THE INTERSTELLAR MEDIUM: VI
Tracers of H_2 : CO rotational lines

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Outline

- Background.
- The CO molecule and rotational transitions.
- Radiative transfer issues.
- The critical density at high optical depths.
- Inferring the H_2 column density from CO line studies.
- *Caveat emptor*!

BACKGROUND

- Molecules: Electronic, vibrational, rotational, … transitions.
  Electronic: UV/optical; Vibrational: mid-IR; Rotational: mm.

- Rotational lines = $B_v\, J(J+1)$; $B_v = \hbar^2/2m_r r_0^{\,2}$; $J \rightarrow J\text{-}1$: $2B_v J$.

- H_2: No electric dipole moment for rotational/vibrational lines.

- Rotational and vibrational H_2 lines at mid-IR wavelengths (~ 2.1 μm, 28μm). $h\nu/k > 500$ K ⇨ Not seen in typical clouds.

- H_2 detectable in electronic UV absorption against stars/quasars.

- N_{HI} threshold for H_2 formation: $N_{HI} \sim 6 \times 10^{20}$ cm^{-2} (Milky Way).
  Metallicity-dependent threshold; higher threshold in LMC/SMC.

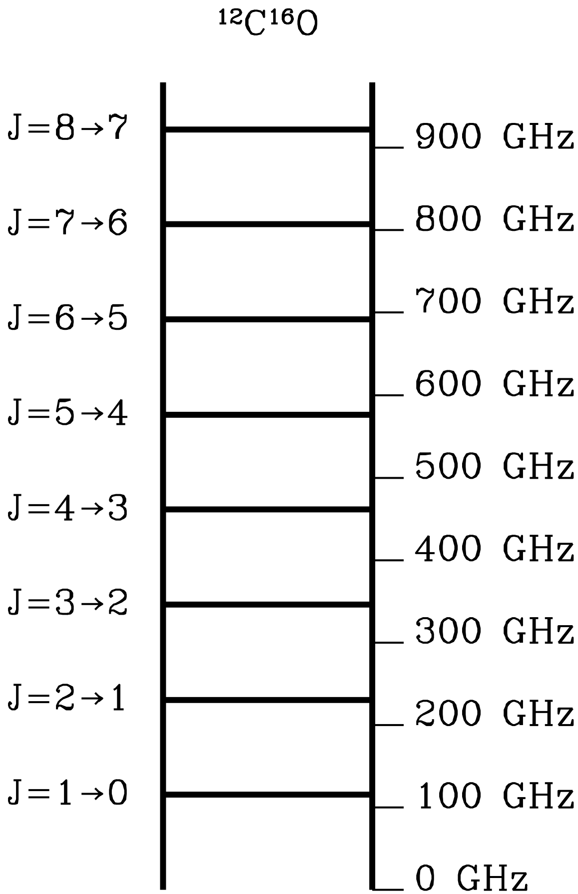
- Correlation between total H column density ($N_H = N_{HI} + 2N_{H_2}$) and reddening: $N_H = 5.8 \times 10^{21}\, E_{B-V}$ cm^{-2} mag^{-1}.

TRACING MOLECULAR GAS: CO LINES

- C, O most abundant species after H and He! O/H ~ 4.9×10^{-4}, C/H ~ 2.7×10^{-4} ⇨ CO most abundant molecule after H_2.

- Large molecular mass: Rotational line frequencies in mm-band! Energy $(J \rightarrow J-1) = \hbar^2 J / m_r r_0^2$ ⇨ $\nu(1 \rightarrow 0) = 115.271$ GHz.

- Low centrifugal distortions: Rotational ladder. Lowest three lines observable from ground!



(NRAO)

- $A_{ul} = (64\pi^4/3hc^3)\, \nu^3 \mu^2\, [J/(2J+1)]$ ⇨ $A_{ul} \propto \nu^3$.
  ⇨ High-J lines have higher Einstein A's.

- $(h\nu_{10}/k) \sim 5.5$ K ⇨ Easily excited in the ISM. $A_{10} \sim 7 \times 10^{-8}\ s^{-1}$ ⇨ Critical density ~ 1100 cm^{-3}.

- Isotopic species: ^{13}CO (110.20 GHz), $C^{18}O$ (109.78 GHz)...

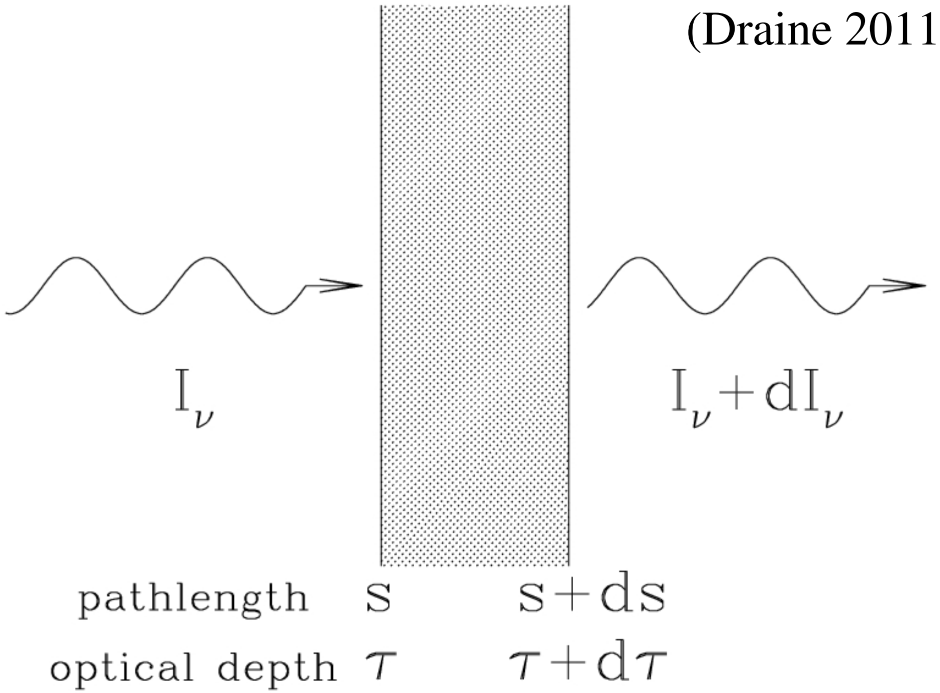
Rotational Lines: Radiative Transfer

- For a uniform medium, with level populations given by T_R.

- Equation of radiative transfer:

$$dI_\nu = -I_\nu \kappa_\nu ds + j_\nu ds$$

(Draine 2011)



- Define optical depth, $d\tau_\nu = \kappa_\nu\, ds$

$$\Rightarrow \quad dI_\nu = -I_\nu\, d\tau_\nu + (j_\nu/\kappa_\nu)\, d\tau_\nu$$

- $I_\nu = I_\nu(0)\, e^{-\tau_\nu} + {}_0\int^{\tau_\nu} e^{-(\tau_\nu - \tau)}\, B_\nu(T_R)\, d\tau.$

$$\Rightarrow \quad I_\nu = I_\nu(0)\, e^{-\tau_\nu} + B_\nu(T_R)\,(1 - e^{-\tau_\nu})$$

- At millimetre wavelengths, the radiation field is the CMB!

$$\Rightarrow \quad I_\nu = B_\nu(T_{CMB})\, e^{-\tau_\nu} + B_\nu(T_R)\,(1 - e^{-\tau_\nu})$$

$$\Rightarrow \quad T_A = (h\nu/k)\,\{[e^{h\nu/kT_{CMB}} - 1]^{-1} e^{-\tau_\nu} + [e^{h\nu/kT_R} - 1]^{-1}(1 - e^{-\tau_\nu})\}\ .$$

Rotational Lines: Radiative Transfer

- The antenna temperature measured towards the cloud is

$$T_A = (h\nu/k)\,\{[e^{h\nu/kT_{CMB}} - 1]^{-1} e^{-\tau_\nu} + [e^{h\nu/kT_R} - 1]^{-1}(1-e^{-\tau_\nu})\}.$$

- The antenna temperature measured away from the cloud is

$$T_{A,OFF} = (h\nu/k)\,\{[e^{h\nu/kT_{CMB}} - 1]^{-1}.$$

- The excess antenna temperature due to the cloud is then

$$\Delta T_A = T_A - T_{A,OFF} = (h\nu/k)(1-e^{-\tau_\nu})\{[e^{h\nu/kT_R} - 1]^{-1} - [e^{h\nu/kT_{CMB}} - 1]^{-1}\}$$

- $T_R > T_{CMB}$ ⇨ Emission.
  $T_R < T_{CMB}$ ⇨ Absorption.
  $T_R = T_{CMB}$ ⇨ $\Delta T_A = 0$. No spectral line.

Critical Densities of Molecules

- $\Delta T_A = (h\nu/k)\,(1\text{-}e^{-\tau_\nu})\,\{[e^{h\nu/kT_R} - 1]^{-1} - [e^{h\nu/kT_{CMB}} - 1]^{-1}\}$.

- $T_R > T_{CMB}$ ⇨ Emission. $T_R = T_{CMB}$ ⇨ No spectral line.

- Collisional & radiative excitation / de-excitation: 2-level system

  $$(n_1/n_0) = [n_c k_{01} + n_\gamma (g_1/g_0) A_{10}] / [n_c k_{10} + (1 + n_\gamma) A_{10}].$$

- Critical density: $n_{crit,u} = [\Sigma_{l<u} (1 + n_\gamma) A_{ul}] / [\Sigma_{l<u} k_{ul}]$

  If $n_c \gg n_{crit,u}$ ⇨ $T_R = T_K$; if $n_c \ll n_{crit,u}$ ⇨ $T_R = T_{CMB}$.

  Lines detected in emission for $n \geq n_{crit}$ ⇨ Density tracer!

- $n_{crit} \approx 1100$ cm^{-3} for CO (1→0), $n_{crit} \approx 4.6 \times 10^4$ for CS (1→0), $n_{crit} \approx 10^6$ for HCN (1→0),...

- $A_{ul} = (64\pi^4/3hc^3)\,\nu^3\,\mu^2\,[J/(2J+1)]$ ⇨ Higher n_{crit} for high-J lines.

Opacity Issues: Radiative Trapping

- For $\tau \gg 1$, stimulated emission critical in determining T_R.
- "Escape probability approximation": Assume that photons are emitted and absorbed at the *same* location. (Scoville & Solomon 1974)
- For a uniform medium, with level populations given by T_R.

$$\Rightarrow \; I_\nu = I_\nu(0)\, e^{-\tau_\nu} + B_\nu(T_R)\,(1 - e^{-\tau_\nu})$$

- $n_\gamma \equiv (c^2/2h\nu^3) I_\nu \;\Rightarrow\; n_\gamma = n_\gamma(0)\, e^{-\tau_\nu} + [n_0 g_1/n_1 g_0 - 1]^{-1}(1-e^{-\tau_\nu})$.
- "Escape probability" $\beta_\nu \equiv e^{-\tau_\nu}$.
- Averaging over directions and integrating over the line profile

$$\Rightarrow \; \langle n_\gamma \rangle = n_\gamma(0).\langle\beta\rangle + [n_0 g_1/n_1 g_0 - 1]^{-1}(1- \langle\beta\rangle).$$

- $(dn_1/dt) = n_0[n_c k_{01} + n_\gamma (g_1/g_0) A_{10}] - n_1[n_c k_{10} + (1 + n_\gamma) A_{10}]$.

$$\Rightarrow = n_0\{n_c k_{01} + n_\gamma(0).(g_1/g_0).\langle\beta\rangle.A_{10}\} - n_1\{n_c k_{10} + [1 + n_\gamma(0)]\langle\beta\rangle A_{10}\}.$$

Opacity Issues: Radiative Trapping

- For collisional and radiative excitation and de-excitation:

$$(dn_1/dt) = n_0[n_c k_{01} + n_\gamma (g_1/g_0)A_{10}] - n_1[n_c k_{10} + (1 + n_\gamma)A_{10}].$$

- Replacing $\langle n_\gamma \rangle = n_\gamma(0).\langle\beta\rangle + [n_0 g_1/n_1 g_0 - 1]^{-1}(1- \langle\beta\rangle)$ ⇨

$$(dn_1/dt) = n_0\{n_c k_{01} + n_\gamma(0).(g_1/g_0).\langle\beta\rangle.A_{10}\} - n_1\{n_c k_{10} + [1 + n_\gamma(0)]\langle\beta\rangle A_{10}\}.$$

- This is the equation for (dn_1/dt) *if* (1) there's no internally produced radiation field, (2) the cloud is transparent to $I_\nu(0)$, and (3) the Einstein A-coefficient is $\langle\beta\rangle A_{10}$.

- $(n_1/n_0) = [n_c k_{01} + n_\gamma(0).(g_1/g_0).\langle\beta\rangle A_{10}] \,/\, \{n_c\, k_{10} + (1 + n_\gamma(0)].\langle\beta\rangle A_{10}\}.$

- Critical density *reduced*: $n_{crit,u} = [\Sigma_{l<u} (1 + n_\gamma).\langle\beta\rangle A_{ul}] \,/\, [\Sigma_{l<u} k_{ul}].$

- $\langle\beta\rangle$ depends on the geometry and velocity structure. For a homogenous sphere and Gaussian velocities, $\langle\beta\rangle \approx (1 + 0.5\tau_0)^{-1}$.

Opacity Issues: The CO $J=1\rightarrow 0$ Line

- $\nu \sim 115.271$ GHz; $A_{10} \sim 7 \times 10^{-8}\ s^{-1}$ ⇨ $n_{crit} \sim A_{10}/k_{10} \approx 1100\ cm^{-3}$.
- For a Gaussian velocity distribution, the attenuation coefficient:

  $\kappa_\nu = n_0.\ [1 - (n_1 g_0/n_0 g_1)]\ .(\lambda^2/8\pi).\ (g_1/g_0).\ A_{10}.\pi^{-1/2}.\ (\lambda/b).\ e^{-(\Delta v/b)^2}$
- The line-centre optical depth, $\tau_0 = \kappa_{\nu,0} \times R$ (Cloud radius $\equiv$ R).

  ⇨ $\tau_0 \approx 0.02\ (n_H/1000)\ (R/3\ pc)\ [n_0/n_H]\ (2/b)\ [1 - (n_1 g_0/n_0 g_1)]$.
- One needs to know T_R and $[n_0/n]$ to determine τ_0 !
- The fraction of CO in the J^{th} rotational level is

  $[n_J/n_{CO}] = (2J+1)e^{-B_0 J(J+1)/kT_R} / \Sigma_J\ (2J+1)\ e^{-B_0 J(J+1)/kT_R}$.
- The partition function $\Sigma_J\ (2J+1)\ e^{-B_0 J(J+1)/kT_R} \approx [1+(kT_R/B_0)^2]^{1/2}$.
- For $T_R \approx 8$ K, $\tau_0 \approx 46\ (n_H/1000)\ (R/3\ pc)\ [[n_{CO}/n_H]/(7\times 10^{-5})]\ (2/b)$

  ⇨ $\langle\beta\rangle \approx (1 + 0.5\tau_0)^{-1} \approx 0.04$ ⇨ $n_{crit} \sim \langle\beta\rangle A_{10}/k_{10} \approx 50\ cm^{-3}$!!!

THE CO COLUMN DENSITY

- The general expression for the attenuation coefficient, κ_ν :

  $\kappa_\nu = n_l . [1 - (n_u g_l / n_l g_u)] .(\lambda^2/8\pi). (g_u/g_l). A_{ul}.\phi_\nu$; $\int \phi_\nu d\nu = 1.$

- The column density in the lower level $N_l = \int n_l \, ds$

  $\Rightarrow N_l = (8\pi/\lambda^2) . (g_l/g_u) . (1/A_{ul}) . \int \tau_\nu/[1 - e^{h\nu/kT_R}] \, d\nu$

  $= 93.28(g_l/g_u).(\nu/GHz)^3.(1/A_{ul}).[1 - e^{h\nu/kT_R}]^{-1}. \int \tau_\nu \, (dv/ \, km \, s^{-1})$

- $A_{ul} = (64\pi^4/3hc^3) \, \nu^3 \mu^2 \, [J/(2J+1)] = 1.165 \times 10^{-11} \nu^3 \mu^2 \, [J/(2J+1)]$

  $\Rightarrow N_l = 8.0 \times 10^{12}. \mu^{-2}. [(2J-1)/J]. [1 - e^{h\nu/kT_R}]^{-1}. \int \tau_\nu \, dv$

- Measured $T_B = (h\nu/k) \, (1-e^{-\tau_\nu}) \, \{[e^{h\nu/kT_R} - 1]^{-1} - [e^{h\nu/kT_{CMB}} - 1]^{-1}\}$

- Problems: (1) Both τ_ν and T_R are unknown, and (2) $\tau_\nu \geq 1$!

The CO Column Density: LTE

- $N_l = 8.0 \times 10^{12} . \mu^{-2} . [(2J-1)/J] . [1 - e^{h\nu/kT_R}]^{-1} . \int \tau_v \, dv$
- Measured $T_B = (h\nu/k)(1-e^{-\tau_v}) \{ [e^{h\nu/kT_R} - 1]^{-1} - [e^{h\nu/kT_{CMB}} - 1]^{-1} \}$
- LTE approximation: *Assume* $T_R = T_K$, for all rotational levels!
- *Assume* ^{13}CO and ^{12}CO have same T_R! Note $\tau_v(^{13}CO) \ll 1$!
- $\tau_v(^{12}CO) \gg 1 \Rightarrow T_R = 5.5/\ln\{1 + 5.5/(T_B + 0.82)\}$
- The fraction of ^{13}CO in the J^{th} rotational level is

  $[n_J/n_{CO}] = (2J+1)e^{-B_0J(J+1)/kT_R} / \Sigma_J (2J+1)\, e^{-B_0J(J+1)/kT_R}$

  $N(^{13}CO) = [\Sigma_J (2J+1)\, e^{-B_0J(J+1)/kT_R}] . e^{+B_0J(J+1)/kT_R} . N_J/(2J+1)]$

- Partition function $\Sigma_J(2J+1)e^{-B_0J(J+1)/kT_R} \approx [1+(kT_R/B_0)^2]^{1/2} \approx T_R/2.76$

  $\Rightarrow N(^{13}CO) = 2.85 \times 10^{14} . T_R/(1 - e^{-5.3/T_R}) . \int \tau_v(^{13}CO) \, dv$

  Finally, $N(^{12}CO) \approx 90 \times N(^{13}CO)$ and $N(H_2) \approx 10^4 \times N(^{12}CO)$.

Caveat Emptor!!!

- CO is a "nice" molecule!!! A high line intensity, a low dipole moment (and hence a low A_{10} and a low critical density), an excitation close to LTE, and a large molecular abundance.

- Many isotopomers: At least one optically thin (^{13}CO, $C^{18}O$...).

- Correlation between measured $N(^{13}CO)$ or $N(C^{18}O)$ and E_{B-V}

  $N(H_2) = 4.4 \times 10^6 \; N(C^{18}O) \; cm^{-2}$ $\qquad N(H_2) < 1.5 \times 10^{22} \; cm^{-2}$.

  $N(H_2) = 3.8 \times 10^5 \; N(^{13}CO) \; cm^{-2}$ $\qquad N(H_2) < 5 \times 10^{21} \; cm^{-2}$.

- But.... ^{12}CO & ^{13}CO may not arise in the same gas ?

  High-J levels not thermalized: Errors in partition function ?

  Less abundant isotopes sub-thermally excited ($T_R < T_K$) ?

- Still one of the best ways of estimating CO and H_2 column densities! But probably only good to an order of magnitude.