

Modeling the molecular rotational transitions of gas components with Gaussian velocity distributions

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1. Introduction

This essay describes how to model the molecular rotational spectra of a gas tracer given its basic physical properties (e.g. column density, excitation temperature, velocity dispersion, etc.). Most of the theoretical framework of this essay is referred to Mangum & Shirley (2015), PASP, 127:266 (hereafter Paper I). Based on the algorithm described in this essay I built a Python package `spectra_rot` dedicated to fit the spectral data and derive the relevant physical properties.

2. Symbols

The symbols used throughout the essay are listed below.

Symbol	Type	Description
J	Transitional	Total angular momentum quantum number.
K	Transitional	Projected angular momentum quantum number.
E_u	Transitional	Upper energy level.
ν_0	Transitional	Rest frequency of the transition.
δv_j	Transitional	Velocity shift of the j th hyperfine line relative to ν_0 . Radio velocity convention used.
R_j	Transitional	Relative strength of the j th hyperfine line. $\sum_j R_j = 1$.
S	Transitional	Line strength.
g_J, g_K, g_I	Transitional	Degeneracies related to the J, K, I (nuclear spin) quantum numbers.
g_u	Transitional	Degeneracy of the upper energy level, $\equiv g_{J_u} g_{K_u} g_{I_u}$
Q_{rot}	Transitional	Rotational partition function.
μ	Molecular	Electric dipole moment of a molecule.
A_0, B_0, C_0	Molecular	Rigid rotor constants of a molecule.
σ	Molecular	Symmetry number of a molecule.
N	Macroscopic	Total column density of a gas tracer.
T_{ex}	Macroscopic	Excitation temperature of a gas tracer.
v_0	Macroscopic	Central line-of-sight velocity of a Gaussian velocity component.
σ_v	Macroscopic	1- σ velocity dispersion of a Gaussian velocity component.
T_{bg}	Macroscopic	Background brightness temperature.

3. Assumptions

The following assumptions and restrictions are made for the rotational transition model.

1. Only linear or symmetric top molecules were considered in this essay.
2. There are no interactions between the different kinds of quantum energy states of the molecule, and the molecule is in ground states of electronic and vibrational energies. In this way, $Q_e = Q_v = 1$ and $Q_{\text{rot}} = Q_r Q_n$.

3. Rigid rotor approximation.
4. McDowell's approximation for calculating Q_{rot} (see below).
5. For symmetric top molecules, we are only interested in one nuclear spin state (e.g. para- NH_3), i.e. $g_I = 1$.
6. The gas materials along the line-of-sight (los) can be decomposed into multiple components with Gaussian los velocity profile

$$f_i(v) = \frac{1}{\sigma_{vi} \sqrt{2\pi}} e^{-\frac{(v-v_{0i})^2}{2\sigma_{vi}^2}}. \quad (1)$$

7. All the velocity components share the same T_{ex} (Otherwise the information of the 3D gas distribution is needed to integrate the radiative transfer equation).

4. Theory

In this section we derive the modeled spectral intensity as a function of los velocity, $\Delta I_\nu(v)$, given the parameters $\{T_{\text{ex}}, N_i, v_{0i}, \sigma_{vi}\}$ of the velocity components and the constants related to the transition and the molecule.

According to Eq. 32 of Paper I (see their derivations), the opacity of the j th hyperfine line of the i th velocity component as a function of v can be written as

$$\tau_{\nu ij}(v) = \frac{4\sqrt{2}\pi^{5/2} S \mu^2 R_j g_u}{3h\sigma_{vi} Q_{\text{rot}}(T_{\text{ex}})} N_i e^{-\frac{(v-v_{0i}-\delta v_j)^2}{2\sigma_{vi}^2} - \frac{E_{\text{u}}}{k_{\text{B}} T_{\text{ex}}}} \left(e^{\frac{h\nu_0}{kT_{\text{ex}}}} - 1 \right). \quad (2)$$

The total opacity

$$\tau_\nu(v) = \sum_{ij} \tau_{\nu ij}(v). \quad (3)$$

The intensity

$$\Delta I_\nu(v; T_{\text{ex}}, N_i, v_{0i}, \sigma_{vi}, T_{\text{bg}}) = (B_\nu(T_{\text{ex}}) - B_\nu(T_{\text{bg}})) (1 - e^{-\tau_\nu(v)}). \quad (4)$$

Now we calculate the constants of the transitions for **linear and symmetric top** molecules.

4.1 Line strength S

1. For $(J, K) - (J-1, K)$ transitions,

$$S = \frac{J^2 - K^2}{J(2J+1)}. \quad (5)$$

2. For $(J, K) - (J, K)$ transitions,

$$S = \frac{K^2}{J(J+1)}. \quad (6)$$

3. For $(J, K) - (J+1, K)$ transitions,

$$S = \frac{(J+1)^2 - K^2}{(J+1)(2J+1)}. \quad (7)$$

For linear molecules, set $K = 0$ for the above equations.

4.2 Degeneracy g_u

Degeneracy of the upper energy state $g_u \equiv g_{J_u} g_{K_u} g_{I_u}$. For linear and symmetric top molecules, $g_{J_u} = 2J_u + 1$. For $K = 0$ or linear molecules, $g_{K_u} = 1$; for $K \neq 0$ in symmetric top molecules, $g_{K_u} = 2$. If you are only interested in one nuclear spin state (e.g. para-NH₃), $g_{I_u} = 1$.

4.3 Rotational partition function

With assumption 2 in Sect. 3,

$$Q_{\text{rot}} = Q_{\text{r}} Q_{\text{n}} = \sum_{J,K,I} g_J g_K g_I e^{-\frac{E_{JK}}{k_B T_{\text{ex}}}}. \quad (8)$$

Here we use McDowell's approximation (see the references in Paper I) to evaluate Q_{rot} . For linear molecules,

$$Q_{\text{rot,linear}} \approx \frac{k_B T_{\text{ex}}}{hB_0} e^{\frac{hB_0}{3k_B T_{\text{ex}}}}. \quad (9)$$

This equation is more accurate at higher temperatures. For $\frac{hB_0}{k_B T_{\text{ex}}} < 0.2$, error is less than 0.01%.

For symmetric top molecules,

$$Q_{\text{rot,sym}} \approx \frac{\sqrt{m\pi}}{\sigma} e^{\frac{hB_0(4-m)}{12k_B T_{\text{ex}}}} \left(\frac{k_B T_{\text{ex}}}{hB_0} \right)^{3/2} \left[1 + \frac{1}{90} \left(\frac{hB_0(1-m)}{k_B T_{\text{ex}}} \right)^2 \right], \quad (10)$$

where $m = B_0/A_0$ for prolate molecules and $m = B_0/C_0$ for oblate molecules. For the calculation of σ , see Sect. 2 of [this paper](#).

5. Numerical implementation

This section describes how the spectral model (essentially Eq. 2, 4, 9, 10) is numerically evaluated in `spectra_rot`. We introduce the following dimensionless intermediate variables.

$$C_N = \frac{4\sqrt{2}\pi^{5/2} S\mu^2 R_j g_u}{3h} \frac{\text{cm}^{-2}}{\text{km s}^{-1}} \quad (11)$$

$$C_{T1} = \frac{E_u}{k_B \text{K}} \quad (12)$$

$$C_{T2} = \frac{h\nu_0}{k_B \text{K}} \quad (13)$$

$$C_I = \frac{2h\nu_0^3}{c^2} \frac{1}{\text{Jy sr}^{-1}} \quad (14)$$

$$C_{Q1} = \frac{hB_0}{k_B \text{K}} \quad (15)$$

$$C_{Q2} = \frac{\sqrt{m\pi}}{\sigma} \left(\frac{k_B \text{K}}{hB_0} \right)^{3/2} \quad (16)$$

$$C_{Q3} = \frac{hB_0(4-m)}{12k_B \text{K}} \quad (17)$$

$$C_{Q4} = \frac{1}{90} \left(\frac{hB_0(1-m)}{k_B \text{K}} \right)^2 \quad (18)$$

Eq. 2, 4, 9, 10 can be numerically expressed as the following equations, respectively.

$$\tau_{vij}(v) = C_N \left(\frac{N_i}{\text{cm}^{-2}} \right) \left(\frac{\sigma_{vi}}{\text{km s}^{-1}} \right)^{-1} \frac{1}{Q_{\text{rot}}(T_{\text{ex}})} e^{-\frac{(v-v_{0i}-\delta v_j)^2}{2\sigma_{vi}^2} - C_{T1} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} \left(e^{C_{T2} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} - 1 \right) \quad (19)$$

$$\frac{\Delta I_\nu(v)}{\text{Jy sr}^{-1}} = C_I \left(\frac{1}{e^{C_{T2} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} - 1} - \frac{1}{e^{C_{T2} \left(\frac{T_{\text{bg}}}{\text{K}} \right)^{-1}} - 1} \right) (1 - e^{-\tau_\nu(v)}) \quad (20)$$

$$Q_{\text{rot,linear}} = \frac{1}{C_{Q1}} e^{\frac{C_{Q1}}{3} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} \quad (21)$$

$$Q_{\text{rot,sym}} = C_{Q2} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{1.5} e^{C_{Q3} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} \left[1 + C_{Q4} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-2} \right] \quad (22)$$

We can also calculate the modeled spectrum in brightness temperature

$$T_b = C_{T2} \ln^{-1} \left[1 + (1 - e^{-\tau_\nu})^{-1} \left(\frac{1}{e^{C_{T2} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} - 1} - \frac{1}{e^{C_{T2} \left(\frac{T_{\text{bg}}}{\text{K}} \right)^{-1}} - 1} \right)^{-1} \right]. \quad (23)$$

For the optically thin limit, replace $(1 - e^{-\tau_\nu})$ with τ_ν in Eq. 4, 20, 23.

The mean opacity of a velocity component, $\bar{\tau}_i$, can be given as

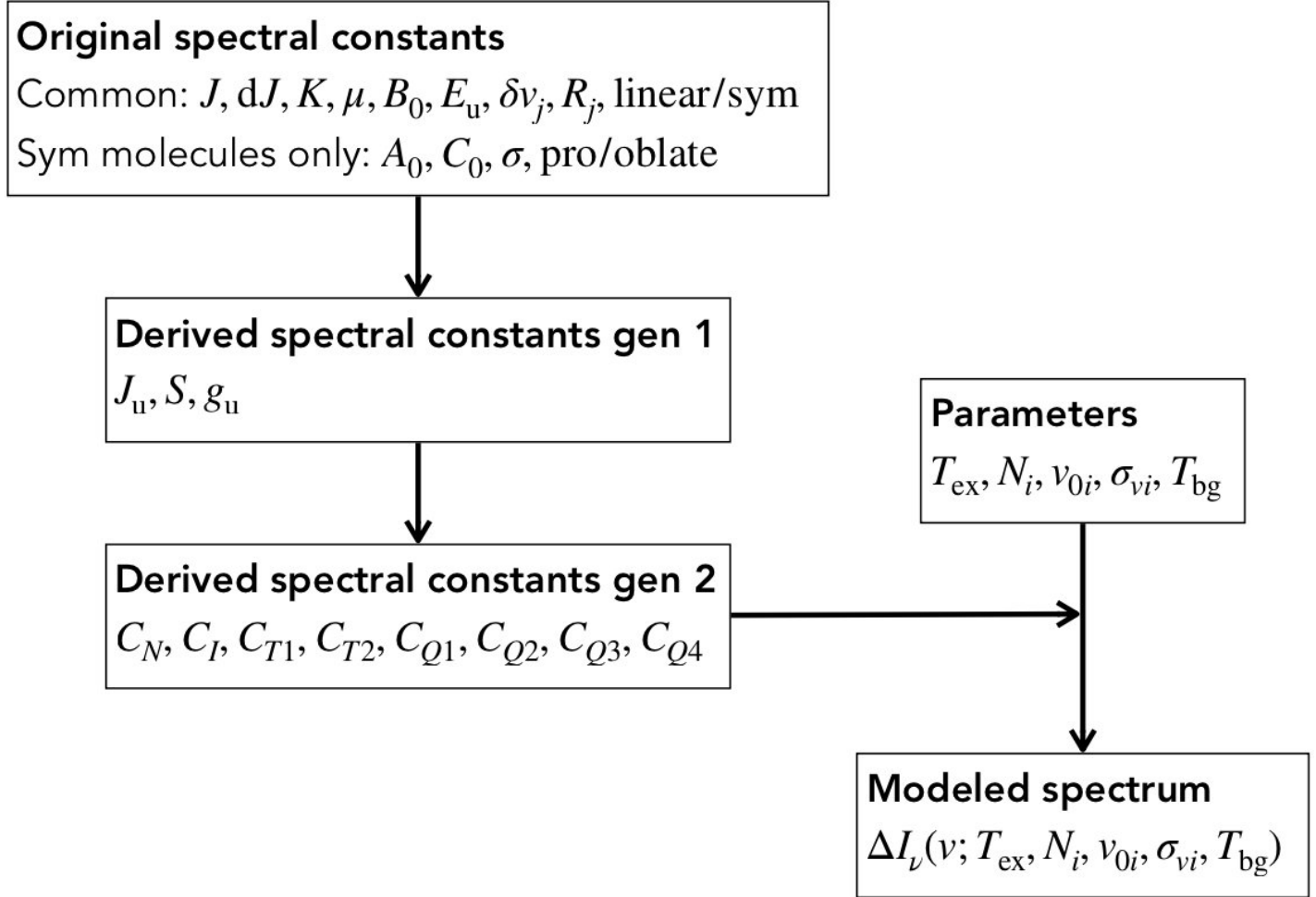
$$\begin{aligned} \bar{\tau}_i &= \frac{1}{2\sqrt{2\ln 2}\sigma_{vi}} \int \sum_j \tau_{vij}(v_i) dv = \\ &= \frac{\sqrt{\pi}}{2\sqrt{\ln 2}} \sum_j C_{Nj} \left(\frac{N}{\text{cm}^{-2}} \right) \left(\frac{\sigma_v}{\text{km s}^{-1}} \right)^{-1} \frac{1}{Q_{\text{rot}}(T_{\text{ex}})} e^{-C_{T1} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} \left[e^{C_{T2} \left(\frac{T_{\text{ex}}}{\text{K}} \right)^{-1}} - 1 \right]. \end{aligned} \quad (24)$$

In this way Eq (3) can be written as

$$\tau_\nu(v) = 2\sqrt{\frac{\ln 2}{\pi}} \sum_{ij} R_j \bar{\tau}_i e^{-\frac{(v-v_{0i}-\delta v_j)^2}{2\sigma_{vi}^2}}. \quad (25)$$

If you want to calculate the mean opacity within a velocity range Δv (e.g. a velocity channel), replace σ_v in Eq (24) with $\Delta v/(2\sqrt{2\ln 2})$.

6. Diagram of `spectra_rot`



7. Some discussions

Here we discuss the behavior of the peak intensity $\Delta I_{\nu,p}$ of the modeled spectrum as a function of N and T_{ex} . For simplicity we make the following restrictions.

1. Only consider linear molecules.
2. One velocity component and one hyperfine line.
3. $T_{\text{bg}} = 0$.

In this way $\Delta I_{\nu,p}(N)$ is similar to the function $1 - e^{-x}$, which saturates at high N . $\Delta I_{\nu,p}(T'_{\text{ex}})$ is similar to the function $(1 - e^{-1/x(e^{1/x}-1)})/(e^{1/x} - 1)$. When $x \gg 1$ (high T_{ex}), it is close to $1/x$; when $x \ll 1$ (low T_{ex}), it is close to $e^{-1/x}$. These functions are demonstrated below.

