Molecular Excitation & Radiation Transfer

José Pablo Fonfría
jpablo.fonfria@csic.es

Instituto de Física Fundamental (IFF)
Consejo Superior de Investigaciones Científicas (CSIC)

UAM Master in Astrophysics
Radiative Processes in Astrophysics

Madrid, 10 October 2025

INSTITUTO DE FÍSICA FUNDAMENTAL

CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

Outline

Outline

1. Radiation transfer: A brief introduction
2. Molecular excitation
3. Solving the Statistical Equilibrium Equations (SEE) and the Radiation transfer problem
4. Line profiles
5. Summary and final remarks

Radiation transfer: A very brief introduction [7, 9]

- The radiation transfer equation is:

$$\frac{dI_\nu}{dl} = -k_\nu I_\nu + \varepsilon_\nu \Longrightarrow \frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu,$$

where I_ν is the intensity of the incident light, k_ν and ε_ν are the total opacity and the emissivity of the medium under study, τ_ν is the optical depth, and S_ν is the source function defined as:

$$\tau_\nu = \int k_\nu dl \qquad \text{and} \qquad S_\nu = \frac{\varepsilon_\nu}{k_\nu}$$

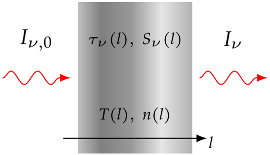
- The solution of the radiation transfer equation for a plane-parallel layer is:

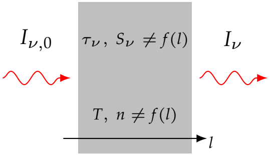
$$I_\nu = I_{\nu,0} e^{-\tau_\nu} + e^{-\tau_\nu} \int_0^{\tau_\nu} dt S_\nu(t) e^t.$$

- For a layer with constant temperature and density, $S_\nu = \text{const.}$:

$$I_\nu = I_{\nu,0} e^{-\tau_\nu} + S_\nu(T)\left(1 - e^{-\tau_\nu}\right).$$

Units (usually CGS):
$[l]$: cm
$[I_\nu]$: erg s^{-1} cm^{-2} Hz^{-1} sr^{-1}
$[k_\nu]$: cm^{-1}
$[\varepsilon_\nu]$: erg s^{-1} cm^{-3} Hz^{-1} sr^{-1}
$[S_\nu]$: erg s^{-1} cm^{-2} Hz^{-1} sr^{-1}





Radiation transfer: A very brief introduction [7, 9]

$$I_\nu = I_{\nu,0} e^{-\tau_\nu} + S_\nu(T)\left(1 - e^{-\tau_\nu}\right) \quad ; \quad F_\nu = \int_{4\pi} P(\phi,\theta) I_\nu(\phi,\theta) d\omega \simeq \langle I_\nu \rangle \Omega$$

Optically *thin* regime

$$\tau_\nu \ll 1$$

$$I_\nu \simeq I_{\nu,0} + \left[S_\nu(T) - I_{\nu,0}\right] \tau_\nu$$

$$F_\nu \simeq \langle I_{\nu,0} + \left[S_\nu(T) - I_{\nu,0}\right] \tau_\nu \rangle \Omega$$

$$\Omega = \text{solid angle}$$

Optically *thick* regime

$$\tau_\nu \gg 1$$

$$I_\nu \simeq S_\nu(T)$$

$$F_\nu \simeq \langle S_\nu(T) \rangle \Omega$$

Radiation transfer: The two-level approximation [7, 9]

- A photon with a given frequency interacting with a quantum system with multiple energy levels could excite levels with an energy distance different than the photon energy, although with a small probability.
- The *two-level approximation* assumes that this is not possible and a photon only can produce a transition if its energy matches up with the energy difference between two levels.

collisional rates

Collisional coefficients
$$\left\{\begin{aligned} \gamma_{lu} &= \frac{g_u}{g_l}\gamma_{ul}e^{-h\nu/k_B T_K} \\ C_{ul} &= n\gamma_{ul} \\ C_{lu} &= n\gamma_{lu} \end{aligned}\right.$$

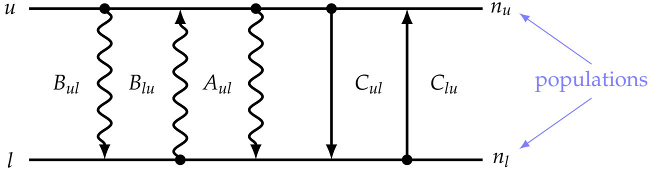
$$\gamma_{ul} = \left(\frac{8k_B T_k}{\pi\mu}\right)^{1/2}\left(\frac{1}{k_B T_k}\right)e^{E_u/k_B T_k}\int_0^{\infty}\sigma_{ul}(E)(E-E_u)e^{-E/k_B T_k}dE$$

$$\left.\begin{aligned} A_{ul} &= \frac{4\pi}{c}\frac{2h\nu^3}{c^2}B_{ul} \\ B_{ul} &= \frac{g_l}{g_u}B_{lu} \end{aligned}\right\}$$
Einstein coefficients

spontaneous emission

induced emission

induced absorption



Radiation transfer: The equation with molecular transitions [7, 9]

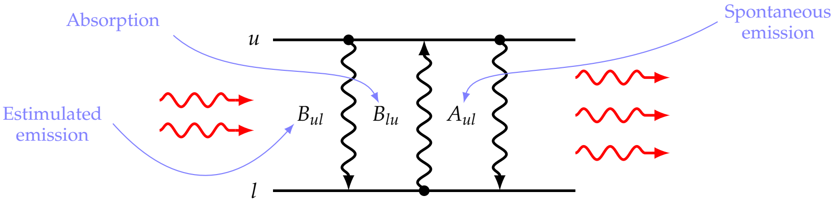
- The radiation transfer equation in its general form can be used to describe the absorption and emission of different materials and gases

$$\frac{dI_\nu}{dl} = -k_\nu I_\nu + \varepsilon_\nu$$

- For the particular case of molecules (or atoms) it can be written using the Einstein coefficients in this way:

$$\frac{dI_\nu}{dl} = \underbrace{\frac{h\nu}{4\pi}A_{ul}n_u + \frac{h\nu}{c}B_{ul}I_\nu n_u}_{emission} - \underbrace{\frac{h\nu}{c}B_{lu}I_\nu n_l}_{absorption}$$

Einstein coefficients



Radiation transfer: Opacity of a molecular line [7, 9]

- For a given molecule with an abundance x and m transitions:

absorption profile (normalized)

$$k_\nu = \frac{c^2}{8\pi}\frac{n_g x}{Z}\sum_{i=1}^{m}\frac{g_{u,i}A_i}{\nu_i^2}\left(\frac{g_{0,i}n_{l,i}}{g_{l,i}n_{0,i}}\right)\left(1-\frac{g_{l,i}n_{u,i}}{g_{u,i}n_{l,i}}\right)\phi_i(\nu-\nu_i)$$

gas density

A-Einstein coefficient

partition function

degeneracy of the upper level

- Assuming that the populations of the levels are described with Boltzmann factors ($\frac{g_u}{g_l}e^{-\Delta E/k_B T_{\rm exc}}$), which are controlled by the excitation temperature, $T_{\rm exc}$:

$$k_\nu = \frac{c^2}{8\pi}\frac{n_g x}{Z}\sum_{i=1}^{m}\frac{g_{u,i}A_i}{\nu_i^2}e^{-E_{l,i}/k_B T_{\rm exc}}\left(1-e^{-h\nu_i/k_B T_{\rm exc}}\right)\phi_i(\nu-\nu_i)$$

$$\int_0^\infty \phi_i(\nu-\nu_i)d\nu = 1 \quad\Rightarrow\quad \phi_i(\nu-\nu_i) = \frac{1}{\sigma_i\sqrt{\pi}}e^{-(\nu-\nu_i)^2/\sigma_i^2}$$

Usually taken as the profile for the Maxwell velocity distribution associated to T_k. The fundamental Lorentzian line profile is too narrow

There are several on-line databases available to find molecular spectroscopic parameters: (mm/submm) MADEX, CDMS, JPL, Splatalogue, (IR) HITRAN, GEISA, (IR/visible) ExoMol…

Radiation transfer: Opacity of a molecular line [7, 9]

- For a given molecule with an abundance x and m transitions:

absorption profile (normalized)

$$k_\nu = \frac{c^2}{8\pi}\frac{n_g x}{Z}\sum_{i=1}^{m}\frac{g_{u,i}A_i}{\nu_i^2}e^{-E_{l,i}/k_B T_{\rm exc}}\left(1 - e^{-h\nu_i/k_B T_{\rm exc}}\right)\phi_i(\nu - \nu_i)$$

gas density

A-Einstein coefficient

partition
function

degeneracy of
the upper level

- The opacity of a given line is positive if

$$\zeta = 1 - e^{-E_{l,i}/k_B T_{\rm exc}} > 0 \Longrightarrow \frac{n_u}{n_l} < \frac{g_u}{g_l} \Longrightarrow T_{\rm exc} > 0 \Longrightarrow k_\nu > 0,$$

resulting in thermal emission, and negative if

$$\zeta = 1 - e^{-E_{l,i}/k_B T_{\rm exc}} < 0 \Longrightarrow \frac{n_u}{n_l} > \frac{g_u}{g_l} \Longrightarrow T_{\rm exc} < 0 \Longrightarrow k_\nu < 0,$$

producing maser emission (*population inversion*).

Radiation transfer: Source function of a molecular line [7, 9]

- For a given molecule with an abundance x and m transitions:

$$S_\nu = \frac{2h}{c^2} \sum_{i=1}^{m} \frac{k_{\nu,i}}{k_\nu} \nu_i^3 \left[\frac{g_{u,i} n_{l,i}}{g_{l,i} n_{u,i}} - 1 \right]^{-1}$$

gas opacity
per line

total gas opacity

- Assuming that T_{exc} controls the populations:

$$S_\nu = \frac{2h}{c^2} \sum_{i=1}^{m} \frac{k_{\nu,i}}{k_\nu} \nu_i^3 \frac{1}{e^{h\nu_i / k_B T_{\text{exc}}} - 1} = \sum_{i=1}^{m} \frac{k_{\nu,i}}{k_\nu} B_{\nu_i}(T_{\text{exc}})$$

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu / k_B T} - 1} \qquad \text{: Planck's function}$$

The process followed to derive k_ν and S_ν can be strightforwardly extended to include other molecules.

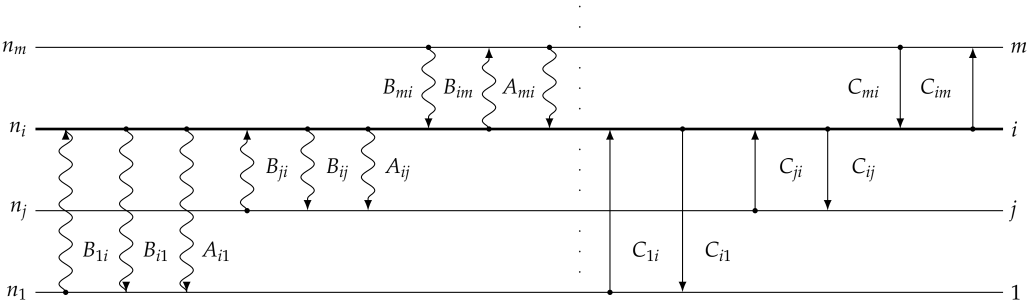
Outline

1. Radiation transfer: A brief introduction
2. Molecular excitation
3. Solving the Statistical Equilibrium Equations (SEE) and the Radiation transfer problem
4. Line profiles
5. Summary and final remarks

Molecular excitation: Statistical Equilibrium

steady-state regime

$$
\begin{aligned}
\frac{dn_i}{dt} = 0 = & \sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i && \text{: radiative, spontaneous} \\
& + \sum_{j\neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j\neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i && \text{: radiative, induced} \\
& + \sum_{j\neq i} C_{ji} n_j - \sum_{j\neq i} C_{ij} n_i && \text{: collisional}
\end{aligned}
$$



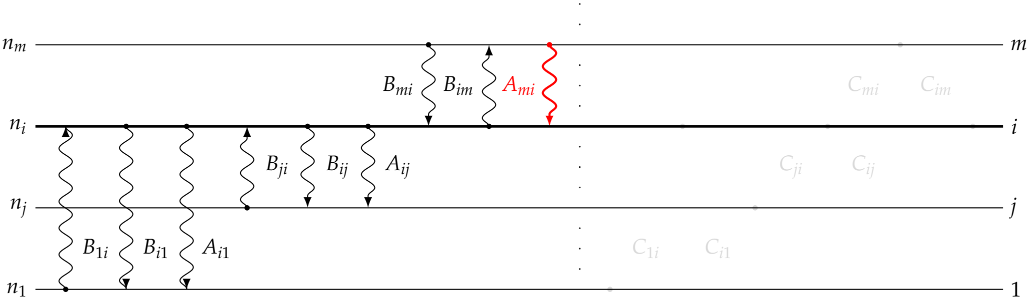
Molecular excitation: Statistical Equilibrium

steady-state regime

$$\frac{dn_i}{dt} = 0 = \sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i \qquad \text{: radiative, spontaneous}$$

$$+ \sum_{j\neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j\neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i \qquad \text{: radiative, induced}$$

$$+ \sum_{j\neq i} C_{ji} n_j - \sum_{j\neq i} C_{ij} n_i \qquad \text{: collisional}$$



Molecular excitation: Statistical Equilibrium

steady-state regime

$$\frac{dn_i}{dt} = 0 = \sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i$$

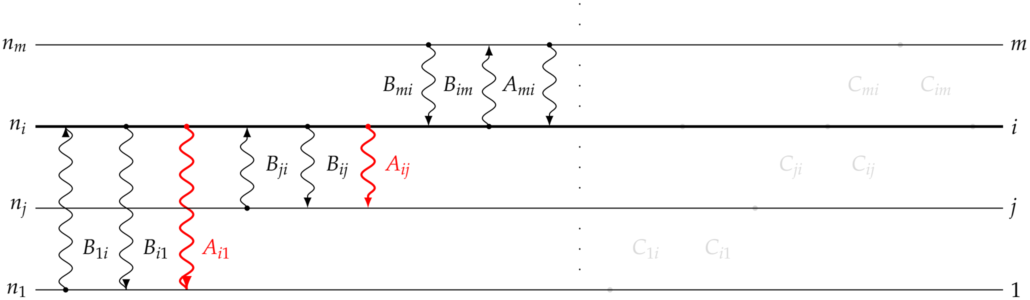
: radiative, spontaneous

$$+ \sum_{j\neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j\neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i$$

: radiative, induced

$$+ \sum_{j\neq i} C_{ji} n_j - \sum_{j\neq i} C_{ij} n_i$$

: collisional



Molecular excitation: Statistical Equilibrium

steady-state regime

$$\frac{dn_i}{dt} = 0 = \sum_{j>i} A_{ji}n_j - \sum_{j<i} A_{ij}n_i$$

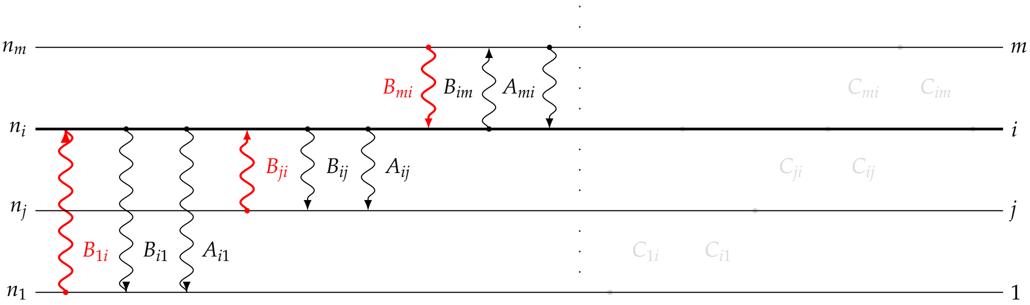
$$+ \sum_{j\neq i} B_{ji}4\pi\bar{J}(\nu_{ji})n_j - \sum_{j\neq i} B_{ij}4\pi\bar{J}(\nu_{ij})n_i$$

: radiative, induced

$$+ \sum_{j\neq i} C_{ji}n_j - \sum_{j\neq i} C_{ij}n_i$$

: collisional

$$\boxed{\bar{J}_\nu = \frac{1}{4\pi}\int_{4\pi} I_\nu(\omega)d\omega}$$



Molecular excitation: Statistical Equilibrium

steady-state regime

$$\frac{dn_i}{dt} = 0 = \sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i$$

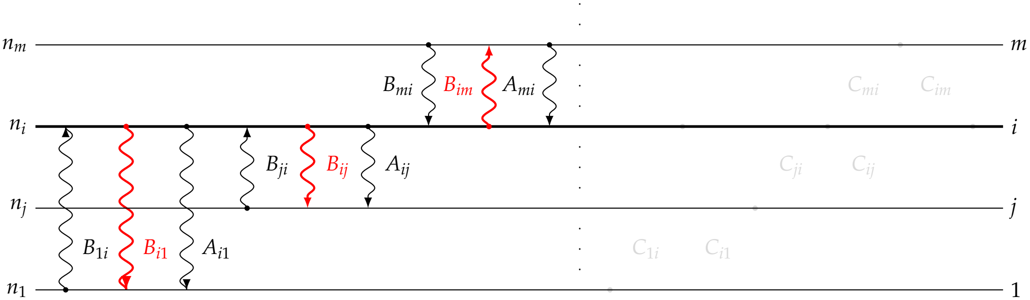
$$+ \sum_{j\neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j\neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i$$

$$\boxed{\bar{J}_\nu = \frac{1}{4\pi} \int_{4\pi} I_\nu(\omega) d\omega}$$

: radiative, induced

$$+ \sum_{j\neq i} C_{ji} n_j - \sum_{j\neq i} C_{ij} n_i$$

: collisional



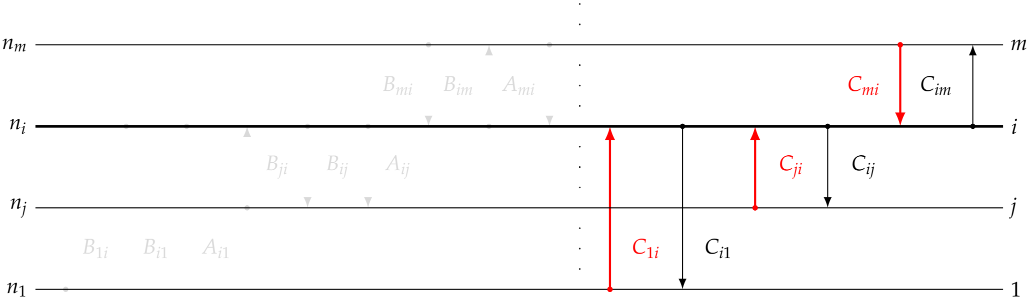
Molecular excitation: Statistical Equilibrium

steady-state regime

$$\frac{dn_i}{dt} = 0 = \sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i \qquad \text{: radiative, spontaneous}$$

$$+ \sum_{j \neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j \neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i \qquad \text{: radiative, induced}$$

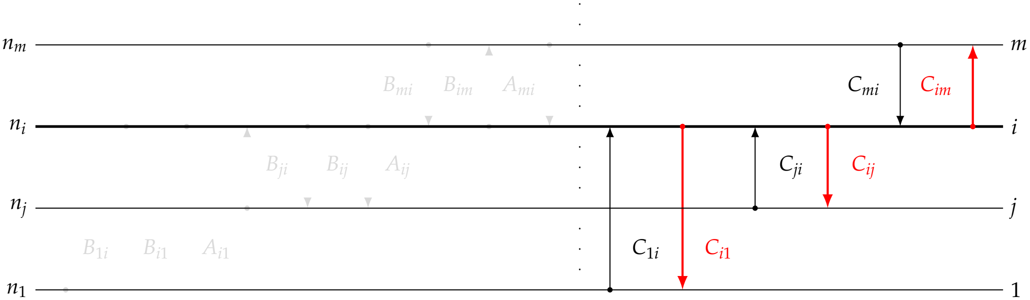
$$+ \sum_{j \neq i} C_{ji} n_j - \sum_{j \neq i} C_{ij} n_i \qquad \text{: collisional}$$



Molecular excitation: Statistical Equilibrium

steady-state regime

$$
\begin{aligned}
\frac{dn_i}{dt} = 0 = & \sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i && \text{: radiative, spontaneous} \\
& + \sum_{j\neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j\neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i && \text{: radiative, induced} \\
& + \sum_{j\neq i} C_{ji} n_j - \sum_{j\neq i} C_{ij} n_i && \text{: collisional}
\end{aligned}
$$



Molecular excitation: Temperatures

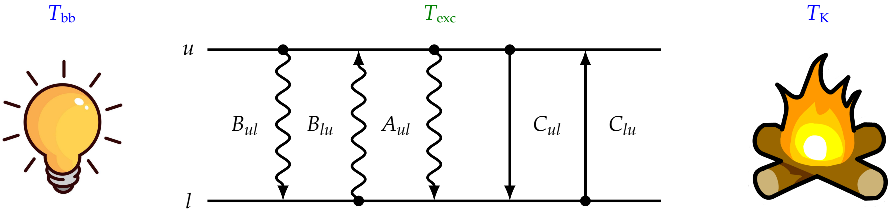
- Kinetic temperature (T_k): $\langle E_k \rangle = \frac{3}{2} k_B T_k$
- Black-body temperature ($T_{\rm bb}$): $B_\nu(T_{\rm bb}) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/k_B T_{\rm bb}} - 1}$
- Excitation temperature ($T_{\rm exc}, T_{\rm rot}, T_{\rm vib}, \ldots$): $\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-(E_u - E_l)/k_B T_{\rm exc}}$

Boltzmann population distribution

$$e^{-h\nu/k_B T_{\rm exc}} = \frac{1 + (n/n_{\rm crit}) e^{-h\nu/k_B T_{\rm K}} \left(e^{h\nu/k_B T_{\rm bb}} - 1\right)}{e^{h\nu/k_B T_{\rm bb}} + (n/n_{\rm crit}) \left(e^{h\nu/k_B T_{\rm bb}} - 1\right)} \quad , \quad \frac{n_{\rm crit}}{n} = \frac{A_{ul}}{C_{ul}}$$

critical density

$$\boxed{T_{\rm bb} \leq T_{\rm exc} \leq T_{\rm K} \quad \text{or} \quad T_{\rm K} \leq T_{\rm exc} \leq T_{\rm bb}}$$



Molecular excitation: $T_{\rm exc}$ and critical density

- $n_{\rm crit}$ is the density at which the change of regime occurs
- $n_{\rm crit}$ is different for every transition:

$$n_{\rm crit} = A_{ul}/\gamma_{ul} \quad , \quad n_{\rm crit} = n_{\rm crit}(\mu)$$

- Boltzmann regime: Excitation is dominated by collisions (collisional LTE)

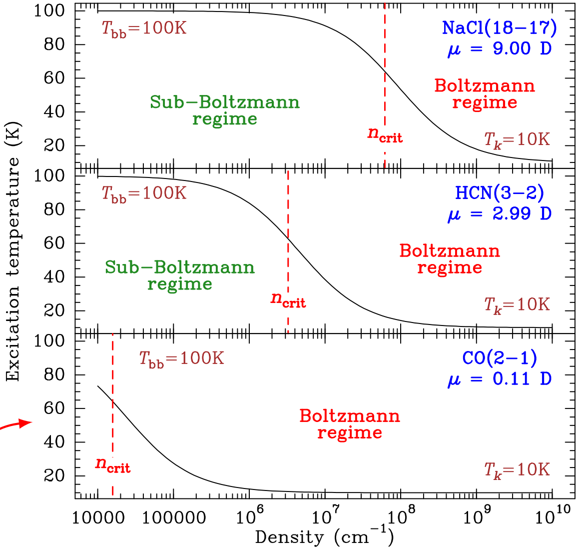
$$n \gg n_{\rm crit} \Longrightarrow T_{\rm exc} \simeq T_k$$

- Sub-Boltzmann regime: Excitation is dominated by radiation (radiative LTE)

$$n \ll n_{\rm crit} \Longrightarrow T_{\rm exc} \simeq T_{\rm bb}$$

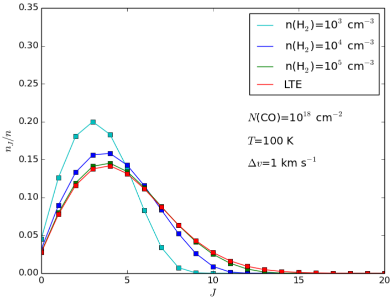
- When $n \simeq n_{\rm crit}$, $T_{\rm exc}$ strongly depends on the balance of the physical conditions

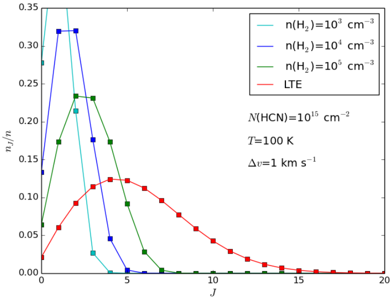
CO is easily thermalized which makes it one of the best molecules to trace T_k

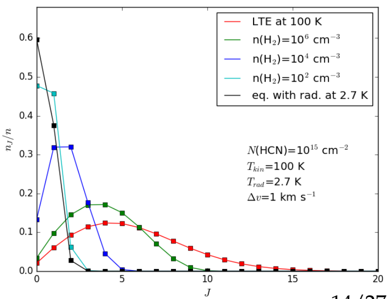


Molecular excitation: Dependence of rotational level populations with density

- The J of the strongest line depends on $T_{\rm exc}$
- $T_{\rm exc}$ depends on the gas density
- The CO rotational level are under collisional LTE for densities higher than $\sim 10^4 - 10^5$ cm^{-3}
- Gas density in molecular clouds $\sim 10^2 - 10^6$ cm^{-3}. Higher than $\sim 10^4$ cm^{-3} around evolved stars
- The behavior strongly changes for HCN ($\mu(\mathrm{HCN}) \simeq 30\mu(\mathrm{CO})$)
- HCN lines are more sensitive to change in density than those of CO for intermediate densities
- Molecules tend to de-excitate to the ground state (rotational relaxation)
- However, the population of the rotational levels have a lower limit determined by the Cosmic Microwave Background (CMB)
- The Boomerang Nebula is the only environment in the known Universe with a temperature lower than the $T_{\rm CMB} \simeq 2.73$ K [13]

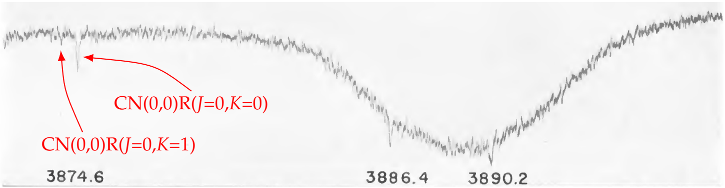




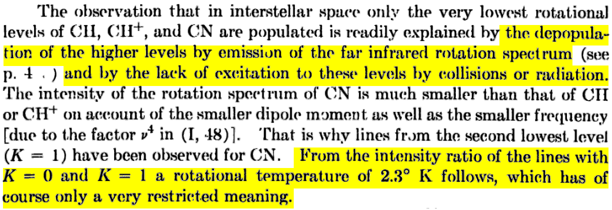


Molecular excitation: A piece of History of Science

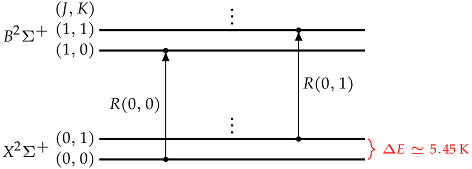
- Optical observations were taken from Mount Wilson of the ζ Oph
- 1940: McKellar presented the analysis of the data with the identifications of two weak CN lines with $J = 0$ $K = 0$ and $J = 0$ $K = 1$ of the R branch of the vibronic band $B^2\Sigma^+ - X^2\Sigma^+$ [8]
- 1941: Adams presented the observations [1]
- 1950: The Nobel Prize winner G. Herzberg estimated the intensity ratio for these lines deriving a rotational $T_{\rm exc} \simeq 2.3$ K [6]
- 1965: Penzias & Wilson [11] detected the Cosmic Microwave Background



Adapted from [8, 1]


The observation that in interstellar space only the very lowest rotational levels of CH, CH$^+$, and CN are populated is readily explained by the depopulation of the higher levels by emission of the far infrared rotation spectrum (see p. 4 .) and by the lack of excitation to these levels by collisions or radiation. The intensity of the rotation spectrum of CN is much smaller than that of CH or CH$^+$ on account of the smaller dipole moment as well as the smaller frequency [due to the factor ν^4 in (I, 48)]. That is why lines from the second lowest level ($K = 1$) have been observed for CN. From the intensity ratio of the lines with $K = 0$ and $K = 1$ a rotational temperature of 2.3° K follows, which has of course only a very restricted meaning.

Taken from [6], p. 496



Outline

1. Radiation transfer: A brief introduction
2. Molecular excitation
3. Solving the Statistical Equilibrium Equations (SEE) and the Radiation transfer problem
4. Line profiles
5. Summary and final remarks

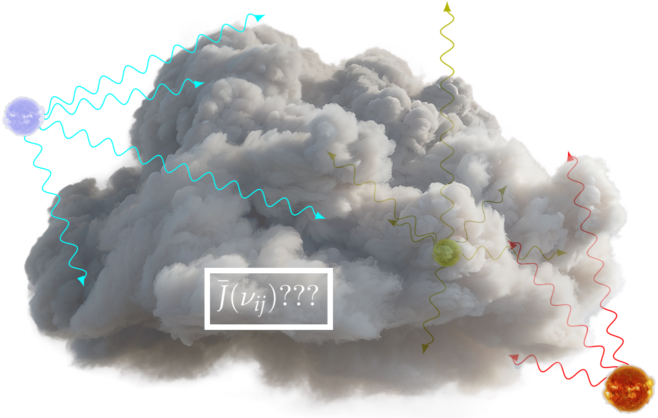
Solving the Statistical Equilibrium Equations (SEE)

$$\sum_{j>i} A_{ji}n_j - \sum_{j<i} A_{ij}n_i + \sum_{j\neq i} B_{ji}4\pi\bar{J}(\nu_{ji})n_j - \sum_{j\neq i} B_{ij}4\pi\bar{J}(\nu_{ij})n_i + \sum_{j\neq i} C_{ji}n_j - \sum_{j\neq i} C_{ij}n_i = 0$$

- We know the quantities A_{ij}, B_{ij}, C_{ij}, n
- Add a conservation condition:

$$\sum_i n_i = n$$

- This is an algebraic linear system of equations with all equations independent
- Can be solved with typical methods (system matrix decomposition – e.g., LU — or iterative methods – e.g., Jacobi)
- Main problem: calculate $\bar{J}(\nu_{ij}) \Longrightarrow$ Radiation transfer equation (SEE+RT; RT: Ray Tracing)



Radiation transfer: Solving methods

- Accelerated Λ iteration (ALI): It uses the Λ operator to calculate iteratively the total intensity and the source function at any point of the modeled environment ($J_\nu^{\mathrm{new}} = \Lambda S_\nu^{\mathrm{old}}$) [12, 17].

- Large Velocity Gradient (LVG; Sobolev method): A photon can escape from the region where it has been emitted due to differences in velocity with other close regions. It is the ALI method with $\Lambda = 1 - \beta$ [14, 3].

- Monte Carlo: A number of model photons (comprising many "real" photons) related to an initial source function travel through the modeled environment modifying the population of the molecular levels. The process is repeated to reach convergence [2, 16].

- Gauss-Seidel algorithm: The population of the molecular levels in a shell are recalculated once the total intensity for this shell is known. It is not necessary to solve the SSE for all the environment at the same time [15, 10, 4].

- Coupled escape probability (CEP): The molecular level populations are calculated without knowing the total radiation intensity in every point of the environment to model [5].

Radiation transfer: Solving methods (Large Velocity Gradient, LVG) [14, 3]

$$\sum_{j>i} A_{ji} n_j - \sum_{j<i} A_{ij} n_i + \sum_{j\neq i} B_{ji} 4\pi \bar{J}(\nu_{ji}) n_j - \sum_{j\neq i} B_{ij} 4\pi \bar{J}(\nu_{ij}) n_i + \sum_{j\neq i} C_{ji} n_j - \sum_{j\neq i} C_{ij} n_i = 0$$

$$\sum_{i} n_i = n$$

$$\boxed{n_i}$$

$$\boxed{\bar{J}_\nu}$$

$$\bar{J}_\nu = (1-\beta)\, S_\nu + \beta I_\nu^0 \qquad , \qquad \beta = \frac{1-e^{-\tau_\nu}}{\tau_\nu},$$

β: escape probability

Radiation transfer: Ray Tracing

- We integrate the emission along the line-of-sight by summing the contribution of each volume in the discretized cloud

$$I_\nu = I_\nu^{\rm bg} e^{-\tau_\nu} + S_\nu \left(1 - e^{-\tau_\nu}\right)$$

⬇

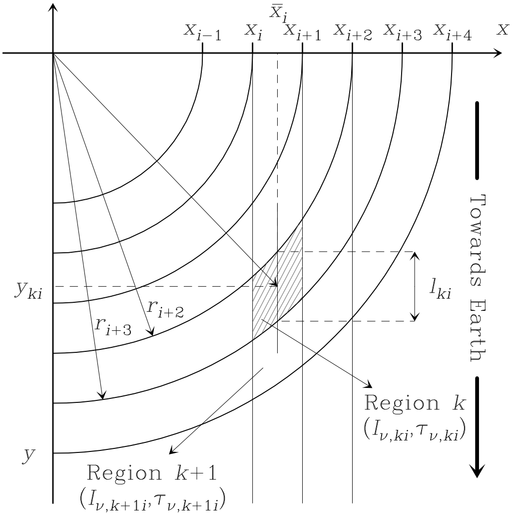
$$I_\nu(x_i) = \sum_{k=m_{x_i}}^{1} S_{\nu,k} \left(1 - e^{-\tau_{\nu,k}}\right) e^{-\sum_{j=1}^{k-1} \tau_{\nu,j}},$$

being m_{x_i} the number of discretized volumes for the x_i coordinate

- Finally, the flux is calculated along with the effect of the PSF of the telescope on the synthetic emission

$$F_\nu = \sum_{i=1}^{n_{\rm layers}} I_\nu(x_i) P(x_i) \delta w_i,$$

where δw_i is the solid angle subtended by the i-th layer



Outline

1. Radiation transfer: A brief introduction
2. Molecular excitation
3. Solving the Statistical Equilibrium Equations (SEE) and the Radiation transfer problem
4. **Line profiles**
5. Summary and final remarks

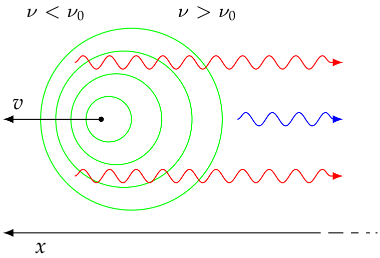
Line profiles: Doppler velocity

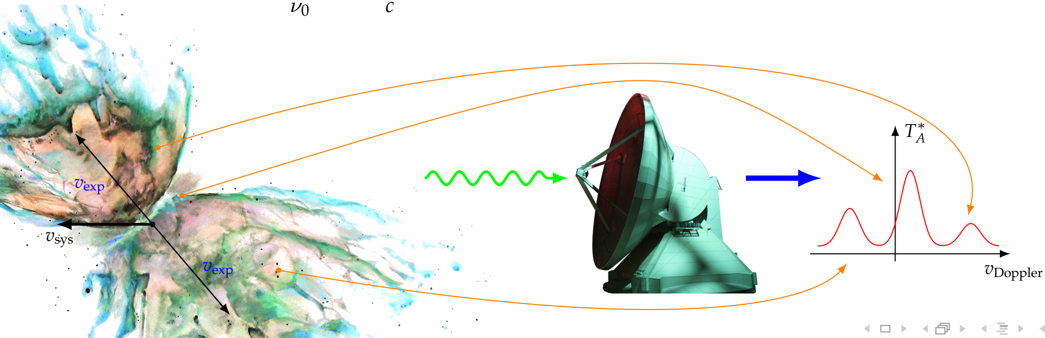
Relativistic Doppler effect

$$\underbrace{\frac{\nu-\nu_0}{\nu_0}}_{z} = \sqrt{\frac{1-v/c}{1+v/c}} - 1$$

Non-relativistic Doppler effect

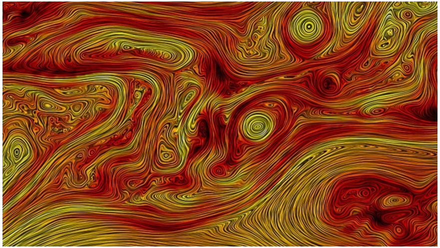
$$\frac{\nu-\nu_0}{\nu_0} \simeq -\frac{v}{c}$$





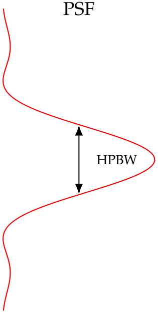
Line profiles: Turbulence and gas kinematics

Observed environment



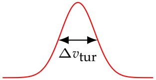
+

PSF

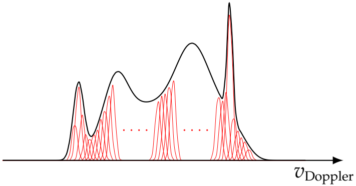


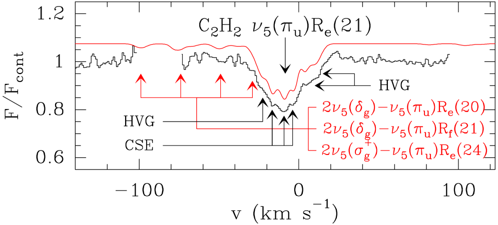
=

Gaussian
velocity profile



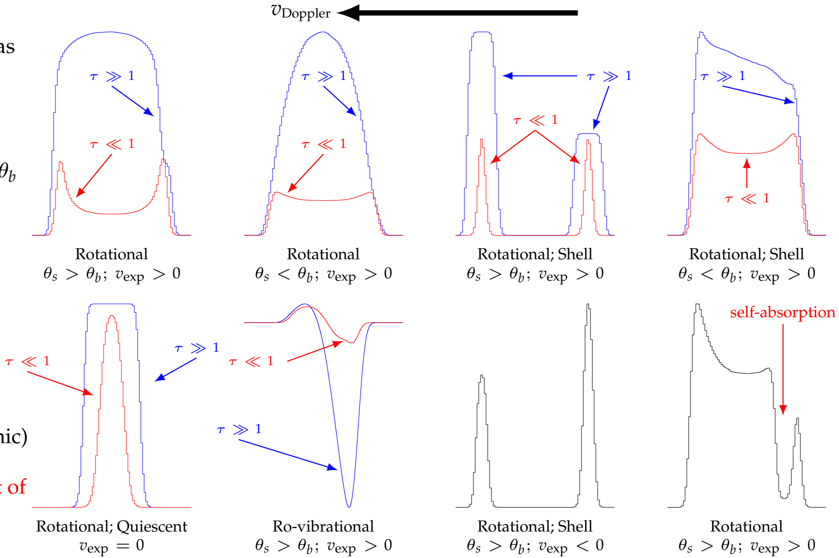
$$v_{\rm Doppler} = \frac{1}{\Delta v_{\rm tur}} \sqrt{\frac{4 \ln 2}{\pi}} \times e^{-v^2 4 \ln 2 / \Delta v_{\rm tur}^2}$$





Line profiles: Typical profiles

- Consider a spherically symmetric cloud with gas expanding radially
- Expansion velocity: v_{exp}
- Source diameter: θ_s
- HPBW of the telescope: θ_b
- Line profiles strongly depends on:
  - Physical conditions (T_k, T_{bb}, n)
  - Expansion velocity (v_{exp})
  - Turbulence (v_{tur})
  - Type of transition (rotational, vibrational, electronic)
  - Size of the source compared with that of the PSF



Outline

1. Radiation transfer: A brief introduction
2. Molecular excitation
3. Solving the Statistical Equilibrium Equations (SEE) and the Radiation transfer problem
4. Line profiles
5. Summary and final remarks

Summary and final remarks

- Understanding radiation transfer is essential to derive useful information about the observed environment
- Light interacts with the gas-phase and solid state material absorbing and re-emitting photons that modifies the radiation field
- This radiation-matter interaction can only be understood with quantum mechanics
- Einstein coefficients (excitation, spontaneous and induced de-excitation) are used to analyze the effect of radiation on molecules
- Molecular excitation depends on the radiation field ($T_{\rm bb}$) and on collisions (T_k)
- Level populations are widely described by Boltzmann factors depending on an excitation temperature, $T_{\rm exc}$
- $T_{\rm exc}$ along with the critical density, $n_{\rm crit}$, qualitatively explains excitation in a given scenario
- Populations can be determined by solving the statistical equilibrium equations
- The combinations of these equations and the radiation transfer equations allow us to solve the problem and derive the physical and chemical conditions from astronomical observations

Use numerical codes to reproduce the observations and $T_{\rm exc}$ and $n_{\rm crit}$ to interpret them

References

[1] Adams, 1941, ApJ, 93, 11

[2] Bernes, 1979, A&A, 73, 67

[3] Castor, 1970, MNRAS, 149, 111

[4] Daniel & Cernicharo, 2008, A&A, 488, 1237

[5] Elitzur & Asensio-Ramos, 2006, MNRAS, 365, 779

[6] Herzberg, Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules, D. Van Nostrand Company, Canada, 1950, p. 496

[7] Ivanov, “Transfer of radiation in spectral lines”, NBS Special Publication, Washington: US Department of Commerce, National Bureau of Standards, 1973, English language edition

[8] McKellar, 1940, PASP, 52, 187

[9] Mihalas, “Stellar atmospheres”, 2nd edition, Freeman, San Francisco, 1978

[10] Paletou & Léger, 2007, J. Quant. Spec. Rad. Trans., 103, 53

[11] Penzias & Wilson, 1965, ApJ, 142, 419

[12] Rybicki & Hummer, 1991, A&A, 245, 171

[13] Sahai & Nyman, 1997, ApJ, 487, L155

[14] Sobolev, “Moving envelopes of stars”, Chap. 1, Harvard Univ. Press, Cambridge, 1960

[15] Trujillo-Bueno & Fabiani-Bendicho, 1995, ApJ, 455, 646

[16] van Zadelhoff et al., 2002, A&A, 395, 373

[17] Uitenbroek, 2001, ApJ, 557, 389