Introduction to molecular excitation and radiative transfer

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Outline

The two-level approximation

Following Quantum Physics, 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.

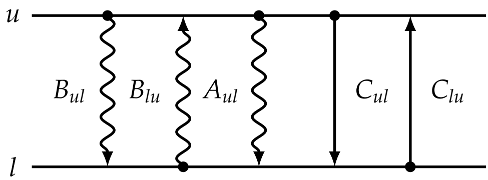
$$\left.\begin{aligned} A_{ul} &= \frac{4\pi}{c}\frac{2h\nu^3}{c^2}B_{ul} \\ B_{ul} &= \frac{g_l}{g_u}B_{lu} \end{aligned}\right\} \text{ Einstein coefficients}$$

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

induced absorption

induced emission

spontaneous emission



Boltzmann population distribution

We use three different temperatures:

- kinetic temperature (T_K): $\langle E_\mathrm{kinetic} \rangle = \frac{3}{2} k_B T_\mathrm{K}$
- black-body temperature (T_bb): $B_\nu(T_\mathrm{bb}) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/k_B T_\mathrm{bb}} - 1}$
- excitation temperature (T_exc, T_rot, T_vib,...): $\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-(E_u - E_l)/k_B T_\mathrm{exc}}$

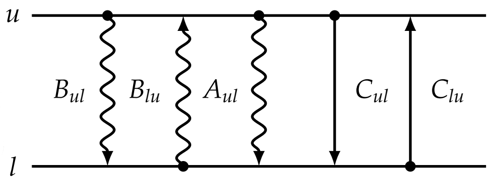
$$e^{-h\nu/k_B T_\mathrm{exc}} = \frac{1 + (n/n_\mathrm{crit}) e^{-h\nu/k_B T_\mathrm{K}} \left(e^{h\nu/k_B T_\mathrm{bb}} - 1\right)}{e^{h\nu/k_B T_\mathrm{bb}} + (n/n_\mathrm{crit}) \left(e^{h\nu/k_B T_\mathrm{bb}} - 1\right)} \quad , \quad \frac{n_\mathrm{crit}}{n} = \frac{A_{ul}}{\gamma_{ul}}$$

critical density

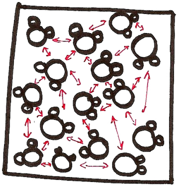
$$\boxed{T_\mathrm{bb} \le T_\mathrm{exc} \le T_\mathrm{K} \quad \text{or} \quad T_\mathrm{K} \le T_\mathrm{exc} \le T_\mathrm{bb}}$$

T_bb

T_exc



T_K

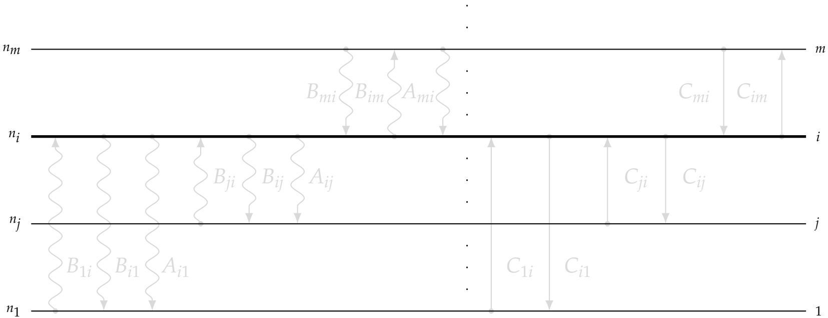


steady-state regime

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

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

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



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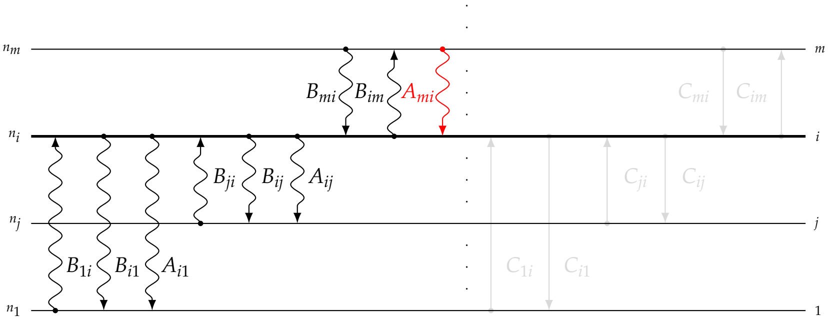

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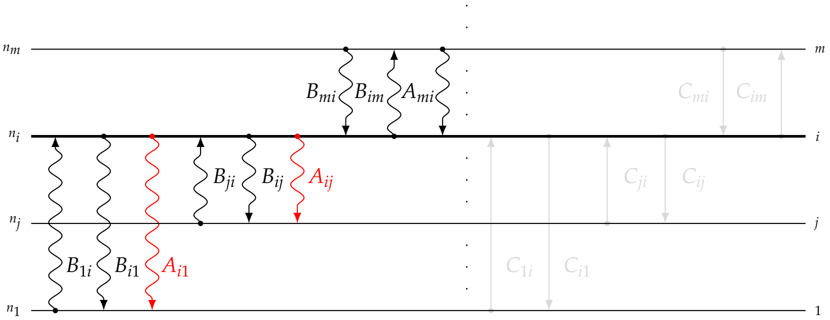

steady-state regime

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

ntaneous

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

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

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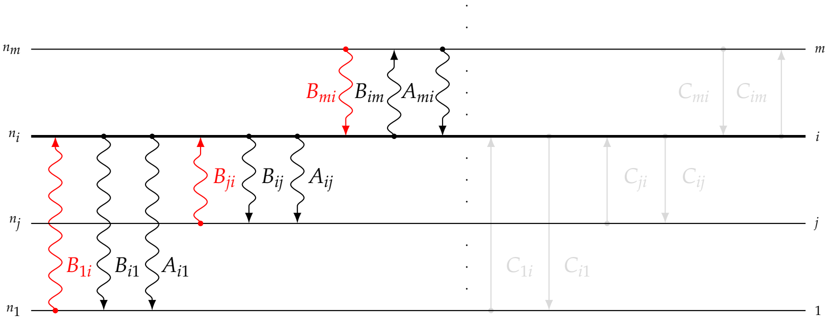

Statistical Equilibrium

steady-state regime

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

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

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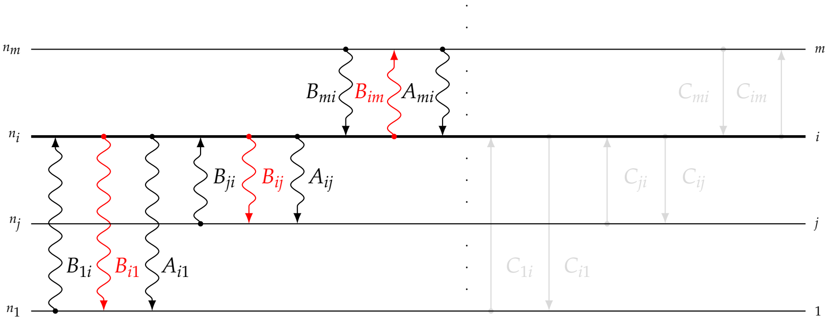

steady-state regime

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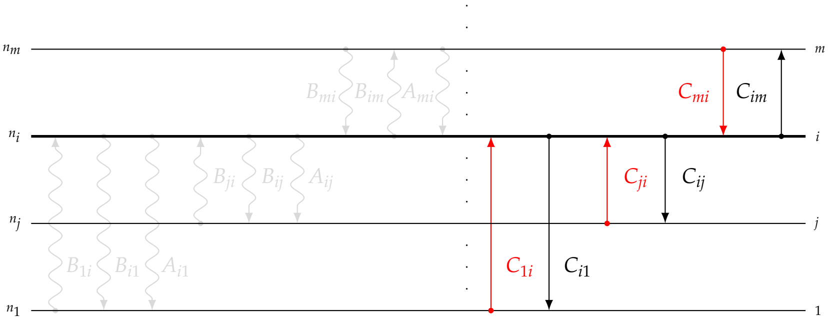

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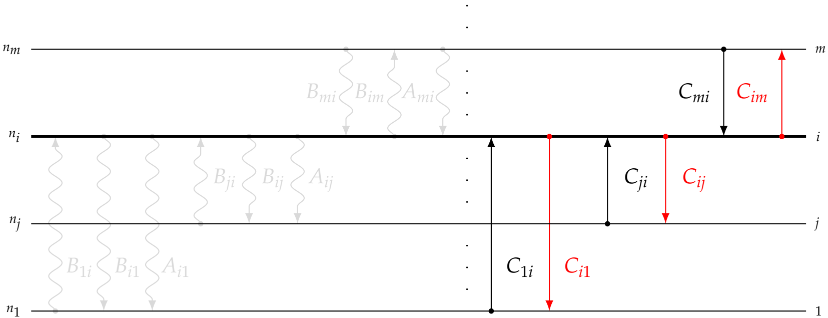
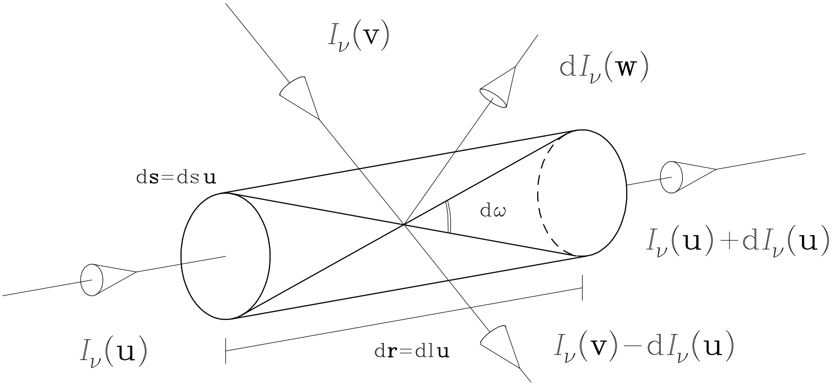
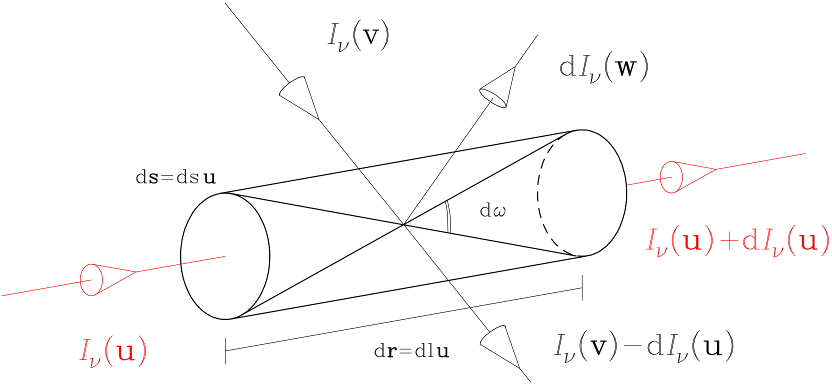




$$\begin{aligned}
I_\nu(\mathbf{r}+d\mathbf{r},\mathbf{u})d\omega ds d\nu &= I_\nu(\mathbf{r},\mathbf{u})d\omega ds d\nu dl + dI_\nu(\mathbf{r},\mathbf{u})d\omega ds d\nu \\
&= I_\nu(\mathbf{r},\mathbf{u})d\omega ds d\nu dl - \mathscr{A}^g_\nu(\mathbf{r},\mathbf{u}) - \mathscr{A}^d_\nu(\mathbf{r},\mathbf{u}) + \mathscr{E}^g_\nu(\mathbf{r},\mathbf{u}) \\
&\quad + \mathscr{E}^d_\nu(\mathbf{r},\mathbf{u}) + \mathscr{S}^g_{\star\to\nu}(\mathbf{r},\star\to\mathbf{u}) + \mathscr{S}^d_{\star\to\nu}(\mathbf{r},\star\to\mathbf{u}) \\
&\quad - \mathscr{S}^g_{\nu\to\star}(\mathbf{r},\mathbf{u}\to\star) - \mathscr{S}^d_{\nu\to\star}(\mathbf{r},\mathbf{u}\to\star)
\end{aligned}$$



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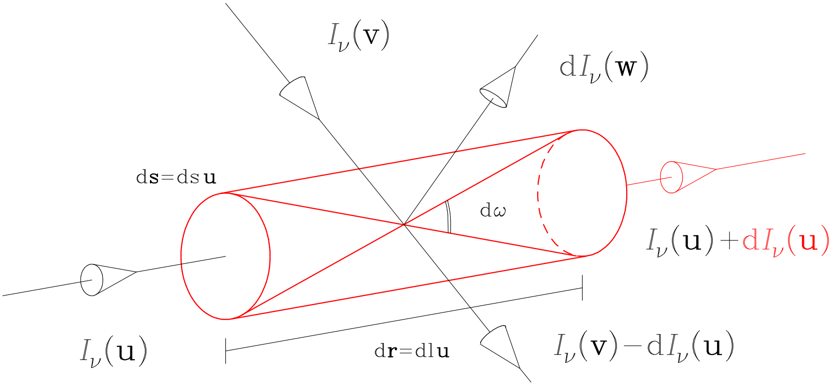
$$



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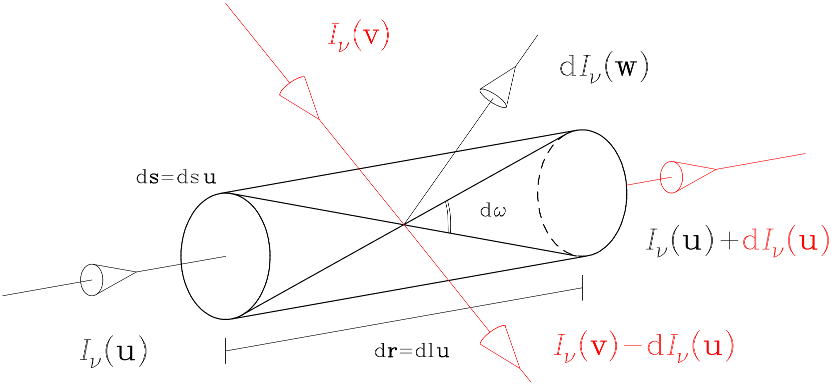

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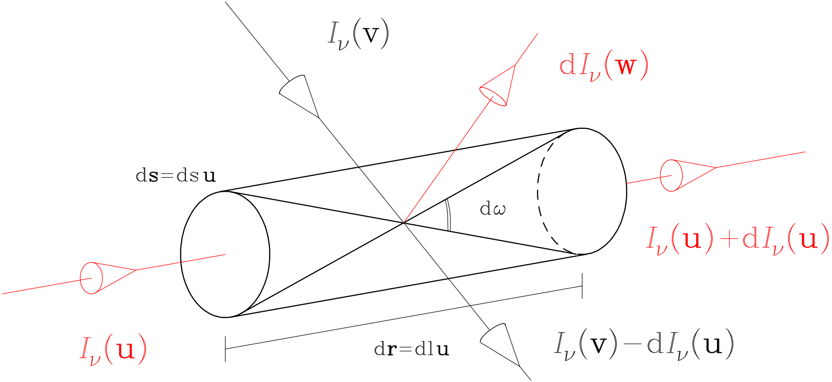

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\end{aligned}
$$

Radiative transfer[2, 3] — The equation

$$
\begin{aligned}
dI_\nu(\mathbf{r},\mathbf{u})d\omega ds d\nu = & -\mathscr{A}^g_\nu(\mathbf{r},\mathbf{u}) - \mathscr{A}^d_\nu(\mathbf{r},\mathbf{u}) + \mathscr{E}^g_\nu(\mathbf{r},\mathbf{u}) \\
& + \mathscr{E}^d_\nu(\mathbf{r},\mathbf{u}) + \mathscr{S}^g_{\star\to\nu}(\mathbf{r},\star\to\mathbf{u}) + \mathscr{S}^d_{\star\to\nu}(\mathbf{r},\star\to\mathbf{u}) \\
& - \mathscr{S}^g_{\nu\to\star}(\mathbf{r},\mathbf{u}\to\star) - \mathscr{S}^d_{\nu\to\star}(\mathbf{r},\mathbf{u}\to\star)
\end{aligned}
$$

- $\mathscr{S}^g_{\star\to\nu}(\mathbf{r},\star\to\mathbf{u})$ and $\mathscr{S}^g_{\nu\to\star}(\mathbf{r},\mathbf{u}\to\star)$: Rayleigh scattering, Compton effect, etc., can be neglected in the CSM and ISM. We assume *complete frequency redistribution* [4, 5, 6, 7].
- $\mathscr{S}^d_{\star\to\nu}(\mathbf{r},\star\to\mathbf{u})$ and $\mathscr{S}^d_{\nu\to\star}(\mathbf{r},\mathbf{u}\to\star)$: Scattering by dust grains is not important for wavelengths larger than $\simeq 8\ \mu$m.

$$
dI_\nu(\mathbf{r},\mathbf{u})d\omega ds d\nu \simeq -\mathscr{A}^g_\nu(\mathbf{r},\mathbf{u}) - \mathscr{A}^d_\nu(\mathbf{r},\mathbf{u}) + \mathscr{E}^g_\nu(\mathbf{r},\mathbf{u}) + \mathscr{E}^d_\nu(\mathbf{r},\mathbf{u})
$$

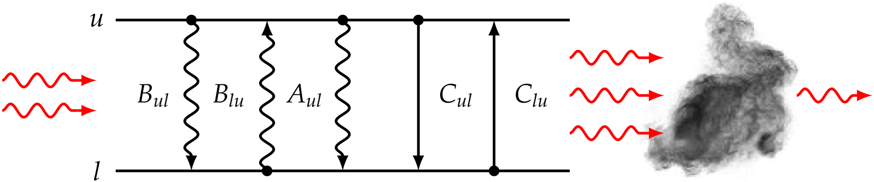
$$\left.\frac{dI_\nu}{dl}\right|_{\text{molecule}} = \underbrace{\frac{h\nu}{4\pi}A_{ul}n_u + \frac{h\nu}{c}B_{ul}I_\nu n_u}_{emission} - \underbrace{\frac{h\nu}{c}B_{lu}I_\nu n_l}_{absorption}$$

Einstein coefficients

The colisional constants C_{ul} and C_{lu} modify the population of the molecular levels, affecting the emitted and absorbed intensity.

$$\left.\frac{dI_\nu}{dl}\right|_{\text{dust}} = \underbrace{n_d\sigma_\nu S_\nu(T_d)}_{emission} - \underbrace{n_d\sigma_\nu I_\nu}_{absorption}$$

Absorption cross section



Molecules Dust

If the observed environment comprises molecular gas and dust:

$$\frac{dI_\nu}{dl} = -\left[k_\nu^g + k_\nu^d\right] I_\nu + \varepsilon_\nu^g + \varepsilon_\nu^d.$$

The typical form of the radiation transfer equation is:

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

source function

optical depth $(d\tau_\nu = k_\nu dl)$

total opacity

$$k_\nu = k_\nu^g + k_\nu^d$$

$$S_\nu = \frac{\varepsilon_\nu}{k_\nu} = \frac{\varepsilon_\nu^g + \varepsilon_\nu^d}{k_\nu^g + k_\nu^d} = \frac{k_\nu^g}{k_\nu^g + k_\nu^d}\frac{\varepsilon_\nu^g}{k_\nu^g} + \frac{k_\nu^d}{k_\nu^g + k_\nu^d}\frac{\varepsilon_\nu^d}{k_\nu^d}$$

$$= \frac{k_\nu^g}{k_\nu} S_\nu^g + \frac{k_\nu^d}{k_\nu} S_\nu^d$$

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

absorption profile (normalized)

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

gas density

A-Einstein coefficient

partition function

degeneracy of the upper level

Assuming local termodynamical equilibrium (LTE, $T_{\rm exc} = T_{\rm K} = T$):

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

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

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

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

absorption profile (normalized)

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

gas density

A-Einstein coefficient

partition function

degeneracy of the upper level

The opacity of a given line is positive if

$$\zeta = 1 - \frac{g_l n_u}{g_u n_l} > 0 \Longrightarrow \frac{n_u}{n_l} < \frac{g_u}{g_l} \Longrightarrow T_{\rm exc} > 0,$$

resulting in thermal emission, and negative if

$$\zeta = 1 - \frac{g_l n_u}{g_u n_l} < 0 \Longrightarrow \frac{n_u}{n_l} > \frac{g_u}{g_l} \Longrightarrow T_{\rm exc} < 0,$$

producing maser emission (*population inversion*).

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

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

gas opacity per line

total gas opacity

Assuming LTE ($T_{\rm exc} = T_{\rm K} = T$):

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

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

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

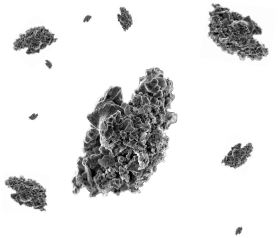
Radiative transfer[2, 3] — k_ν and S_ν of a dust grain

For a solid state material which accounts for a fraction y of each grain:

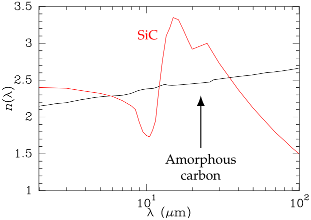
$$
\begin{aligned}
k_\nu^d &= n_d y \sigma_{\nu,i} = n_d y \sigma_g Q_{\text{abs,i}}(\lambda) \\
&= n_d y \sigma_g \frac{\tilde{Q}_{\text{abs,i}}(\lambda)}{\lambda} \\
&= n_d y \sigma_g \frac{1}{\lambda} \underbrace{\left\{ -8\pi r_g \mathrm{Im}\left[\frac{m^2-1}{m^2+1}\right] \right\}}_{\boxed{\text{Mié Theory [8]}}}
\end{aligned}
$$

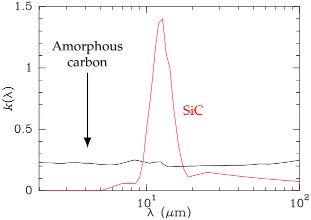
absorption efficiency

geometrical section



Optical properties (refraction index: $m = n + ik$) [9, 10, 11, 12, 13, 14]



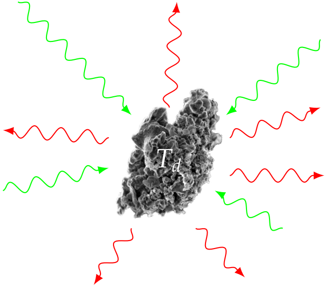


For a solid state material which accounts for a fraction y of each grain:

$$
\begin{aligned}
k_\nu^d &= n_d y \sigma_{\nu,i} = n_d y \sigma_g Q_{\text{abs,i}}(\lambda) \\
&= n_d y \sigma_g \frac{\tilde{Q}_{\text{abs,i}}(\lambda)}{\lambda} \\
&= n_d y \sigma_g \frac{1}{\lambda}\left\{-8\pi r_g \mathrm{Im}\left[\frac{m^2-1}{m^2+1}\right]\right\}
\end{aligned}
$$

absorption efficiency

geometrical section



$$\boxed{\text{Thermal equilibrium + Gray body } (S_\nu^d = B_\nu(T_d))}$$

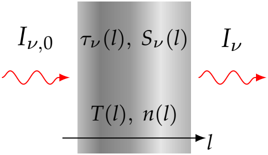
Total absorption = Total emission $+$ $\varepsilon_\nu \simeq k_\nu^d B_\nu(T_d)$

$$\int_0^\infty d\nu k_\nu^d \underbrace{\int_{4\pi} d\omega I_\nu(\omega)}_{4\pi \bar{J}_\nu:\ \text{total intensity}} = 4\pi \int_0^\infty d\nu \varepsilon_\nu^d \simeq 4\pi \int_0^\infty d\nu k_\nu^d B_\nu(T_d) \quad \Longrightarrow \quad T_d$$

A plane-parallel layer

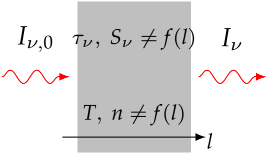
The solution of the radiation transfer equation for a plane-parallel layer is:

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



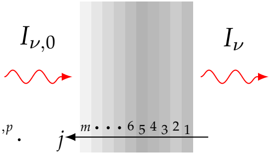
For a layer with constant temperature and density, $S_\nu = \text{const.}$:

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



The numerical solution of the radiation transfer equation is based on the discretization of the target environment in m layers with constant physical quantities:

$$I_\nu = I_{\nu,0} e^{-\sum_{j=1}^{m} \tau_{\nu,j}} + \sum_{j=1}^{m} S_\nu(T_j)\left(1 - e^{-\tau_{\nu,j}}\right) e^{-\sum_{p=1}^{j-1} \tau_{\nu,p}} .$$



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

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

$$\tau_\nu \gg 1$$

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

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

Assuming we have observed a set of rotational lines of a molecule and they are optically thin [15]:

$$F_\nu^{\text{observed}} \simeq \langle I_\nu \rangle \frac{\pi}{4}\left(\theta_s^2 + \theta_b^2\right) = \frac{2k_B\nu^2 T_{mb}}{c^2}\frac{\pi}{4}\left(\theta_s^2 + \theta_b^2\right) \quad , \quad T_{mb} = \frac{F_{\text{eff}}}{B_{\text{eff}}} T_{\text{A}}^*$$

$$F_\nu^{\text{emitted}} \simeq \frac{2k_B\nu^2 T_B}{c^2}\frac{\pi}{4}\theta_s^2 = \frac{h\nu}{4\pi} g_u A_{ul} \frac{N_{\text{col}}}{Z} e^{-E_u/k_B T_{\text{rot}}} \phi_\nu \frac{\pi}{4}\theta_s^2$$

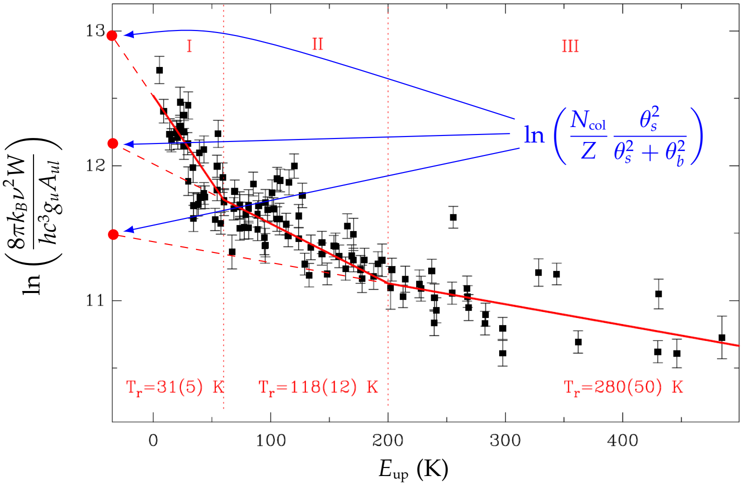
$$W = \int_0^\infty T_{mb} dv \simeq \frac{hc^3 g_u A_{ul}}{8\pi k_B \nu^2} \frac{N_{\text{col}}}{Z} e^{-E_u/k_B T_{\text{rot}}} \frac{\theta_s^2}{\theta_s^2 + \theta_b^2}$$

$$\boxed{\ln\left(\frac{8\pi k_B \nu^2 W}{hc^3 g_u A_{ul}}\right) \simeq \ln\left(\frac{N_{\text{col}}}{Z}\frac{\theta_s^2}{\theta_s^2 + \theta_b^2}\right) - \frac{E_u}{k_B T_{\text{rot}}}}$$

In the optically thick regime, the additional quantity $\ln\left[\underbrace{(1 - e^{-\tau})/\tau}_{\text{escape probability } (\beta)}\right]$ needs to be added to the right hand term.

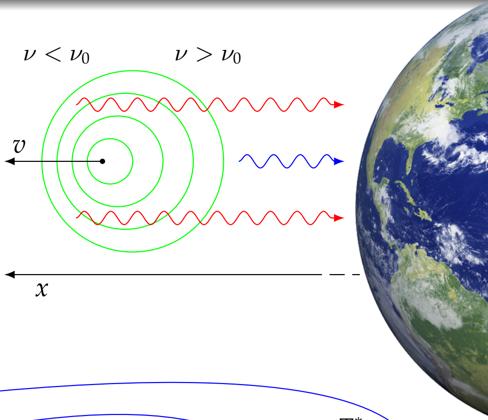
escape probability (β)[20, 21, 22, 23, 3, 24]

Assuming we have observed a set of rotational lines of a molecule and they are optically thin [26]:



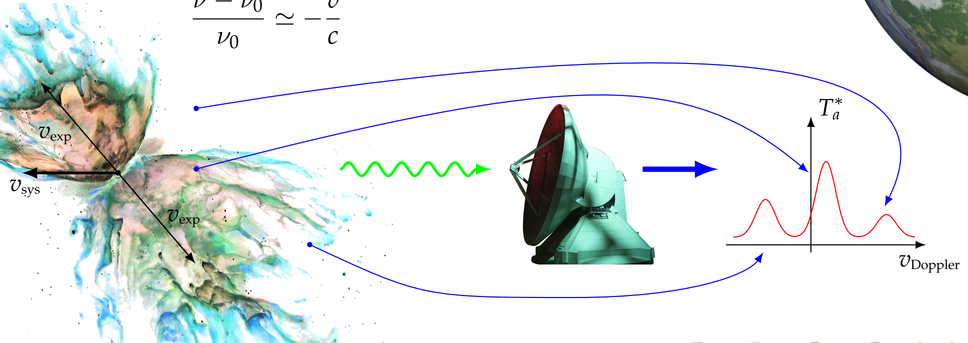
Relativistic Doppler effect

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

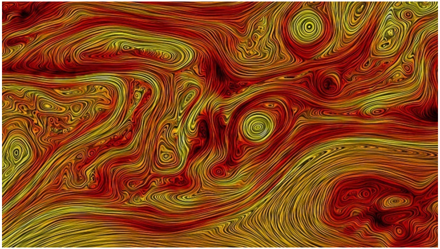


Non-relativistic Doppler effect

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



Observed environment



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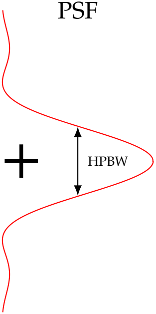
PSF



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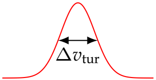
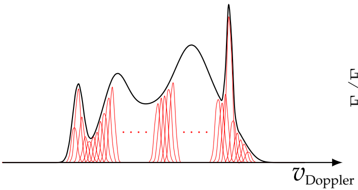
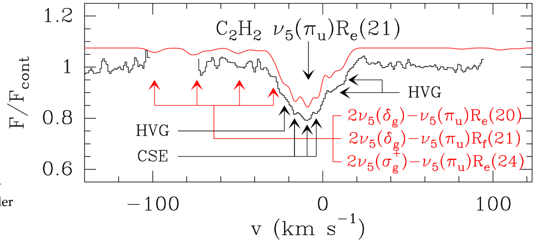
Gaussian velocity profile



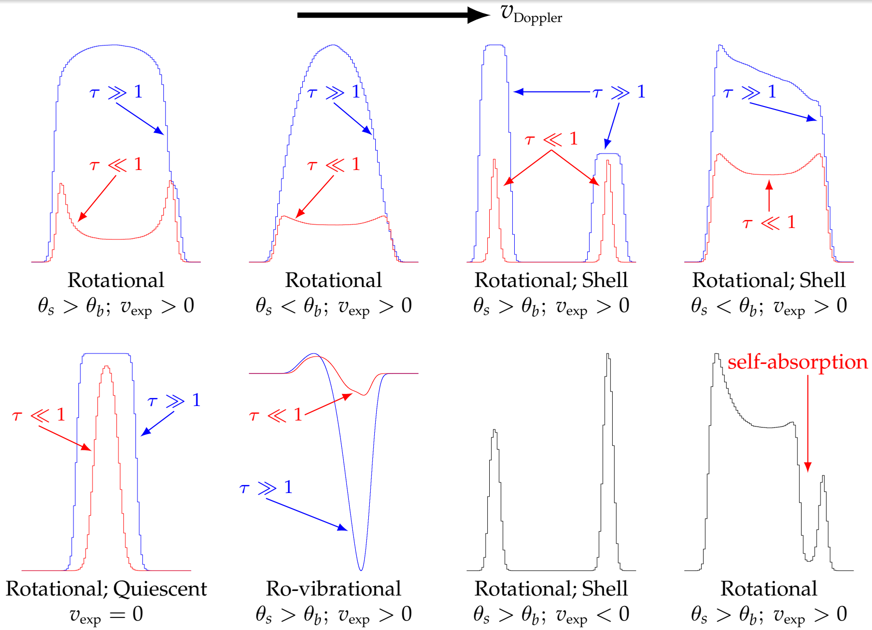
$$v_{\rm Doppler} = \frac{1}{\Delta v_{\rm tur}}\sqrt{\frac{4\ln 2}{\pi}} \times e^{-v^2 4\ln 2/\Delta v_{\rm tur}^2}$$





- Accelerated Λ iteration (ALI) [17, 30]: It uses the Λ_{ij} operator to calculate iteratively the total intensity and the source function at any point of the modeled environment.
- Large Velocity Gradient (LVG; Sobolev method) [22, 25]: 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 $\Lambda_{ij} = 1 - \beta$.
- Monte Carlo [18, 28]: 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.
- Gauss-Seidel algorithm [31, 32, 16]: 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.
- Coupled escape probability (CEP) [34]: The molecular level populations are calculated without knowing the total radiation intensity in every point of the environment to model.

Typical resulting lines



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