Introduction to radiative transfer and molecular excitation

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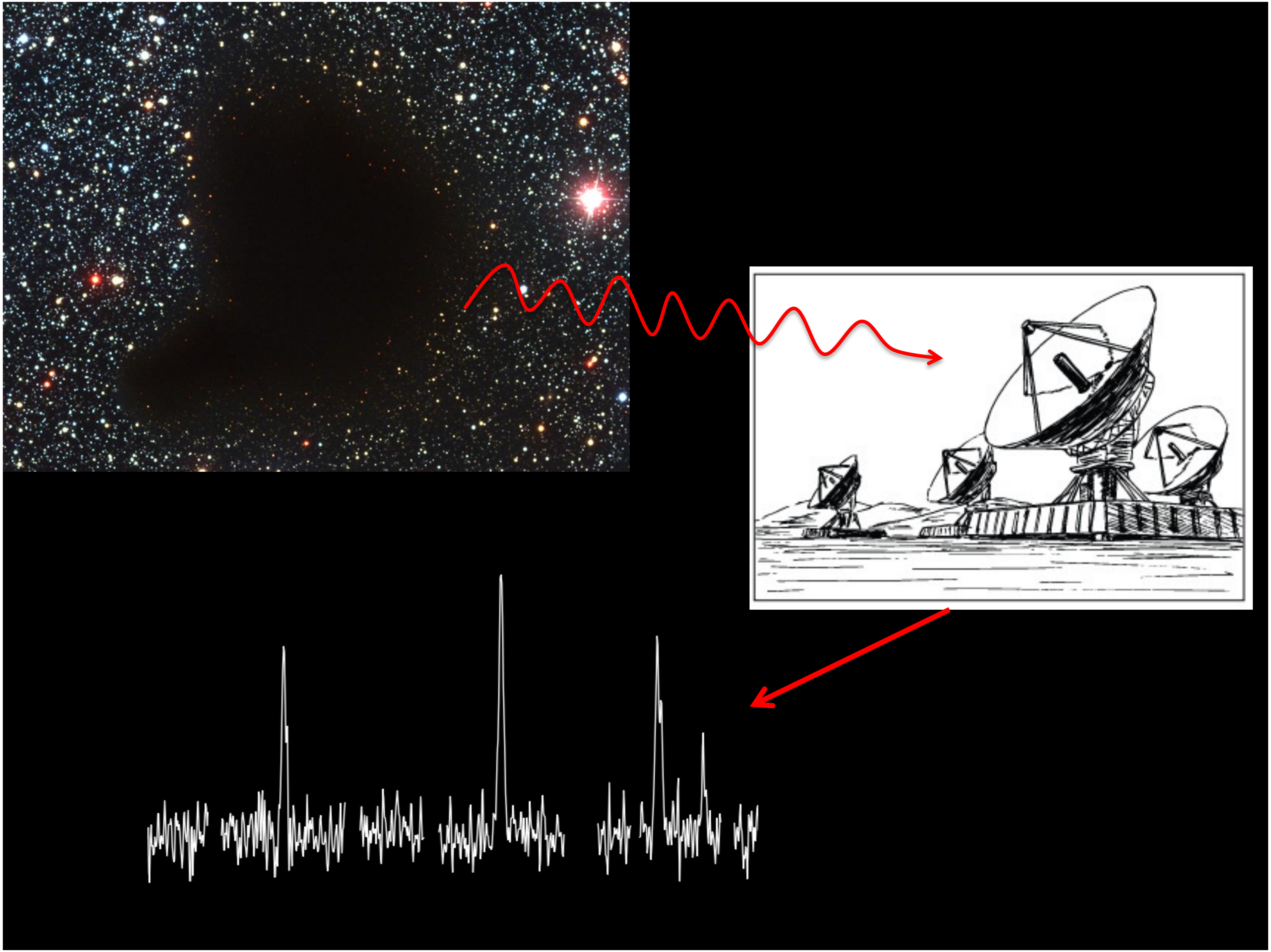


Organization of this lesson

1) Introduction to radiative transfer

2) Introduction to molecular excitation

3) Line profiles

1) Introduction to radiative transfer

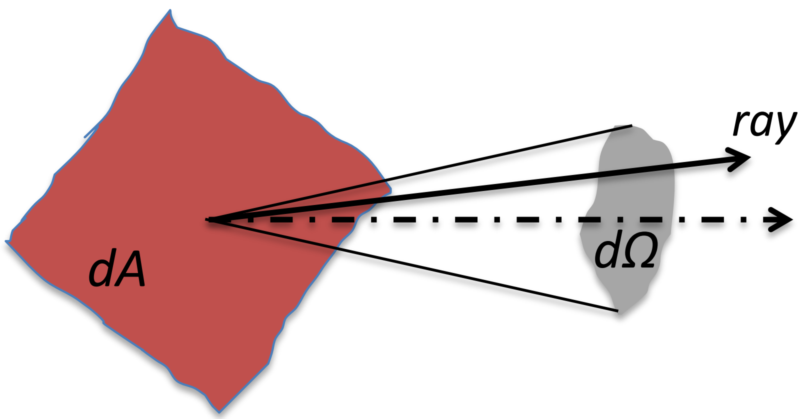
A good introduction can be found for example in chapter 1 of
"*Radiative Processes in Astrophysics"* by Rybicki and Lightman

A key quantity: *the specific intensity* I_ν

I_ν is the energy carried out by a set of rays within a solid angle $d\Omega$ crossing an area dA perpendicular to the direction of propagation in a time interval dt within a frequency range $d\nu$

$$dE = I_\nu \, dt \, dA \, d\nu \, d\Omega$$

$$I_\nu = energy\ (time)^{-1}\ (area)^{-1}\ (frequency)^{-1}\ (solid\ angle)^{-1} = erg\ s^{-1}\ cm^{-2}\ Hz^{-1}\ sr^{-1}$$



I_ν is conserved along a ray in empty space

$$\frac{dI_\nu}{ds} = 0$$

I_ν depends on the position in space and on the direction

A key equation: *the equation of radiative transfer*

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu$$

defining τ_ν and S_ν as:

$$d\tau_\nu = \alpha_\nu \, ds \qquad S_\nu = \frac{j_\nu}{\alpha_\nu}$$

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

s path length of propagation of ray (=) cm

α_ν absorption coefficient (=) cm^{-1}

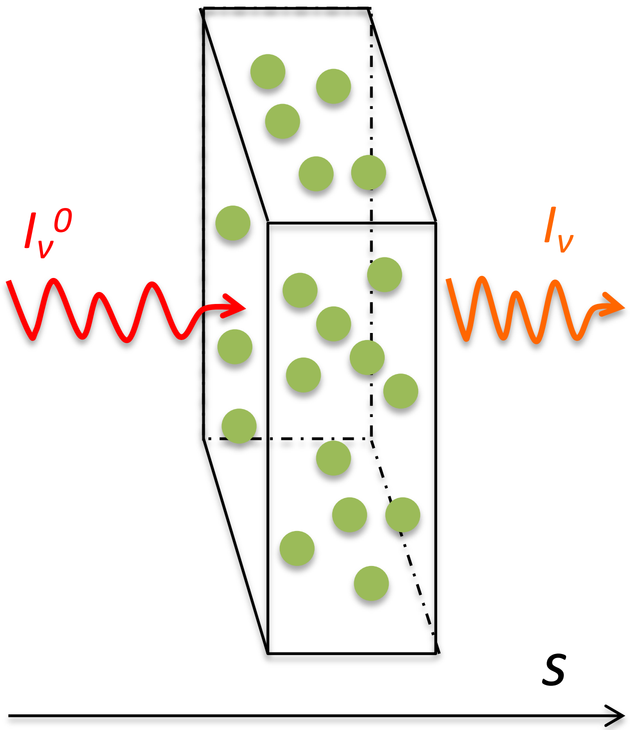
j_ν emission coefficient (=) $erg\ s^{-1}\ cm^{-3}\ Hz^{-1}\ sr^{-1}$

formal solution of the equation of radiative transfer:

$$I_\nu(\tau_\nu) = I_\nu(0)\, e^{-\tau_\nu} + \int_0^{\tau_\nu} S_\nu(\tau_\nu')\, e^{-(\tau_\nu-\tau_\nu')}\, d\tau_\nu'$$

solution for an homogeneous medium:

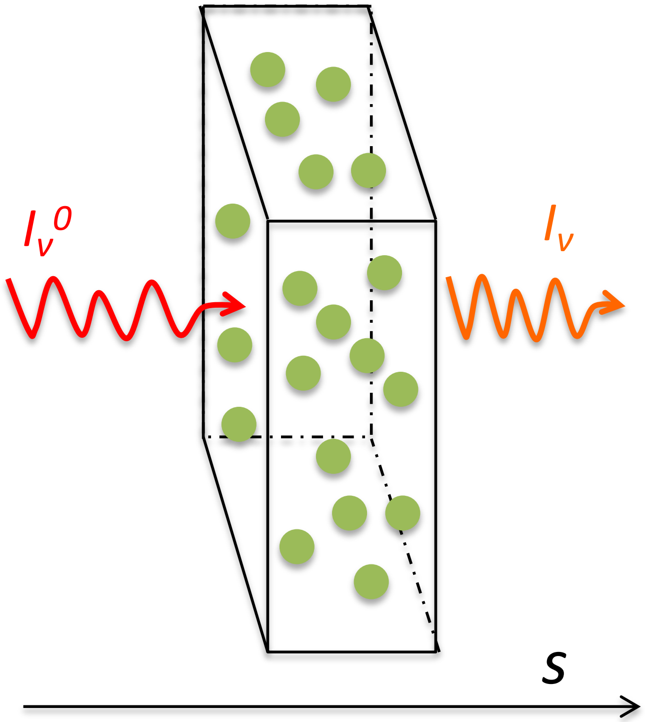
$$I_\nu = I_\nu^0\, e^{-\tau_\nu} + S_\nu (1 - e^{-\tau_\nu})$$



Limiting cases (τ_ν)

radiative transfer equation
for an homogeneous medium

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



$\tau_\nu \to 0 \quad \Rightarrow \quad I_\nu = I_\nu^0 + [S_\nu - I_\nu^0]\, \tau_\nu$ optically thin emission

$\tau_\nu \to \infty \quad \Rightarrow \quad I_\nu = S_\nu$ optically thick emission

Limiting cases (τ_ν)

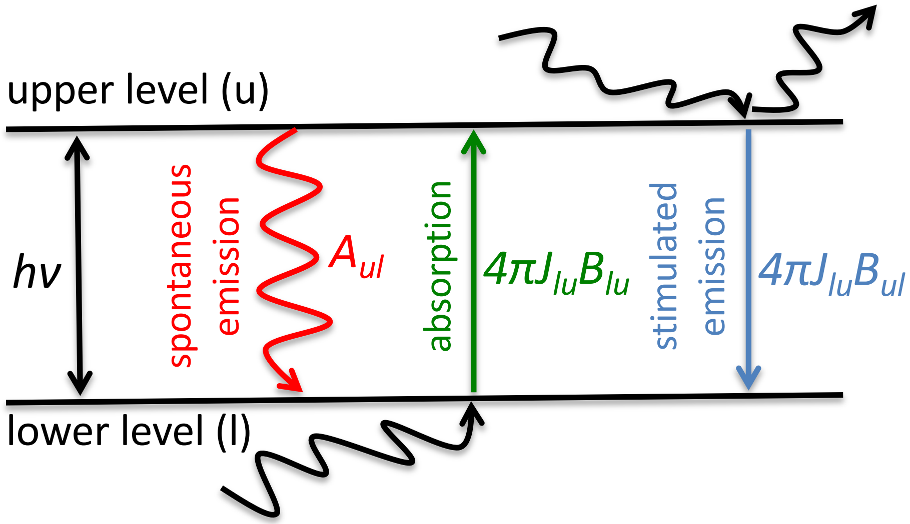
Transparent **Opaque**

$\tau_\nu \rightarrow 0$ ➔ $I_\nu = I_\nu^0 + [S_\nu - I_\nu^0]\,\tau_\nu$ optically thin emission

$\tau_\nu \rightarrow \infty$ ➔ $I_\nu = S_\nu$ optically thick emission

From macroscopic ($\alpha_\nu\, j_\nu$) to microscopic quantities

A_{ul}	*spontaneous emission rate*	$[=]\ s^{-1}$
$4\pi J B_{lu}$	*absorption rate*	$[=]\ s^{-1}$
$4\pi J B_{ul}$	*stimulated emission rate*	$[=]\ s^{-1}$



relations between Einstein coefficients

$$A_{ul} = 4\pi \frac{2h\nu^3}{c^2} B_{ul} \qquad g_l B_{lu} = g_u B_{ul}$$

$g_l\ g_u$ *statistical weight of lower and upper level*

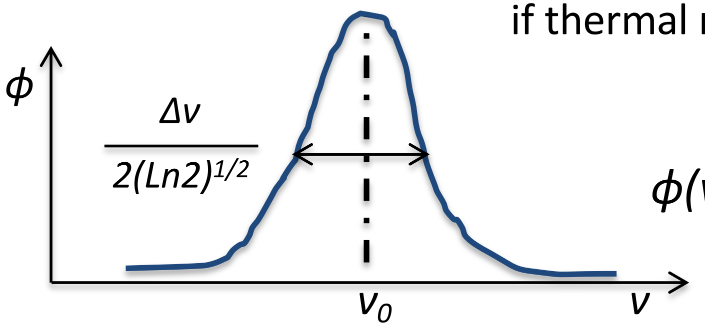
average radiation field J

$$J = \frac{1}{4\pi} \int_{4\pi} d\Omega \int_0^\infty I_\nu\, \phi(\nu)\, d\nu$$

intrinsic line profile function $\phi(\nu)$ $[=]\ Hz^{-1}$

normalized such as:

$$\int_0^\infty \phi(\nu)\, d\nu = 1$$



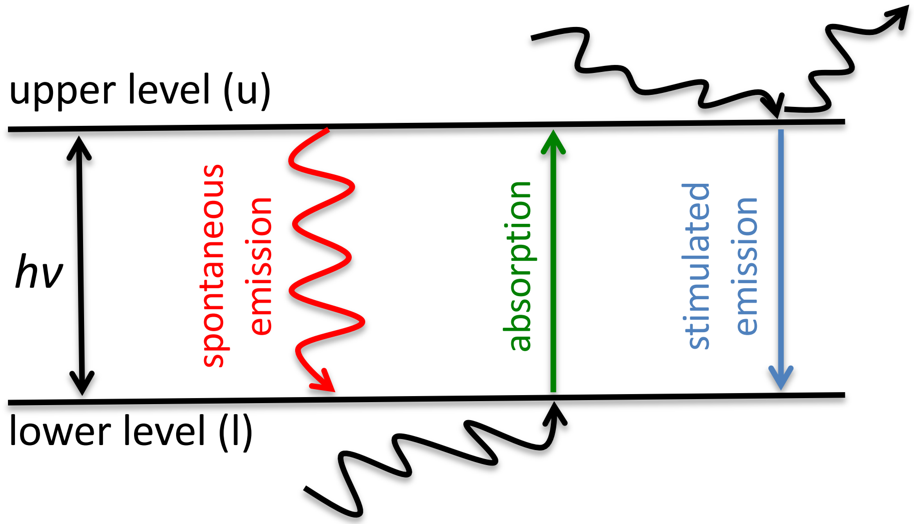
if thermal motions or turbulence dominate:
gaussian line profile

$$\phi(\nu) = \frac{1}{\Delta\nu\, \pi^{1/2}} \exp\left\{-\left(\frac{\nu-\nu_0}{\Delta\nu}\right)^2\right\}$$

From macroscopic (α_ν j_ν) to microscopic quantities

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\alpha_\nu = \frac{c^2 A_{ul} n_u}{8\pi\nu^2} \left(\frac{n_l/g_l}{n_u/g_u} - 1 \right) \phi(\nu)$$



A_{ul} *Einstein coefficient of spontaneous emission* $[=]\ s^{-1}$

$g_l\ g_u$ *statistical weight of lower and upper level*

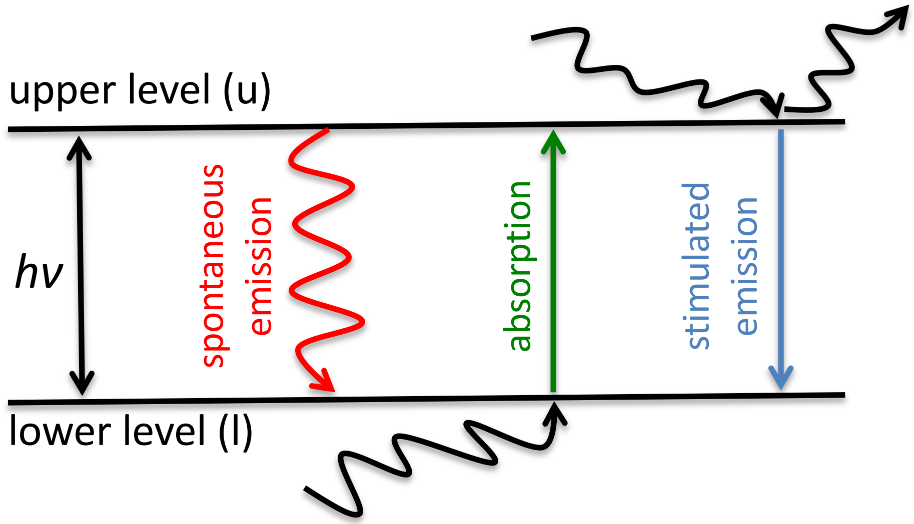
$\phi(\nu)$ *line profile function* $[=]\ Hz^{-1}$

$n_l\ n_u$ *population of lower and upper level* $[=]\ cm^{-3}$

The excitation temperature T_{ex}

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\alpha_\nu = \frac{c^2 A_{ul} n_u}{8\pi\nu^2} \left(\frac{n_l/g_l}{n_u/g_u} - 1 \right) \phi(\nu)$$



we define T_{ex} as in Boltzmann law $$\frac{n_u/g_u}{n_l/g_l} = exp(-h\nu/kT_{ex})$$

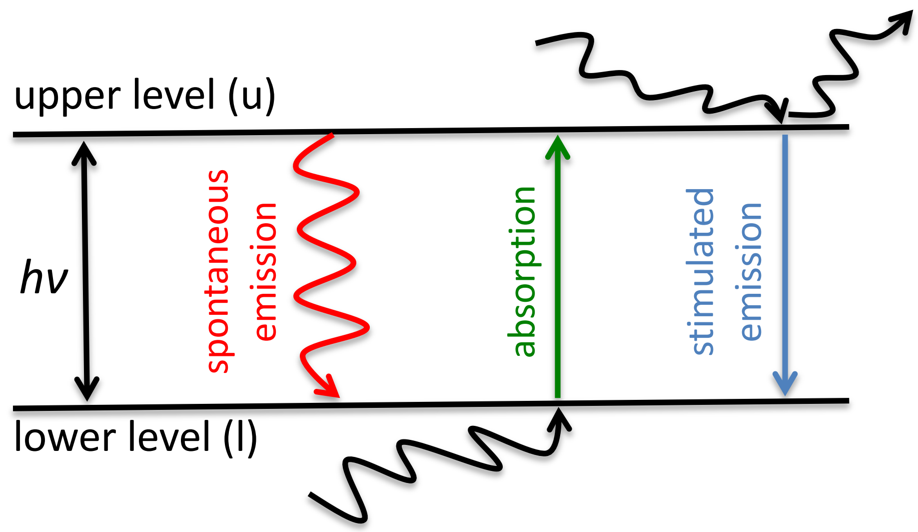
$T_{ex} > 0$ ➔ $n_l/g_l > n_u/g_u$ ➔ $\alpha_\nu > 0$ ➔ $\tau_\nu > 0$ normal populations "thermal emission"

$T_{ex} < 0$ ➔ $n_u/g_u > n_l/g_l$ ➔ $\alpha_\nu < 0$ ➔ $\tau_\nu < 0$ inverted populations maser emission

The source function S_ν

$$j_\nu = \frac{h\nu}{4\pi} n_u A_{ul} \phi(\nu)$$

$$\alpha_\nu = \frac{c^2 A_{ul} n_u}{8\pi\nu^2} \left(\frac{n_l/g_l}{n_u/g_u} - 1 \right) \phi(\nu)$$



$$\frac{n_u/g_u}{n_l/g_l} = exp(-h\nu/kT_{ex})$$

$$S_\nu = \frac{j_\nu}{\alpha_\nu} = \frac{2h\nu^3}{c^2} \frac{1}{\left(\frac{n_l/g_l}{n_u/g_u} - 1 \right)} = \underbrace{\frac{2h\nu^3}{c^2} \frac{1}{exp(h\nu/kT_{ex}) - 1}}_{\text{Planck law at } T=T_{ex}}$$

$$S_\nu = B_\nu(T_{ex})$$

1) Introduction to radiative transfer: Summary

A key quantity: *the specific intensity* I_ν

A key equation: *the equation of radiative transfer*

From macroscopic ($\alpha_\nu\ j_\nu$)
to microscopic quantities ($A_{ul}\ g_u\ g_l$)
and level populations ($n_u\ n_l$)

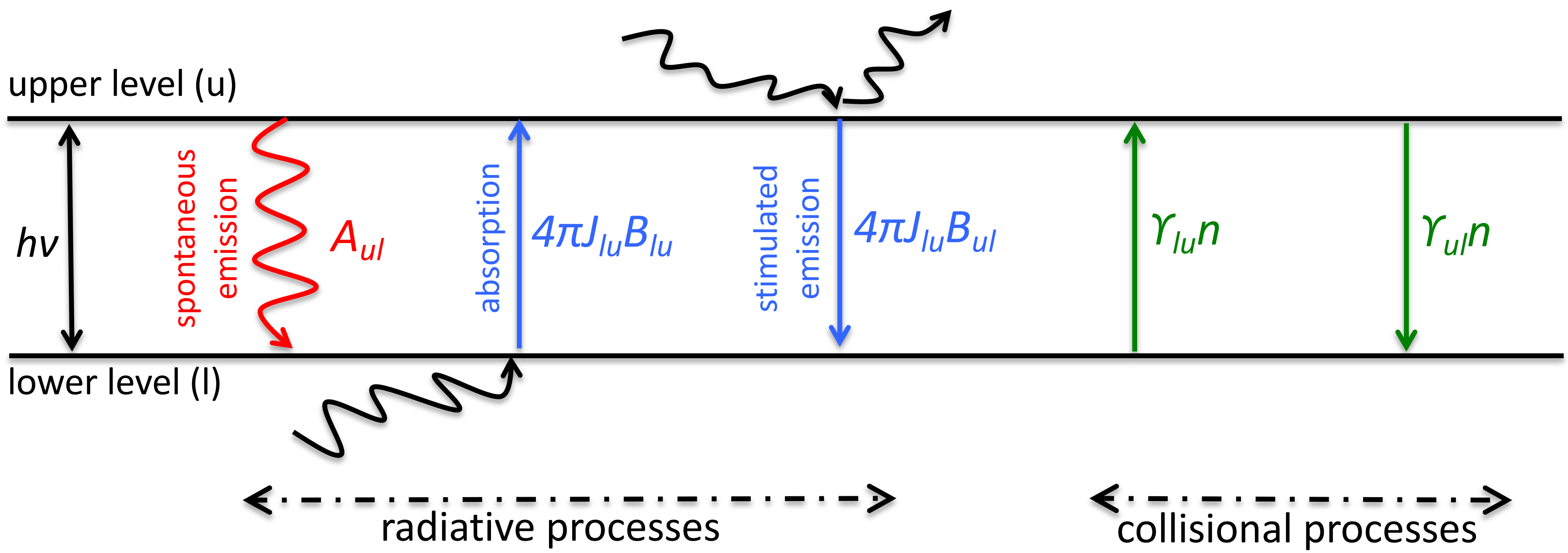
How are these level populations ($n_u\ n_l$) determined?

2) Introduction to molecular excitation

Statistical equilibrium

$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j (4\pi J_{ij} B_{ji} + \Upsilon_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i} (4\pi J_{ij} B_{ij} + \Upsilon_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$

$\Upsilon_{ij} n$	*collisional excitation rate for transition i → j per unit time*	$[=]\ s^{-1}$
Υ_{ij}	*collisional rate coefficient for transition i → j*	$[=]\ cm^3 s^{-1}$
n	*number of particles of buffer gas per unit volume*	$[=]\ cm^{-3}$

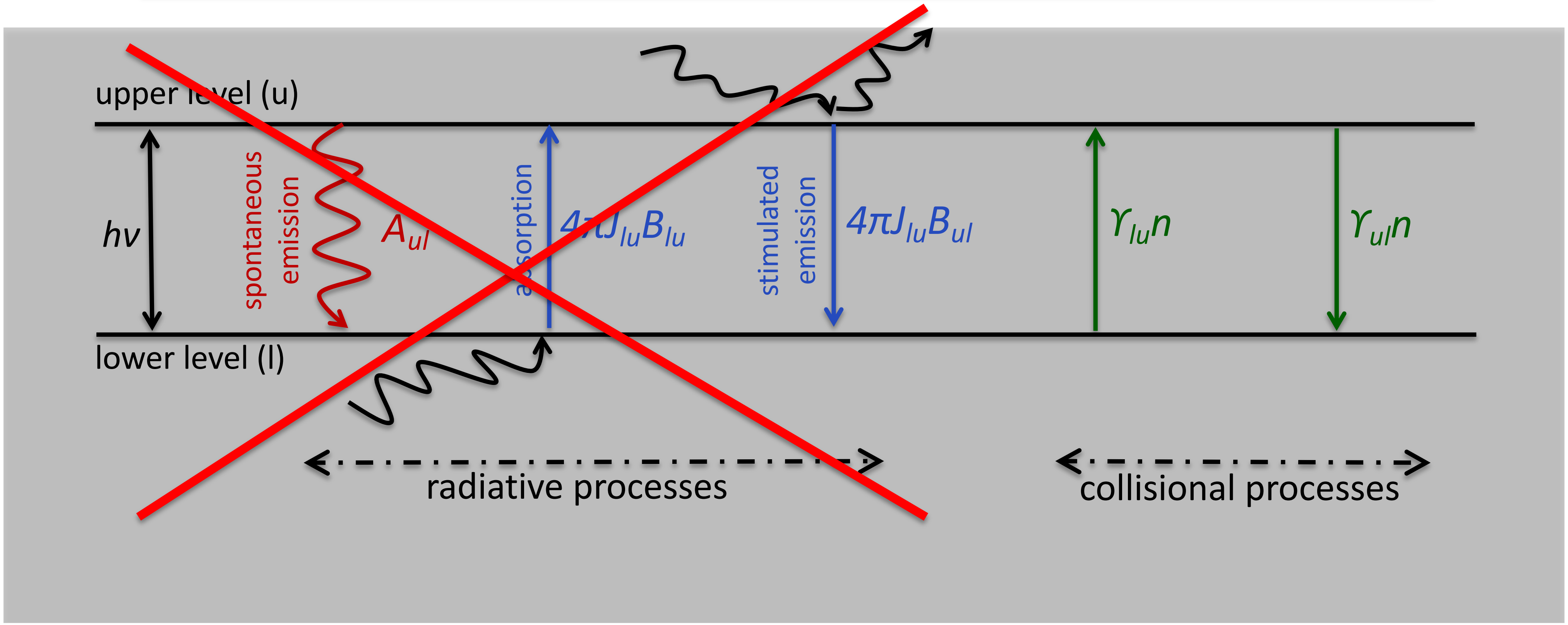


Limiting case: collisional rates >> radiative rates → LTE

$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j (4\pi J_{ij} B_{ji} + \Upsilon_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i} (4\pi J_{ij} B_{ij} + \Upsilon_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$

$\Upsilon_{lu}\, g_l = \Upsilon_{ul}\, g_u \exp(-h\nu/kT_{kin})$ collisional rate coefficients must fulfil detailed balance

$n_u \Upsilon_{ul}\, n - n_l \Upsilon_{lu}\, n = 0$ → $\frac{n_u/g_u}{n_l/g_l} = \exp(-h\nu/kT_{kin})$ Boltzmann population distribution at T_{kin}



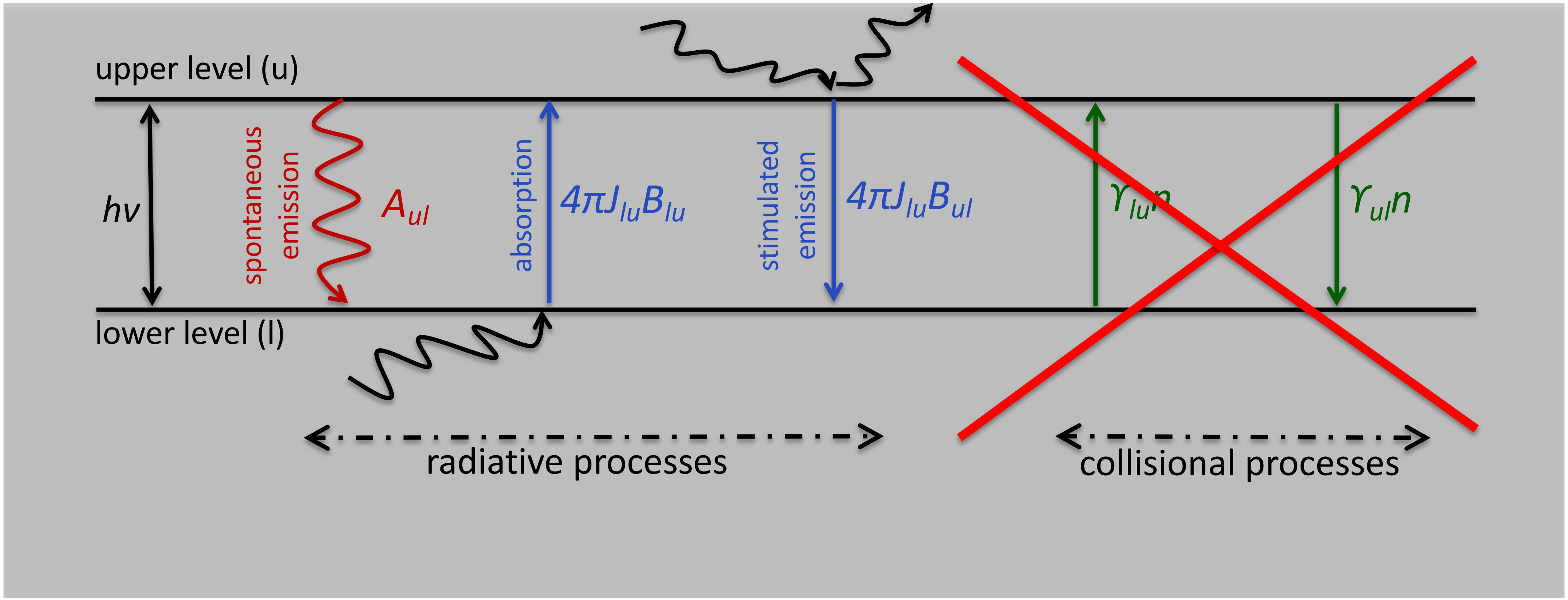
Limiting case: radiative rates >> collisional rates

$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j (4\pi J_{ij} B_{ji} + \Upsilon_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i} (4\pi J_{ij} B_{ij} + \Upsilon_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$

if $J_{ul} = B_\nu(T_{rad})$ *uniform blackbody radiation field at* T_{rad}

$$n_u 4\pi J_{ul} B_{ul} + n_u A_{ul} - n_l 4\pi J_{ul} B_{lu} = 0 \rightarrow \frac{n_u/g_u}{n_l/g_l} = \exp(-h\nu/kT_{rad})$$

Boltzmann population distribution at T_{rad}



2) Introduction to molecular excitation: Remember

One must solve statistical equilibrium

If collisional processes dominate:

→ LTE: Boltzmann distribution at T_{kin}

If radiative processes dominate:

→ LTE: Boltzmann distribution at T_{rad}

Solving statistical equilibrium

Statistical equilibrium

$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j\,(4\pi J_{ij} B_{ji} + \Upsilon_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i} (4\pi J_{ij} B_{ij} + \Upsilon_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$

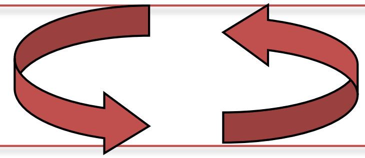
- add a conservation equation: $\sum_i n_i = n$

- linear system of algebraic equations: to be solved numerically (Gauss-Jordan, …)

- knowns: $\boldsymbol{A_{ij}}$, $\boldsymbol{B_{ij}}$, $\boldsymbol{\Upsilon_{ij}}$ *(spectroscopic and collisional microscopic quantities)*
  $\boldsymbol{n}$ (density of particles of buffer gas)
- unknowns: $\boldsymbol{n_i}$ (level populations)
- to be evaluated: $\boldsymbol{J_{ij}}$ (radiation field, depends on the unknown $\boldsymbol{n_i}$)

Large Velocity Gradient (LVG) method

$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j\,(4\pi J_{ij} B_{ji} + \gamma_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i} (4\pi J_{ij} B_{ij} + \gamma_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$



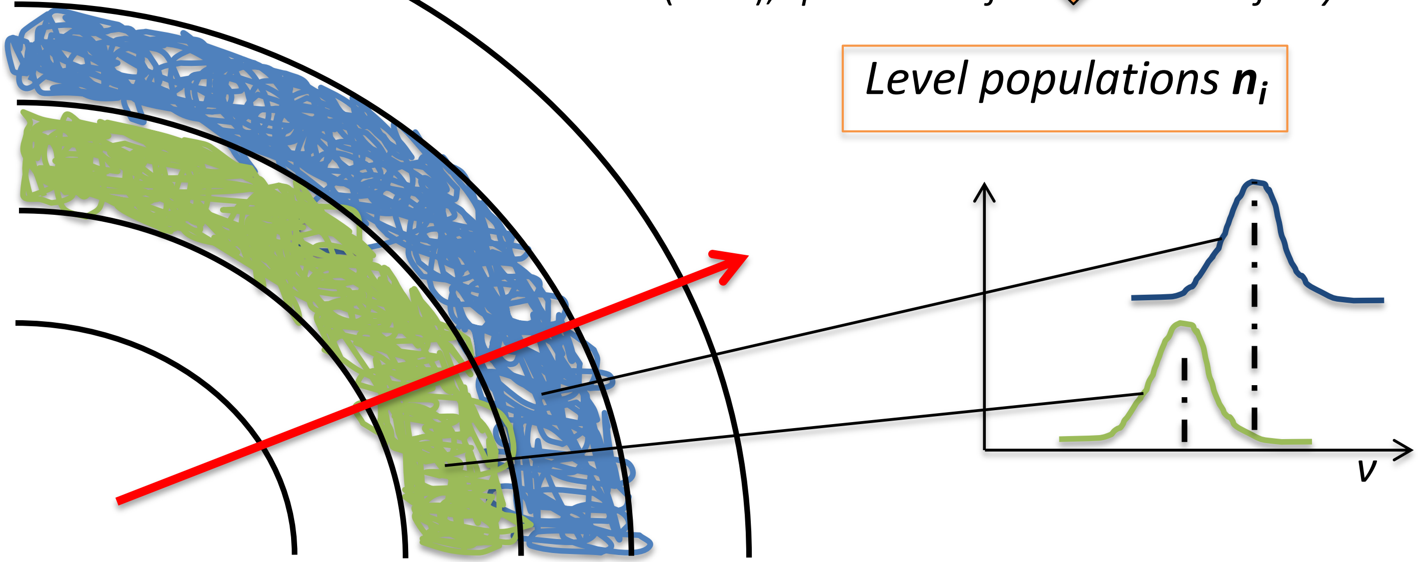
$$J = (1-\beta)\, S_\nu + \beta I_\nu^0$$

β: escape probability

$$\beta = \frac{1-e^{-\tau_\nu}}{\tau_\nu}$$

See the complete derivation in:
Sobolev (1960), *Moving envelopes of stars*, Harvard Univ. Press
Castor (1970), *Spectral line formation in Wolf-Rayet envelopes*, MNRAS, 149, 111

Level populations $\boldsymbol{n_i}$



Shells radiatively decoupled due to Doppler shift

Radiation field J can be Evaluated locally in each shell

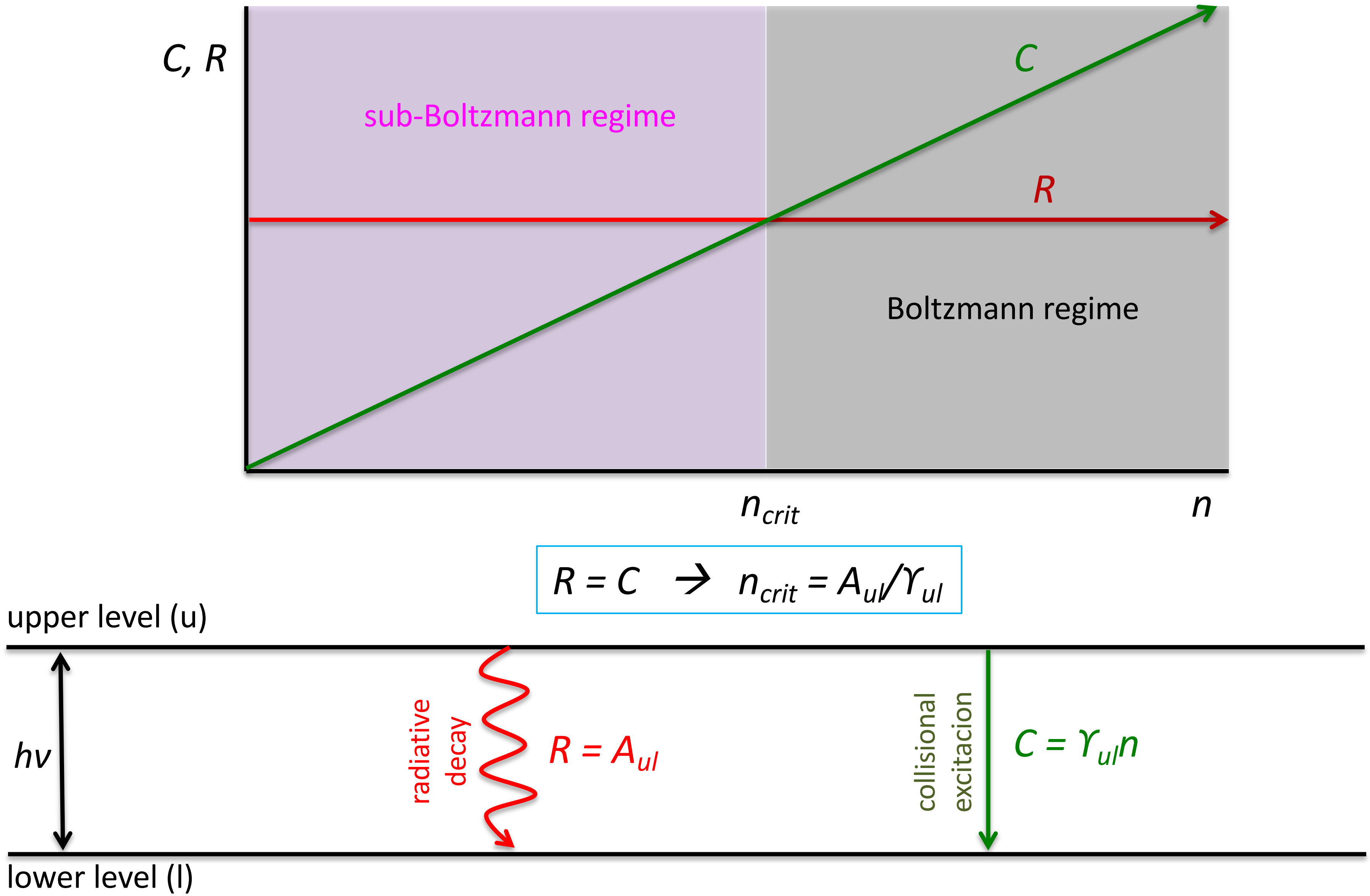
More advanced methods

$$\frac{dn_i}{dt} = \sum_{j\neq i} n_j (4\pi J_{ij} B_{ji} + \Upsilon_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j\neq i} (4\pi J_{ij} B_{ij} + \Upsilon_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$

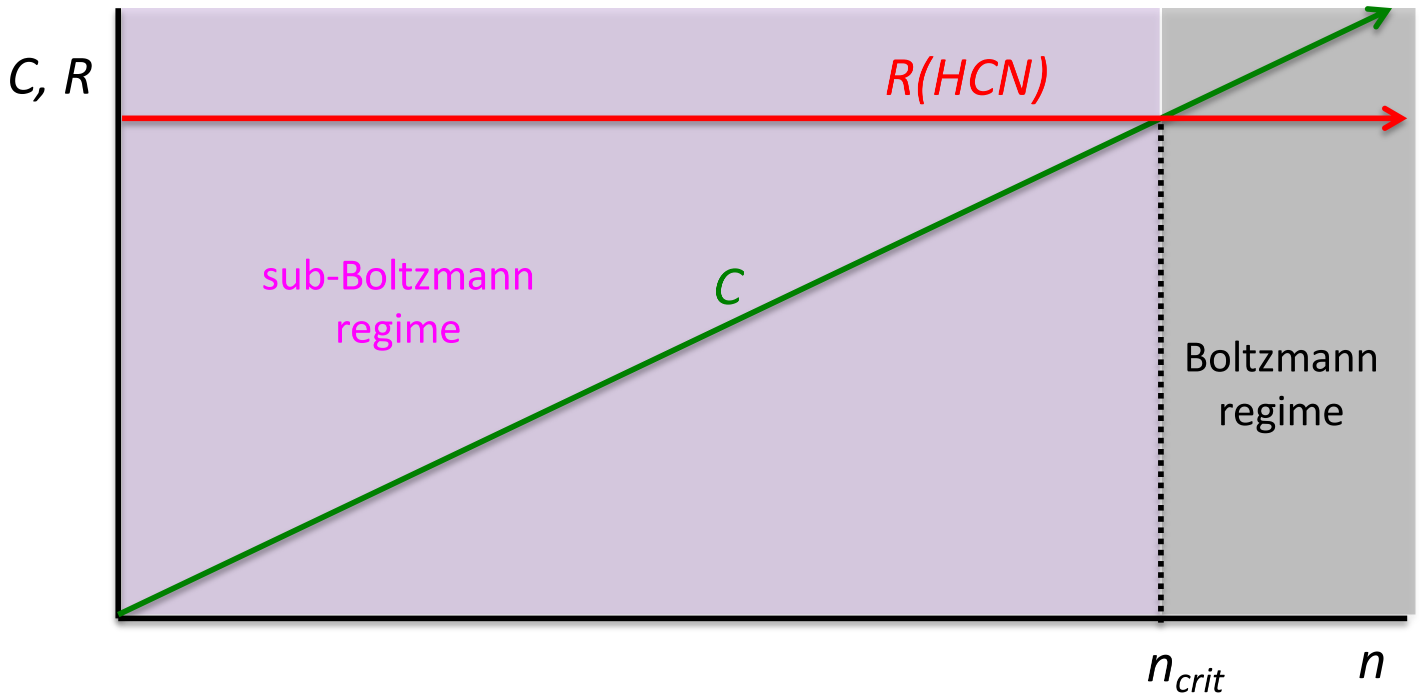
More advanced methods to get the level populations:

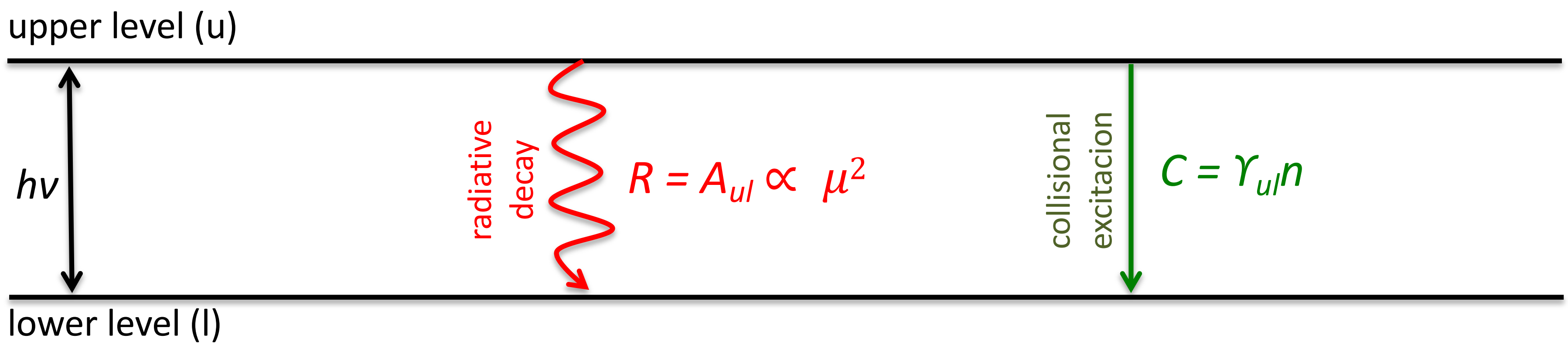
- Monte Carlo: Bernes 1979, A&A, 73, 67
  Hogerheijde & van der Tak 2000, A&A, 362, 697
- Accelerated Λ Iteration (ALI): Rybicki & Hummer 1991, A&A, 245, 171
- Gauss-Seidel algorithm: Trujillo Bueno & Bendicho 1995, ApJ, 455, 646
  Daniel & Cernicharo 2008, A&A, 488, 1247
- Coupled escape probability (CEP): Elitzur & Asensio Ramos 2006, MNRAS, 365, 779

Statistical equilibrium
collisional vs radiative excitation

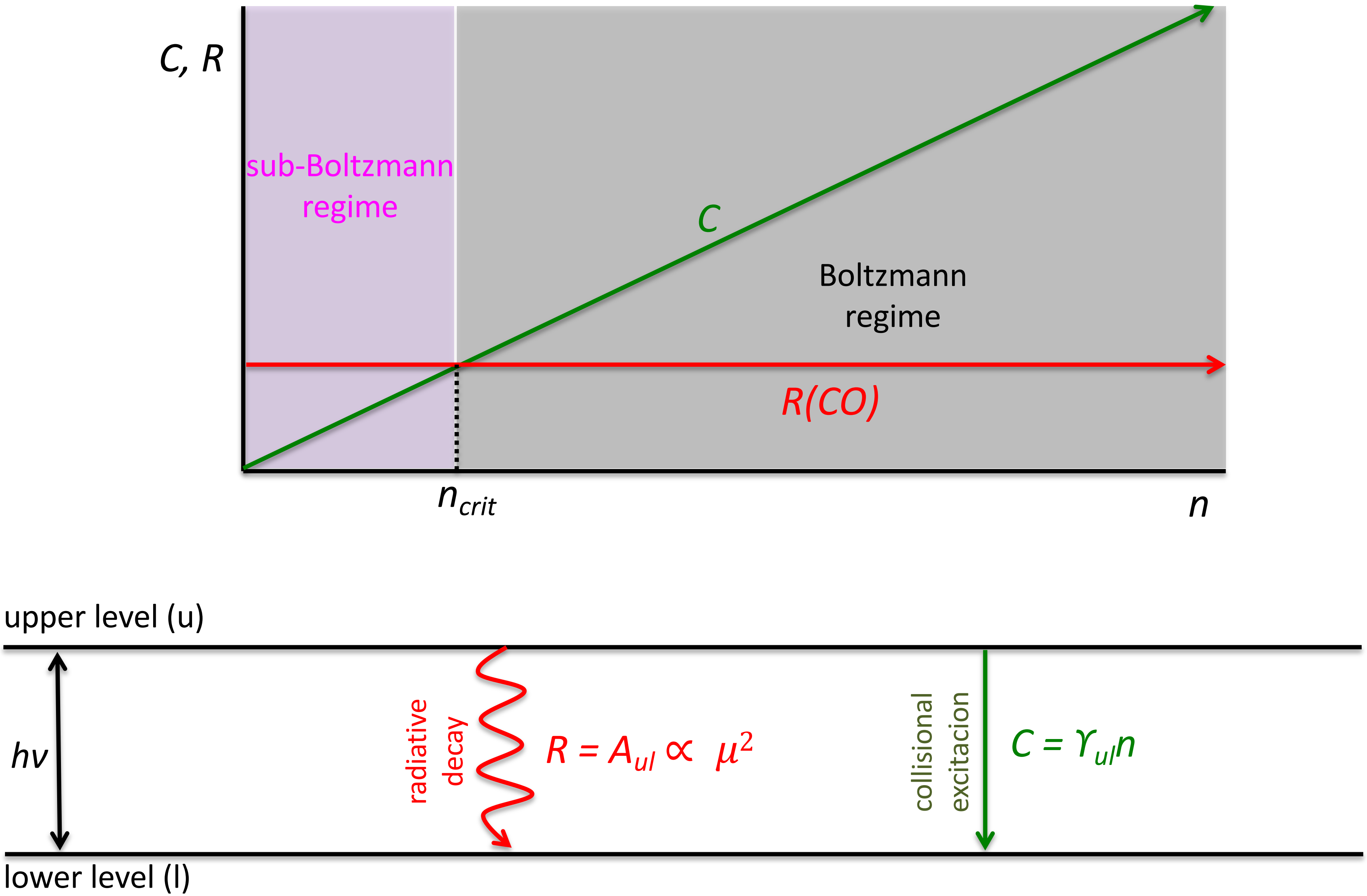


Statistical equilibrium
collisional vs radiative excitation



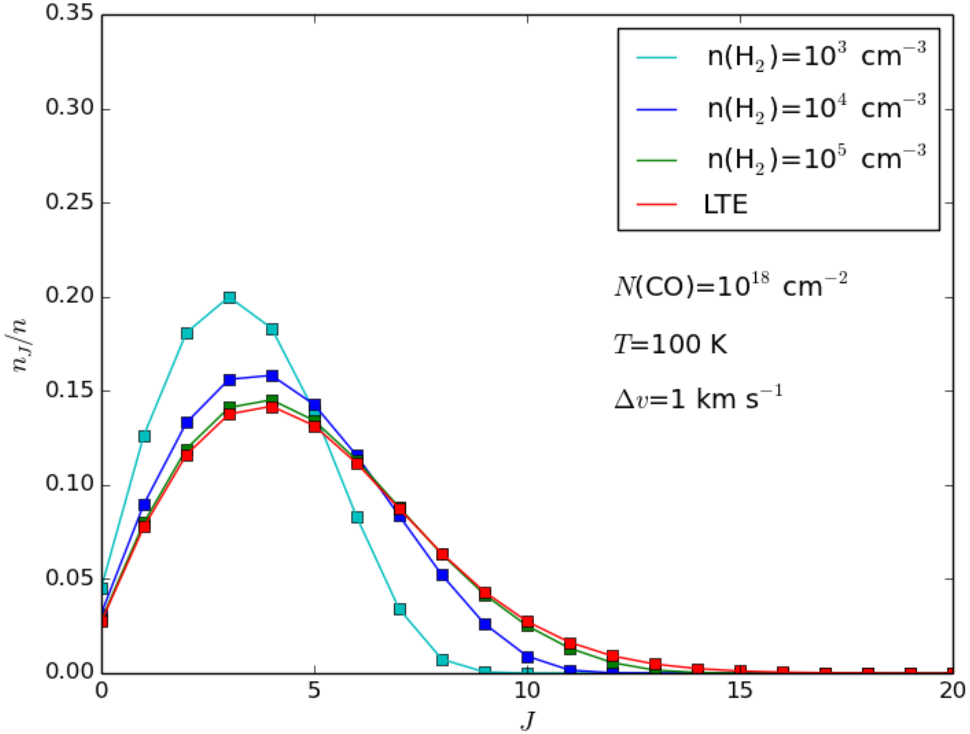


Statistical equilibrium
collisional vs radiative excitation

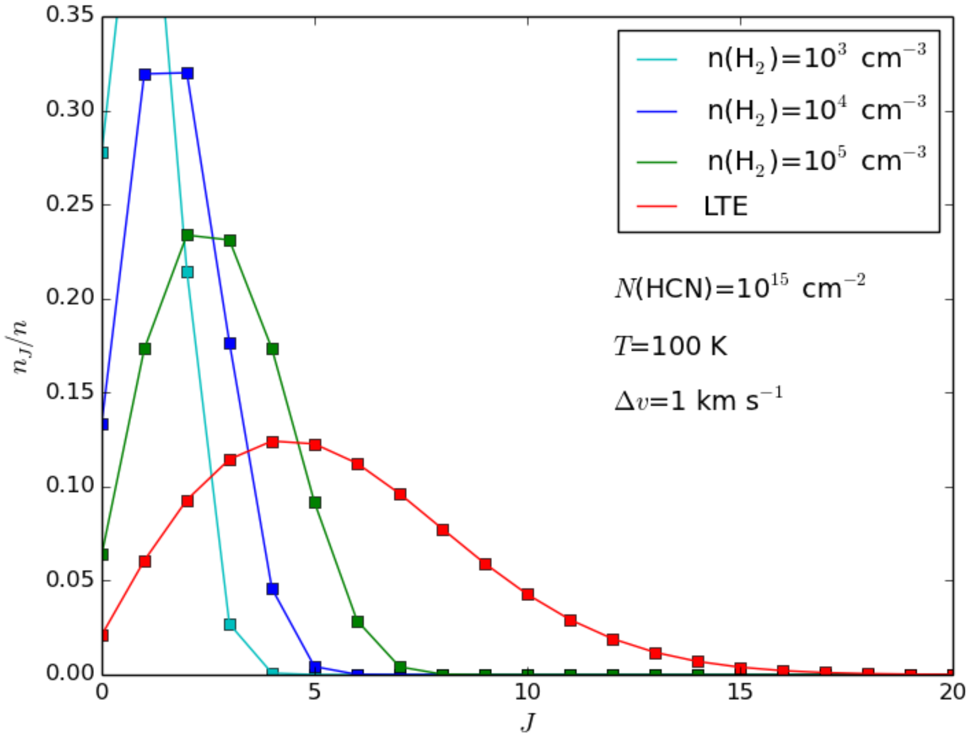


Statistical equilibrium
Limiting case towards LTE

CO: μ=0.11 Debye



HCN: μ=2.99 Debye



- At high densities, level populations tend towards a Boltzmann distribution at T_{kin} (LTE)
- The critical density of thermalization depends on the dipole moment of the molecule

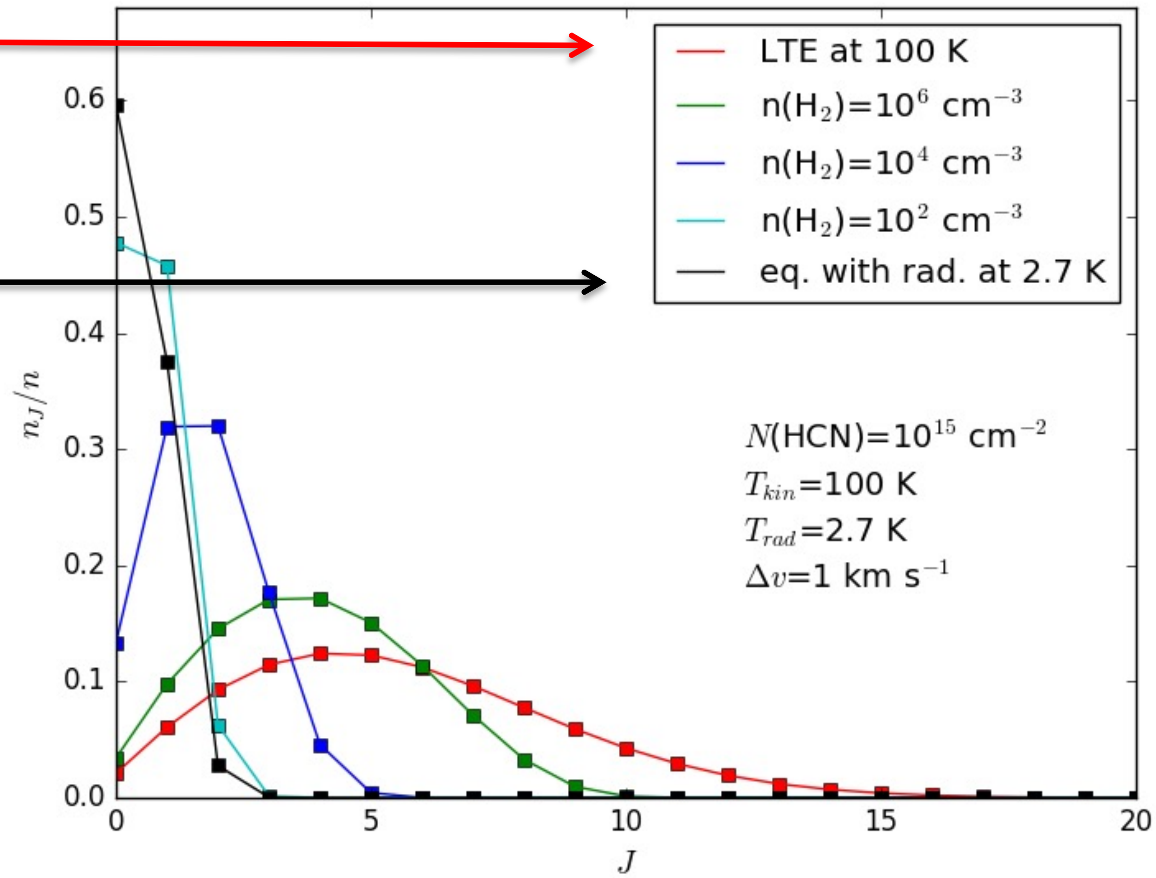
- CO is a good tracer of T_{kin} : easily thermalized

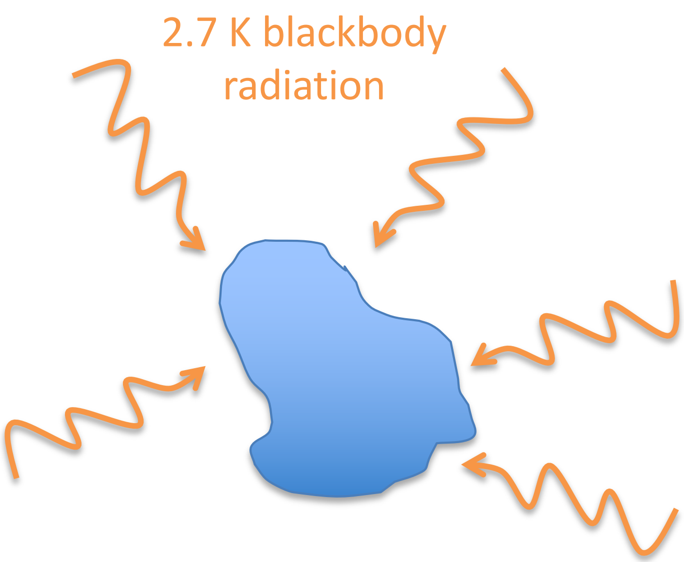
- HCN is a good tracer of $n(H_2)$: thermalises at high densities

Statistical equilibrium
Limiting case with strong surrounding radiation field

high $n(H_2)$: thermalisation at T_{kin}

low $n(H_2)$: equilibrium with surrounding radiation field



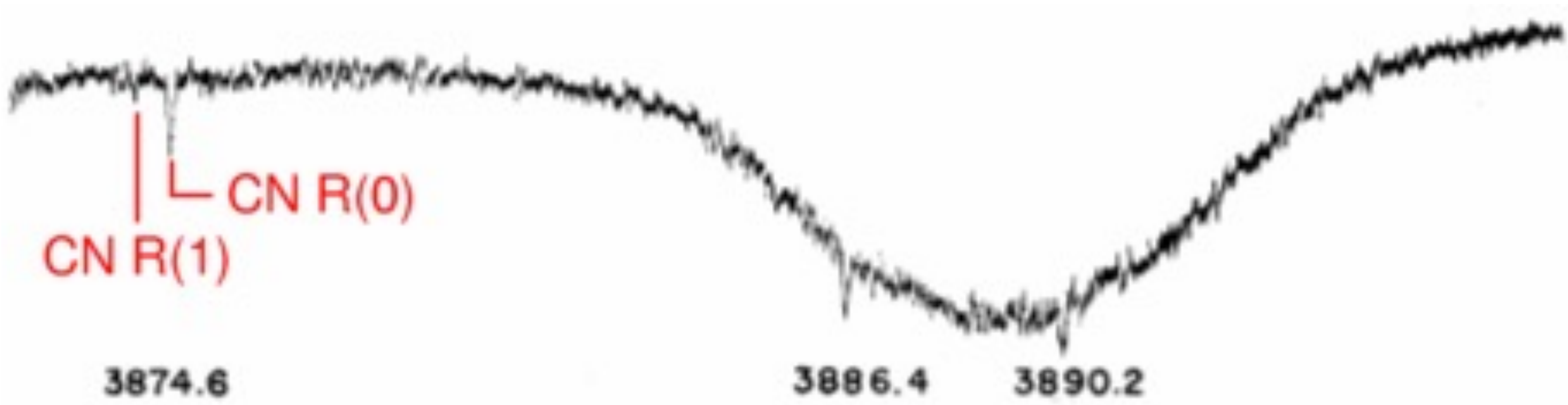


CMB discovered by Penzias & Wilson in 1965.

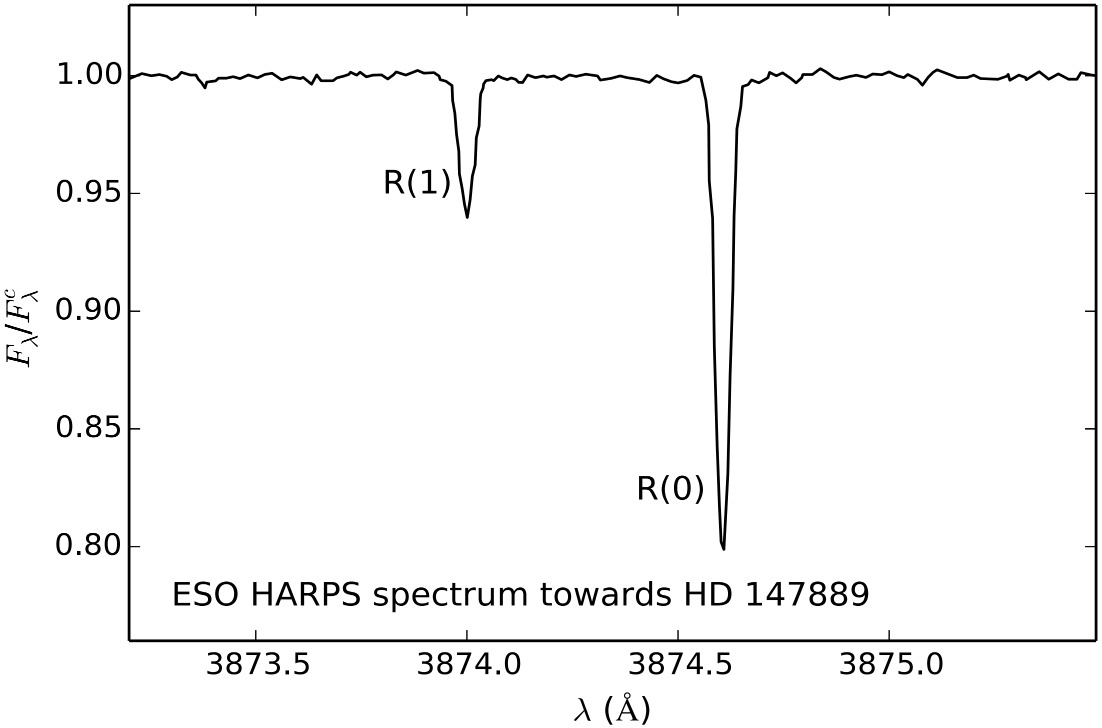
First observations of CMB by McKellar using interstellar molecules in 1940, although he did not realized of the meaning at that time.

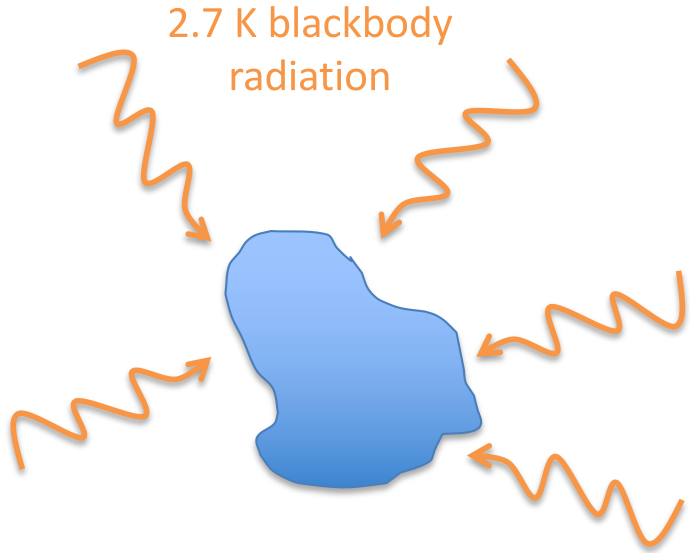
In 1950 the Nobel-prize winning physicist Gerhard Herzberg wrote in his book *Spectra of Diatomic Molecules*:

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.

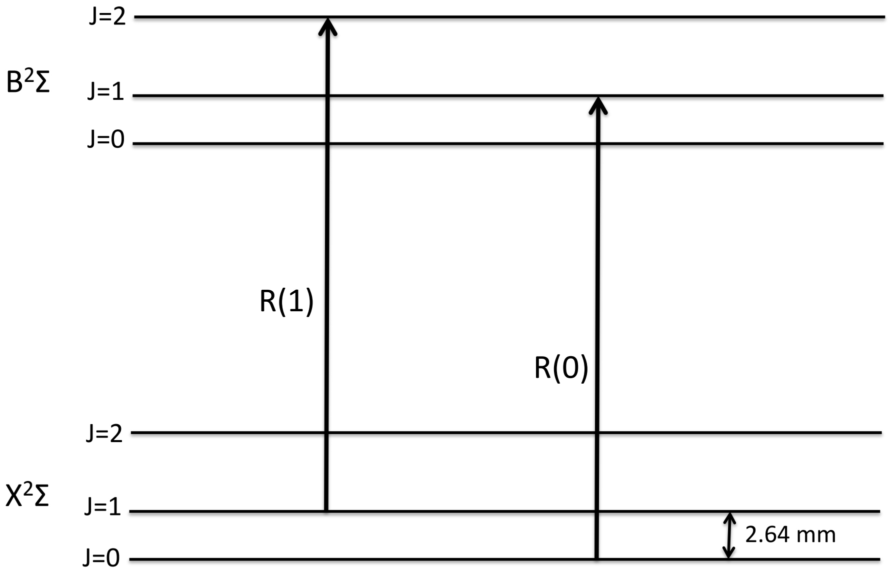


Spectrum towards zeta Oph taken in 1940 by McKellar.





$N(\mathrm{CN}) = 10^{13}\ \mathrm{cm^{-2}}$
$T_k = 50$ K
$\Delta v = 1\ \mathrm{km\ s^{-1}}$



$n(H_2)$ [cm^{-3}]	T_{ex} [K]
10	2.73
100	2.73
1000	2.77
10^4	3.15
10^5	7.15

2) Introduction to molecular excitation: Summary

One must solve statistical equilibrium

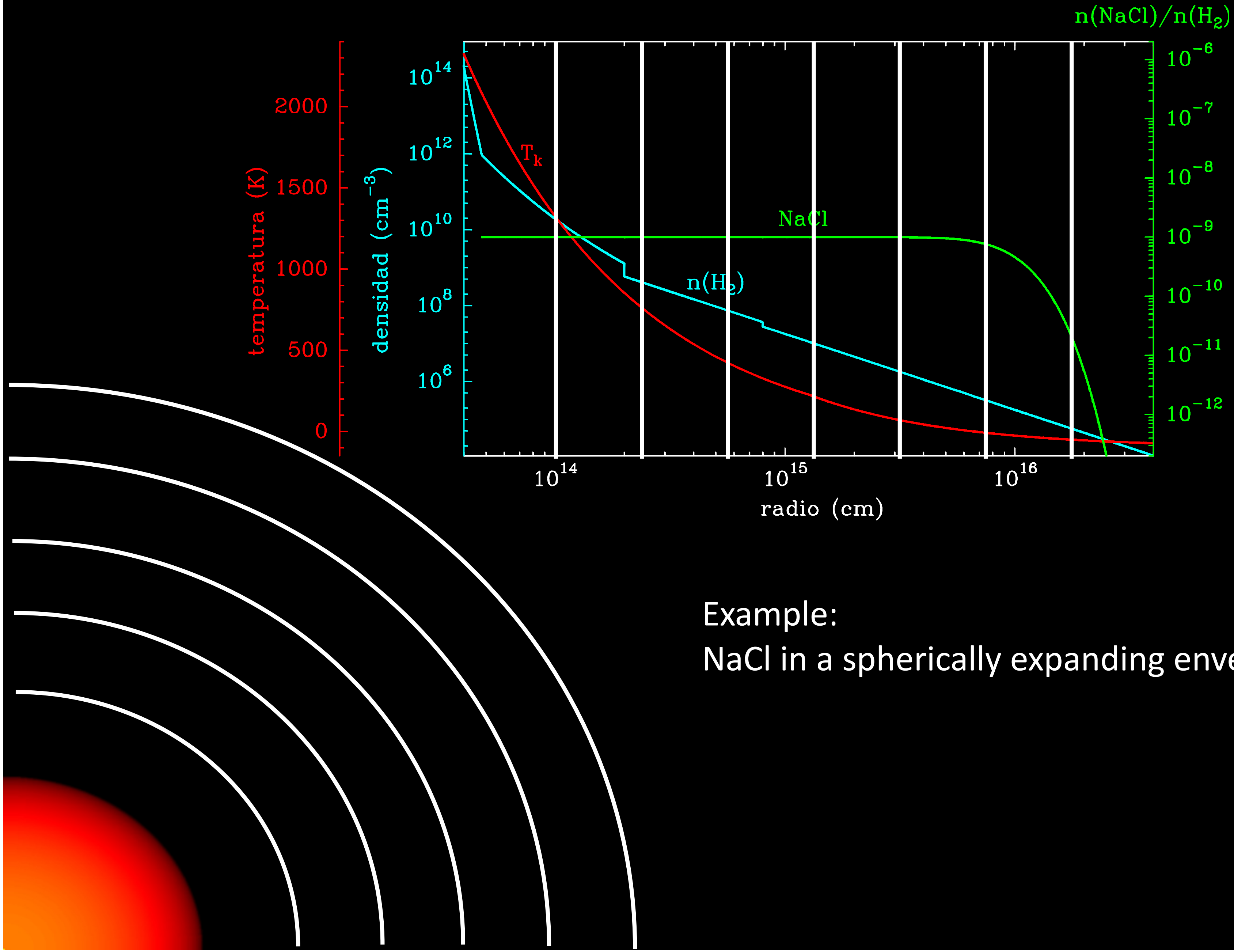
If collisional processes dominate:

→ LTE: Boltzmann distribution at T_{kin}

If radiative processes dominate:

→ LTE: Boltzmann distribution at T_{rad}

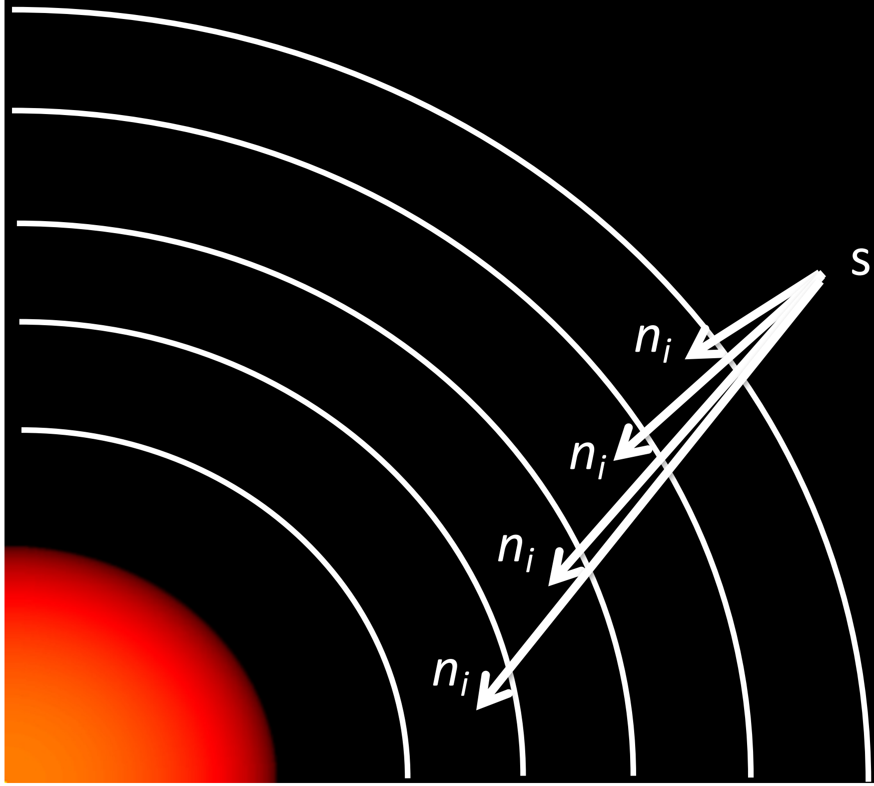
Radiative model: statistical equilibrium + ray-tracing



Example:
NaCl in a spherically expanding envelope

Radiative model: statistical equilibrium + ray-tracing

$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j (4\pi J_{ij} B_{ji} + \Upsilon_{ji} n) + \sum_{j>i} n_j A_{ji} - n_i \sum_{j \neq i} (4\pi J_{ij} B_{ij} + \Upsilon_{ij} n) - n_i \sum_{j<i} A_{ij} = 0$$

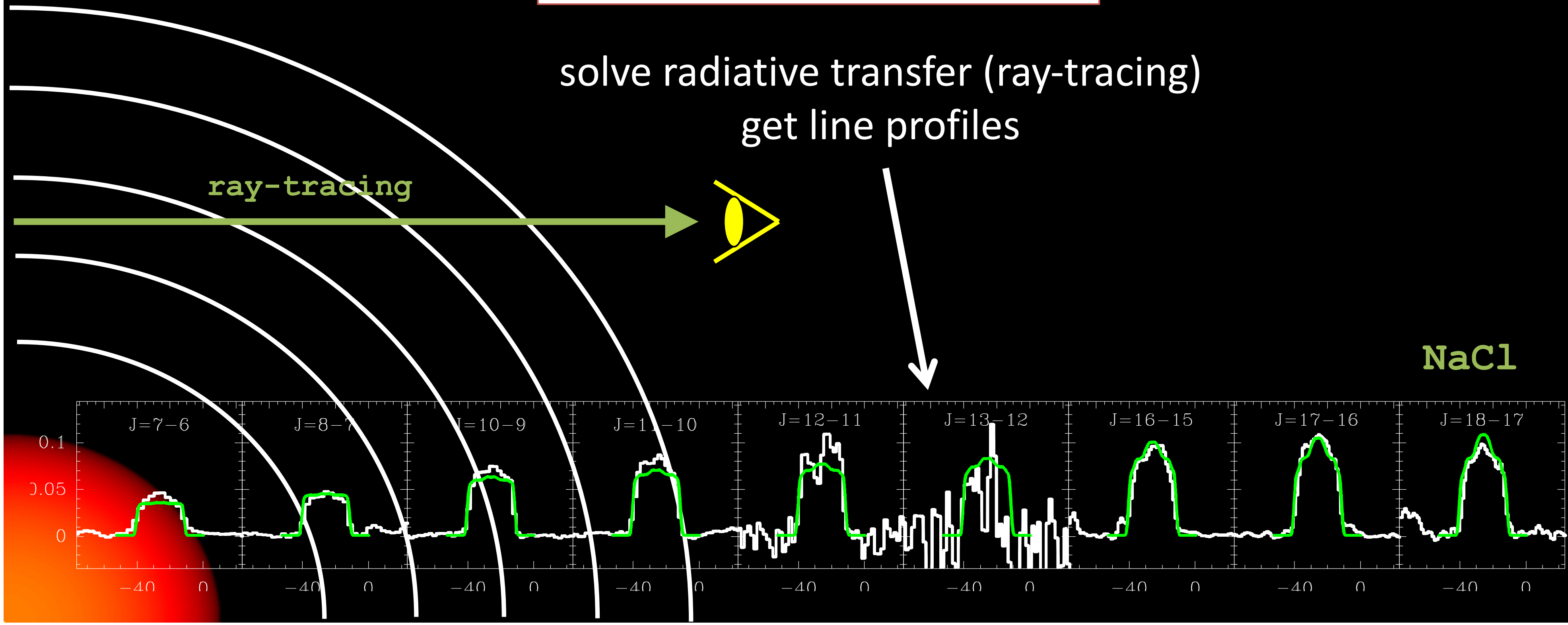


solve statistical equilibrium (LVG)
get level populations

Radiative model: statistical equilibrium + ray-tracing

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

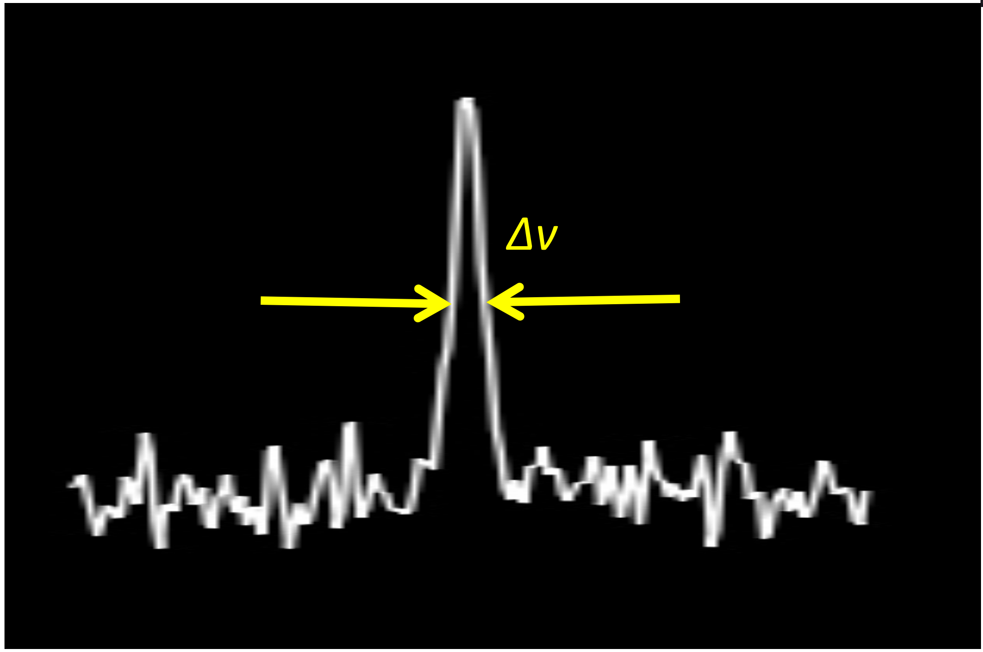
solve radiative transfer (ray-tracing)
get line profiles



3) Line profiles

Line profiles

Macroscopic motions: NO
 - quiescent source



gaussian line profile:

- thermal broadening → T_{kin}

$$\Delta v = \sqrt{\frac{8 \, Ln2 \, kT_{kin}}{m}}$$

- microturbulence broadening

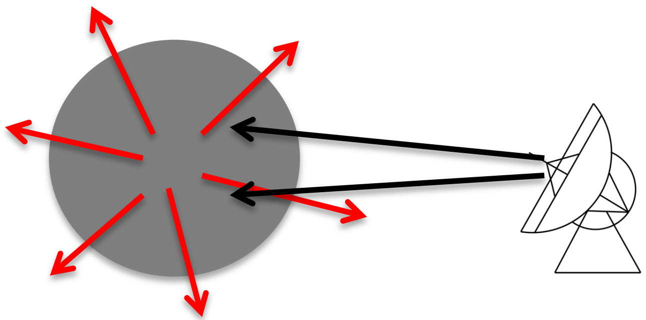
Line profiles

Macroscopic motions: NO

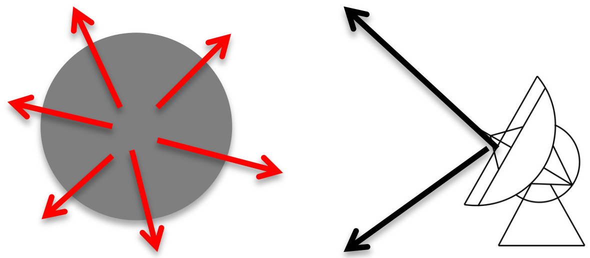
- quiescent source

Macroscopic motions: YES

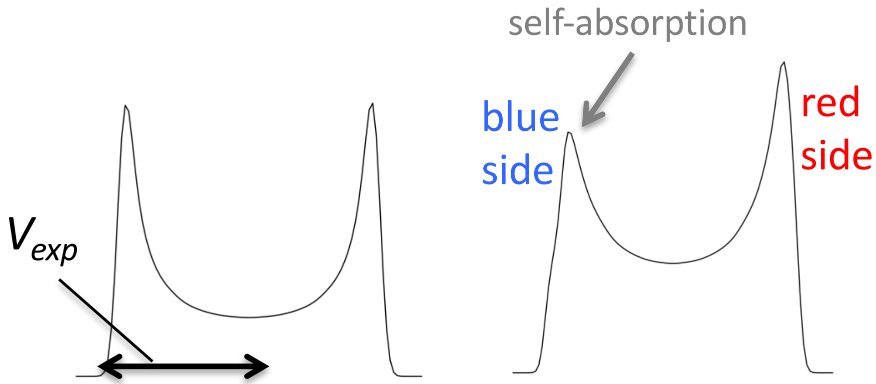
- expanding cloud



source resolved by telescope

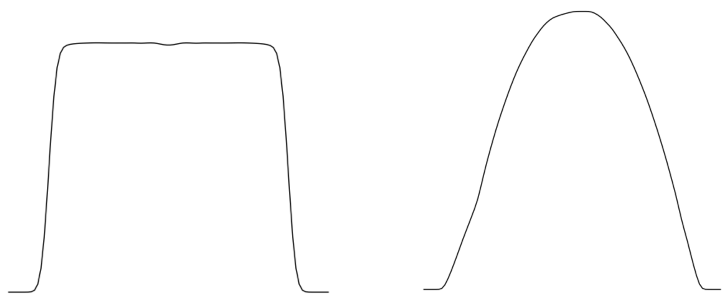


source not resolved by telescope



optically thin

optically thicker

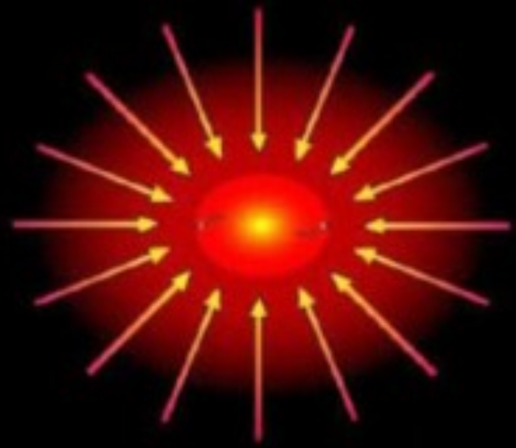


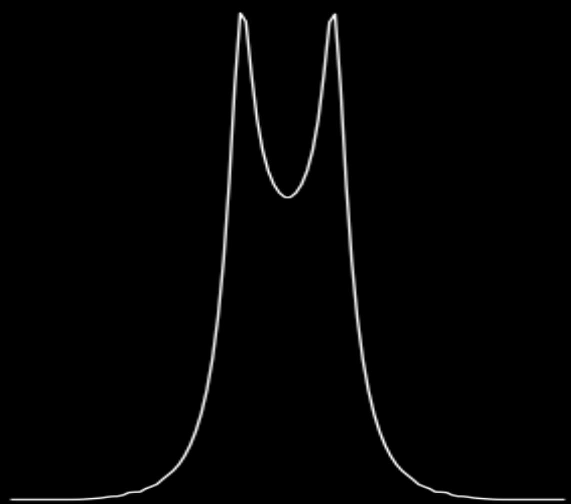
optically thin

optically thick

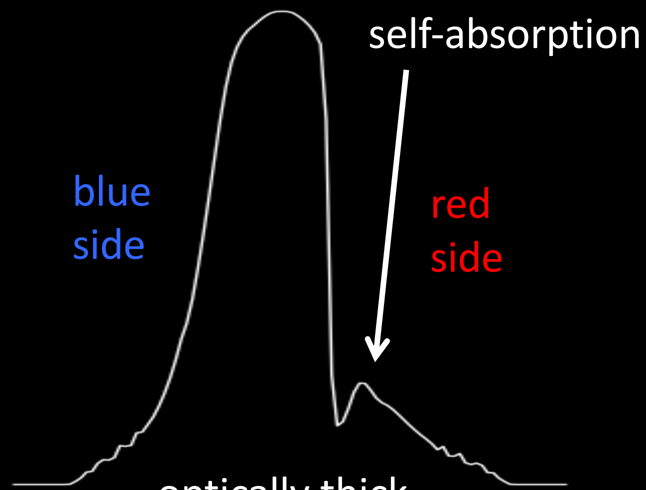
Line profiles

Macroscopic motions: NO
 - quiescent source
Macroscopic motions: YES
 - expanding cloud
 - collapsing cloud





optically thin



optically thick

Remember !

Radiative transfer model:

(1) Solve statistical equilibrium to get level populations
(LVG, MC, ALI, …)

(2) Solve radiative transfer equation (ray-tracing) to get line profiles

Astronomical observation + radiative transfer model

You can retrieve - physical structure of the source
(temperature, density, kinematics)

- chemical composition of the source
(molecular abundances)