Formalism for the CASSIS software

Charlotte VASTEL

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I. Radiative transfer

The intensity of a source emitting in the interstellar medium along a line of sight I_ν, will change if the radiation is absorbed or emitted, and this change can be described by the equation of transfer:

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu \tag{1}$$

where $\frac{dI_\nu}{ds}$ represents the change of the intensity I_ν at the corresponding frequency ν through a slab of material of thickness s. It depends on the absorption coefficient α_ν and the emissivity j_ν.

In Local Thermodynamic Equilibrium (LTE) the intensities of emitted and absorbed radiation are not independant. The Einstein coefficients give a convenient means to describe the interaction of radiation with matter by the emission and absorption of photons.

Consider a gas containing atoms with discrete energy levels E_u and E_l. According to Einstein (1916), a system in the excited state E_u will return spontaneously to the lower level E_l with a certain probability A_{ul} such that $n_u A_{ul}$ is the number of such spontaneous transitions per second in a unit volume, with n_u the density of state u. The difference in energy between transition u and l results in a frequency $\nu = (E_u - E_l)/h$. The absorption line will be described by a line profile function $\Phi(\nu)$ which is peaked and normalized:

$$\int_0^\infty \Phi(\nu) d\nu = 1 \tag{2}$$

If the intensity of the radiation field is I_ν, we can define an average intensity by:

$$\bar{I} = \int_0^\infty I_\nu \Phi(\nu) d\nu \tag{3}$$

The probability of the absorption of a photon is $B_{lu}\bar{U}$ such that the number of absorbed photons is $n_l B_{lu}\bar{U}$ where $\bar{U} = 4\pi\bar{I}/c$ is the average energy density of the radiation field. Einstein found that in order to derive Planck's law, another emission process was needed: $n_u B_{ul}\bar{U}$ that is the number of photons emitted by stimulated emission. If the system is in a stationary state, the number of absorbed and emitted photons must be equal:

$$n_u A_{ul} + n_u B_{ul}\bar{U} = n_l B_{lu}\bar{U} \tag{4}$$

We can express j_ν and α_ν by:

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \Phi(\nu) \tag{5}$$

$$\alpha_\nu = \frac{h\nu}{c} \left(n_l B_{lu} - n_u B_{ul} \right) \Phi(\nu) \tag{6}$$

Let's define the opacity τ of a line by:
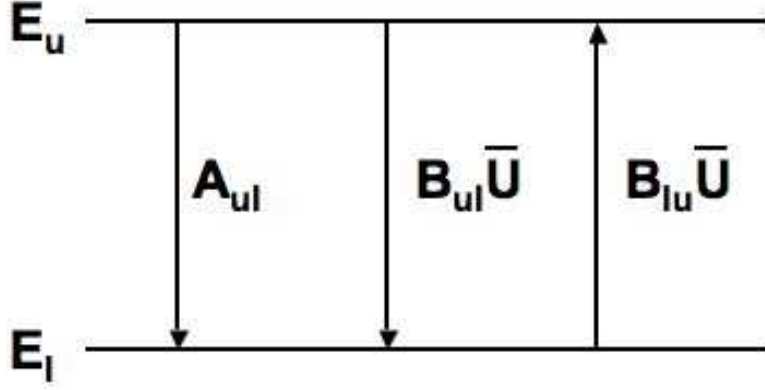
$$d\tau = \alpha_\nu ds \tag{7}$$

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

and the source function by :

$$S_\nu = \frac{j_\nu}{\alpha_\nu} \tag{8}$$

Then we get :

$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu \tag{9}$$

$$\frac{dI_\nu}{d\tau_\nu} e^\tau + I_\nu e^\tau = S_\nu e^\tau \tag{10}$$

$$\frac{d}{d\tau_\nu}(I_\nu e^\tau) = S_\nu e^\tau \tag{11}$$

We can then integrate this equation between 0 and τ_ν :

$$\int_0^{\tau_\nu} \frac{d}{d\tau_\nu}(I_\nu e^\tau)\, d\tau_\nu = \int_0^{\tau_\nu} S_\nu e^\tau\, d\tau_\nu \tag{12}$$

Assuming that the source function is constant, we then get :

$$I_\nu = S_\nu + e^{-\tau_\nu}(I_{\nu_0} - S_\nu) \tag{13}$$

where I_{ν_0} represents the cosmic microwave background (CMB) at 2.7 K. The emitted intensity of an astronomical source is coupled to the CMB. In order to compare the intensity of the observed signal with the original intensity of the emitting source in absence of the intervening interstellar medium ($I_\nu(0)$), we get :

$$I_{\nu_{obs}}(s) = I_\nu(s) - I_\nu(0) = (S_\nu(T) - I_\nu(0))(1 - e^{-\tau_\nu}) \tag{14}$$

With this equation, we assume that the source function does not vary as a function of the opacity, namely it does not vary throughout the cloud. The source function can be described as:

$$S_\nu = \frac{\frac{h\nu}{4\pi} n_u A_{ul}}{\frac{h\nu}{c} \left(n_l B_{lu} - n_u B_{ul} \right)} \tag{15}$$

We can describe an excitation temperature, T_{ex}, which characterizes the population levels:

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-\frac{h\nu}{kT_{ex}}} \tag{16}$$

Then:

$$S_\nu = \frac{A_{ul}c}{4\pi} \frac{1}{\frac{g_l}{g_u} e^{E_{ul}/kT_{ex}} B_{lu} - B_{ul}} \tag{17}$$

In LTE, the brightness distribution is described by the Planck function, which depends only on the thermodynamic temperature T of the surroundings (blackbody radiation):

$$S_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \tag{18}$$

$$I_\nu(0) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/2.7k} - 1} \tag{19}$$

From equations 17, 18 and 19, we find that the Einstein coefficients A_{ul}, B_{ul} and B_{lu} are not independent and must obey:

$$g_l B_{lu} = g_u B_{ul} \tag{20}$$

$$A_{ul} = \frac{8\pi h\nu^3}{c^3} B_{ul} \tag{21}$$

We note that the previous equation defines B in terms of radiation density per unit frequency interval. The intensity of radiation at frequency ν, observed by a telescope, is given by:

$$I_{obs} = (I(T_{ex}) - I(T_{CMB}))(1 - e^{-\tau_\nu}) \tag{22}$$

where T_{ex} is the excitation temperature in the cloud and T_{CMB} is the cosmic microwave background at 2.7 K. In the Rayleigh-Jeans limit (namely $\frac{T_0}{T} \ll 1$ where $T_0 = h\nu/k$),

$$I_\nu = \frac{2kT}{\lambda^2} \tag{23}$$

It is the custom in radioastronomy to measure the brightness of a source by its brightness temperature, T_b. This is the temperature which would result in the given brightness if inserted into the Rayleigh-Jeans law.

Equation 22 then becomes:

$$T_b(v) = T_0 \left(\frac{1}{e^{T_0/T_{ex}} - 1} - \frac{1}{e^{T_0/2.7} - 1} \right) (1 - e^{-\tau(v)}) \tag{24}$$

where $T_0 = h\nu/k$.

When a background continuum source (T_{dust}, τ_{dust}) is coupled to the molecular/atomic cloud (T_{ex}, τ) along the line of sight, the previous equation must take into account the dust temperature and opacity, as well as the cosmic microwave background (CMB). In a on-off observation, the resulting brightness temperature obtained from the telescope is:

$$T_b = J_\nu(CMB)e^{-\tau_{dust}}e^{-\tau} + \Omega_{dust}J_\nu(T_{dust})(1-e^{-\tau_{dust}})e^{-\tau} + \Omega J_\nu(T_{ex})(1-e^{-\tau}) - J_\nu(CMB) \tag{25}$$

where $J_\nu(T) = (h\nu/k)/(1-e^{h\nu/kT}-1)$ is the radiation temperature, Ω_{dust} represents the dilution factor for the continuum source and Ω represents the dilution factor for the molecular/atomic cloud. In the case where $\tau_{dust} = 0$ and $\Omega = 1$, the equation becomes:

$$T_b = (J_\nu(T_{ex}) - J_\nu(CMB))(1 - e^{-\tau}) \tag{26}$$

In the case where $\Omega = \Omega_{dust} = 1$, then:

$$T_b = (J_\nu(CMB)e^{-\tau_{dust}} + J_\nu(T_{dust})(1-e^{-\tau_{dust}}))e^{-\tau} + T_{ex}(1-e^{-\tau}) - J_\nu(CMB) \tag{27}$$

Outside the line, towards the continuum source, the continuum obtained in the on-off observation is defined by:

$$T_C = (J_\nu(CMB)e^{-\tau_{dust}} + J_\nu(T_{dust})(1 - e^{-\tau_{dust}})) - J_\nu(CMB) \tag{28}$$

Combining equations 27 and 28 give a resulting brightness temperature that is used for the CASSIS formalism:

$$\mathrm{T_b} = \mathrm{T_C}e^{-\tau} + (1 - e^{-\tau})(J_\nu(T_{ex}) - J_\nu(CMB)) \tag{29}$$

- For emission lines:

$$T_b - T_C = \Delta T = (1 - e^{-\tau})(J_\nu(T_{ex}) - J_\nu(CMB) - T_C) \tag{30}$$

- For absorption lines:

$$T_C - T_b = T_{abs} = (1 - e^{-\tau})(T_C - J_\nu(T_{ex}) + J_\nu(CMB)) \tag{31}$$

The line opacity can be expressed as a function of the column density and the excitation temperature, that we assume to be constant on the line of sight:

$$\int \tau dv = \int \frac{h\nu\Phi_\nu}{c}(B_{lu}n_l - B_{ul}n_u)dv = \frac{g_u}{g_l}\frac{A_{ul}c^3 n_l}{8\pi\nu^3}(1 - exp(-h\nu/kT_{ex})) \tag{32}$$

Where Φ_ν is the line profile with $\int \Phi(\nu)d\nu = 1$.

For a gaussian line shape, we can express the opacity as a function of the cloud's depth:

$$\tau_{ul}(z) = \frac{A_{ul}c^3}{8\pi\nu_{ul}^3 \Delta v \sqrt{\pi}/2\sqrt{ln2}} \int_0^z n_u \left(\frac{n_l g_u}{n_u g_l} - 1\right) dz' \tag{33}$$

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where Δv (velocity units) is the full width at half maximum of the observed line. Integrating on the line of sight, we get, at the line center :

$$\tau_0 = \frac{g_u}{g_l} \frac{c^2}{8\pi\nu^2 \Delta\nu \sqrt{\pi}/2\sqrt{ln2}} A_{ul} N_l \left(1 - e^{-h\nu/kT_{ex}}\right) \qquad (34)$$

where $\Delta\nu$ (frequency units) is the full width at half maximum of the observed line, and N_l is the column density in the lower state.

This equation can also be expressed as:

$$\tau_0 = \frac{c^2 A_{ul} N_u}{8\pi\nu^2 \Delta\nu \sqrt{\pi}/2\sqrt{ln2}} \left(e^{h\nu/kT_{ex}} - 1\right) \qquad (35)$$

This can be related to the total column density:

$$N_{tot} = N_{lowest} Q(T_{ex})/g_{lowest} = N_u Q(T_{ex}) e^{E_u/kT_{ex}}/g_u. \qquad (36)$$

where $Q(T_{ex})$ is the partition function for an excitation temperature T_{ex} and the index "lowest" represents the lowest level associated to the molecule and its form (ortho, para, ...). E_u is the upper level of the transition compared to the ground level (different from zero when orho, para or meta forms). When the collision rate between molecules is high (in LTE), $T_{ex} \rightarrow T_b \rightarrow T_K$. By choosing a column density such that $\tau \gg 1$ at the line center, the line will therefore saturate, the temperature at the line center will become constant, and will result in a non-negligeable line broadening (see Equation 24). At T_{ex} = 20 K, for the ^{12}CO molecule, we get T_b = 16.5 K for the $1 \rightarrow 0$ transition and T_b = 14.8 K for the $2 \rightarrow 1$ transition. Figure 2 presents the line profiles of the ^{12}CO molecule for transitions $1 \rightarrow 0$ and $2 \rightarrow 1$ at T_{ex} = 20 K, FWHM = 1 km s^{-1}, τ = 10 and τ = 0.5 at the line center.

Several mechanisms can broaden spectral lines. The most important involves the Doppler effect. Individual atoms are in random, chaotic motion. The hotter the gas, the faster the random thermal motions of the atoms. When a photon is emitted by an atom in motion, the frequency of the detected photon is changed by the Doppler effect. The photon is then not recorded at the precise frequency predicted by atomic physics but rather at a slightly shifted. Throughout the whole cloud, atoms move in every possible direction, resulting in a broadening of the line. From Fuller & Myers (1992) :

$$(\Delta v)^2 = 8ln(2)\frac{kT}{m} \qquad (37)$$

where Δv is the full width at half maximum, k is the Boltzmann constant, T is temperature in the gas, and m is the mass of the atom (or molecule). For example, in the case of the D_2H^+ molecule, at a temperature of 8 K, the thermal linewidth will be 0.27 km/s. Note that turbulence can also result in the broadening of a spectral line.

For CASSIS: by defining a column density and an excitation temperature, we get from 32 $\int \tau dv$. Then, using a linewidth (before broadening
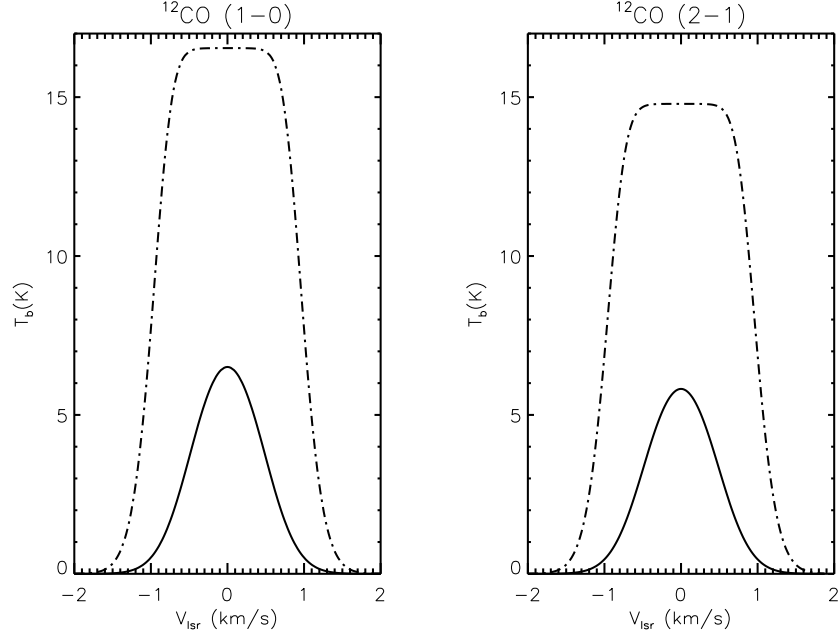
Figure 2: Line profiles for the ^{12}CO transitions $1 \rightarrow 0$ and $2 \rightarrow 1$ at $T_{ex} = 20$ K, Δv = 1 km s^{-1} and $\tau = 0.5$ (plain lines) and 10 (dot-dashed lines) at the line center.

due to optical depth), we get $\tau(v)$ (as a function of velocity), which has a gaussian profile:

$$\tau(v) \;=\; \tau_0 exp(-\frac{(v - v_0)^2}{2\sigma^2}) \qquad (38)$$

where v_0 is the velocity in the local standard of rest (V_{LSR}),
σ(km/s) $= \Delta$v(km/s)$/(2\sqrt{2ln2})$, where Δv is the full-width at half maximum. Then from 24 we get T_b as a function of velocity. This results in a line profile that is to be included in K6.

II. Molecules (Using the JPL or CDMS catalogs)

1) The Einstein A_{ul} coefficients

The line intensity in the catalogs, $I_{ul}(300K)$ is obtained from:

$$I_{ul}(T) = \frac{8\pi^3}{3hc}\nu_{ul}S_{ul}\mu^2[e^{-E_l/kT} - e^{-E_u/kT}]/Q_{rs}(T) \tag{39}$$

where ν_{ul} is the line frequency, S_{ul} is the line strength, μ is the dipole moment along the molecular axis and Q_{rs} is the rotation-spin partition function (using the same zero of energy as E_u and E_l). The units of intensity given in the catalog is $nm^2.MHz$ The average spontaneous emission rate from the upper states into the lower states is:

$$A_{ul} = I_{ul}(T)\nu_{ul}^2\frac{Q_{rs}(T)}{g_u}\frac{1}{e^{-E_l/kT} - e^{-E_u/kT}} \times \frac{8\pi}{c^2} \tag{40}$$

where T = 300 K.

$$A_{ul} = I_{ul}(T)\nu_{ul}^2\frac{Q_{rs}(T)}{g_u}\frac{1}{e^{-E_l/kT} - e^{-E_u/kT}} \times 2.796410^{-16} \ s^{-1} \tag{41}$$

where $I_{ul}(T)$ is in $nm^2.MHz$ and ν is in MHz.

2) The partition functions

In the cold regions of the ISM it is important to consider ortho and para states separately. The energy of the lowest rotational or rotation-hyperfine level is 0 by default. The energy of the lowest level for the other spin-modification(s) is usually given in the documentation. One should consider Q values for the different spin-modifications separately at least at low temperatures. The CDMS database intends to provide this information in the near future.

In the CASSIS database, the new catalog (tagged "VASTEL") takes into account the ortho/para/A/E forms for the H_2O, D_2O, H_2S, D_2S, H_2CO, D_2CO, CH_3CCH, c-C_3H_2, H_2D^+ and D_2H^+ molecules. The JPL catalog has been used for the D_2S, H_2O, D_2O, c-C_3H_2 and H_2S molecules; the CDMS catalog has been used for the H_2CO, D_2CO, D_2O, D_2S, H_2S, H_2O, CH_3CCH, H_2D^+ and D_2H^+ molecules.

A file called catdir.cat is also provided. Each element of this file has the following format:

TAG: the species tag or molecular identifier (8 or 9 on the 5th digit to separate the ortho/para/A/E symmetry). For example 020091 for o–D_2O, means that the CDMS catalog (original D_2O = 020502) has been used (4th digit) to be compared with 20592 for o–D_2O where the JPL database has been used (original D_2O tag= 020001).

NAME: an ASCII name for the species.

NLINE: the number of lines in the catalog.

QLOG: A seven-element vector containing the base 10 logarithm of the partition function for temperatures of 300 K, 225 K, 150 K, 75 K, 37.5 K, 18.75 K, 9.375 K, respectively. The main interest of having those Q(Tex) for each symmetry, is an accurate computation for the column density for a symmetry state, or in the case of CASSIS, computation of the main beam temperature for a line of a certain symmetry.

VERSION: the version of the calculation for this species in the catalog (starts at number 69).

ALOG: the base 10 logarithm of the partition function for temperature of 300 K as found in the CDMS or JPL database, where the ortho and para forms are not disentangled. **This value is necessary to compute the Einstein coefficients.**

1) H_2O and D_2O

H_2O and D_2O are asymmetric top molecules, with the dipole moment along the b-axis. They have ortho and para forms. The notation for the transitions is J,K_a,K_c.

For H_2O:

g_J=3(2J+1) ΣK odd : ortho transitions
g_J=(2J+1) ΣK even : para transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-para})/kT_{ex}}$ where $E_{0-para} = 0$ K

$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$ where $E_{0-ortho} = 34.23$ K
1113342.9640 0.3000 -0.8353 3 0.0000 3 -180031404 1 1 1 0 0 0 0 0
556936.0020 0.0500 -0.8147 3 23.7944 9 -180031404 1 1 0 0 1 0 1 0

For D_2O:

$g_J=6(2J+1)$ ΣK even : ortho transitions
$g_J=3(2J+1)$ ΣK odd : para transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$ where $E_{0-para} = 17.43$ K
$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$ where $E_{0-ortho} = 0$ K
607349.6000 0.2000 -1.3353 3 0.0000 18 -20001 303 1 1 1 0 0 0
316799.8100 0.1200 -2.0408 3 12.1170 9 -20001 303 1 1 0 1 0 1

2) H_2S and D_2S

The H_2S and D_2S molecules are asymmetric top molecules. They have ortho and para forms. The notation for the transitions is J,K_a,K_c.

For H_2S:

$g_J=3(2J+1)$ ΣK odd : ortho transitions
$g_J=(2J+1)$ ΣK even : para transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$ where $E_{0-para} = 0$ K
$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$ where $E_{0-ortho} = 19.78$ K
452390.3300 0.0700 -2.6154 3 0.0000 3 -34002 303 1 1 1 0 0 0
168762.7624 0.0100 -2.8376 3 13.7463 9 -34002 303 1 1 0 1 0 1

For D_2S:

$g_J=6(2J+1)$ ΣK even : ortho transitions
$g_J=3(2J+1)$ ΣK odd : para transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$ where $E_{0-para}=10.01$ K

$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$ where $E_{0-ortho} = 0$ K
91359.1209 0.0230 -4.1358 3 6.9561 9 340 303 1 1 0 1 0 1
237903.6752 0.0581 -3.1702 3 0.0000 18 340 303 1 1 1 0 0 0

3) H_2CO and D_2CO

H_2CO and D_2CO are planar asymetric top molecules but the assymetry is very small: they are therefore almost prolate symmetric top molecules with the dipole moment along the A-axis. The notation for the transitions is J, K_a, K_c.

For H_2CO:

$g_J=(2J+1)$ K_a is even : para transitions
$g_J=3(2J+1)$ K_a is odd : ortho transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-para})/kT_{ex}}$ where $E_{0-para}=0$ K
$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-ortho})/kT_{ex}}$ where $E_{0-ortho} = 15.16$ K
4829.6600 .0010 -5.9024 3 10.5390 9 -30004 303 1 1 0 1 1 1
72837.9480 .0100 -4.1792 3 .0000 3 -30004 303 1 0 1 0 0 0

For D_2CO:

$g_J=6(2J+1)$ K_a is even : ortho transitions
$g_J=3(2J+1)$ K_a is odd : para transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-para})/kT_{ex}}$ where $E_{0-para} = 8.05$ K
$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-ortho})/kT_{ex}}$ where $E_{0-ortho} = 0$ K
6096.0673 .0039 -6.2883 3 5.5983 9 32006 303 1 1 0 1 1 1
58468.6700 .1000 -4.1897 3 .0000 18 -32006 303 1 0 1 0 0 0

4) H_2D^+ and D_2H^+

These molecules are asymmetric top molecules. The notation for the transitions is J, K_a, K_c.

For D_2H^+:

$g_I=6(2I+1)$ ΣK even : ortho transitions (warning: different from the documentation file in the CDMS catalog)
$g_I=3(2I+1)$ ΣK odd : para transitions (warning: different from the documentation file in the CDMS catalog)
The partition function for the ortho transitions will be different than the one for the para transitions. This is necessary in order to estimate the main beam temperature from a column density of a line or to determine the column density from an observation. The need is all the more important as the energy difference between the zero level for the ortho transitions and the zero level for the para transitions is large (see Figure 3).
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-para})/kT_{ex}}$
$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i - E_{0-ortho})/kT_{ex}}$
where E_{0-para} is the fundamental energy of the para level (50.2 K) and $E_{0-ortho}$ is the fundamental energy of the ortho level (0 K).

$Q_{para}(T_{ex}=8K)=9.1$ $Q_{ortho}(T_{ex}=8K)=6.00$
$Q_{para}(T_{ex}=10K)=9.3$ $Q_{ortho}(T_{ex}=10K)=6.02$
$Q_{para}(T_{ex}=12K)=9.6$ $Q_{ortho}(T_{ex}=12K)=6.05$
$Q_{para}(T_{ex}=15K)=10.0$ $Q_{ortho}(T_{ex}=15K)=6.16$

For H_2D^+:

$g_I=3(2I+1)$ K_a odd : ortho transitions
$g_I=1(2I+1)$ K_a even : para transitions
$Q_{para}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-para})/kT_{ex}}$
$Q_{ortho}(T_{ex})=\Sigma g_i e^{-(E_i-E_{0-ortho})/kT_{ex}}$
where E_{0-para} is the fundamental energy of the para level (0 K) and $E_{0-ortho}$ is the fundamental energy of the ortho level (86.4 K).

$Q_{para}(T_{ex}=8K)=1.00$ $Q_{ortho}(T_{ex}=8K)=9.96$
$Q_{para}(T_{ex}=10K)=1.00$ $Q_{ortho}(T_{ex}=10K)=10.51$
$Q_{para}(T_{ex}=12K)=1.01$ $Q_{ortho}(T_{ex}=12K)=11.03$
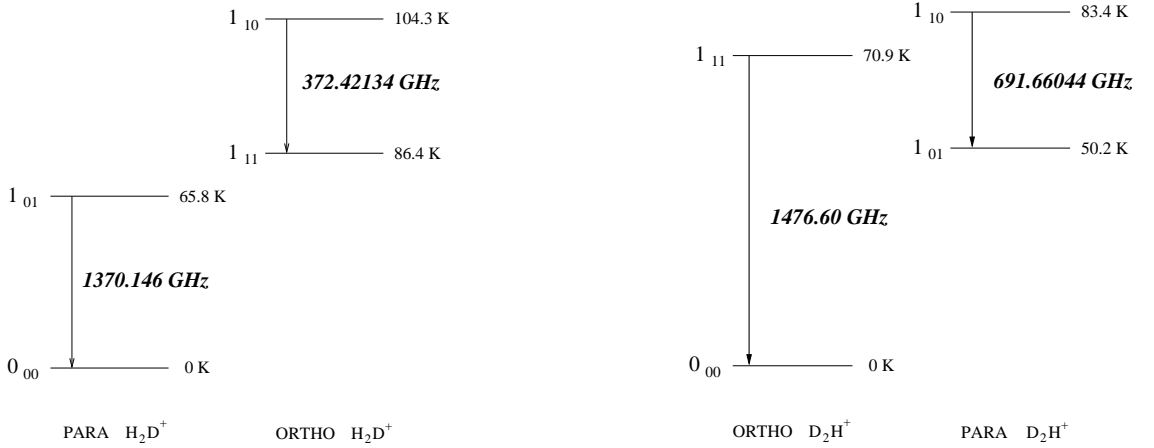$Q_{para}(T_{ex}=15K)=1.04$ $Q_{ortho}(T_{ex}=15K)=11.74$

Figure 3: Lower energy transitions for the H_2D^+ and D_2H^+ molecules.

III. Absorption lines

The determination of column densities from absorption lines is more accurate in general, with respect to the quantities inferred from the analysis of emission lines, because the calculated value does not depend on the excitation temperature of the line, T_{ex}, as long as this is negligeable with respect to the temperature of the background continuum source T_c.

$$N_{tot} = \frac{8\pi\nu^3}{A_{ul}c^3}\Delta v\frac{\sqrt{\pi}}{2\sqrt{\ln 2}}\frac{g_l}{g_u}\tau_0 \tag{42}$$

and,

$$\tau_0 = -\ln(1 - \frac{T_{abs}}{T_C}) \tag{43}$$

where τ_0 is the opacity at the line center, T_{abs} is the temperature of the absorption line and T_C is the temperature of the continuum. The opacity profile is defined as 38. Using T(v) (with the 0 K level reference) we get $T(v) = T_C - T_{abs}(v)$. Absorption lines can then be determined (see Figure 4).

CASSIS take into account the background continuum and the excitation temperature of the lines (see section I) to determine the line intensity (see equation 29):

$$T_b = T_C e^{-\tau} + (1 - e^{-\tau})(J_\nu(T_{ex}) - J_\nu(CMB)) \tag{44}$$

Since N_{tot} can be computed as (see section I):

$$N_{tot} = \frac{8\pi\nu^3}{A_{ul}c^3}\Delta v\frac{\sqrt{\pi}}{2\sqrt{\ln 2}}\frac{\tau_0 Q(T_{ex})}{g_u}\frac{\exp(E_u/kT_{ex})}{[\exp(h\nu/kT_{ex}) - 1]} \tag{45}$$

then, the opacity is deduced and therefore the line profile. NB: E_u is the upper level of the transition compared to the ground level (different from zero when orho, para or meta forms).

Towards SgrB2(M), we get a continuum of $\sim$ 1920 Jy around 692 GHz in a 30" beam and $\sim$ 4000 Jy around 1476 GHz in a 20" beam (Goldsmith, Lis, Hill, Lasenby 1990). The HIFI beam width is $\sim$ 30" at 692 GHz and $\sim$ 13" at 1476 GHz. The conversion from source flux density to antenna temperature is:

$S_\nu(\text{Jansky}) = T_a(K)/(\eta\pi\ D(cm)^2/8k) = 3520 \times \frac{T_A(K)}{\eta_A(D(meters))^2}$

This corresponds, for the Herschel dish diameter of 3.5 m, to a continuum of about 5 K at 692 GHz and $\sim$ 10 K at 1476 GHz.

For a 1.3 10^{13} cm^{-2} D$_2$H$^+$ column density, with FWHM=1 km/s, we get:
1) at 691 GHz, $\tau \sim 0.2$ and $\frac{T_{abs}}{T_C} \sim 0.2$
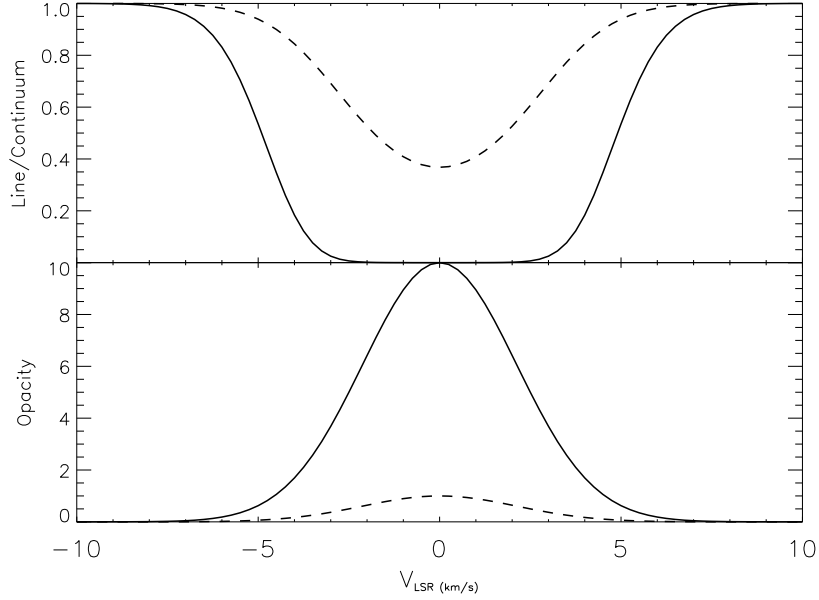2) at 1476 GHz, $\tau \sim 0.36$ and $\frac{T_{abs}}{T_C} \sim 0.3$

Figure 4: Example of absorption lines. The upper plot represents 2 absorption features with an opacity of 10 (plain line) and with an opacity of unity (dashed-line), with a linewidth of 5 km s^{-1} and a continuum normalized to unity. The lower plot represent the opacity profiles for the same lines.

Laboratory measurements: gas cells

The informations concerning the physical conditions in the environment can be deduced from the shape of the observed lines. There are several cause of line broadening, the main being:

Natural broadening: The Uncertainty principle relates the life of an excited state with the precision of the energy, so the same excited level will have slightly different energies in different atoms. This broadening effect is described by a Lorentzian profile.

Thermal Doppler broadening: Atoms will have different thermal velocities, so they will see the photons red or blue shifted, absorbing photons of different energies in the frame of reference of the observer. The higher the temperature of the gas, the larger the velocity differences (and velocities), and the broader the line. This broadening effect is described by a Doppler profile.

Pressure broadening: the collision of other particles with the emitting particle interrupts the emission process. The duration of the collision is much shorter than the lifetime of the emission process. This effect depends on the density of the gas. The broadening effect is described by a Lorentzian profile.

Opacity broadening: considerable reabsorption of emission line photons, an effect known as opacity, often causes line broadening. The line is broadened

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since photons at the line wings have a smaller reabsorption probability than photons at the line center (see previous section).

The combined line profile will be the convolution of the line profiles of each mechanism. For example, a combination of thermal Doppler broadening and pressure broadening will yield a Voigt profile. The natural broadening is usually too small to be taken into account. the Voigt profile must be evaluated by numerical integration.

Let's consider a Lorentzian profile f_L and a Gaussian profile f_G. The resulting line shape will result in a Voigt profile f_V, which can be expressed as the convolution of the first two:

$$f_\nu(\nu - \nu_0, \delta\nu_L, \delta\nu_D) \;=\; f_L \;\otimes\; f_G \;=\; \frac{\sqrt{\ln 2a}}{\pi^{3/2}} \int_{-\infty}^{+\infty} \frac{[-(\ln 2)(\nu' - \nu_0)^2/\delta\nu_D^2]}{(\nu - \nu')^2 + \delta\nu_L^2} d\nu' \quad (46)$$

where $\delta\nu_L$ and $\delta\nu_D$ are half-widths of the Lorentzian and Gaussian profiles respectively, ν is the source frequency, ν_0 is the frequency of the line center and a is the ratio of the profiles width $(\delta\nu_L/\delta\nu_D)$. We used the Liu et al. (2001) empirical analytical approximation to determine the Voigt profile:

$$f_V(\nu - \nu_0, \delta\nu_V) = c_L f_L(\nu - \nu_0, \delta\nu_V) + c_G f_G(\nu - \nu_0, \delta\nu_V) \quad (47)$$

$$= c_L \frac{1}{\pi} \frac{\delta\nu_V}{(\nu - \nu_0)^2 + \delta\nu_V^2} + c_G \frac{\sqrt{\ln 2}}{\sqrt{\pi}\delta\nu_V} \exp\left(\frac{-(\ln 2)(\nu - \nu_0)^2}{\delta\nu_V^2}\right) \quad (48)$$

From Olivero and Longbothum (1977, J. Quant. Spectrosc. Radiati. Transfer):

$$\delta\nu_V = 0.5346\delta\nu_L + \sqrt{0.2166\delta\nu_L^2 + \delta\nu_D^2} \quad (49)$$

Introducing a dimensionless parameter, d=$(\delta\nu_L-\delta\nu_D)/(\delta\nu_L+\delta\nu_D)$, the weigth coefficients are given by:

$$c_L = f_1(d) \;, \qquad c_G = f_2(d) \quad (50)$$

where d is the profile parameter. If d=1 (-1 respectively), we obtain a pure Lorentz profile (Gaussian respectively).

Liu et al. (2001) found from the fitting on 2 molecules that:

$$c_L = 0.68188(17) + 0.61293(31) \times d - 0.18384(39) \times d^2 - 0.11568(44) \times d^3 \quad (51)$$

$$c_G = 0.32460(17) - 0.61825(31) \times d + 0.17681(39) \times d^2 + 0.12109(44) \times d^3 \quad (52)$$

The pressure broadening can be obtained from the HITRAN database. After selecting the molecule and the spectral range you need, the JavaHAWKS software will produce a file output. This file is read by CASSIS as "File output from HITRAN". The γ_{self} parameter (in cm^{-1}.atm^{-1} at 296 K) is then extracted and converted for the needed temperature T and pressure P.

$$\delta\nu_L = \gamma_{self} \times \frac{P(mbar)}{1013.25} \times 299792.45810^5 \times \frac{T}{296} \quad (53)$$

The probability that a molecule in a gas at temperature T has a velocity v in a particular direction is proportional to exp(-mv^2/2kT), where m is the molecular mass. Consequently the line is symmetric and has a half width at half maximum of:

$$\delta\nu_D = \frac{\nu_0}{c}\sqrt{\frac{2(\ln 2)kT}{m}} \qquad (54)$$

Determining the line profile, the absorption coefficient α_{max} (in units of cm^{-1}) can be obtained from I$_{ba}$:

$$\alpha_{max}[L^{-1}] = H[L^2] \times n[L^{-3}] \qquad (55)$$

where H is the line strength, L is the length of the gas cell and n is the density in the gas cell (=P/kT). H can be expressed as a function of I$_{ba}$ (in nm^2.MHz; based on the integral of the absorption cross-section over the spectral line shape: see figure 5):

$$I_{ba} = H \times [\pi\delta\nu_L + \sqrt{\frac{\pi}{ln2}}\delta\nu_D] \qquad (56)$$

Then, we get:

$$\alpha_{max} = H \times n = \frac{I_{ba}}{\pi\delta\nu_L + \sqrt{\frac{\pi}{ln2}}\delta\nu_D} \times \frac{P}{kT} \qquad (57)$$

The power transmission through a uniform medium of length L at the peak of the line is exp(-α_{max}L). The opacity can be computed as α_{max}L.

Example: ^{12}CO (4-3) transition at 461040.7682 MHz, in a 102.54 cm length cell, at T=300 K, and P=3.3 mB [1]. From the HITRAN database $\delta\nu_L = 7451480.17$ Hz. At T=300K $\delta\nu_D = 1076200.38$ Hz.

$$\alpha_{max} = \frac{10^{-3.2657}}{(\pi\delta_L + \sqrt{\frac{\pi}{ln2}}\delta_D) \times 3.02284} \times \frac{3.310^3}{1.3810^{-16} \times 300} \times 10^{-18} \times 10^{-2} \qquad (58)$$

The opacity is then about 0.018 cm^{-1} × 102.54 cm=1.83. In Figure 6 we present a comparaison between the laboratory measure and the result from a convolution between a Gaussian profile (thermal Doppler broadening) and a Lorentzian profile (pressure broadening) assuming that the opacity is equal to . We see that we can't reproduce the observed profile with the given parameters.

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[1] 1 bar = 10^6 baryes, 1 mmHg = 0.00133 bar, 1 Torr = 1mm Hg, 760 mm Hg = 101325 Pa=1 atm=1013.25 mbar. The cgs unit for pressure is barye (1 mB = 10^3 barye).
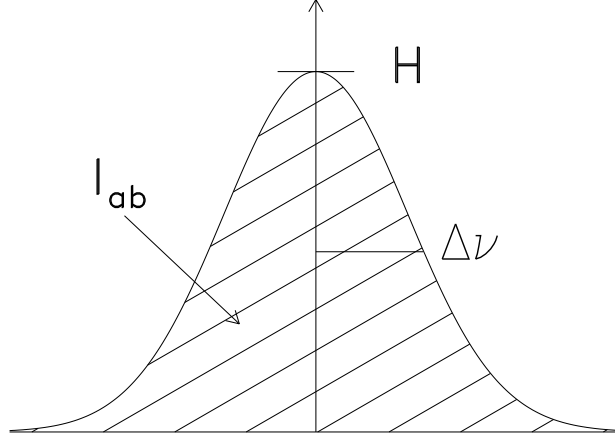
Figure 5: Gaussian line profile, with height H, and half width at half maximum $\delta\nu$ and the integrated profile represented by the I_{ab} parameter (in $nm^2.MHz$) from the JPL and CDMS catalogues.
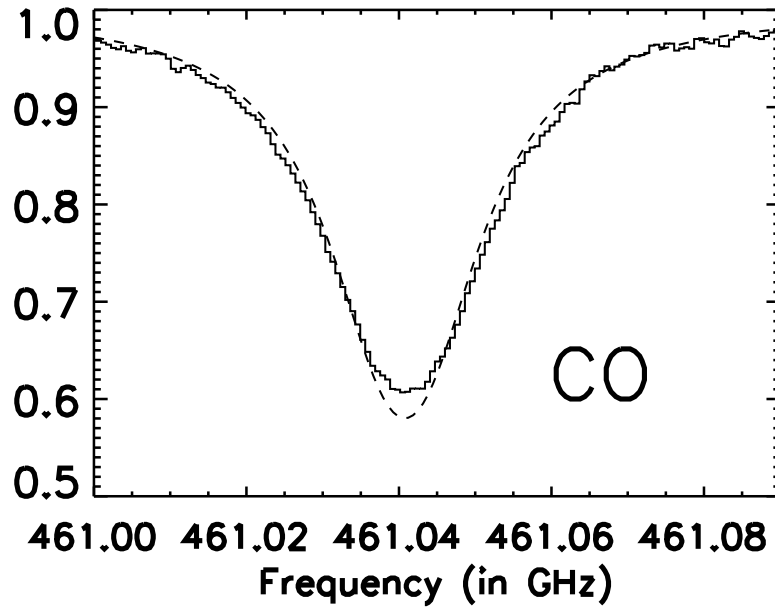

Figure 6: Comparaison between the observed HIFI spectrum (plain line) and the modeled line using the conditions in the gas cell (dashed-line).

IV. Rotational diagram

This term refers to a plot of the column density per statistical weight of a number of molecular energy levels, as a function of their energy above the ground state. In LTE, this corresponds to a Boltzmann distribution, so a plot of the natural logarithm of N_u/g_u versus E_u/k yields a straight line with a slope of $1/T$. The temperature inferred represents the excitation temperature.

From Chapter I., we can write the optical depth of the transition as:

$$\tau = \frac{c^3 A_{ul} N_u}{8\pi\nu^3 \Delta v \sqrt{\pi}/2\sqrt{ln2}}[e^{h\nu/kT_{ex}} - 1] \tag{59}$$

Neglecting the 2.7 K radiation ($h\nu/k \gg 2.7$), we can express the main beam temperature as:

$$T_b = \frac{h\nu}{k}\frac{1}{exp(h\nu/kT_{ex}) - 1}\frac{1 - e^{-\tau}}{\tau} \times \tau \tag{60}$$

Therefore, we can compute the column density in the upper state as:

$$N_u = \int T_b dv \times \frac{8\pi k\nu^2}{hc^3 A_{ul}} \times \frac{\tau}{1 - e^{-\tau}} \tag{61}$$

$$N_u = W \times \frac{8\pi k\nu^2}{hc^3 A_{ul}} \times C_\tau \tag{62}$$

Where W in the integrated area and C_τ is the optical depth correction factor. When the line is optically thin, C_τ is equal to unity.

For a molecule in LTE, all excitation temperatures are the same, and the population of each level is given by:

$$N_u = \frac{N_{tot}}{Q(T_{ex})}g_u e^{-E_u/kT_{ex}} \tag{63}$$

We can rewrite this equation to obtain:

$$ln\frac{N_u}{g_u} = lnN_{tot} - lnQ(T_{ex}) - \frac{E_u}{kT_{ex}} \tag{64}$$

A rotational diagram can be useful to determine whether the emission is optically thick or thin, whether the level populations are described by LTE, and to determine what temperature describe the population distribution in the event that LTE applies. Equation 64 can be written in terms of the observed integrated area W:

$$ln\frac{8\pi k\nu^2 W}{hc^3 A_{ul} g_u} = lnN_{tot} - lnC_\tau - lnQ(T_{ex}) - \frac{E_u}{kT} \tag{65}$$

If we don't take into account the C_τ factor, each of the upper level populations would be underestimated by a factor C_τ, different for each transition. Therefore, the ordinate of the rotation diagram would be below its correct value by the factor ln C_τ. A change in the temperature for lines of different excitation might indicate that the source has different temperature components or that the lines considered are not optically thin and cannot be easily used to obtain a meaningful excitation temperature.

V. Telescopes parameters

By defining the flux density per beam as $S_{\nu,b}=K \times S_{\nu,tot}$ (K being the correction factor: Baars 1973) we get:

$$S_{\nu,b} = \frac{2kT'_A}{A_{eff}} \tag{66}$$

where T$'_A$ is the antenna temperature, only corrected for atmospheric losses:

$$T'_A = T_A exp(-\tau_z A) \tag{67}$$

where τ_z is the opacity at the zenith, and A is the air mass (1/sin(elevation)). It can be converted into antenna temperature (T$^*_A$), corrected for atmospheric attenuation, the forward efficiency and the signal band gain:

$$T'_A = T^*_A \times F_{eff} \tag{68}$$

where F$_{eff}$ is the forward efficiency. The main beam temperature is then the temperature of an equivalent source just filling the main beam:

$$T_{mb} = \frac{F_{eff}}{B_{eff}}T^*_A = \frac{T'_A}{B_{eff}} \tag{69}$$

In equation 66, A$_{eff}$ is the effective antenna area defined by the product between the aperture efficiency η_A and the geometrical area of the aperture, A$_{geom}=\pi(D/2)^2$ where D is the diameter of the telescope. η_A is the ratio of the strength of the signal received from a point source to that which would have been received by a telescope of the same diameter that had no losses or blockage, having uniform illumination, and no surface errors.
Then equation 66 becomes:

$$S_{\nu,b} = \frac{2kT_{mb}B_{eff}}{\eta_A\pi(D/2)^2} \tag{70}$$

in erg/s/cm^2/Hz. Note that 1 Jansky = 10^{-23} erg s^{-1} cm^{-2} Hz^{-1}.
To compare with flux in erg/s/cm^2, we have to multiply this equation by $\Delta\nu=\Delta$v $\times \nu$/c.

$$Flux(erg/s/cm^2) = \frac{2kT_{mb}B_{eff}}{\eta_A\pi(D/2)^2} \times \Delta v \times \frac{\nu}{c} \tag{71}$$

Which means that:

$$T_{mb}\Delta v = Flux(erg/s/cm^2) \times \frac{\pi(D/2)^2}{2k} \times \frac{c}{\nu} \times \frac{\eta_A}{B_{eff}} \tag{72}$$

Another way to compute it is using the Rayleigh-Jeans approximation:

$$B_\nu = \frac{2\nu^2}{c^2}\Omega kT_{mb} \tag{73}$$

$$B_\nu = \frac{2k}{\lambda^3}\Omega \int T_{mb}dv \qquad in \ erg/s/cm^2 \tag{74}$$

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Then:
$$\int T_{mb}dv = Flux(erg/s/cm^2) \times \frac{c^3}{\nu^3} \times \frac{1}{2k\Omega} \qquad (75)$$

For HIFI, with an effective aperture of 3.28 m:
1) telescope apperture efficiency = 64 % at 1.9 THz and 72 % at 500 GHz
leading to a conversion factor of 511 Jy per Kelvin (in T_a^*) at 1.9 THz, and 454 Jy per Kelvin (in T_a^*) at 500 GHz.
2) telescope main beam efficiency = $\sim$ 90 %
leading to a conversion factor of 460 Jy per Kelvin (in T_{mb}) at 1.9 THz, and 408 Jy per Kelvin (in T_{mb}) at 500 GHz..

VI. References

- Kraus (RadioAstronomy, 1986)

- Rohlfs & Wilson (Tools of Radio Astronomy)

- C. Kramer: Calibration of Spectral Line Data at the IRAM 30m Radio
  Telescope, 1997:
  http://www.iram.fr/IRAMES/otherDocuments/manuals/Report/cali_rep_ddo970205.ps

- H. M. Pickett, R. L. Poynter, E. A. Cohen, M. L. Delitsky, J. C. Pearson, and
  H. S. P. Muller; J. Quant. Spectrosc. Radiat. Transfer 60 (1998) 883 890.