# Synthetic Spectra for Interstellar Molecules in LTE and non-LTE regimes

Maitrey Sharma

April 23, 2024

**Abstract**

This work presents a code which can calculate the intensities of atomic and molecular lines produced in a uniform medium, based on statistical equilibrium calculations involving collisional and radiative processes and including radiation from background sources to infer physical and chemical parameters such as temperature, density, and molecular abundances.

## 1 Introduction

Consider a mono-atomic or singly-charged chemical species in gaseous state with $N$ energy levels defined as $E_i$ with $i = 1 \dots N$ in ascending order. Pertaining to the temperature this chemical species exists at, each level will have certain occupation or population. These occupation numbers can change due to collisions between neighboring molecules and if the environment is sufficiently dense and temperatures are sufficiently high, this population distribution can be deemed as thermal and can be expressed as

$$\frac{N_j}{N_i} = e^{-(E_j - E_i)/k_B T} \tag{1}$$

Here, $N_i$ (and $N_j$) represents the level occupation number density of state $i$ (and $j$), $k_B$ is the Boltzmann constant and $T$ is the temperature of the gas. This thermal distribution is basis for the condition of *local thermodynamic equilibrium* or LTE. In other words, the mean free path of the (excited) molecules is much, much less than the scales at which the temperature varies in the medium.

Equation 1 can be modified to include the degeneracies of states through statistical weights, which results in

$$\frac{N_j}{N_i} = \frac{g_j}{g_i} e^{-(E_j - E_i)/k_B T} \tag{2}$$

where $g_i = 2l + 1$, $l$ being the orbital angular momentum of electron in state $i$. And finally, we can obtain the fractional occupational numbers $n_i$ using the partition function $Z(T)$ as

$$n_i = \frac{1}{Z(T)} g_i e^{-E_i/k_B T} \tag{3}$$

## 2 Radiative Transfer

Now, transitions between levels can also be facilitated by the emission or absorption of a photon. This is called a radiative transition, or a spectral line transition.

$$\frac{dI_\nu}{ds} = j_\nu - \alpha_\nu I_\nu \tag{4}$$

where $I_\nu$ is the specific intensity defined as the amount of energy passing through a surface normal to the path, per unit time, surface, bandwidth (measured here in frequency units), and solid angle. $j_\nu$ and $\alpha_\nu$ are the local emission and excitation coefficients. This can be solved to obtain

$$I_\nu = I_\nu(0)e^{\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau'_\nu)e^{-(\tau_\nu - \tau'_\nu)}d\tau'_\nu \tag{5}$$

where $I_\nu(0)$ is the background radiation entering the medium. To calculate the emission and excitation coefficients, we require the Einstein coefficients $A_{ij}$ and $B_{ij}$ along with a function called *line profile* $\phi(\nu)$ which basically defines the susceptibility of the transition to photons of frequency $\nu$.

In the case of LTE, radiative transfer can be performed by using the following data

1. A *line list* This is a list (usually in ASCII format) in which for each line the $A_{ij}$, $E_i$, $\nu_{ij}$, $g_i$, $g_j$ are given.
2. A *partition function table* as a function of temperature.

But if we were to perform a non-LTE radiative transfer, we will need

1. A *level list* in which for each level the $E_i$ and $g_i$ are given.
2. *Collisional rates* $C_{ij}$ between each pair of levels at different temperatures.
3. A *line list* but this time containing, for each line, the index $i$ of the upper and $j$ of the lower level, where these indices refer to the level list mentioned above. Along with, of course, $A_{ij}$ and line profile information.

As collisional rates difficult to measure in lab, for most of the astrophysically relevant species, only LTE radiative transfer is possible.

### 2.1 The Problem of non-LTE transfer

If the level populations $n_i$ are known, the radiative transfer equation can be solved exactly. In particular, under LTE conditions, knowledge of the kinetic gas temperature $T_{\rm kin}$ allows the determination of $n_i$ by virtue of the Boltzmann equation. For many interstellar and circumstellar media, the density is too low to attain LTE, but statistical equilibrium (SE) can often be assumed. Under the condition of SE, for every level $i$ we demand that the rate at which

atoms/molecules are being (de-) excited out of level $i$ is equal to the rate at which level $i$ is being re-populated by (de-) excitation from other levels:

$$\sum_{j>i} n_j A_{ji} - \sum_{j<i} n_i A_{ij} + \sum_j [n_j C_{ji} - n_i C_{ij}] = 0 \tag{6}$$

This must be true for all levels $i$ and therefore, Equation 6 constitutes a coupled set of $N_{\text{lev}}$ linear equations with $N_{\text{lev}}$ unknowns, or in other words, a matrix equation.

## 2.2 Lambda Iteration and Accelerated Lambda Iteration

The Lambda iterative scheme is defined as follows used in order to solve a coupled set of equations:

1. Make an initial guess for the mean intensity
2. Integrate the formal transfer equation along a large number of rays, such that close to every point $x$ a sufficient number of rays pass by that we can make an approximate calculation of the mean intensity
3. Compute mean intensity at all locations, thereby computing the scattering emissivity
4. Go back to 2, until we find a converged solution to mean intensity.

We can rewrite 6 by including the mean intensity $J_{ij}$ as

$$\begin{aligned} &\sum_{j>i} [n_j A_{ji} + (n_j B_{ji} - n_i B_{ij}) J_{ji}] \\ &- \sum_{j<i} [n_i A_{ij} + (n_i B_{ij} - n_j B_{ji}) J_{ij}] \\ &+ \sum_{j \neq i} [n_j C_{ji} - n_i C_{ij}] = 0 \end{aligned} \tag{7}$$

By defining something called the Lambda operator as

$$J_\nu = \Lambda[S_\nu] \tag{8}$$

which basically acts as a function which computes the mean intensity $J$ at some point $\mathbf{x}$ knowing what the source function $S_\nu(\mathbf{x}')$ is for all $\mathbf{x}'$. In principle, the $\Lambda_{ij}$ can be defined as

$$\Lambda_{ij} = \frac{1}{4\pi} \int d\nu \oint d\Omega \phi_{ij}(\nu, \mathbf{x}, \mathbf{n}) \Lambda_{\nu, \mathbf{n}} \tag{9}$$

where $\Lambda_{\nu,\mathbf{n}}$ is the angle-dependent Lambda operator. Equation 7 then becomes

$$\begin{aligned}
&\sum_{j>i}[n_j A_{ji} + (n_j B_{ji} - n_i B_{ij})\Lambda_{ji}[S_{ji}]] \\
&- \sum_{j<i}[n_i A_{ij} + (n_i B_{ij} - n_j B_{ji})\Lambda_{ij}[S_{ij}]] \\
&+ \sum_{j\neq i}[n_j C_{ji} - n_i C_{ij}] = 0
\end{aligned} \tag{10}$$

Now lambda iteration just involves the iteration between solving the set of equations in 7 for given $J_{ij}$, and computing $J_{ij}$ for given $n_i$. Using 10, we can write

$$\begin{aligned}
&\sum_{j>i}[n_j^{m+1} A_{ji} + (n_j^{m+1} B_{ji} - n_i^{m+1} B_{ij})\Lambda_{ji}[S_{ji}^m]] \\
&- \sum_{j<i}[n_i^{m+1} A_{ij} + (n_i^{m+1} B_{ij} - n_j^{m+1} B_{ji})\Lambda_{ij}[S_{ij}^m]] \\
&+ \sum_{j\neq i}[n_j^{m+1} C_{ji} - n_i^{m+1} C_{ij}] = 0
\end{aligned} \tag{11}$$

where $m$-index is the iteration counter. After each iteration you solve the coupled set of linear equations 11 to obtain new set of level populations.

We can improve Lambda iteration by splitting of the $\Lambda$-operator.

$$\Lambda_{ij} = \Lambda_{ij}^* + (\Lambda_{ij} - \Lambda_{ij}^*) \tag{12}$$

as form of separating out the diagonal (or tridiagonal) part of the operator matrix. This gives rise to the accelerated Lambda iteration scheme or ALI and can be summarized as

$$\begin{aligned}
&\sum_{j>i}[n_j^{m+1} A_{ji}(1-\Lambda_{ji}^*) + (n_j^{m+1} B_{ji} - n_i^{m+1} B_{ij})(\Lambda_{ji} - \Lambda_{ji}^*)[S_{ji}^m]] \\
&- \sum_{j<i}[n_i^{m+1} A_{ij}(1-\Lambda_{ij}^*) + (n_i^{m+1} B_{ij} - n_j^{m+1} B_{ji})(\Lambda_{ij} - \Lambda_{ij}^*)[S_{ij}^m]] \\
&+ \sum_{j\neq i}[n_j^{m+1} C_{ji} - n_i^{m+1} C_{ij}] = 0
\end{aligned} \tag{13}$$

## 2.3 The Escape Probability Scheme

Now that we have a mathematical framework to efficiently solve the coupled system of equations, we can return to the problem at hand and analyze it scientifically as well to see if we can make some further approximations. Even with the above iterative schemes, for inhomogeneous or geometrically complex objects, extensive calculations with many grid points are required. However, if only the global properties of the source are of interest then we can introduce a geometrically averaged escape probability $\beta$, the probability that a photon will

escape the medium from where it was created. This probability depends only on the optical depth $\tau$ and is related to the intensity within the medium, ignoring background radiation and any local continuum, through

$$J_{\nu_{ul}} = S_{\nu_{ul}}(1 - \beta) \tag{14}$$

We have included three kinds of geometries in our implementation. The first one comes from Sobolev's Large Velocity Gradient (LVG) approximation for an extending spherical shell. For this case, the probability is given by

$$\beta_{\text{LVG}} = \frac{1}{\tau}\int_0^\tau e^{\tau'} d\tau' = \frac{1 - e^{-\tau}}{\tau} \tag{15}$$

The second geometry is that of a uniform static sphere and escape probability for it is given by

$$\beta_{\text{sphere}} = \frac{1.5}{\tau}\left[1 - \frac{2}{\tau^2} + \left(\frac{2}{\tau} + \frac{2}{\tau^2}\right) e^{-\tau}\right] \tag{16}$$

And lastly, we have a plane-parallel slab geometry, applicable for shocks

$$\beta_{\text{slab}} = \frac{1 - e^{-3\tau}}{3\tau} \tag{17}$$

# 3 Description of the Code

## 3.1 Input to the code

1. The code leverages the Leiden Atomic and Molecular Database (LAMDA) database to get the required data required for non-LTE radiative transfer. Therefore, first input is the LAMDA file for the molecule/species one is interested in.

2. The geometry of the system, as described in the last section to get the correct escape probability scheme.

3. A function to obtain the background radiation. By default, we use the cosmic microwave background, which means basically radiation corresponding to the $T = 2.73$ K.

4. The kinetic temperature of the source. This will be used to calculate the corresponding uprates and downrates of collisional events between particles at different energy levels. Uprates and downrates are linked through detailed balance equation.

5. Densities of the collisional partners. Collisional partners are often the most abundant species such has the hydrogen molecule (present in two forms as spin isomers: ortho and para).

6. The (total) column density of the molecule one is interested in. Column density is basically the integrated number density of a molecular species along a column formed by the line of sight.

7. The full-width half-maximum of the line profile. Line profiles can be Gaussian or rectangular.

### 3.2 Output of the code

1. The code displays results for all transitions. These results include quantum numbers, the upper and lower energy levels, excitation temperature, frequency and wavelength.

2. The line optical depth, defined as the optical depth of the equivalent rectangular line shape.

3. Fractional populations (occupational numbers) for each energy level.

4. The line intensity, defined as the Rayleigh-Jeans equivalent temperature.

5. Once the above items are calculated, few extra inputs can be supplied to calculate more relevant quantities. For example, flux can be computed by providing distance to the observer, radius of the source (as sources are assumed to be spherical or slab-like) and the solid angle subtended by the source. The last one is what links this to actual observations through telescopes.

6. Finally, we can obtain the final synthetic spectrum by using the given input parameters along with the source function.

## 4 Results

## References


[1] T. De Jong, A. Dalgarno, and W. Boland. Hydrostatic models of molecular clouds. *Symposium - International Astronomical Union*, 87:177–181, 1980. URL: http://dx.doi.org/10.1017/S0074180900072491, doi:10.1017/s0074180900072491.

[2] Cornelis P. Dullemond. Zentrum für Astronomie Heidelberg - Institut für Theoretische Astrophysik — ita.uni-heidelberg.de. https://www.ita.uni-heidelberg.de/~dullemond/lectures/radtrans_2012/index.shtml. [Accessed 24-04-2024].

[3] E. A. Gussmann. D. mihalas: Stellar atmospheres. second edition. w. h.freeman &; co., san francisco 1978. xx + 632 p. *Astronomische Nachrichten*, 300(4):221–222, January 1979. URL: http://dx.doi.org/10.1002/asna.19793000416, doi:10.1002/asna.19793000416.

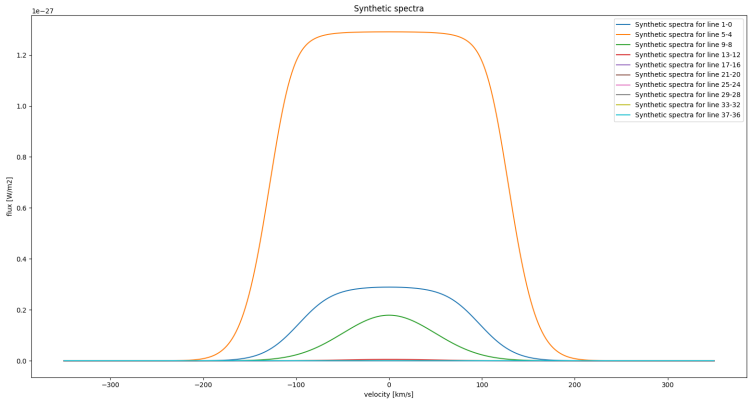


Figure 1: Synthetic spectrum in the non-LTE regime.

[4] Donald E Osterbrock and Gary J Ferland. *Astrophysics Of Gas Nebulae and Active Galactic Nuclei*. University science books, 2006.

[5] F. F. S. van der Tak, J. H. Black, F. L. Schöier, D. J. Jansen, and E. F. van Dishoeck. A computer program for fast non-lte analysis of interstellar line spectra: With diagnostic plots to interpret observed line intensity ratios. *Astronomy &; Astrophysics*, 468(2):627–635, April 2007. URL: `http://dx.doi.org/10.1051/0004-6361:20066820`, `doi:10.1051/0004-6361:20066820`.