solar atmosphere). For a reliable interpretation of spectro-(polarimetric) observations of molecular lines it is often necessary to carry out detailed radiative transfer simulations, both in LTE and in NLTE. Here we present a multilevel radiative transfer code for the synthesis of molecular lines in stellar atmospheres, showing some illustrations of calculations in different astrophysical contexts and considering complex molecules like H$_2$O. We discuss our implementation of highly convergent iterative methods and formal solvers with special emphasis on spherical geometry. We present also a chemical evolution code which is currently allowing us to investigate the approximation of instantaneous chemical equilibrium in the calculation of the abundances of a variety of molecular species.

1. Introduction

Radiative Transfer (RT) in molecular lines is important for obtaining information on the cold Universe from observed molecular spectra. As in the case of atomic RT, it requires to find the populations of the energy levels which are consistent with the radiation field, but with the complication of the very large number of levels that have to be included. The difficulty of the problem is enhanced by the possibility of having populations inversions in maser transitions. Therefore, it is desirable to apply iterative methods like those developed by Trujillo Bueno & Fabiani Bendicho (1995, hereafter TF95). To this end, we have generalized these rapidly convergent methods to spherical geometry and to molecular line transfer. As an illustrative example of a complex problem, we have carried out a NLTE multilevel calculation of an ortho/para-water model in a hot cloud, where we have some interesting maser effects. Astronomical masers may produce some numerical instabilities (due to the exponential increase of the intensity) and a finer discretization has to be used. In Fig. 1 we show some of the emission/absorption profiles obtained for models of ortho and para-water including 40 energy levels.

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The water column density is $N(\text{H}_2\text{O})=1.8\times10^{17}$ cm$^{-2}$. Some of the lines, like that at 183 GHz (first line on the left), are maser transitions.

2. Iterative Methods and Illustrative Examples

In order to investigate the physical conditions in a given object by comparing the observed with the synthetic spectrum, one should solve the RT problem for many different physical conditions in order to carry out a detailed analysis. To this end, it is desirable to apply very fast iterative methods. We have generalized the RT methods based on the Gauss-Seidel and SOR iteration schemes developed by TF95 to spherical geometry. The conceptual idea of the usual methods based on local ALI (Jacobi iteration) and the new RT methods is fairly simple and allows an improvement of up to an order of magnitude in the convergence rate$^1$.

The spherical geometry is depicted in the left panel of Fig. 2. We have applied the impact parameter technique (e.g. Mihalas 1978). The RT equation is solved along each characteristic as in the plane-parallel case starting from the outer boundary. Once all the contributions have been added to the incoming mean intensity, one can apply the inner boundary condition and obtain the radiation field in the deepest layer. Before propagating outwards all the rays, one can build and solve the preconditioned rate equations and obtain a new estimate of the populations in the deepest layer. If this technique is applied for each layer, one ends up with an iterative scheme which can be up to a factor of 4 faster (Gauss-Seidel up and down) than the usual local ALI method. The speed can be improved if the SOR method is used. This method is implemented as the Gauss-Seidel scheme but using an overrelaxation parameter whose value lies between 1 and 2 (see TF95).

$^1$Additional explanations on the convergence properties of these methods can be found in the review paper by Trujillo Bueno (these proceedings).
Figure 2. Geometry used for solving the RT problem in spherical geometry (left panel). The right panel shows typical convergence properties of the original GS-based methods of TF95 (i.e. not the up-and-down improvement described by Trujillo Bueno (these proceedings)).

The typical convergence properties for a problem in which the spherical effects are important are shown in the right panel of Fig. 2. Note that multilevel GS (MUGA) is a factor of 2 faster than multilevel ALI (MALI) and multilevel SOR (MUSOR) brings about an order of magnitude of improvement, therefore allowing us to solve more complicated problems. All these methods based on the operator splitting technique suffer from a deterioration of the convergence rate as the spatial resolution of the grid is increased. Therefore, it may happen that the local ALI method is found to be slowly convergent in a very fine grid that is needed for solving the problem under consideration, but SOR still converges reasonably. Multilevel RT methods which do not suffer from this sensitivity to the spatial resolution of the grid have been developed by Fabiani Bendicho, Trujillo Bueno & Auer 1997. These non-linear multigrid methods are of interest in 3D RT and perhaps for solving problems in which very strong maser action takes place.

3. Chemical Equilibrium

For solving a RT problem for molecular species one has to obtain first the molecular abundance at every point of the model atmosphere. It is usually assumed that this abundance is given by the instantaneous chemical equilibrium approximation. However, this assumption might be incorrect for dynamic scenarios if the dynamical timescales are of the order of the association/dissociation timescales (Ayers & Rabin 1996; Uitenbroek 2000). Both, observations and the radiation-hydrodynamical simulations carried out by Carlsson & Stein (1999) show that the solar chromosphere is very dynamical, with wave propagation and shock formation. Therefore, taking into account the timescale for the formation and destruction of CO in the solar chromosphere (between milliseconds to some days), we conclude that it can be comparable or even higher than the dynamical timescales (of the order of minutes). The assumption of instanta-
Figure 3. Ratio between the abundance of CO obtained following the CO chemistry and the abundance obtained in instantaneous chemical equilibrium for a hot model like FAL-C (left panel) and for a cool model like COOL-C (right panel).

aneous chemical equilibrium seems to be incorrect for a reliable interpretation of some “enigmatic” CO observations (see Ayres & Rabin 1996). To this end, we have developed a chemical evolution code for investigating the reliability of such an approximation. As an example, we show in Fig. 3 the ratio between the abundance obtained following the chemistry and assuming instantaneous chemical equilibrium for two selected models: a relatively hot model like FAL-C (Fontenla et al 1993) in which the timescale is lower than 100 seconds and a relatively cold model like COOL-C (Ayres et al 1986) in which we have timescales up to some days. We are now working on relaxing this assumption in the radiation-hydrodynamical simulations of Carlsson & Stein (1999), including also the cooling produced by CO in order to verify if the discrepancy between the observations and the modeling of the CO fundamental vibro–rotational lines disappears.

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References

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