Highlights of Spanish Astrophysics VII, Proceedings of the X Scientific Meeting of the Spanish Astronomical Society held on July 9 - 13, 2012, in Valencia, Spain. J. C. Guirado, L.M. Lara, V. Quilis, and J. Gorgas (eds.)

SHAPEMOL: the companion to SHAPE in the molecular era of ALMA and HERSCHEL

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Abstract

Modern instrumentation in radioastronomy constitutes a valuable tool for studying the Universe: ALMA will reach unprecedented sensitivities and spatial resolution, while Herschel/HIFI has opened a new window (most of the sub-mm and far infrared ranges are only accessible from space) for probing molecular warm gas ($\sim$50$-$1000 K), complementing ground-based telescopes, which are better suited to study molecular molecular gas with temperatures under $\sim$100 K.

On the other hand, the `SHAPE` software has emerged in the last few years as the standard tool for determinging the morphology and velocity field of different kinds of gaseous nebulae (mainly planetary nebulae, protoplanetary nebulae and nebulae around massive stars, although it can also be applied to H II regions and molecular clouds) via spatio-kinematical modelling. Standard `SHAPE` implements radiative transfer solving, but it is only available for atomic species and not for molecules.

Being aware of the growing importance of the development of tools for easying the analyses of molecular data from new era observatories, we introduce the computer code `shapemol`, a plug-in for `SHAPE` with which we intend to fill the so far empty molecular niche. `shapemol` enables spatio-kinematic modeling with accurate non-LTE calculations of line excitation and radiative transfer in molecular species. This code has been succesfully tested in the study of the excitation conditions of the molecular envelope of the planetary nebula NGC 7027 using data from Herschel/HIFI and IRAM 30m. Currently, it allows radiative transfer solving in the ^{12}CO and ^{13}CO J=1$-$0 to J=17$-$16 lines. `shapemol`, used along `SHAPE`, allows to easily generate synthetic maps to test against interferometric observations, as well as synthetic line profiles to match single-dish observations.

1 ALMA and Herschel: modern era radio observatories

Recent development in radioastronomical instrumentation has lead to outstanding improvements in areas crucial in this field. On the one hand, the Atacama Large Millimeter Array (ALMA) will reach, when completed in 2013, unprecedented spatial resolutions and sensitivities. It will consist of 66 12-m antennas with baselines up to 16 km, which together with a compact array of 12-m and 7-m antennas will reach spatial resolutions as high as $0\farcs006$ at 675 GHz and $0\farcs037$ mas at 110 GHz. As of today, in cycle 1 and with 32 antennas in place (baselines up to $\sim$1 km), ALMA his capable of reaching a spatial resolution of $0\farcs08$ in band 9 (e.g. ^{12}CO and ^{13}CO J=6$-$5 transitions), which already exceeds the highest spatial resolution achievable by HST in the optical (see, as an example of the ALMA capabilities, the recently published cycle 0 data by [1]).

On the other hand, the Heterodyne Instrument for the Far Infrared aboard Herschel (HIFI) is an invaluable tool because it opens a new window from which to probe warm molecular gas ($\sim$50–1000 K). While incapable of generating images of the source and thus lacking information on the spatial distribution of its molecular gas, HIFI produces 1-D high-resolution spectra in the range of 480$-$1250 GHz and 1410-1910 GHz, which includes transitions as high as ^{12}CO and ^{13}CO J=16$-$15, unobservable from the ground —as is most of the sub-mm and far-infrared range. Still in operation till 2013, Herschel+HIFI has contributed to the study of the excitation conditions of the warm molecular gas of many nebulae (e.g. [2]).

The study of nebulae around evolved objects, where molecular gas is very common, can greatly benefit from both ALMA's spatial resolution and sensitivity and Herschel+HIFI ability to probe warm molecular gas. In particular, the spatio-kinematical analyses often performed on protoplanetary (PPNe) and planetary nebulae (PNe) in the optical thanks to software codes such as `SHAPE` [8], the state-of-the-art tool in the field, can be complemented with the study of the excitation conditions through means of radiative transfer solving. With this joint goal in mind we have developed `shapemol`, a plug-in which enables `SHAPE` to work with molecular transitions.

2 SHAPE

`SHAPE` is a user-friendly software tool for building spatio-kinematic models of gaseous nebulae —mainly PPNe/PNe, but also supernova remnants, light echoes, emission nebulae from massive stars, etc. It enables easy implementation of a 3-D structure and a 3-D velocity field to describe the model nebula and generate synthetic images, position-velocity diagrams, 1-D spectral profiles and channel maps for direct comparison with observations. Its versatility has made it the standard tool in the field, where it has proven to be valuable for producing accurate spatio-kinematic descriptions of many planetary nebulae (e.g. [8, 4, 10]).

`SHAPE` implements radiative transfer solving for atomic species, in which the absorption and emission coefficients are easily predictable over a large range of temperatures, densities, and abundances. It is, however, unable, on its own, to work with molecular species, both in thermalized and non-thermalized cases. This is due to the strong dependence of the absorp-

tion and emission coefficients of each grid cell not only on the local abundance, temperature, and density, but also on the size of the emitting structure and the velocity of the grid cell along the line of sight.

We designed `shapemol` to fill this gap. We used a special version (4.51β) of `SHAPE`[1], specifically tailored for usage alongside our own code. In the following, we describe this software and its role in the modeling process.

3 SHAPEMOL

`shapemol` is a GDL/IDL-based code built to be used as a complement for `SHAPE`, enabling radiative transfer solving in molecular transitions. Specifically, it performs non-LTE calculations of line excitation (based on the well-known LVG approximation which allows for a significative simplification of the problem, see below) in order to compute the absorption (κ_ν) and emission (j_ν) coefficients of each individual cell in the grid, for the desired transition and species.

The values of κ_ν and j_ν in spectral lines are given by the populations of the involved energy levels and the line profile shape. In the case of low-frequency transitions requiring relatively low excitation, the profile shape is given by the local velocity dispersion due to thermal dispersion or turbulence. The level populations depend on the collisional transition rates and the radiative excitation and de-excitation rates, which in turn depend on the amount of radiation reaching the nebula point we are considering at the frequency of the line (averaged over angle and frequency within the local line profile). The calculation of such averaged radiation intensity requires a previous knowledge of the absorption and emission coefficients in the whole cloud, in order to solve the radiative transfer equation in all directions and frequencies. Indeed, the populations of a high number of levels must be calculated simultaneously, since the population of each one depends on those of the others, and in all the points of the cloud. So, the solution of the system becomes extremely complex in the general case.

The problem is greatly simplified when there is a large velocity gradient (LVG) in the cloud, introducing important Doppler shifts between points that are sufficiently far away. When this shift is larger than the local velocity dispersions, the points cannot radiatively interact at large scales, so the radiative transfer is basically a local phenomenon. The excitation equations can be then solved, and κ_ν and j_ν calculated in each point, independently of the rest of the cloud, in the frame of the LVG approximation. In any case, the level populations depend in a complex way on the (local) physical conditions, and the solution requires an iterative process. See [3] for a comprehensive version of the general formalism of this issue. The LVG approximation includes the main ingredients of the problem (collisional and radiative rates, trapping when opacities are high, population transfer between different levels, etc.) and gives fast, sensible solutions. These excitation calculations are quite accurate, even when the LVG conditions are barely satisfied, at least for the case of molecular lines from shells around evolved stars (e.g. [9, 5]). The approximation itself is not necessary

[1] `SHAPE` is available on http://bufadora.astrosen.unam.mx/shape/

to derive the resulting line profiles, which can be calculated solving the standard, full transfer equation using the level populations derived from the LVG approximation and a local velocity dispersion, as indeed we have done using `SHAPE`.

According to the LVG approximation, κ_ν and j_ν depend in a heavily non-linear way on the density n and the temperature T of the grid cell, and almost linearly on the product $\frac{r}{V}X$, where r is the distance of a given point (or code cell) to the central star, V its velocity and X the abundance of the desired species. Besides these three parameters, the results of the LVG depend on the logarithmic velocity gradient, $\epsilon = \mathrm{d}V/\mathrm{d}r\, r/V$, but only slightly. In its current state, `shapemol` lets the user select values of $\epsilon = 0.2$, 1 and 3. The calculations done by `shapemol` are considerably simplified in the most common case, when $\epsilon = 1$, i.e. a linear dependence of V on r, since the escape probability of a photon in that case is given by a simple analytical function of the opacity. Such velocity fields are found in many young planetary nebulae, which are basically expanding at high velocity following a 'Hubble' velocity law.

The approach of `shapemol` consists of relying on a set of pre-generated tables of κ_ν and j_ν as functions of n and T, each table corresponding to a species, and values of ϵ and the $\frac{r}{V}X$ product. The values of κ_ν and j_ν in each table are individually computed for each pair of n and T by iteratively solving a set of equations via the convergence algorithm typical of LVG codes. In all calculations 40 rotational levels were taken into account, allowing accurate calculations for temperatures up to at least 1000 K, and we used collisional rates from the Leiden Atomic and Molecular Database (LAMDA; see [6]). For a set of physical conditions, `shapemol` selects the table with the closest value of $\frac{r}{V}X$. Once a table has been selected, `shapemol` computes κ_ν and j_ν by linear interpolation between the values for the two adjacent tabulated values of n and T. The steps in n and T were specifically chosen to be small enough so as to guarantee that a 1^{st} order interpolation is a good approximation between two consecutive values. Finally, given the roughly linear dependence of κ_ν and j_ν on the product $\frac{r}{V}X$, the software scales the computed absorption and emission coefficients according to the ratio of the desired value of $\frac{r}{V}X$ to that of the selected table; to avoid significant errors, calculations were performed for a large number of values of this parameter. As mentioned, the absorption and emission coefficients calculated in this way for each cell of the model nebula are used to solve the standard radiative transfer equation and calculate the line profile leaving the nebula in a given direction; at this level, we must assume values of the local velocity dispersion in each point.

The current version of `shapemol` is available from the first author. At its present state, it is able to compute the J= 1−0, 2−1, 3−2,... up to the 17−16 transitions of the ^{12}CO and ^{13}CO species. There are 199 values of T and 21 values of n in the available pre-generated tables, ranging from 10 to 1000 K in steps of 5 K for the temperature, and from 10^2 cm^{-3} to 10^7 cm^{-3} in multiplicative factors of $\sqrt[4]{10}$ for the density. A more refined version, where we will consider including more species, is under progress and will be presented by Santander-García et al. (in preparation).

With respect to the computational errors, we tested `SHAPE`+`shapemol` by matching its results against analytic theoretical predictions in a spherical nebula under several circumstances of abundances, thicknesses, turbulence, velocity distributions and beam sizes. In particular, we modeled a stationary nebula with an abundance range large enough to make it

optically thin or thick; a nebula expanding at a constant velocity and another one following a Hubble-like expansion pattern, for which analytical predictions can be made with the help of the LVG approximation. Also, we explored the flux measured off-center with a small beam size in all the previous scenarios and compared it with the theoretical predictions. All the previous tests were performed for different values of the abundance, velocities and micro-turbulence values, always fulfilling the relation $V > \delta_{\rm V}$, as the LVG approximation demands. In all cases, the error of the model with respect to the predicted intensity was <10%. This error includes numerical errors due to the grid size, limited by the RAM memory of the system, as well as the rounding errors of computational algorithms.

The current version of `shapemol` has been successfully used to study the excitation conditions of the molecular gas of the young PNe NGC 7027, where the synthetic profiles have been matched against data from Herschel/HIFI and the IRAM 30-m radiotelescope [7].

3.1 Modeling process using shapemol

The modeling process using `SHAPE` and `shapemol` is as follows:

1. We model a nebula with several distinct outflows or structures using the standard tools in `SHAPE`. The nebula is then diced in a large number of cells (∼tens of thousands) using a 3-D grid. Each cell in this 3-D grid is characterized by a identification code (unique per each structure), a position, a velocity, a density and a temperature. These values are dumped into an ascii text file, one line per grid cell.

2. `shapemol` reads the text file and let us select the desired ϵ, molecular species and transition, the molecular abundance of each different structure and a value for the micro-turbulence, $\delta_{\rm V}$. The software then computes the absorption and emission coefficients using the LVG approximation and adds them to the text file along with the frequency of the selected transition and the micro-turbulence value.

3. `SHAPE` reads the text file generated by `shapemol` and performs full radiative transfer solving for the whole 3-D grid, creating a data-cube consisting of a stack of images of the nebula, one per frequency resolution element (i.e. spectral channel). The radiative transfer solving used in this step is exact and implements no approximations. This data-cube is then convolved, channel by channel, with the telescope beam, which is simulated by a Gaussian with a FWHM equal to the telescope beam HPBW. The profiles from the central four pixels are added, and the intensity I in each channel is divided by the projected area of the four cells on the plane of the sky. A final profile is then shown, in units of W s^{-1} Hz^{-1} m^{-2} str^{-1}, which once converted to $T_{\rm mb}$ allows for direct comparison with observations.

Acknowledgments

We acknowledge Wolfgang Steffen and Nico Koning for their invaluable help with adapting `SHAPE` to be used along with `shapemol`. This work was partially supported by Spanish MICINN within

the program CONSOLIDER INGENIO 2010, under grant Molecular Astrophysics: The Herschel and ALMA Era ASTROMOL (ref.: CSD2009-00038).

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