

The Large Velocity Gradient Approach

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I. Radiative transfer

In the document "Formalism for the CASSIS software" we have only considered molecules populated under LTE conditions. We now start a more general analysis. Let P_{ij}^k be the transition probability for the transition $i \rightarrow j$ caused by the process k , and let n_i be the number density in the state i . Then:

$$\frac{dn_i}{dt} = -n_i \sum_j \sum_k P_{ij}^k + \sum_j n_j \sum_k P_{ji}^k \quad (1)$$

For a stationary situation $dn_i/dt=0$. For a two-level system that is:

$$n_u(A_{ul} + B_{ul}\bar{U} + C_{ul}) = n_l(B_{lu}\bar{U} + C_{lu}) \quad (2)$$

where \bar{U} is the average radiation field intensity (see document "Formalism for the CASSIS software"):

$$\bar{U} = \frac{4\pi}{c} \times \bar{I} = \frac{8\pi h\nu^3}{c^3} \frac{1}{\exp(h\nu/kT_{bg}) - 1} \quad (3)$$

where T_{bg} is the background temperature. The rates C_{ij} are the collision rates per second per molecule of the species of interest. They depend on the density of the collision partner (exemple H_2 , H or He):

$$C_{ij} = \gamma_{ij} \times n_{collision} \quad (4)$$

where $n_{collision}$ is the density of the collision partner. γ_{ij} is the velocity-integrated collision cross section in $cm^3 s^{-1}$. Those rate coefficients depend on the temperature. If collisions dominate, then:

$$\frac{C_{lu}}{C_{ul}} = \frac{n_u}{n_l} = \frac{g_u}{g_l} \exp\left(-\frac{h\nu}{kT_k}\right) \quad (5)$$

where T_k is the kinetic temperature.

From equation (2), (3) and (5) we obtain:

$$\frac{n_u g_l}{n_l g_u} = \exp\left(-\frac{h\nu}{kT_{ex}}\right) = \frac{A_{ul} + C_{ul} \exp(-h\nu/kT_k)(\exp(h\nu/kT_{bg}) - 1)}{A_{ul} \exp(h\nu/kT_{bg}) + C_{ul}(\exp(h\nu/kT_{bg}) - 1)} \quad (6)$$

If we neglect the background radiation field ($h\nu \gg kT_{bg}$) then:

$$T_{ex} = \frac{h\nu/k}{h\nu/kT_k + \ln(1 + A_{ul}/C_{ul})} \quad (7)$$

When collisions dominate ($C_{ul} \gg A_{ul}$), then $T_{ex} \rightarrow T_k$ (LTE regime).

For a molecule in LTE, all excitation temperatures are the same, and N_u can be expressed as a fonction of N_{tot} . For non LTE excitation, a different excitation temperature may characterize the population of each level relative to that of the

ground state or relative to that of any other level.

The optical depth τ_0 in the line at line center is related to the fractional populations (f_u , f_l , that can be solved by the statistical equilibrium equations) by:

$$\tau_0 = \frac{A_{ul}c^3 N_{tot}}{8\pi\nu^3 \Delta\nu} \left[\frac{g_u}{g_l} f_l - f_u \right] \quad (8)$$

where N_{tot} is the total column density, and $\Delta\nu$ is the linewidth.

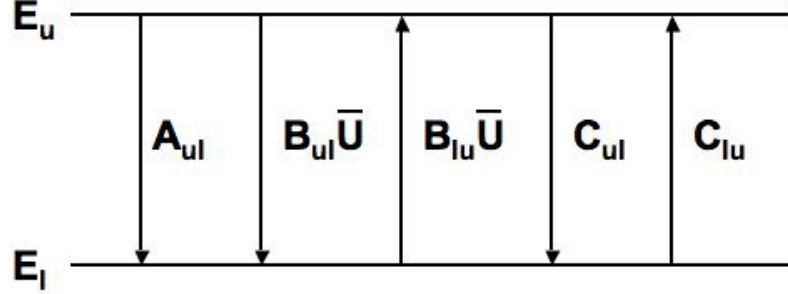


Figure 1: Transitions between the states up (u) and low (l).

II. The Large Velocity Gradient approach

In the following, we present the most widely used method of radiative transfer which satisfactorily accounts for photon transport when lines are optically thick. This is the Large Velocity Gradient (or LVG) approximation.

We need to estimate \bar{U} to calculate the level population. We can define a probability β that a photon emitted in the transition at a radius r will escape from the cloud. Then, $\bar{U} = S(1-\beta)$ where S is the source function and depends on the molecular level population:

$$S_\nu = \frac{A_{ul}}{B_{ul} \frac{n_l g_u}{n_u g_l} - 1} \quad (9)$$

If all the photons escape, then $\beta=1$ and \bar{U} is the blackbody radiation field intensity. If no photons escape from the cloud, then \bar{U} is the source function. From equation (1) the statistical equilibrium equations get a more simple form for a two-level state:

$$\frac{dn_1}{dt} = -n_1 C_{12} + n_2 C_{21} + \beta n_2 A_{21} \quad (10)$$

$$\frac{dn_2}{dt} = n_1 C_{12} - n_2 C_{21} - \beta n_2 A_{21} \quad (11)$$

The β parameter can be expressed as a function of the optical depth τ :

$$\beta = \frac{1 - e^{-\tau}}{\tau} \quad \text{for a radially expanding sphere} \quad (12)$$

$$\beta = \frac{1 - e^{-3\tau}}{3\tau} \quad \text{for an homogeneous slab} \quad (13)$$

The excitation temperature can then be expressed as:

$$T_{ex} = \frac{h\nu/k}{h\nu/kT_k + \ln(1 + A_{ul}\beta/C_{ul})} \quad (14)$$

III. The code

1. Introduction

The code included into CASSIS is an adaptation of the LVG method described in Castets et al. (1990). The original code is from J. Cernicharo. At this stage it only treats linear molecules. In the future, we plan to introduce non-linear molecules and use the frequencies and the Einstein coefficients from the JPL and CDMS catalogs.

The energy levels for diatomic and linear polyatomic molecules are quantified to first order according to:

$$E_{rot} = BJ(J+1) \quad (15)$$

where B is the rotational molecular constant. These rotational energy levels can be defined by their rotational quantum number J and their statistical weight are:

$$g = 2J + 1 \quad (16)$$

The computed frequency between level J+1 and level J is:

$$\nu_{J+1,J} = 2B(J+1) \quad (17)$$

The corresponding Einstein coefficient can therefore be computed using this frequency and the dipole moment μ quoted in Table 1:

$$A_{ul} = \frac{64\pi^4\nu^3}{3hc^3} |\mu_{ul}|^2 \quad (18)$$

2. Input

To run the on-line version of the LVG code, one must supply the following parameters:

- Any molecule in the list of table 3.
- The number density of H₂ molecules in the cloud (in cm⁻³). Collision with He are taken into account when the helium abundance is given. By default, the Helium abundance is taken to the interstellar medium value (He/H₂ = 0.2).
- The ortho-to-para ratio for the H₂ molecules. Presently this parameter only matters for the CO molecule where collisional rate coefficients exist for both spin states.

Table 1: List of the adopted molecular constant and dipole moments from the JPL and CDMS catalogs for the linear molecules used.

Molecule	B [Hz]	μ [Debye]
^{12}CO	$5.7635968 \cdot 10^{10}$	0.11011
^{13}CO	$5.5101012 \cdot 10^{10}$	0.11046
C^{18}O	$5.4891421 \cdot 10^{10}$	0.11049
HCO^+	$4.459441 \cdot 10^{10}$	3.9
DCO^+	$3.601977 \cdot 10^{10}$	3.9
H^{13}CO^+	$4.33773 \cdot 10^{10}$	3.9
CS	$2.449556 \cdot 10^{10}$	1.958
^{13}CS	$2.312385 \cdot 10^{10}$	1.958
C^{34}S	$2.410355 \cdot 10^{10}$	1.958
C^{33}S	$2.429333 \cdot 10^{10}$	1.958
N_2H^+	$4.658688 \cdot 10^{10}$	3.4
HC_3N	$4.549059 \cdot 10^9$	3.73172
HC_5N	$1.3313327 \cdot 10^9$	4.33
HC_7N	$5.640011 \cdot 10^8$	4.82
HC_9N	$2.905183 \cdot 10^8$	5.2
C_4H	$4.758656 \cdot 10^9$	0.87
C_3N	$4.94762 \cdot 10^9$	2.85
HCN	$4.4315976 \cdot 10^{10}$	2.9852
H^{13}CN	$4.3170127 \cdot 10^{10}$	2.9852
DCN	$3.6207462 \cdot 10^{10}$	2.9908
HNC	$4.533198 \cdot 10^{10}$	3.05
HN^{13}C	$4.354561 \cdot 10^{10}$	2.699
C_2H	$4.367453 \cdot 10^{10}$	0.769
DNC	$3.815299 \cdot 10^{10}$	3.05
HCS^+	$2.133714 \cdot 10^{10}$	1.958
OCS	$6.081492 \cdot 10^9$	0.7152
OC^{34}S	$5.93283 \cdot 10^9$	0.7154
O^{13}CS	$6.06192 \cdot 10^9$	0.7153
HC_{11}N	$1.69063 \cdot 10^8$	5.47

- The kinematic temperature of the molecular cloud.
- The width of the molecular lines.
- The column density of the molecule (in cm^{-2}).
- The collision rates available for the linear molecule selected (see table 2). Presently, only one database is selected by default in the on-line version. In the future CASSIS will offer the possibility to choose between many collision databases. Note that in the LVG computation the kinetic temperature must be within the range chosen for the corresponding molecule (see table 2.)
- The geometry used: sphere or slab.
- The Velocity in the Standard of Rest for each components.
- The filling factor for each molecule in the beam.

Note that the excitation temperature (left to the kinetic temperature) quoted in the CASSIS interface will have no effect for the LVG computation. In the same way, the excitation temperature quoted will have no effect for the LTE computation.

In the future, CASSIS will be able to introduce a background source (temperature and filling factor) and compute the contamination for the emission of the foreground molecular cloud. Presently we only consider the contribution of the cosmic blackbody radiation, set equal to 2.7 K in all calculations.

The molecules available in the LVG code are listed in table 3:

- Same collision rates for ^{13}CO and C^{18}O as for ^{12}CO .
- Same collision rates for ^{13}CS , C^{33}S and C^{34}S as for CS .
- Same collision rates for DCO^+ and H^{13}CO^+ as for HCO^+ .
- Same collision rates for H^{13}CN , HCN , DCN , DNC , HN^{13}C and C_2H as for HCN .
- Same collision rates for C_3N and C_4H as for HC_3N .
- Same collision rates for OC^{34}S and O^{13}CS as for OCS .
- Interpolation with the HC_3N collision rates for HC_5N , HC_7N , HC_9N and HC_{11}N .

3. Output

From the input parameters listed in the previous section, the LVG computation returns the values for the opacity of the line at the line center, and the excitation

Table 2: List of molecular collisional data used in the code.

Molecule	Collision partner	Temperature [K]	Reference
CO	p-H ₂	10 – 250	Flower (2001)
	o-H ₂	10 – 100	Flower (2001)
CS	p-H ₂	2 – 100	Turner et al. (1992)
HCO ⁺	p-H ₂	5 – 30	Flower (1999)
N ₂ H ⁺	He	5 – 50	Daniel et al. (2005)
HCN	He	5 – 100	Green & Thaddeus (1974)
HC ₃ N	He	10 – 20	Green & Chapman (1978)
HCS ⁺	He	10 – 60	Monteiro (1984)
OCS	p-H ₂	10 – 100	Green & Chapman (1978)

Table 3: List of molecules available in the code.

CO	CS	HCO ⁺	N ₂ H ⁺	HCN	HC ₃ N	HC ₅ N	HCS ⁺	OCS
¹³ CO	¹³ CS	DCO ⁺		H ¹³ CN	C ₃ N	HC ₇ N		OC ³⁴ S
C ¹⁸ O	C ³³ S	H ¹³ CO ⁺		HNC	C ₄ H	HC ₉ N		O ¹³ CS
	C ³⁴ S			DCN		HC ₁₁ N		
				DNC				
				HN ¹³ C				
				C ₂ H				

temperature. Using equations (24) and (31) from the document "Formalism for the CASSIS software", the interface will display the spectrum in the frequency range selected.