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RADIATIVE TRANSFER TOOLS FOR THE GTC

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RESUMEN

En esta contribución presentamos códigos que permiten la rápida solución de problemas de transporte radiativo y que pueden ser de gran interés para la interpretación de espectros obtenidos con GTC y su instrumentación post-foco. Tales códigos están basados en los métodos iterativos de transporte radiativo introducidos por Trujillo Bueno & Fabiani Bendicho (1995). Presentamos resultados de la generalización de estos métodos a transiciones moleculares y a geometría esférica con campos de velocidad macroscópicos. Mostramos el interés de tener un espectrógrafo de media–alta resolución para poder resolver la estructura rotacional de las bandas. Mostramos observaciones espectropolarimétricas de líneas de OH realizadas con el polarímetro TIP (Tenerife Infrared Polarimeter) desarrollado en el IAC y su interpretación teórica.

ABSTRACT

We present very fast radiative transfer tools of interest for the interpretation of future spectroscopic observations taken with the GTC and its post-focus instrumentation. Our radiative transfer codes are based on the iterative methods introduced by Trujillo Bueno & Fabiani Bendicho (1995). Taking into consideration spherical geometry and macroscopic velocity fields, we present results from the application of these fast radiative transfer methods. We show why it is of interest to develop a medium–high resolution spectrograph in order to be able to resolve the rotational structure of the molecular bands. We show some spectropolarimetric observations made with the Tenerife Infrared Polarimeter (TIP), developed at the IAC and the theoretical modeling done with the theoretical tools we have developed.

Key Words: **METHODS: NUMERICAL — SUN: MAGNETIC FIELDS — TECHNIQUES: POLARIMETRIC**

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1. INTRODUCTION

Radiative transfer tools are fundamental for the correct interpretation of observed spectra and allow us to calculate synthetic spectra and make detailed comparisons with spectroscopic observations. In order to carry out this synthesis, some ingredients are necessary. First, a thermodynamical model of the object's atmosphere (temperature, atomic or molecular hydrogen density, macroscopic velocity fields, etc.). The other ingredient is a model of the atom or molecule one is interested in. This model has to include all the relevant energy levels in the given problem, the radiative transitions among the levels with their transition probabilities given by their Einstein coefficients and the collisional rates. With this information, we can then solve the problem using either approximate methods (local thermodynamic equilibrium—LTE—or large velocity gradient—LVG) or a more general approach (non-local thermodynamic equilibrium—NLTE). The approximate methods are very fast and are useful for certain physical conditions (LTE when the populations of the levels are given by Saha–Boltzmann statistics and LVG when the velocity gradients in the medium are very high), allowing synthetic spectra to be obtained that include millions of atomic and molecular lines. On the other hand, the exact NLTE approach requires high computational power because, in this case, one has to solve both the rate equations and the radiative transfer equations for each radiative transition that takes place in the assumed atomic or molecular model. In order to solve the problem, it is necessary to develop and apply iterative methods because the problem is not only non-local but also non-linear. Very fast iterative methods have been developed by

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Trujillo Bueno & Fabiani Bendicho (1995) for the solution of radiative transfer problems in Cartesian geometries and for atomic transitions. Because these NLTE methods can solve the problem with an order of magnitude of improvement with respect to the so-called accelerated lambda iteration (ALI) method, they allow the possibility of investigating more complex problems, such as those encountered in molecular astrophysics. An illustration of the convergence properties of the methods is shown in Figure 1, where we give the maximum relative change versus the iteration number of the Gauss–Seidel (GS) and successive over-relaxation (SOR) methods of Trujillo Bueno & Fabiani Bendicho (1995) compared with the ALI method. Over the past few years, we have generalized the GS and SOR methods to spherical geometry, including macroscopic velocity fields, and to molecular transitions.

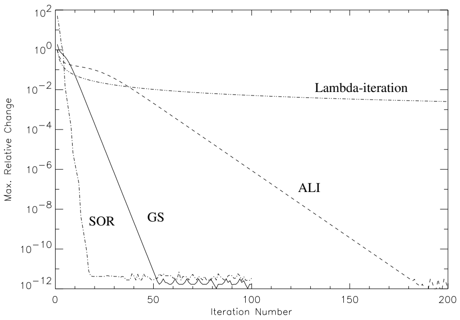

Fig. 1. Typical convergence properties of the various iterative schemes are shown for the case of the NLTE line transfer problem.

2. EXAMPLES OF SOLAR AND STELLAR SPECTROSCOPY

In this section, we shall show some examples of the published work carried out with the aid of those very fast radiative transfer tools. The first example is related to the determination of stellar abundances via NLTE syntheses in realistic 3D hydrodynamical models of the stellar atmosphere (Shchukina & Trujillo Bueno 2001). In Figure 2a, we show a snapshot of the 3D temperature structure of the solar photospheric model at a given time. The authors built an iron atomic model including around 500 levels and solved the ensuing Fe I–Fe II–Fe III NLTE problem. In Figure 2b, we show the difference in the spatially averaged profiles when solving the NLTE problem (solid line) and when using the LTE approximation (dashed line). In the case of the Sun, the derived iron abundance difference between the two approaches is only 0.1 dex, but it can be higher for metal-poor stars.

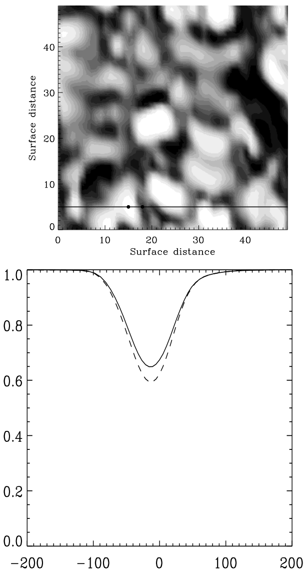

Fig. 2. Surface variation of the gas kinetic temperature at a geometrical height $h = 1$ km in the 3D hydrodynamical simulation of the solar atmosphere (left panel) and the averaged emerging profile normalized to the true mean continuum intensity in NLTE (solid line) and in LTE (dashed line).

Another example concerns the synthesis of the G band in the Sun (Sánchez Almeida et al. 2001). The G band in the solar spectrum is around 4300 Å and is caused by absorption produced by CH. In Figur ee3, we show very high resolution observations of the spectral region around 4300 Å, together with the modeling of the G band, taking into account the CH opacity and all the atomic lines. The synthetic spectrum, which was obtained assuming LTE because this is a very good approximation for the formation of this band, gives us information about the thermodynamic conditions in the deeper zones of the atmosphere and about the formation of the G band bright points in small-scale magnetic flux concentrations in the solar atmosphere.

3. POSSIBLE APPLICATIONS TO FUTURE GTC OBSERVATIONS

In the previous section, we showed some applications of radiative transfer tools for the interpretation of observed spectra in solar-type stars. We now turn to the possible application of these tools to future observations with the GTC and its post-focus instrumentation. The projected instrumentation for the GTC covers a spectral region between 3600 Å and 24 μm with a gap between 2.5 and 8 μm. Although the visible spectral region is of great interest,

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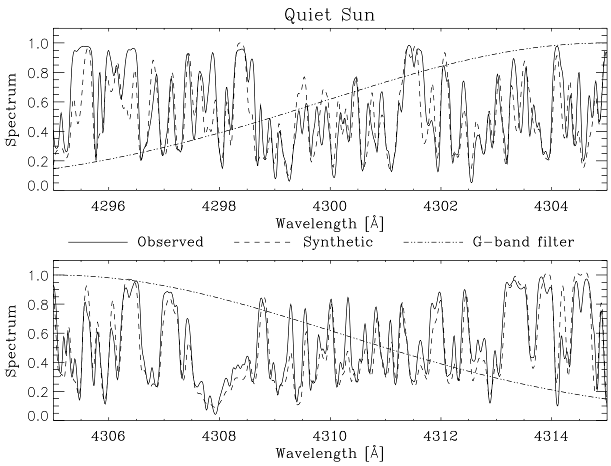

Fig. 3. Comparison between the observed G band spectrum of the Sun and the modeled spectrum with an LTE code from Sánchez Almeida et al. (2001).

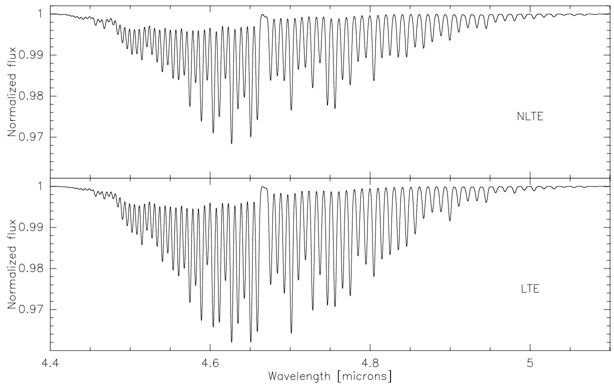

Fig. 4. Synthetic spectrum at a resolution of 2000 for the fundamental CO band showing the difference between the full NLTE calculation and the approximate LTE solution for a circumstellar envelope with a mass loss rate of 10^{-4} $M_\odot$ yr^{-1}.

we shall focus on the infrared (IR region, which is particularly interesting for the diagnostics of physical conditions via molecular spectroscopy. In fact, the region between 1 and 24 μm is full of molecular bands, although these can be found in other spectral regions as well, as we have seen with the G band produced by CH. The opacity between 1 and 2.5 μm is predominantly molecular in nature. In this spectral region, we find important bands of water vapor (H_2O), the fundamental and some of the overtone bands of CO at 4.67, 2.33, and 1.17 μm, which are important temperature indicators and are of fundamental importance in cooling. We also have vibrational bands of SiO, bands of oxides, such as TiO and VO, some bands of methane, CH_4, and important bands of hydrides, such as OH, SiH, FeH, MgH, and CaH. This spectral region is of particular interest for the study of the coldest bodies of the Universe (brown dwarfs, planets, envelopes of evolved stars, molecular clouds, etc.). However, we must not forget that molecules can be observed even in "hot" media, such the atmosphere of the Sun. One of our interests with the GTC is to use the power of a 10 m class telescope to study these objects in detail via atomic and molecular spectroscopy.

An important point that has to be taken into account is the spectral resolution of the instrumentation. Molecular bands in the IR are produced by the vibration of the molecules. The simultaneous rotation of the molecule, because of its energy, is observed as fine structure in the vibrational band. If one is able to observe this rotational structure of a molecular band, then a detailed study of the abundances and physical conditions is possible. The spectral coverage of CanariCam is very interesting, but its spectral resolution is not sufficient for detecting the rotational structure of molecular emission/absorption. On the other hand, the resolution of EMIR is high enough to obtain the fine structure of the molecular bands between 1 and 2.5 μm.

As an example of the application of radiation transfer tools to possible observations with the GTC, we have solved the NLTE problem for a CO molecular model in an expanding circumstellar shell with a very high mass loss of 10^{-4} $M_\odot$ yr^{-1}. The radial variation of the thermodynamical conditions is taken from the usual models for a circumstellar envelope (e.g., González-Alfonso & Cernicharo 1999). The model molecular model includes the first three vibrational levels ($v = 0 \ldots 2$) and 41 rotational levels in each vibrational level ($J = 0 \ldots 40$), where v and J are the vibrational and rotational quantum numbers, respectively. For these 123 levels we have 160 radiative transitions and a total of 3992 transitions (including radiative and collisional). The synthetic band for $R = 2000$ in NLTE and LTE is shown in Figure 4, although this spectral region cannot be observed with the GTC with the planned Day One instrumentation. An interesting point to note is that, with this resolution, which is possible for some wavelengths with the planned GTC instrumentation, it is possible to detect the rotational structure of the band.

4. SPECTROPOLARIMETRY

We have looked at some examples of the application of radiation transfer tools to observed spectra

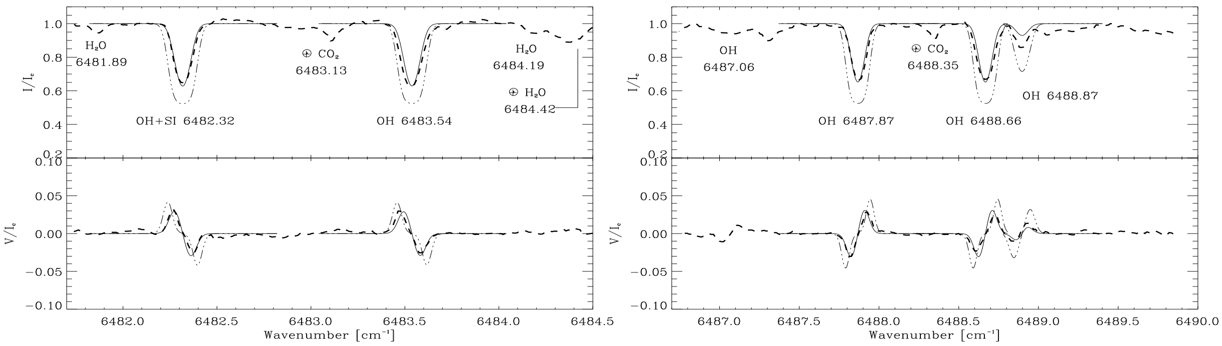

Fig. 5. Comparison between the observed intensity (top panels) and circular polarization (bottom panels) of OH lines in sunspots (dashed line) and the modeled spectrum with an LTE code using a relatively hot (solid line) and cool (dashed–dotted line) model of the magnetized sunspot atmosphere.

where the spectra contains only the intensity. We wish now to stress the utility of spectropolarimetry, which is a very promising technique that can take advantage of 10 m class telescopes (see Trujillo Bueno, Moreno-Insertis, & Sánchez 2002) . Nowadays, spectropolarimetry is being applied with great success in solar physics with instruments like TIP (Tenerife Infrared Polarimeter) built at the IAC and mounted at the Vacuum Tower Telescope (VTT) (see Trujillo Bueno et al. 2002) and in radio astronomy with instrumentation like the spectropolarimeter at the IRAM 30 m telescope at Pico Veleta. Spectropolarimetry allows us to obtain all the information that light carries from the source, because it accounts not only for the total flux but also for the polarization properties of the light. Polarization is generated and modified by any anisotropy (the presence of magnetic fields, anisotropic illumination, etc.). We have also developed the necessary tools for the modeling of Stokes profiles caused by the magnetic field arising from the Zeeman effect for atomic and molecular transitions. This allows us to diagnose spectropolarimetric observations and obtain important information about the magnetic field strength and topology in magnetized atmospheres. We also plan to develop radiative transfer tools for modeling scattering polarization in molecular lines applying the polarization transfer methods of Trujillo Bueno & Manso Sainz (1999).

As an example, we show TIP observations of four OH lines around 1.54 μm, first observed in a sunspot by Harvey (1985). A sunspot is a very cool, magnetized stellar atmosphere, and the presence of a magnetic field whose direction is preferentially radial leads to important circular polarization signals. Figure 5 shows the intensity (Stokes I) and circular polarization (Stokes V) for the four OH lines, revealing a polarization reversal that can been explained with the aid of the theory of Zeeman effect for diatomic molecules developed by Schadee (1978; see Berdyugina & Solanki 2001; Asensio Ramos, Trujillo Bueno & Collados, in preparation). With the aid of the radiation transfer tools for the Stokes parameters we have developed, we have synthesized the emergent profiles in cool and hot umbra models obtained by Collados et al. (1994) by the inversion of atomic lines. We show that the hot model gives a nice fit to the observations while the cool one does not. This is related to the relation between the size of the sunspot and its average temperature. This example illustrates that we have now the RT tools for the interpretation of molecular spectra in astrophysical plasmas.

5. CONCLUSIONS

The GTC will achieve a great advance in our knowledge of the Universe. We consider that, in many situations, it is necessary to complement the observations with powerful numerical tools (not only for radiative transfer, but also for chemical evolution, chemical equilibrium, MHD simulations, etc.) for a rigorous interpretation of the observed spectra. The Day One instrumentation is capable of detecting very faint objects, and their spectral coverage in the IR is interesting for the study of molecular bands in brown dwarfs, evolved stars, etc. We have developed these necessary tools and we are carrying out interesting studies in molecular and atomic astrophysics covering a broad kind of objects. Finally, we demonstrate that spectropolarimetry is a very promising technique that can take advantage of 10 m class telescopes in the same way as it is being

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successfully applied to solar magnetism.

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REFERENCES

Asensio Ramos, A., Trujillo Bueno, J., & Collados, M., in preparation

Berdyugina, S. V., & Solanki, S. K. 2001, A&A, 380, L5

González-Alfonso, E., & Cernicharo, J. 1999, ApJ, 525, 845

Harvey, J. W. 1985, in Measurement of Solar Vector Magnetic Fields, ed. M. J. Hagyard, NASA, CP-2374, 109

Sánchez Almeida, J., Asensio Ramos, A., Trujillo Bueno, J., & Cernicharo, J. 2001, ApJ, 555, 978

Schadee, A. 1978, JQSRT, 19, 517

Shchukina, N., & Trujillo Bueno, J. 2001, ApJ, 550, 970

Trujillo Bueno, J., & Fabiani Bendicho, P. 1995, ApJ, 455, 646

Trujillo Bueno, J., Landi Degl'Innocenti, E., Collados, M., Merenda, L., & Manso Sainz, R. 2002, Nat, 415, 403

Trujillo Bueno, J., & Manso Sainz, R. 1999, 516, 436

Trujillo Bueno, J., & Moreno-Insertis, F., & Sánchez, F. (eds) 2002, Astrophysical Spectropolarimetry (Cambridge: Cambridge University Press)

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