

Derivation of the total column of a dipole molecule assuming LTE

I derive the total column density of a dipole molecule assuming LTE and $\tau \ll 1$, which are standard assumptions for many molecules, particularly CO isotopologues (or is it isotopomers? can never remember...) and ^{12}CO in outflow line wings. I then show a few examples for CO.

This exercise has previously been performed for the CO 1-0 line in Bourke et al. (1997); Garden et al. (1991); Cabrit & Bertout (1990), and probably many others, but to the best of my knowledge has not been done for higher transitions.

1. Radiative Transfer in a Dipole Line

Equation of Radiative Transfer (Wilson et al. 2009, eqn 1.9):

$$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + \epsilon_\nu \quad (1)$$

Definition of optical depth (Wilson et al. 2009, eqn 1.15):

$$d\tau_\nu = -\kappa_\nu ds \quad (2)$$

Spontaneous Emission (Wilson et al. 2009, eqn 12.15): n_u is the volume density of molecules in the upper state.

$$\epsilon_\nu = \frac{h\nu_{ul}A_{ul}n_u}{4\pi}\varphi(\nu) \quad (3)$$

Absorption:

$$dE = -\frac{h\nu_{ul}B_{lu}n_l}{c}I_\nu \varphi(\nu) \quad (4)$$

Stimulated Emission:

$$dE = \frac{h\nu_{ul}B_{ul}n_u}{c}I_\nu \varphi(\nu) \quad (5)$$

From (1), κ_ν should be the leading factor in front of I_ν . This is how Wilson et al. (2009) eqn 12.17 is derived.

$$\kappa_\nu = \frac{h\nu_{ul}B_{ul}n_u}{c}\varphi(\nu) - \frac{h\nu_{ul}B_{lu}n_l}{c}\varphi(\nu) \quad (6)$$

The A and B values are related by

$$A_{ul} = \frac{8\pi h\nu_{ul}^3}{c^3}B_{ul} \quad (7)$$

and

$$B_{ul} = \frac{g_l}{g_u}B_{lu} \quad (8)$$

In LTE, Kirchoff's law is equal to the blackbody function (Wilson et al. 2009, eqns 1.14, 12.8, 12.9)

$$\frac{\epsilon_\nu}{\kappa_\nu} = \frac{2h\nu^3}{c^2} \left(\frac{g_u n_l}{g_l n_u} - 1 \right)^{-1} = \frac{2h\nu^3}{c^2} \left[\exp \left(\frac{h\nu}{k_B T} \right) - 1 \right]^{-1} \quad (9)$$

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp \left(\frac{-h\nu_{ul}}{k_B T_{ex}} \right) \quad (10)$$

Plugging equations (10) and (7) into (6) we get Wilson et al. (2009) equation 12.17:

$$\kappa_\nu = \frac{c^2}{8\pi\nu_{ul}^2} \frac{g_u}{g_l} n_l A_{ul} \left[1 - \exp \left(\frac{-h\nu_{ul}}{k_B T_{ex}} \right) \right] \varphi(\nu) \quad (11)$$

However, that is not the most useful form of the equation, since we observe *emission*, which is the transition from the upper to lower state; equation 12.17 makes sense theoretically because it is defining an absorption coefficient. This form is more useful (where we have replaced n_l with n_u using (10)):

$$\kappa_\nu = \frac{c^2}{8\pi\nu_{ul}^2} n_u A_{ul} \left[\exp \left(\frac{h\nu_{ul}}{k_B T_{ex}} \right) - 1 \right] \varphi(\nu) \quad (12)$$

We then return to the optical depth (2) and integrate over ν :

$$\int \tau_\nu d\nu = \frac{c^2}{8\pi\nu_{ul}^2} A_{ul} \left[\exp \left(\frac{h\nu_{ul}}{k_B T_{ex}} \right) - 1 \right] \int \varphi(\nu) d\nu \int n_u ds \quad (13)$$

($\int \varphi(\nu) d\nu \equiv 1$ Wilson et al. 2009, eqn 12.1)

Convert to column:

$$\int n ds = N \quad (14)$$

Therefore the column of molecules in the upper state is

$$N_u = \frac{8\pi\nu_{ul}^2}{c^2 A_{ul}} \left[\exp \left(\frac{h\nu_{ul}}{k_B T_{ex}} \right) - 1 \right]^{-1} \int \tau_\nu d\nu \quad (15)$$

Convert from column to an observable, T_B (or T_B^* - that is up to the observer to fill in with correction factors etc, particularly because CO tends to be extended, and other dipole molecules might as well). Start with Wilson et al. (2009) equation 15.29, which is the conversion of brightness temperature to the full blackbody form times the thin-cloud component of the radiative transfer equation:

$$T_B(\nu) = \frac{h\nu}{k_B} \left(\left[e^{h\nu/k_B T_{ex}} - 1 \right]^{-1} - \left[e^{h\nu/k_B T_{CMB}} - 1 \right]^{-1} \right) (1 - e^{-\tau_\nu}) \quad (16)$$

Rearrange to solve for τ_ν :

$$\tau_\nu = -\ln \left[1 - \frac{k_B T_B}{h\nu} \left(\left[e^{h\nu/k_B T_{ex}} - 1 \right]^{-1} - \left[e^{h\nu/k_B T_{CMB}} - 1 \right]^{-1} \right)^{-1} \right] \quad (17)$$

The population of the upper state in terms of the observable T_B :

$$N_u = \frac{8\pi\nu_{ul}^2}{c^2 A_{ul}} \left[\exp\left(\frac{h\nu_{ul}}{k_B T_{ex}}\right) - 1 \right]^{-1} \int -\ln \left[1 - \frac{k_B T_B}{h\nu_{ul}} \left(\left[e^{h\nu_{ul}/k_B T_{ex}} - 1 \right]^{-1} - \left[e^{h\nu_{ul}/k_B T_{CMB}} - 1 \right]^{-1} \right)^{-1} \right] d\nu \quad (18)$$

Convert to km s^{-1} with $d\nu = \frac{\nu}{c} dv$

$$N_u = \frac{8\pi\nu_{ul}^3}{c^3 A_{ul}} \left[\exp\left(\frac{h\nu_{ul}}{k_B T_{ex}}\right) - 1 \right]^{-1} \int -\ln \left[1 - \frac{k_B T_B}{h\nu_{ul}} \left(\left[e^{h\nu_{ul}/k_B T_{ex}} - 1 \right]^{-1} - \left[e^{h\nu_{ul}/k_B T_{CMB}} - 1 \right]^{-1} \right)^{-1} \right] dv \quad (19)$$

Use the first term of the Taylor expansion: $\ln(1+x) \approx x - \frac{x^2}{2} + \frac{x^3}{3} \dots$

$$N_u = \frac{8\pi\nu_{ul}^3}{c^3 A_{ul}} \left[\exp\left(\frac{h\nu_{ul}}{k_B T_{ex}}\right) - 1 \right]^{-1} \int \frac{k_B T_B}{h\nu_{ul}} \left(\left[e^{h\nu_{ul}/k_B T_{ex}} - 1 \right]^{-1} - \left[e^{h\nu_{ul}/k_B T_{CMB}} - 1 \right]^{-1} \right)^{-1} dv \quad (20)$$

This can be simplified:

$$\frac{\left[e^{h\nu_{ul}/k_B T_{ex}} - 1 \right]^{-1}}{\left[e^{h\nu_{ul}/k_B T_{ex}} - 1 \right]^{-1} - \left[e^{h\nu_{ul}/k_B T_{CMB}} - 1 \right]^{-1}} = \frac{e^{h\nu_{ul}/k_B T_{CMB}} - 1}{e^{h\nu_{ul}/k_B T_{CMB}} - e^{h\nu_{ul}/k_B T_{ex}}} \quad (21)$$

Which yields:

$$N_u = \frac{8\pi\nu_{ul}^2 k_B}{c^3 A_{ul} h} \frac{e^{h\nu_{ul}/k_B T_{CMB}} - 1}{e^{h\nu_{ul}/k_B T_{CMB}} - e^{h\nu_{ul}/k_B T_{ex}}} \int T_B dv \quad (22)$$

This can be converted to use μ instead of A_{ul} using Wilson et al. (2009) equation 15.20
 $A_{ul} = \frac{64\pi^4}{3hc^3} \nu^3 \mu_{ul}^2$:

$$n_u = \frac{3}{8\pi^3 \mu_e^2} \frac{k_B}{\nu_{ul}} \frac{2J_l + 3}{J_l + 1} \frac{e^{h\nu_{ul}/k_B T_{cmb}} - 1}{e^{h\nu_{ul}/k_B T_{cmb}} - e^{h\nu_{ul}/k_B T_{ex}}} \int T_B dv \quad (23)$$

or in terms of J_u :

$$N_u = \frac{3}{8\pi^3 \mu_e^2} \frac{k_B}{\nu_{ul}} \frac{2J_u + 1}{J_u} \frac{e^{h\nu_{ul}/k_B T_{cmb}} - 1}{e^{h\nu_{ul}/k_B T_{CMB}} - e^{h\nu_{ul}/k_B T_{ex}}} \int T_B dv \quad (24)$$

Stepping back, (16) can be simplified if one assumes that the CMB contribution to the brightness temperature is negligible. This assumption is very safe for high-lying transitions and high excitation temperatures, only exceeding 5% for $T_{ex} < 10, 6$, and 4 K for the CO 1-0, 2-1, and 3-2 transitions (see figure 2).

$$T_B(\nu) = \frac{h\nu}{k_B} \left[e^{h\nu/k_B T_{ex}} - 1 \right]^{-1} (1 - e^{-\tau_\nu}) \quad (25)$$

Which can be solved for τ_ν again:

$$\tau_\nu = -\ln \left(1 - \frac{k_B T_B}{h\nu} \left[e^{h\nu/k_B T_{ex}} - 1 \right] \right) \approx \frac{k_B T_B}{h\nu} \left[e^{h\nu/k_B T_{ex}} - 1 \right] \quad (26)$$

This equation can be used following the above steps to derive a result in the form of (22):

$$N_u \approx \frac{8\pi\nu_{ul}^2}{c^2 A_{ul}} \frac{k_B}{h\nu_{ul}} \int T_B dv = \frac{8\pi\nu_{ul} k_B}{c^3 A_{ul} h} \int T_B dv = \frac{3k_B}{8\pi^3 \mu_{ul}^2 \nu_{ul}^2} \frac{2J_l + 3}{J_l + 1} \int T_B dv \quad (27)$$

Note that (19) is the full solution assuming LTE with *no* approximations.

2. Partition Function

We are interested in the total number (or column) of molecules, not that in a single state:

$$n_{tot} = \sum_{J=0}^{\infty} n_J \quad (28)$$

The Boltzmann distribution defines the distribution of molecular excitation states in LTE:

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} \exp \left(\frac{-E_{ul}}{k_B T_{ex}} \right) \quad (29)$$

$$E_{ul} = hB_e J_u (J_u + 1) \quad (30)$$

$$g_J = 2J + 1 \quad (31)$$

By approximating the sum over all states as an integral, we can solve for the number in the ground state, which can in turn be used to solve for the number in any state:

$$n_{tot} = \sum_{J=0}^{\infty} n_J = n_0 \sum_{J=0}^{\infty} (2J + 1) \exp \left(-\frac{J(J + 1)B_e h}{k_B T_{ex}} \right) \quad (32)$$

$$\approx \int_0^{\infty} n_0 (2J + 1) \exp \left(-\frac{J(J + 1)B_e h}{k_B T_{ex}} \right) dJ \quad (33)$$

$$= \left[n_0 \frac{k_B T_{ex}}{B_e h} \exp \left(-\frac{J(J + 1)B_e h}{k_B T_{ex}} \right) \right]_0^{\infty} \quad (34)$$

$$= n_0 \frac{k_B T_{ex}}{B_e h} \quad (35)$$

Rearrange to acquire

$$n_0 = n_{tot} \frac{B_e h}{k_B T_{ex}} \quad (36)$$

Plug back in to the Boltzmann distribution (29)

$$n_J = n_{tot} \frac{B_e h}{k_B T_{ex}} (2J + 1) \exp \left(-\frac{J(J + 1)B_e h}{k_B T_{ex}} \right) \quad (37)$$

and finally rearrange

$$n_{tot} = n_J \frac{k_B T_{ex}}{(2J+1)B_e h} \exp\left(\frac{J(J+1)B_e h}{k_B T_{ex}}\right) \quad (38)$$

Note that n can be converted to N by multiplying both sides by the path length.

The numerical solution is acquired from plugging (29) into (32)

$$n_J = \left[\sum_{j=0}^{j=j_{max}} (2j+1) \exp\left(-\frac{j(j+1)B_e h}{k_B T_{ex}}\right) \right] (2J+1) \exp\left(-\frac{J(J+1)B_e h}{k_B T_{ex}}\right) \quad (39)$$

REFERENCES

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- Cabrit, S., & Bertout, C. 1990, ApJ, 348, 530
- Garden, R. P., Hayashi, M., Hasegawa, T., Gatley, I., & Kaifu, N. 1991, ApJ, 374, 540
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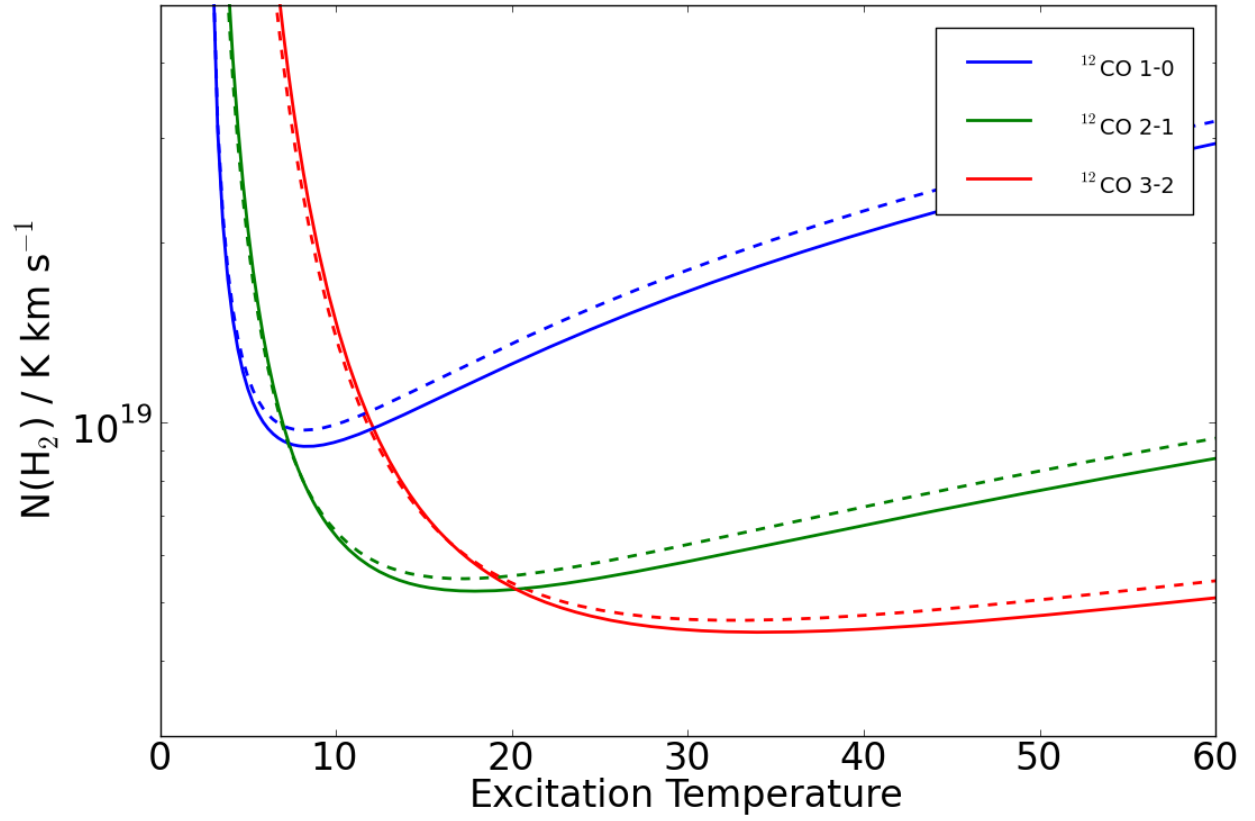


Fig. 1.— Using (22) (i.e. assuming $\tau_\nu \ll 1$) and a numerical treatment of the partition function out to $J = 200$, the conversion from $T_B(^{12}\text{CO})$ to $N(\text{H}_2)$ vs T_{ex} . We assume $X_{\text{CO}} = 10^{-4}$ and LTE.

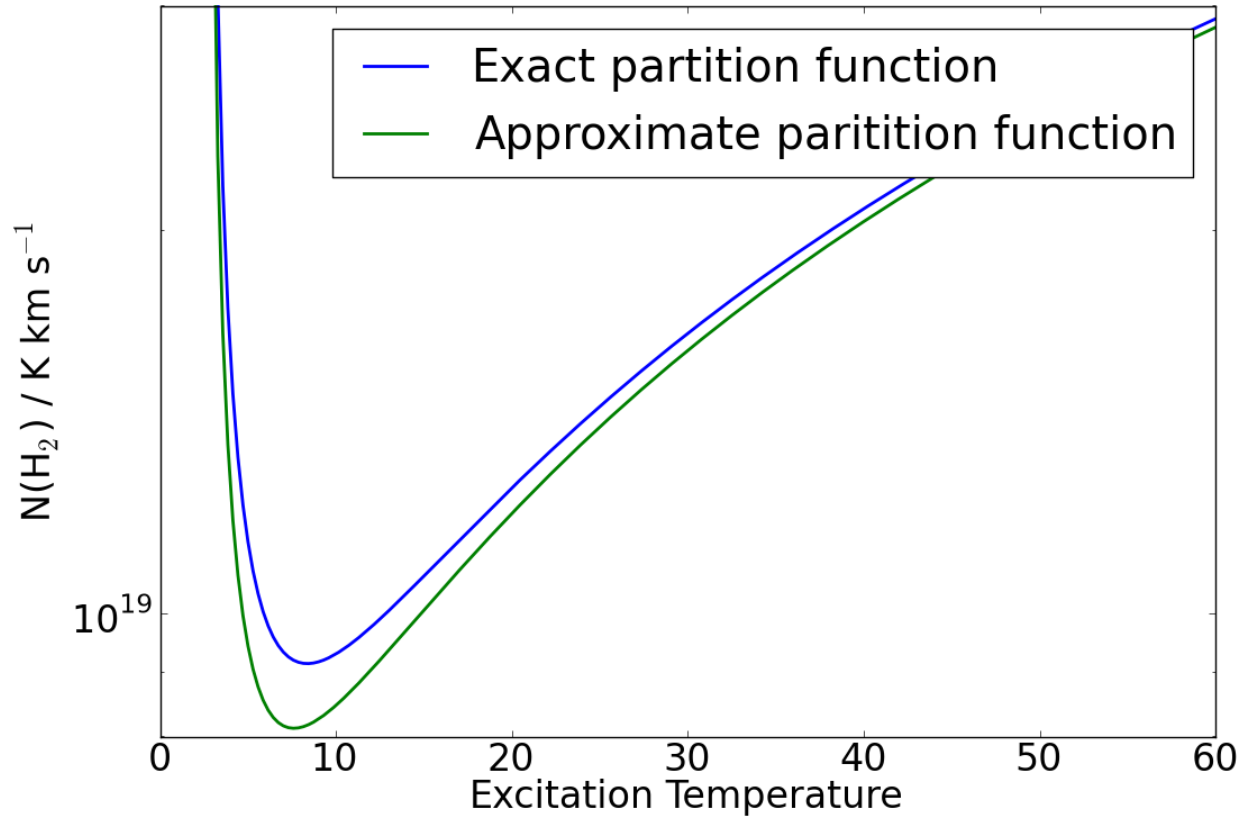


Fig. 2.— Comparison of the approximate to the exact (numerical) solutions of the partition function. The approximate partition function is calculated using the approximation in (32). The exact (numerical) solution sums the population in all states out to $J = 200$.

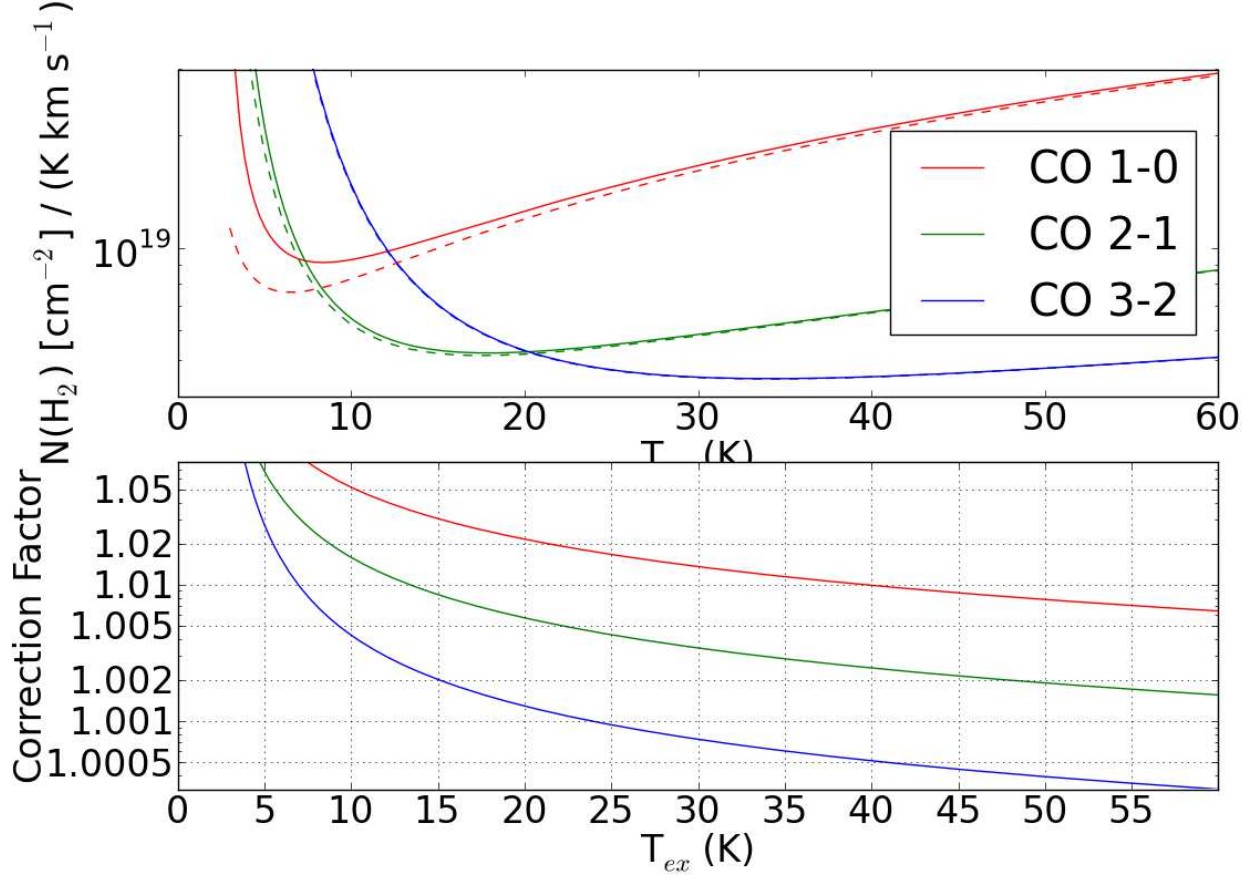


Fig. 3.— *Top*: Comparison of a full treatment of the optical depth including the contribution of the CMB as in (19) with an approximation that ignores the CMB, (27). *Bottom*: Equation (19)/Equation (27), which is the Correction Factor that needs to be applied to the approximate version to recover the full version. Note that the correction factor is $< 5\%$ for most reasonable excitation temperatures.