Monte Carlo methods for molecular line observations at (sub)mm wavelengths

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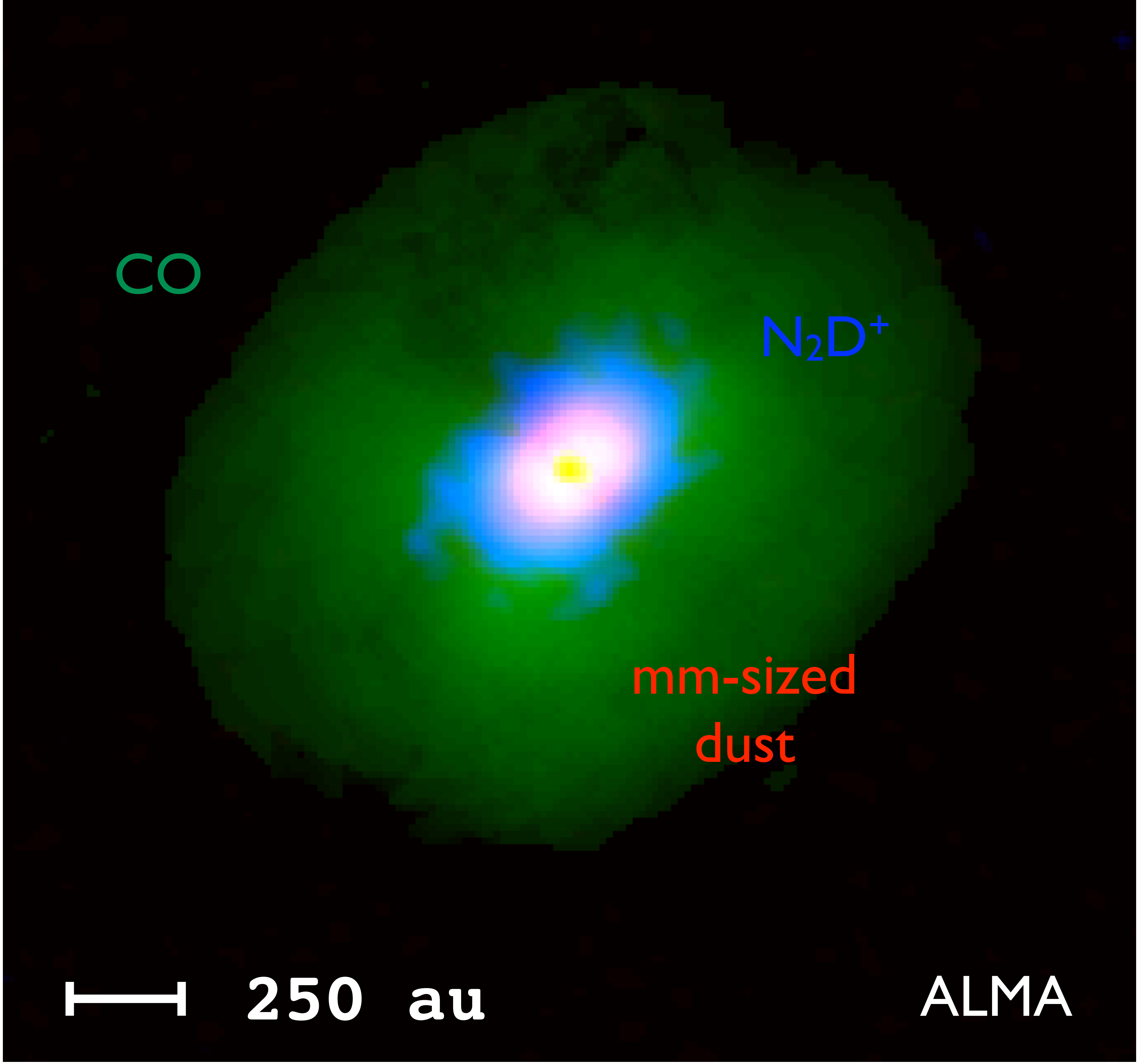
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Outline

- Lecture 1:
  - How does molecular line transfer and non-LTE excitation work?
- Lecture 2:
  - How can Monte Carlo methods help?
  - How does LIME work?
  - Practical work with LIME Q&A (tomorrow)

Non-LTE excitation and the formation of molecular lines at (sub) millimeter wavelengths

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Outline

- Molecular energy levels and transitions
- The equation of radiative transfer
- Molecular excitation
- The coupled problem, and some ways to solve it that are *not* Monte Carlo methods

Molecular energy levels and transitions

An excursion to quantum mechanics

- Molecular energy levels are found by solving the Schrödinger equation $H\Psi = E\Psi$,

- where H is the Hamiltonian describing the interactions within the system, and Eigenvalues E are the energy levels of the system

- For molecules we need to include in the Hamiltonian

  - the interaction of the electrons with the atomic nuclei
  - the interaction of the electrons with each other
  - the interactions of the nuclei with each other

- Let's recap what the simpler H-atom looks like...

a) The H-atom

Structure of H atom (or any 1-electron system) can be solved exactly quantum mechanically by solving the Schrödinger equation $H\Psi = E\Psi$,

$$H = \frac{p^2}{2\mu} + V(r) = -\frac{\hbar^2}{2\mu}\nabla^2 - \frac{Ze^2}{r}$$

with μ the reduced mass,

$$\mu \equiv \frac{Am_p \cdot m_e}{Am_p + m_e} \approx m_e$$

Z the nuclear charge (1 for H, 2 for He$^+$, 3 for Li^{++}…),
and A the nuclear mass

Solution for the H-atom

- Discrete energy levels for $E<0$, characterized by three quantum numbers n, l, m

  $n=1, 2, 3, 4, \ldots$ principal quantum number

  $l=0, 1, 2, \ldots n-1$ angular quantum number

  $m=l, l-1, \ldots -l+1, -l$ magnetic quantum number

- Energy levels independent of l and m, each one degenerate with n^2 substates

$$E = -\frac{\mu e^4}{2\hbar^2}\frac{1}{n^2} \equiv -hcR_H\frac{1}{n^2}$$

with R_H=109,677.585 cm^{-1} : Rydberg constant for H

Selection rules

- Radiative (electric dipole) transitions are only possible between pairs of levels that adhere to so-called ‘selection rules’
- This can be understood by conservation of angular momentum between the initial and the final state, which includes the photon (spin 1)
- Formally one has to calculate quantum mechanical transition matrix elements
- For hydrogen $\Delta l = \pm 1$; $\Delta m = 0, \pm 1$; no limitations on Δn

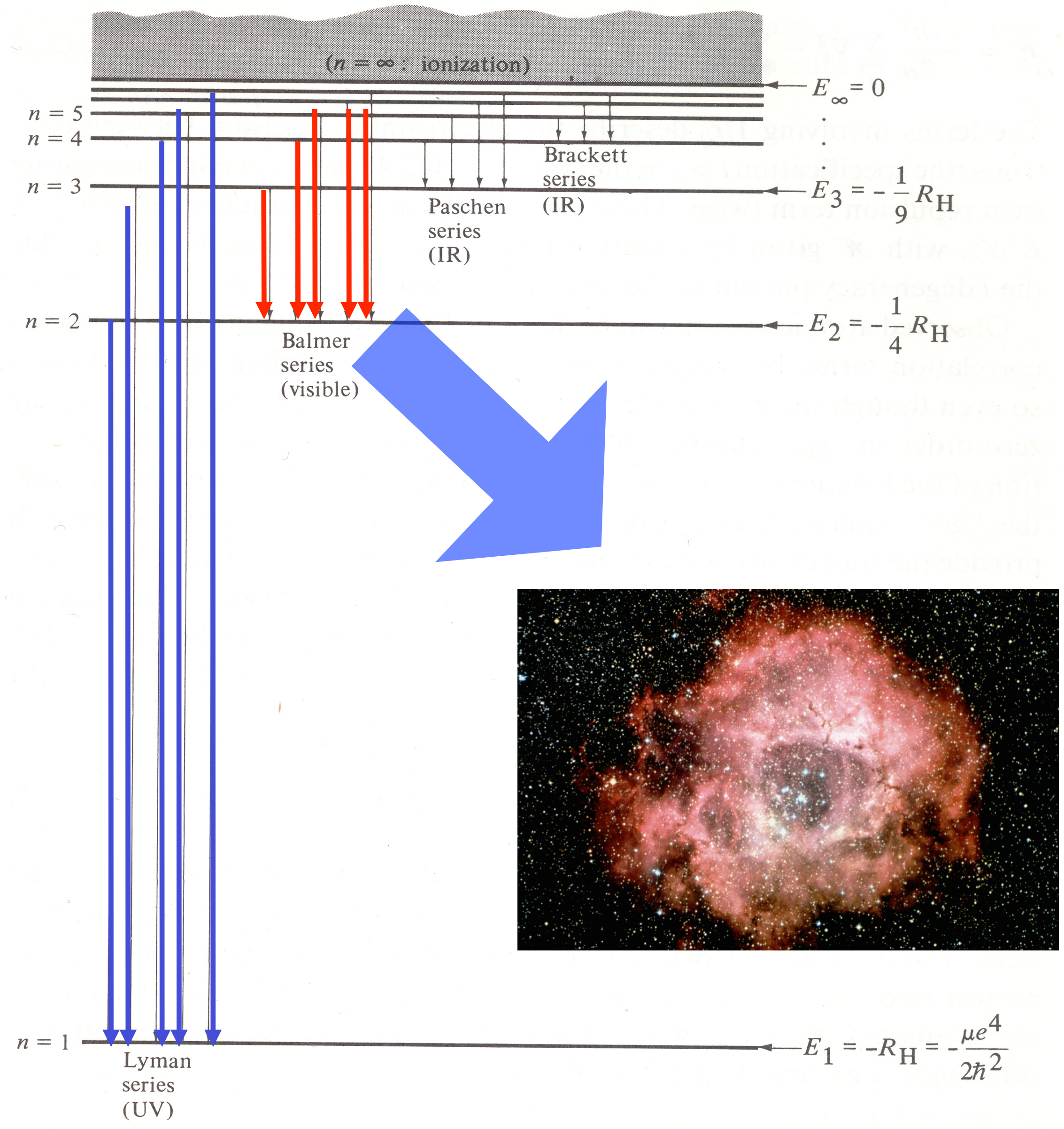
$1/\lambda = R_H(1 - 1/n^2)$ $n = 2, 3, 4, \ldots$ Lyman series

$1/\lambda = R_H(1/2^2 - 1/n^2)$ $n = 3, 4, 5, \ldots$ Balmer series

$1/\lambda = R_H(1/3^2 - 1/n^2)$ $n = 4, 5, 6, \ldots$ Paschen series

$1/\lambda = R_H(1/4^2 - 1/n^2)$ $n = 5, 6, 7, \ldots$ Bracket series

$1/\lambda = R_H(1/5^2 - 1/n^2)$ $n = 6, 7, 8, \ldots$ Pfund series



b) Molecular energy levels

- All information about molecule is contained in Schrödinger equation ($R \equiv$ positions of nuclei, $x \equiv$ positions of electrons):

$$H\,\Psi(\vec{x},\vec{R}) = E\,\Psi(\vec{x},\vec{R})$$

- Hamilton operator:

$$\begin{aligned} H &= T_N + T_e + V_{Ne} + V_{ee} + V_{NN} \\ &\equiv T_N + H^{el} \end{aligned}$$

Born-Oppenheimer approximation (1927)

- Mass of nuclei ≫ mass of electrons ⇒ nuclei move slowly compared with electrons ⇒
- Separate wave function into electronic and nuclear part, and determine motion of electrons first with nuclei held fixed

$$\Psi(\vec{x},\vec{R}) = \Psi^{el}(\vec{x};\vec{R})\,\Psi^{nuc}(\vec{R})$$

$$H^{el}\,\Psi^{el}(\vec{x};\vec{R}) = \underset{\uparrow}{E^{el}}\,\Psi(\vec{x};\vec{R})$$

Electronic potential energy surface

- Electronic + nuclear levels
  - Nuclear level consist of vibrational levels and rotational levels

Nuclear motion

- Born-Oppenheimer: $$\left(T_N + E^{el}(\vec{R}) - E\right)\Psi^{nuc}(\vec{R}) = 0$$

where it is assumed that $$T_N\,\Psi^{el}\,\Psi^{nuc} \approx \Psi^{el}\,T_N\,\Psi^{nuc}$$

- Diatomic molecule in center-of-mass system:

$$T_N = -\frac{1}{2\mu R^2}\underset{\substack{\uparrow\\ \text{Radial part}}}{\frac{\partial}{\partial R}}\left(R^2\frac{\partial}{\partial R}\right) + \underset{\substack{\uparrow\\ \text{Angular part}}}{\frac{J^2}{2\mu R^2}}$$

  - J = nuclear angular momentum operator
  - μ= reduced mass of system

- Assume $$\Psi^{nuc}(\vec{R}) = \underset{\substack{\uparrow\\ \text{Angular}}}{Y(\hat{R})}\,\underset{\substack{\uparrow\\ \text{Radial}}}{\chi(R)}/R$$

Nuclear motion (cont'd)

$$\left(\frac{J^2}{2\mu R^2} - E^{rot}\right) Y_{JM}(\hat{R}) = 0$$

Rotational equation

$$\left(-\frac{1}{2\mu}\frac{d^2}{dR^2} + E^{el}(R) + \frac{J(J+1)}{2\mu R^2} - E^{vib}\right)\chi(R) = 0$$

Vibrational equation

Vibration

- Take vibrational equation and assume that $E^{\mathrm{el}}(R)$ is bound.
  Take $J = 0$, and expand $E^{\mathrm{el}}(R)$ around minimum

$$\left(-\frac{1}{2\mu}\frac{d^2}{dR^2} + E^{el}(R) + \frac{J(J+1)}{2\mu R^2} - E^{vib}\right)\chi(R) = 0$$

- Harmonic oscillator equation, solution:

$$\begin{aligned} E^{el}(R) &= E^{el}_{\min}(R_e) + \frac{1}{2}\frac{d^2}{dR^2}E^{el}\bigg|_{R_e}(R-R_e)^2 + \ldots \\ &= -D_e + \frac{1}{2}k(R-R_e)^2 \Rightarrow \end{aligned}$$

$$E = -D_e + E^{vib}, \quad E^{vib} = \hbar\omega_e(v+\frac{1}{2}), \quad \omega_e = \sqrt{\frac{k}{\mu}}$$

v=0, 1, 2, …

Rotation

- If nuclei fixed at R_e ⇒ rigid rotator equation

$$\left(\frac{J^2}{2\mu R^2} - E^{rot}\right) Y_{JM}(\hat{R}) = 0$$

$$\Rightarrow E^{rot} = \frac{\hbar^2}{2\mu R_e^2} J(J+1) = B_e J(J+1)$$

$J=0, 1, 2, \ldots$

- Moment of inertia: $I = \mu R_e^2$
- Rotational constant: $B_e = \frac{\hbar^2}{2\mu R_e^2}$

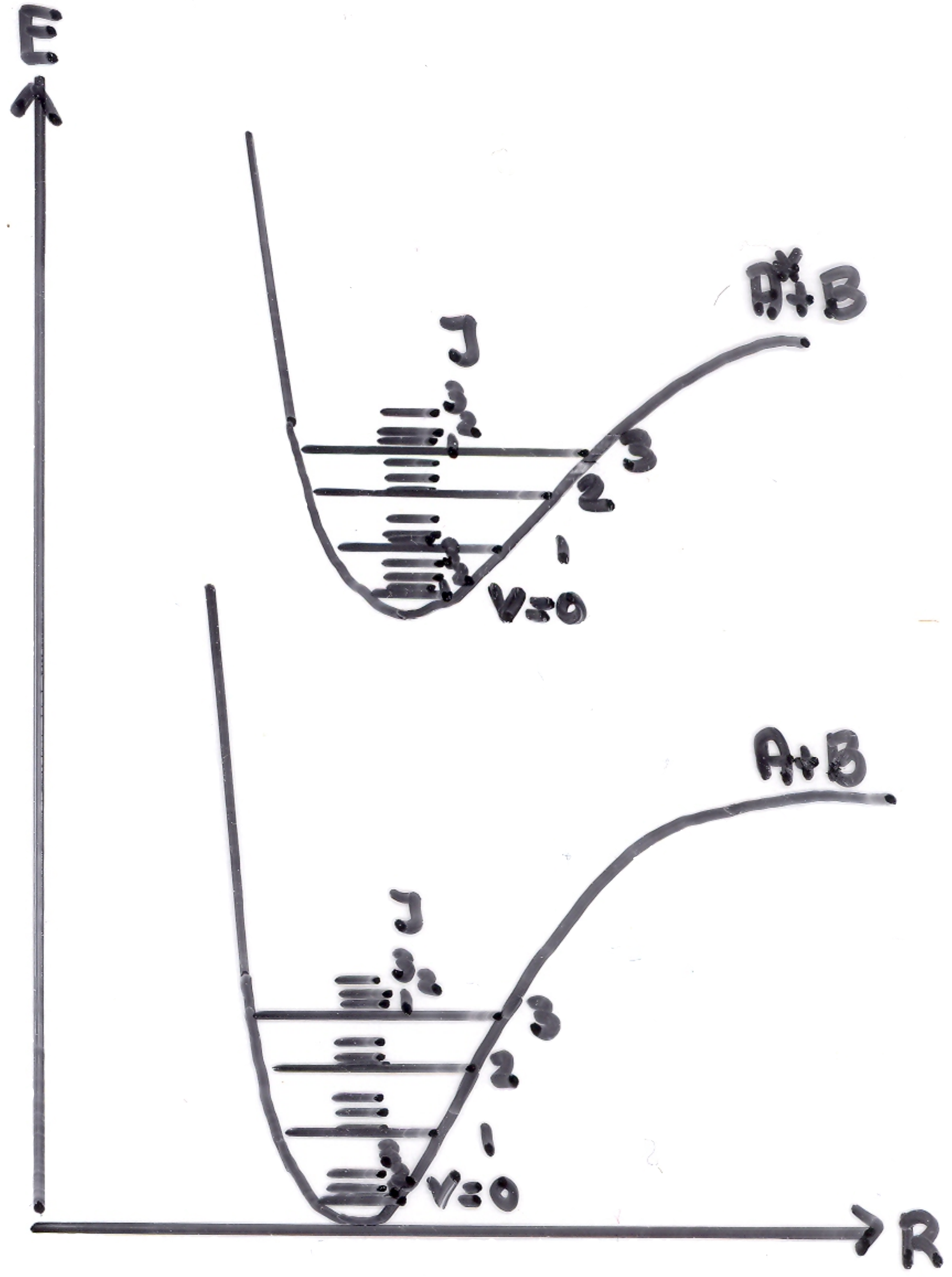
- ΔE between adjacent J levels increases with J, depends on μ:

$$\Delta E^{rot}(J) = 2B_e(J+1)$$

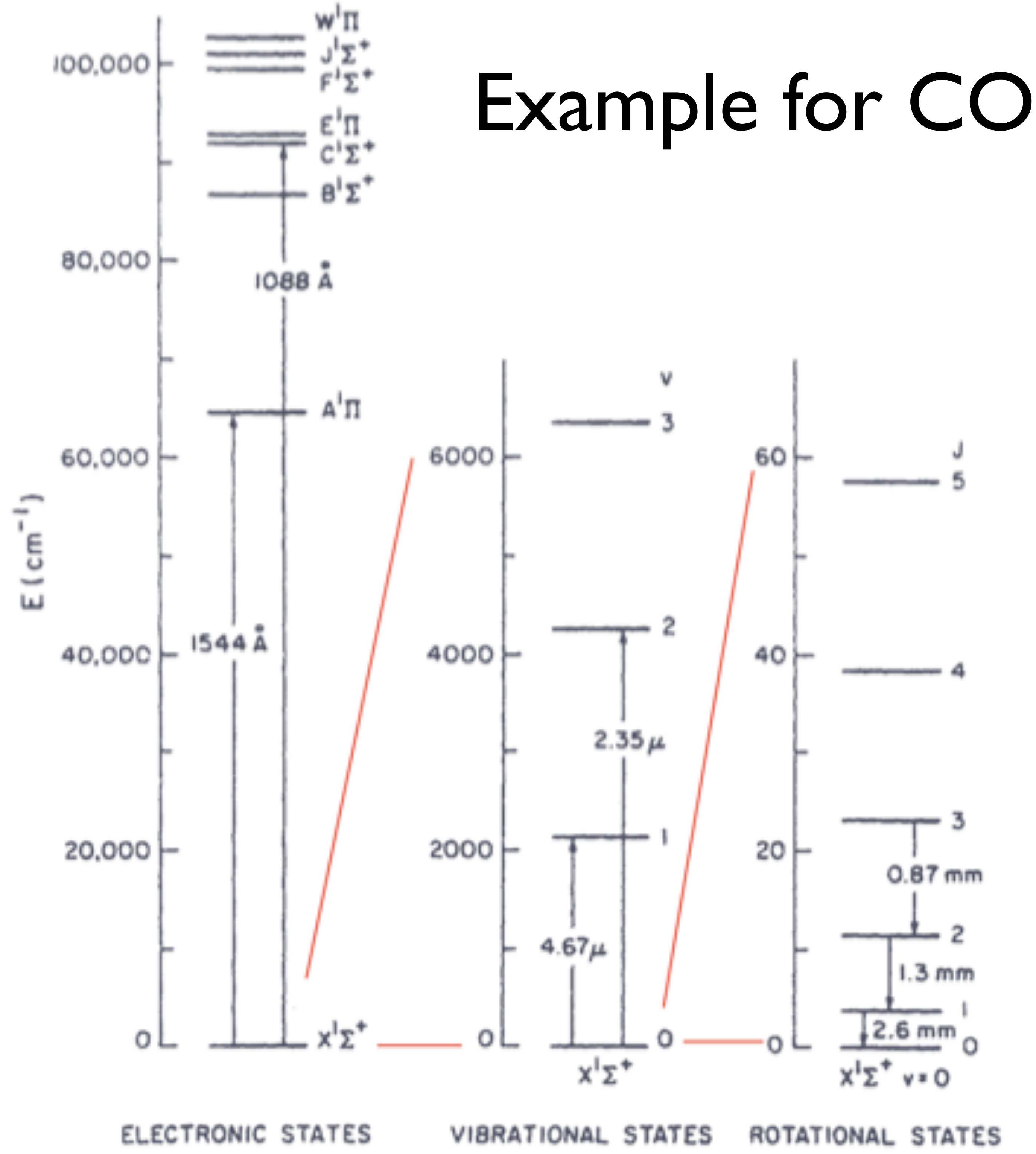
Molecular transitions (summary)

- The nuclear and electronic motions in molecules are nearly decoupled (Born-Oppenheimer approximation)
- $$E = E^{el}_{\mathrm{min}} + E^{vib} + E^{rot} \quad \text{with } E^{el} \gg E^{vib} \gg E^{rot}$$
- $$E^{el} : E^{vib} : E^{rot} = 1 : \sqrt{\frac{m_e}{\mu}} : \frac{m_e}{\mu}$$
- Energy difference two electronic states typically a few eV → VIS and UV wavelengths
- Energy difference two vibrational states typically 0.1–0.3 eV → 500–3000 cm^{-1} → IR wavelengths
- Energy difference two rotational states typically 0.001 eV → few cm^{-1} → (sub)millimeter wavelengths

Summary energy levels



Example for CO



c) Examples
Rotational Spectra

- CO J=1–0 ν = 115 GHz ⇔ λ = 2.6 mm
  J=2–1 ν = 230 GHz ⇔ λ = 1.3 mm
  J=3–2 ν = 345 GHz ⇔ λ = 0.87 mm
- Typically λ a few mm for J=1–0 in heavy diatomics (CS, SiO, SO, …)
- Hydrides have much higher rotational frequencies (near λ = 400 μm) because μ is much smaller

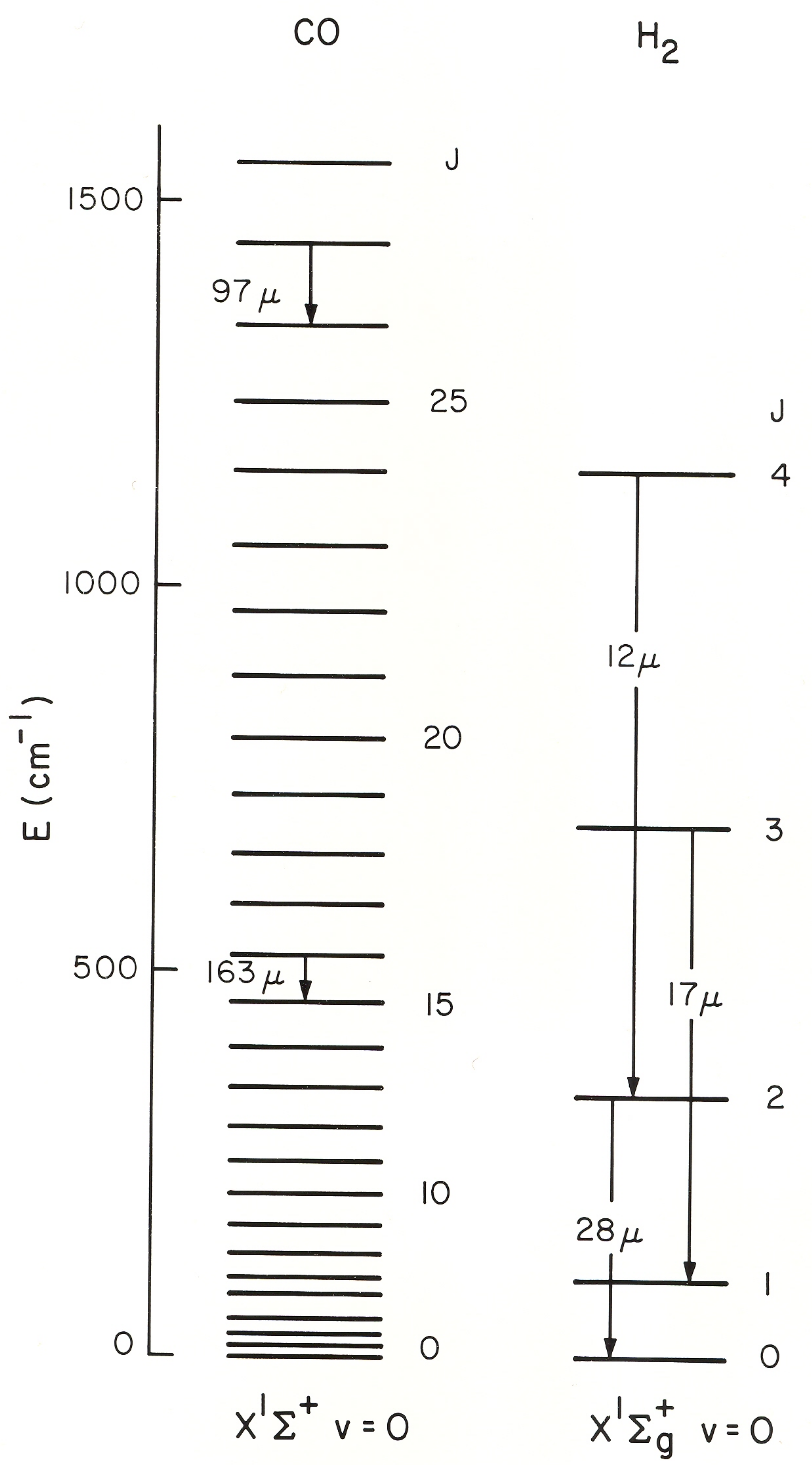
$$\mu = \frac{m_1 m_2}{m_1 + m_2} = \frac{16 \cdot 12}{16 + 12} \approx 7 \quad \text{for } {}^{12}\mathrm{C}^{16}\mathrm{O}$$

$$= \frac{16 \cdot 1}{16 + 1} \approx 1 \quad \text{for } {}^{16}\mathrm{OH}$$

Selection rules

- Molecule must have permanent dipole moment ⇒ no strong rotational spectra observed for H_2, C_2, O_2, CH_4, C_2H_2, …
- $\Delta J = 1$ ⇒ only transitions between adjacent levels
- For symmetric molecules like H_2, only quadrupole transitions occur with $\Delta J = 2$, e.g.
  - $J = 2 \rightarrow 0$ $\lambda = 28\ \mu m$
  - $J = 3 \rightarrow 1$ $\lambda = 17\ \mu m$
  - $J = 4 \rightarrow 2$ $\lambda = 12\ \mu m$

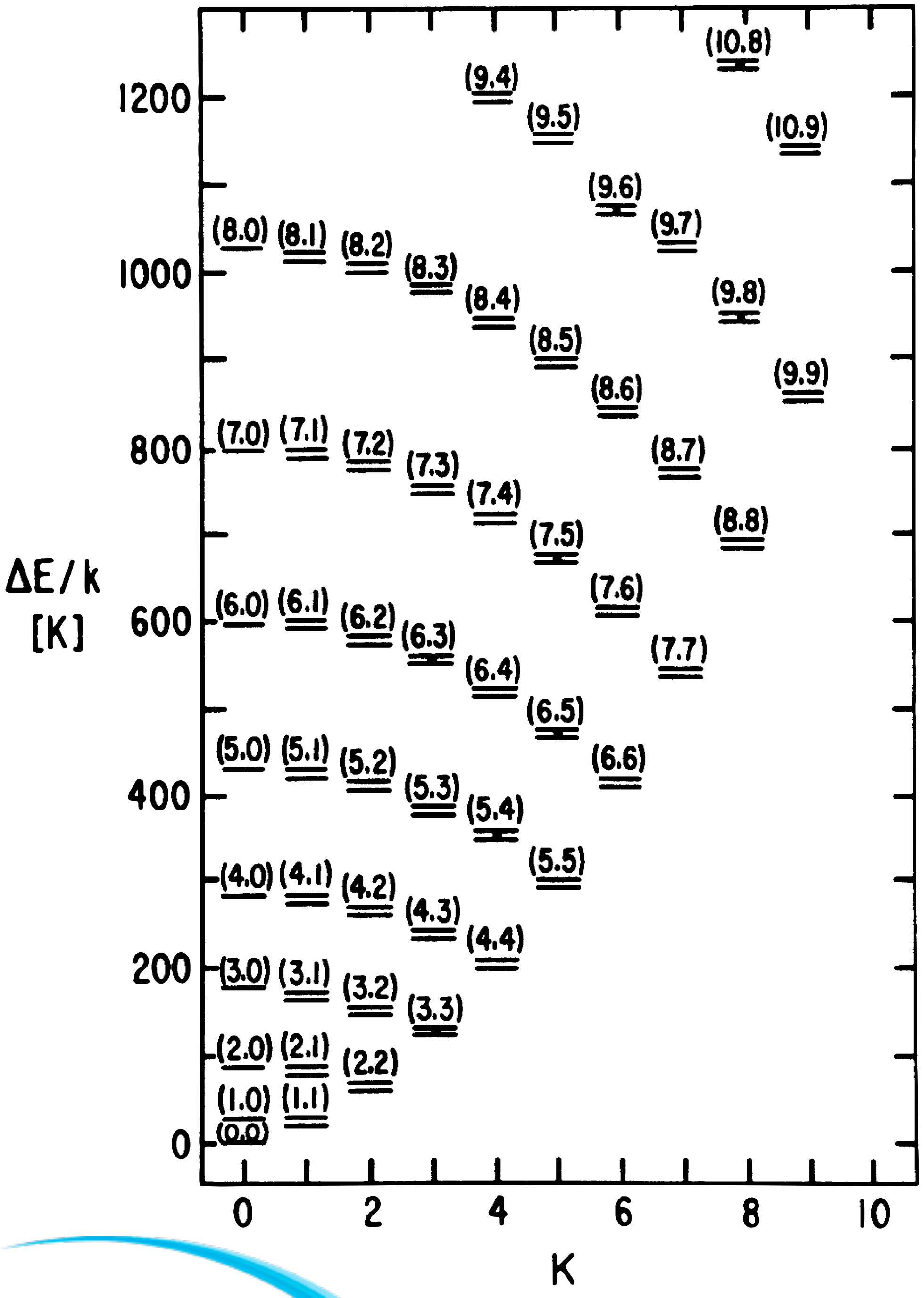
CO vs H_2 rotational levels

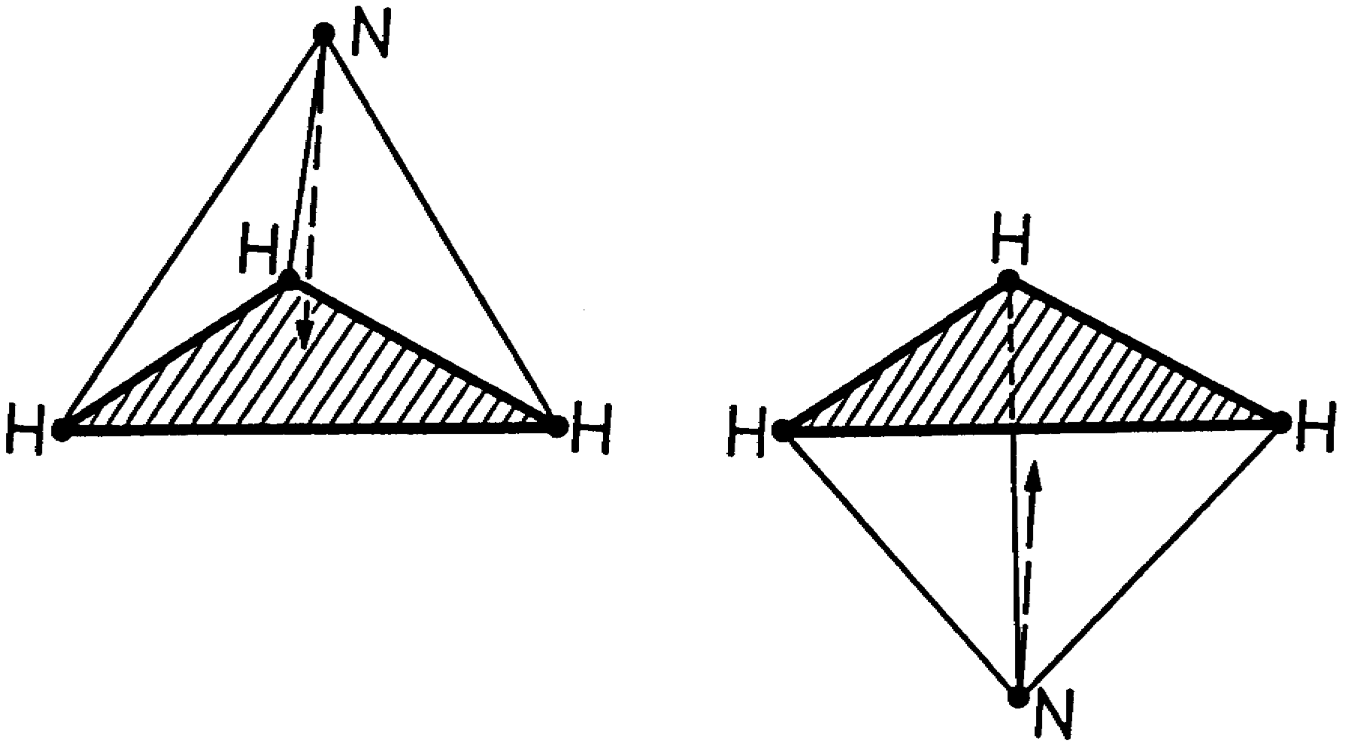


Note much wider spacing for H_2 compared with CO

Energy levels of NH_3

Rotational energy levels of symmetric-top molecules

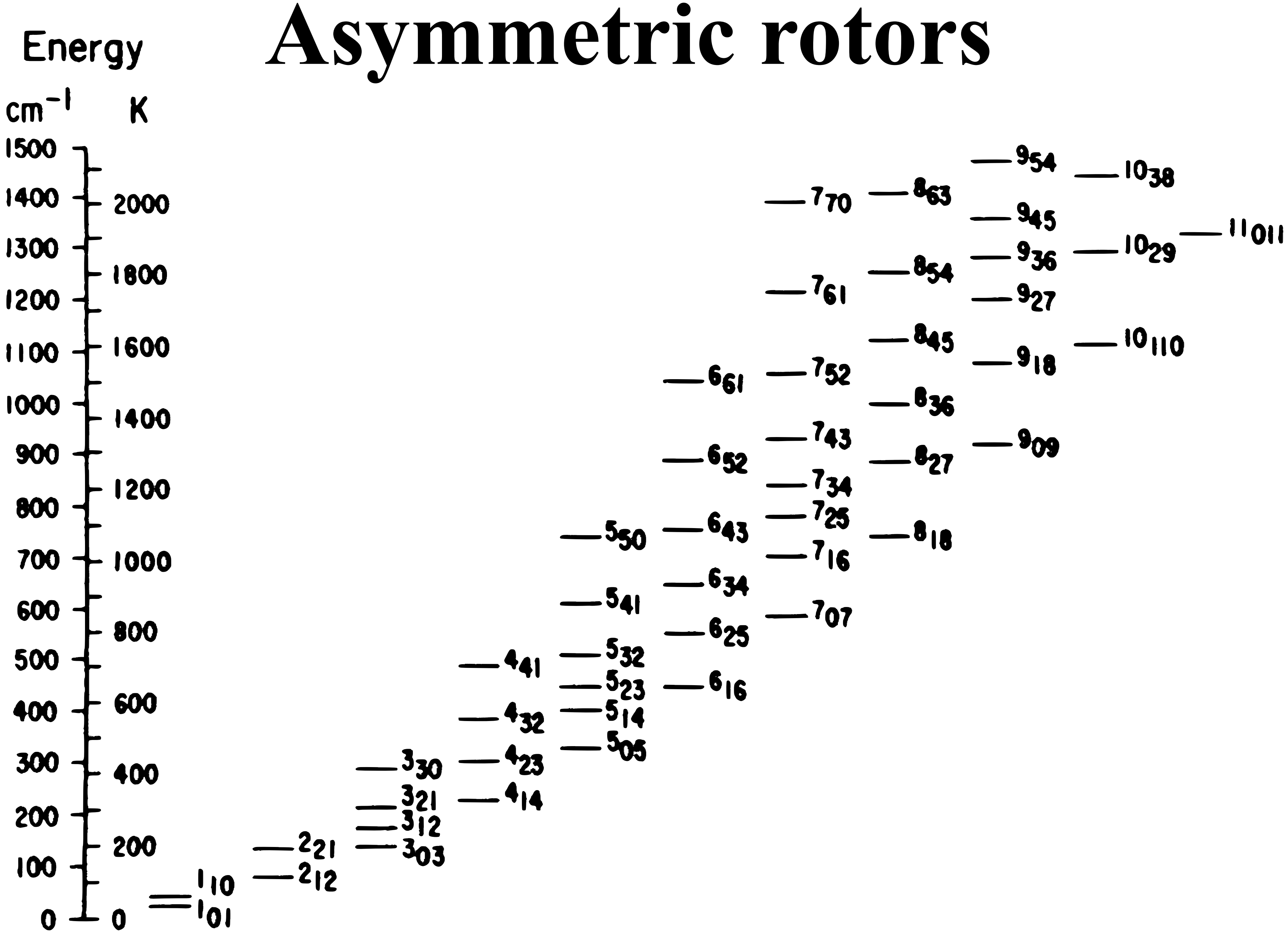




- Inversion doubling of rotational transitions
- Frequency about 23 GHz
- Used to build first masers

Rotational levels of ortho-H_2O

Asymmetric rotors



The equation of radiative transfer

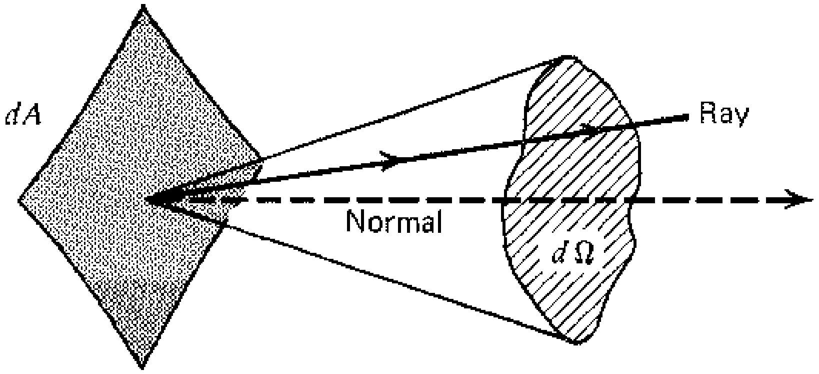
An excursion to basic radiative transfer theory

- The first step in solving radiative transfer, is to do a proper bookkeeping of the *emitted* or *received* radiation
- Flux F defined as energy emitted/received per unit area per unit of time (per unit of frequency or wavelength)

(Specific) (energy) **flux** F_ν
units: W $\mathrm{m^{-2}\ Hz^{-1}}$ or erg $\mathrm{s^{-1}\ cm^{-2}\ Hz^{-1}}$

$$dE = F_\nu \, dA \, dt \, d\nu$$

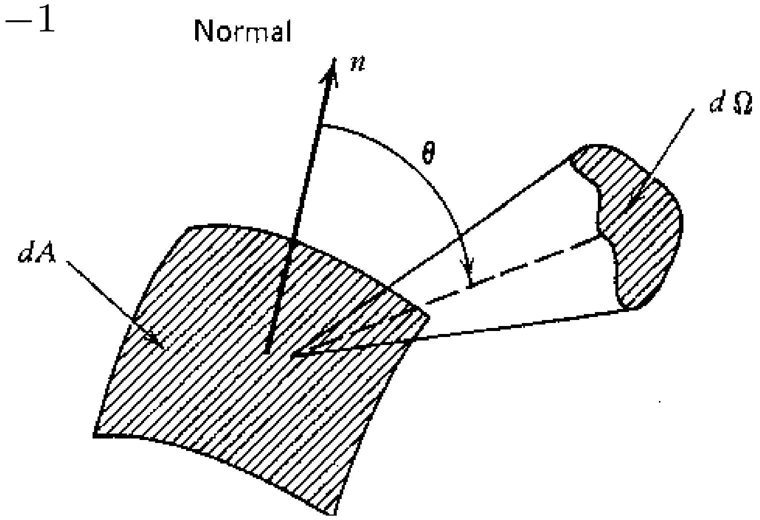
Conservation of energy $\Rightarrow \; F_\nu \propto r^{-2}$



- Intensity I defined as flux emitted/received per unit solid angle

(Specific) **intensity** I_ν
units: W $\mathrm{m^{-2}\ Hz^{-1}\ sr^{-1}}$ or erg $\mathrm{s^{-1}\ cm^{-2}\ Hz^{-1}\ sr^{-1}}$

$$dE = I_\nu \, dA \, dt \, d\nu \, d\Omega$$
$$\Rightarrow F_\nu = \int I_\nu \, \cos\theta \, d\Omega$$

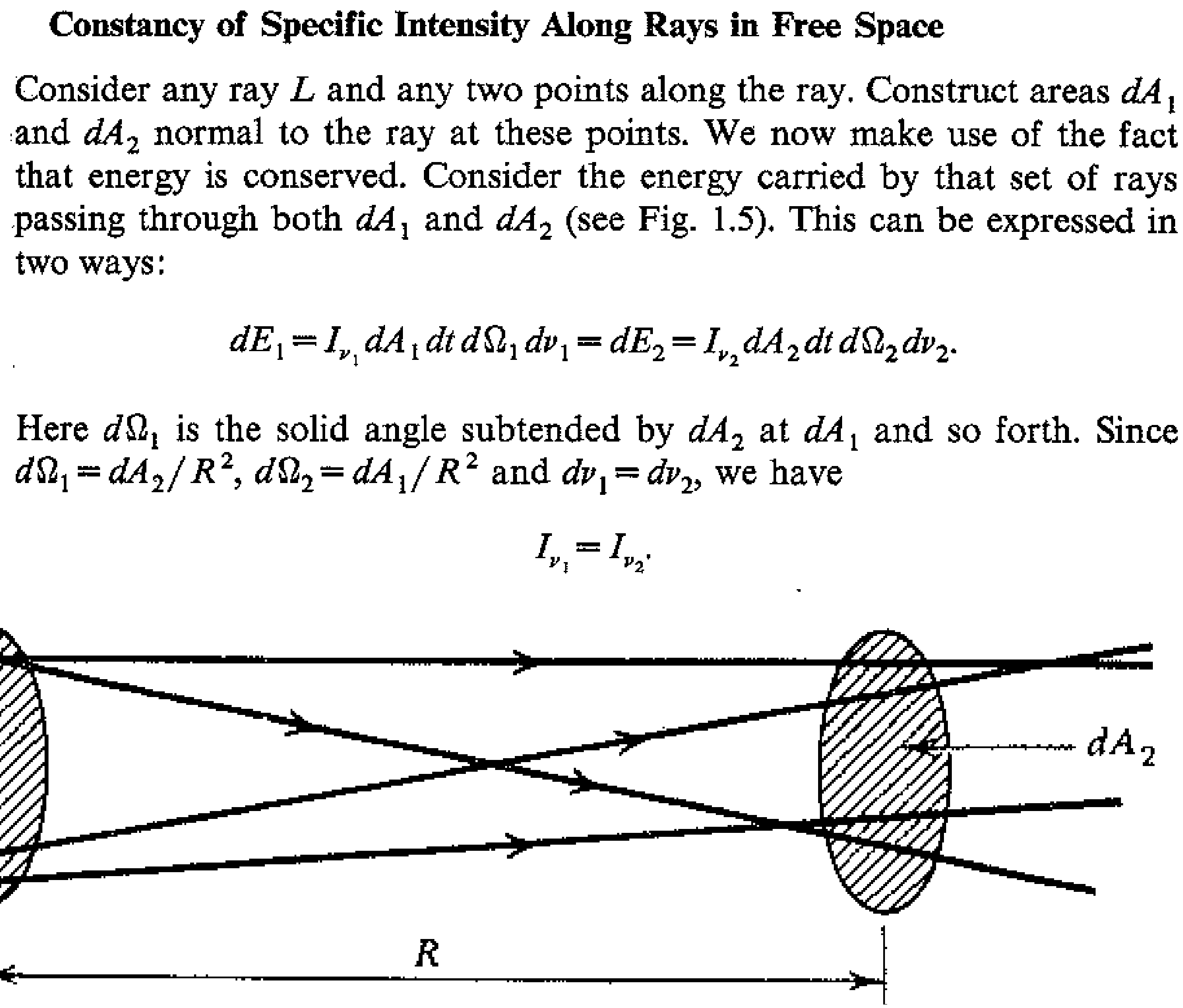


Conservation of intensity

- Unless some process adds energy (photons) or takes away energy (photons), *intensity* is conserved along a ray.

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

  - *Flux* decrease as r^{-2}



Constancy of Specific Intensity Along Rays in Free Space

Consider any ray L and any two points along the ray. Construct areas dA_1 and dA_2 normal to the ray at these points. We now make use of the fact that energy is conserved. Consider the energy carried by that set of rays passing through both dA_1 and dA_2 (see Fig. 1.5). This can be expressed in two ways:

$$dE_1 = I_{\nu_1} dA_1\, dt\, d\Omega_1\, d\nu_1 = dE_2 = I_{\nu_2} dA_2\, dt\, d\Omega_2\, d\nu_2.$$

Here $d\Omega_1$ is the solid angle subtended by dA_2 at dA_1 and so forth. Since $d\Omega_1 = dA_2/R^2$, $d\Omega_2 = dA_1/R^2$ and $d\nu_1 = d\nu_2$, we have

$$I_{\nu_1} = I_{\nu_2}.$$

The equation of radiative transfer

- If there is emission or absorption along the line of sight, this changes to

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

with **emission coefficient** j_ν in W m^{-3} sr^{-1} Hz^{-1} and **absorption coefficient** α_ν in m^{-1}.
This is the **equation of radiative transfer**.

Source funtion and opacity

With **optical depth**

$$d\tau_\nu \equiv \alpha_\nu \, ds$$

and **source function**

$$S_\nu \equiv \frac{j_\nu}{\alpha_\nu}$$

we can rewrite the radiative transfer equation as

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

Formal solution

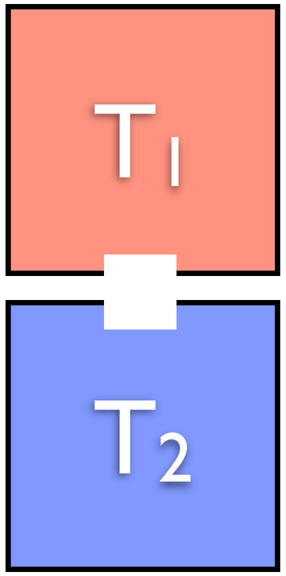
This has the **formal** solution

$$I_\nu(\tau_\nu) = I_0 e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-(\tau_\nu - \tau'_\nu)}\, S_\nu(\tau'_\nu)\, d\tau'_\nu$$

Evaluating this expression is not trivial and can often only be done numerically!!
If S_ν is *independent* of location,

$$I_\nu(\tau_\nu) = I_0 e^{-\tau_\nu} + S_\nu\,(1 - e^{-\tau_\nu}) = S_\nu + e^{-\tau_\nu}(I_0 - S_\nu)$$

Thermal radiation



Thermal emission is radiation emitted by material in thermal equilibrium (TE); blackbody radiation (BB) is thermal emission that is in TE itself.

BB is independent of material, shape, color, direction, flavor, or country of origin. It only depends on temperature and wavelength (or frequency)

$$I_\nu = f(\nu, T) \equiv B_\nu(T). \tag{2.14}$$

Kirchhoff's Law: material emitting thermal radiation has

$$S_\nu = B_\nu(T), \tag{2.15}$$

and therefore

$$j_\nu = \alpha_\nu \, B_\nu(T). \tag{2.16}$$

Useful distinction: Thermal radiation has $S_\nu = B_\nu$ and blackbody radiation has $I_\nu = B_\nu$. Thermal radiation becomes blackbody radiation for $\tau \to \infty$.

The Planck spectrum

$$B_\nu(T) = \frac{2hv^3/c^2}{\exp(h\nu/kT) - 1}$$

or

$$B_\lambda(T) = \frac{2hc^2/\lambda^5}{\exp(hc/\lambda kT) - 1}.$$

Radiative transfer with molecules: absorption and emission of line photons

Einstein coefficients

Linking Kirchhoff's Law (macroscopic) with microscopic properties.

- For a two-level system with levels $E_2 > E_1$, $E_2 - E_1 = h\nu_0$, and degeneracies g_1 and g_2, define
  - probability for spontaneous emission (s^{-1}) $= A_{21}$.
  - probability for absorption $= B_{12}\bar{J}$, where $\bar{J} \equiv \int_0^\infty J_\nu \phi(\nu) d\nu$ and $\phi(\nu)$ is the *profile function*. It describes the finite width around the frequency ν_0 where absorption can take place. For a slowly varying average intensity J_ν (like the Planck function), $\phi(\nu)$ can be approximated as a δ-function, and $\bar{J} = J_\nu$.
  - probability for stimulated emission $= B_{21}\bar{J}$.
- The Einstein coefficents A_{21}, B_{21}, and B_{12} are related by

$$\boxed{g_1 B_{12} = g_2 B_{21}} \tag{2.25}$$

and

$$\boxed{A_{21} = \frac{2h\nu^3}{c^2} B_{21}.} \tag{2.26}$$

- The macroscopic emission and absorption coefficients can be written in terms of the *microscopic* Einstein coefficients as

$$\boxed{j_\nu = \frac{h\nu_0}{4\pi} n_2 A_{21} \phi(\nu)} \tag{2.27}$$

and

$$\boxed{\alpha_\nu = \frac{h\nu_0}{4\pi}(n_1 B_{12} - n_2 B_{21})\phi(\nu).} \tag{2.28}$$

Here, *absorption* also includes stimulated emission (as negative absorption).

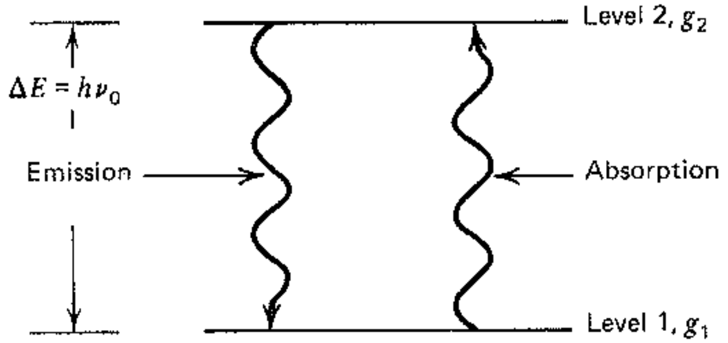


Figure 1.12a ***Emission and absorption from a two level atom.***

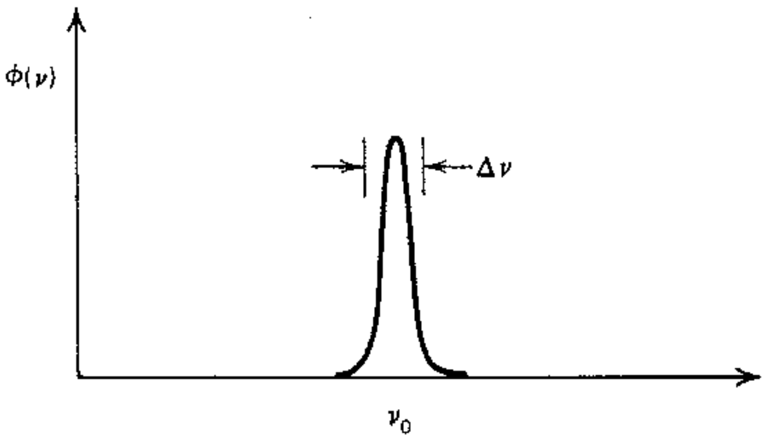


Figure 1.12b ***Line profile for 12a.***

Line formation: broadening

- Quantum mechanical uncertainty principle causes each transition to have a finite width around the frequency given by *E*=*hv*

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu-\nu_0)^2 + (\gamma/4\pi)^2}$$

- Thermal motions of the molecules cause a Gaussian broadening of the line

$$\phi(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} e^{-(\nu-\nu_0)/\Delta\nu_D^2},$$

$$\Delta\nu_D \equiv \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}}$$

  - Random, turbulent motions further broaden the line

$$\Delta\nu_D \equiv \frac{\nu_0}{c}\sqrt{\frac{2kT}{m} + \xi^2}.$$

- In planetary and stellar atmospheres, pressure broadening dominates the line profile.

The relation with continuum emission

- For high optical depth, the intensity of *any* emission (& associated absorption) process approaches the Planck function
- For line emission, this happens first at line center
    - Flat topped line + wider line
- Solid material have fewer degrees of freedom than gas-phase (free moving) atoms/molecules
    - Fewer emission frequencies
    - Much wider 'bands' because individual atoms/molecules have slightly different surroundings (energies)
- If energy within a system is completely equilibrated (the system is in TE)
    - emission becomes blackbody

Excitation: T$_{\mathrm{ex}}$ and LTE

- In TE, the populations of two connected levels are given by a Boltzmann distribution

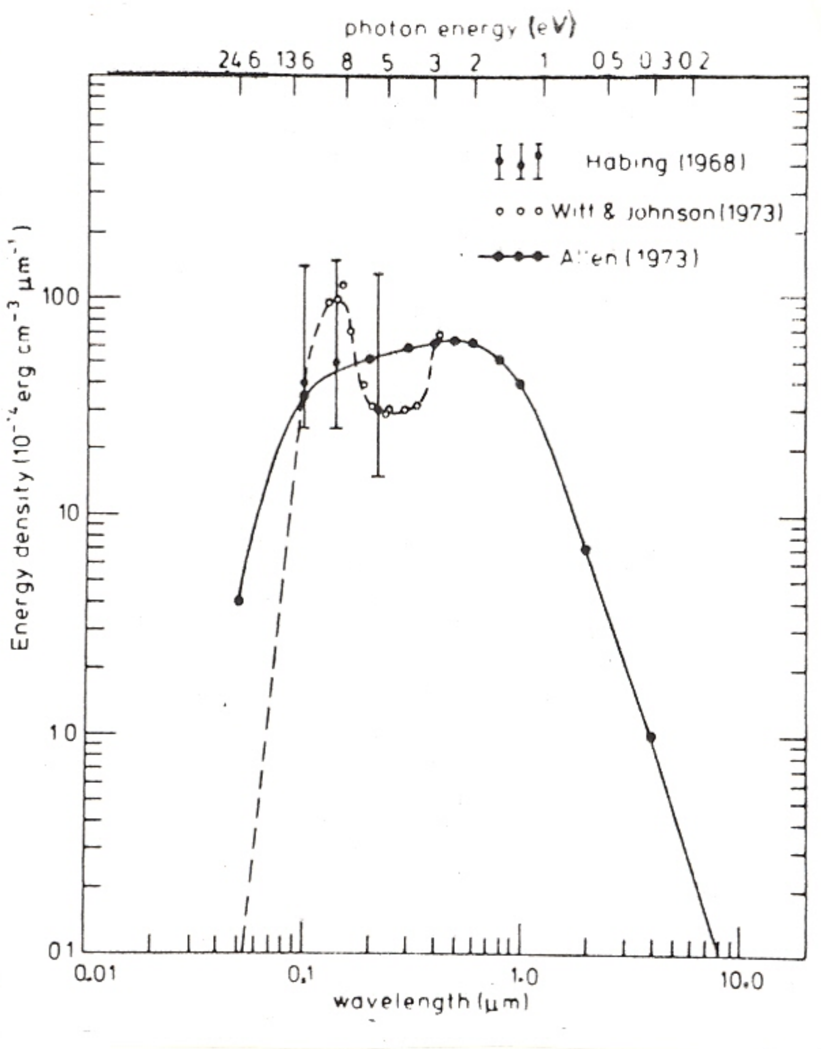
$$\frac{n_i}{n_j} = \frac{g_i}{g_j} e^{-\frac{E_i - E_j}{kT}} .$$

- Even if the excitation is not in TE, for given n_i and n_j one can always define an excitation temperature T_{ex}

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} e^{-\frac{E_i - E_j}{kT_{\mathrm{ex}}}} .$$

Why is ISM is <u>not</u> in Thermal Equilibrium?

- The interstellar radiation field is far from thermal equilibrium
  - peak at 2000 Å →$T_{\rm color}$=10^4 K, but energy content ~1 eV $\rm cm^{-3}$ ≡ 3 K



Spectrum does not
look like a blackbody!

Units in ‘radio’ astronomy

- Express intensity as a temperature of a blackbody that has the same intensity at the observing frequency as your measurement
    - furthermore, approximate Planck function by the Rayleigh-Jeans limit
    - Antenna temperature $T_A = c^2/(2k\nu^2) \times I_\nu$

- Often expressed as ‘main beam antenna temperature’: average intensity observed over the main lobe of the antenna pattern, correcting for the empty sky seen by the sidelobes

- If the emission is optically thin, $T_A <$ true temperature
- In the submillimeter, the RJ limit is generally not valid, and T_A always < true temperature!

- Convert to flux: $F_\nu = (2k\nu^2)/c^2 \times T_A \times \Omega_{\mathrm{beam}}$

Recap of RT

- Intensity along a ray is increased by emission and decreased by absorption

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

- Rewrite as

$$d\tau_\nu \equiv \alpha_\nu \, ds$$

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

$$S_\nu \equiv \frac{j_\nu}{\alpha_\nu}$$

- Emission and absorption takes place within a given frequency response (‘line profile function’), including contributions from the intrinsic line width, thermal, and (micro) turbulent broadening

Recap of RT (2)

- Emission and absorption coefficients are given by
  - the Einstein coefficient for spontaneous emission A_{ij}
  - the derived coefficients for stimulated emission and absorption B_{ij} and B_{ji}.

$$g_1 B_{12} = g_2 B_{21}$$

$$A_{21} = \frac{2h\nu^3}{c^2} B_{21}.$$

  - and the populations of the involved energy levels n_{ij}

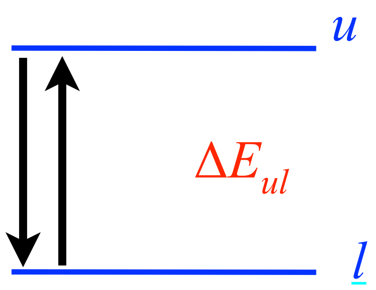
$$j_\nu = \frac{h\nu_0}{4\pi} n_2 A_{21} \phi(\nu)$$

$$\alpha_\nu = \frac{h\nu_0}{4\pi} (n_1 B_{12} - n_2 B_{21}) \phi(\nu).$$

Molecular excitation

Molecular excitation

- *Collisions* can cause the excitation of an atom or molecule to increase or decrease
  - collisions with H_2, He, and e^- dominate
  - collision rates usually given as collision rate coefficient q_{ij}
    - =cross section to collisional (de)excitation averaged over Maxwell distribution at temperature T
    - units $cm^3 s^{-1}$
    - upward and downward rate coefficients related as

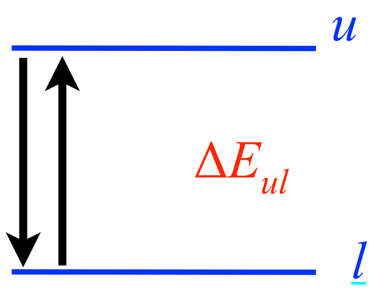


$$q_{lu} = \frac{g_u}{g_l}\, q_{ul}\, e^{\frac{-\Delta E_{ul}}{kT}}$$

    - collision rate (in s^{-1}) obtained after multiplication with density of collision partner: $n(H_2)\, q_{ul}$

Molecular excitation (2)

- *Radiative* transition only exist between levels where they are allowed (dipole, magnetic dipole, quadrupole, etc)
  - De-excitation follows spontaneous emission
    - Sponteneous emission rate A_{ul}
  - De-excitation follows stimulated emission (B_{ul})
  - Excitation follows absorption of a photon of the right frequency (within the line profile function) (B_{lu})



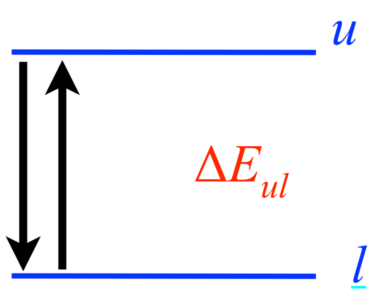
  - Rates for stimulated emission and for absorption depend on the average intensity of the surrounding radiation field

$$J_\nu \equiv \frac{1}{4\pi} \int I_\nu \, d\Omega$$

  - ...which may depend on the photon emitted (and absorbed) by other atoms/molecules of the same species
    - coupling of excitation over large distances.

Critical density

- Consider two levels connected by collisional and radiative transitions, with the system in the excited state at level *u*
  - if the density of collision partners is low, de-excitation will occur via spontaneous emission
  - if the density of collision partners is sufficiently high, collisional excitation will occur before spontaneous emission happens
  - the density where de-excitation through collisions and via spontaneous emission are equally likely is called the critical density



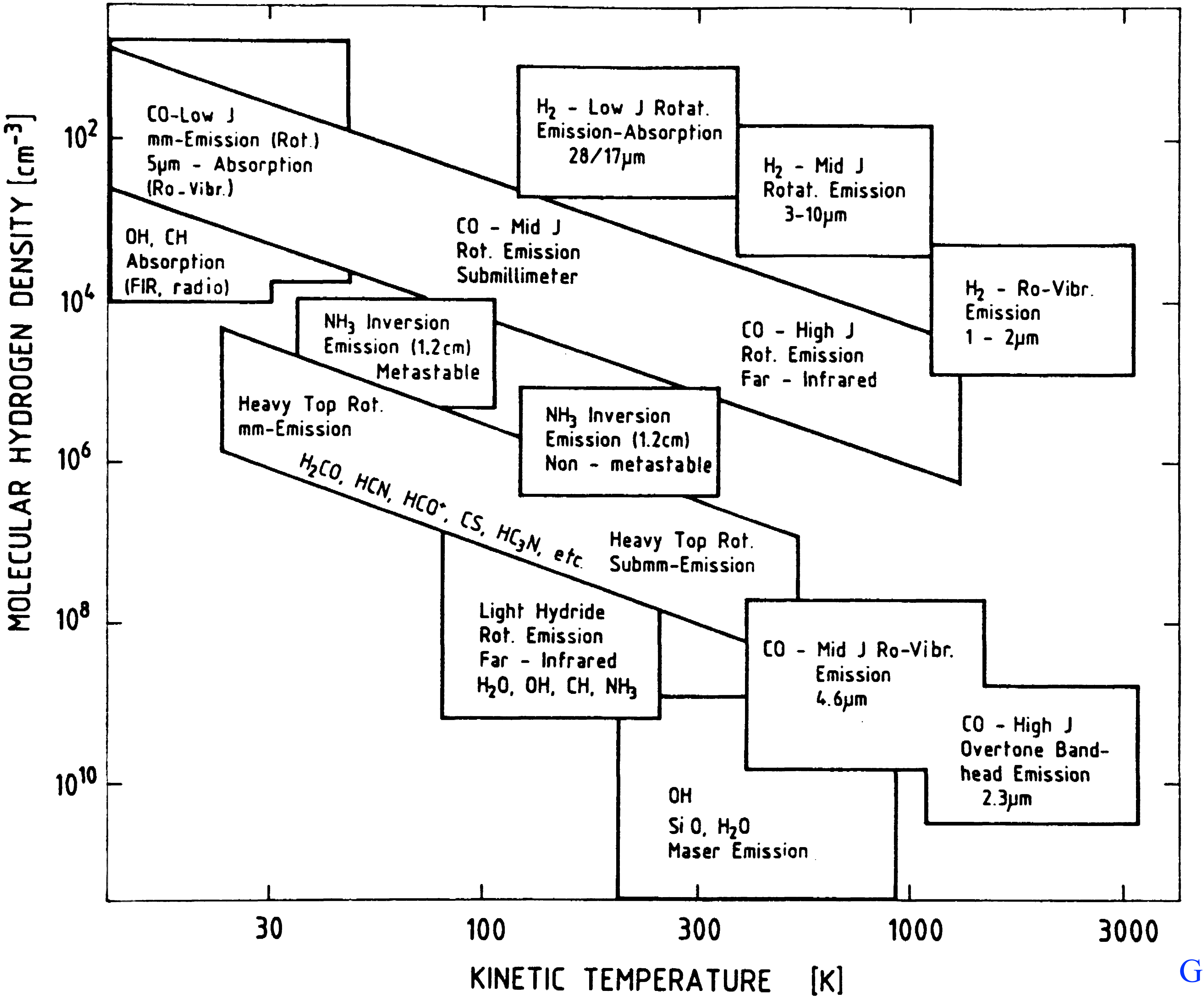
$$n_{crit} \equiv A_{ul}/q_{ul}$$

  - for $n > n_{\mathrm{crit}}$, efficient collisions make sure that the level populations reach thermal equilibrium

$$\frac{n_u}{n_l} = \frac{q_{ul}}{q_{lu}} = \frac{g_u}{g_l} e^{-\frac{\Delta E}{kT}}.$$

  - for $n < n_{\mathrm{crit}}$, we call the excitation regime sub-thermal

The “Genzel” plot



Genzel 1990, 1992

LTE vs Statistical Equilibrium

- For $n > n_{\rm crit}$, efficient collisions make sure that the level populations reach thermal equilibrium

$$\frac{n_u}{n_l} = \frac{q_{ul}}{q_{lu}} = \frac{g_u}{g_l} e^{-\frac{\Delta E}{kT}}.$$

- For $n < n_{\rm crit}$, we call the excitation regime sub-thermal
- Need to solve the *statistical equilibrium* of collisional and radiative excitation and de-excitation of ensemble of atoms / molecules

$$n_l\Big(n_c q_{lu} + B_{lu}\bar{J}_\nu\Big) = n_u\Big(n_c q_{ul} + B_{ul}\bar{J}_\nu + A_{ul}\Big),$$

where

$$\bar{J}_\nu = \frac{1}{4\pi}\int I_\nu d\Omega.$$

- (2-level system, *u*–*l*)
- Can always write the solution as a Boltzmann distribution at $T = T_{\rm ex}$

$$\frac{n_u}{n_l} = \frac{q_{ul}}{q_{lu}} = \frac{g_u}{g_l} e^{-\frac{\Delta E}{kT_{\rm ex}}}$$

Statistical Equilibrium

- For multi-level systems the equation of statistical equilibrium becomes

$$n_l \left[\sum_{k<l} A_{lk} + \sum_{k\neq l} (B_{lk}J_\nu + C_{lk})\right] =$$

$$\sum_{k>l} n_k A_{kl} + \sum_{k\neq l} n_k(B_{kl}J_\nu + C_{kl}).$$

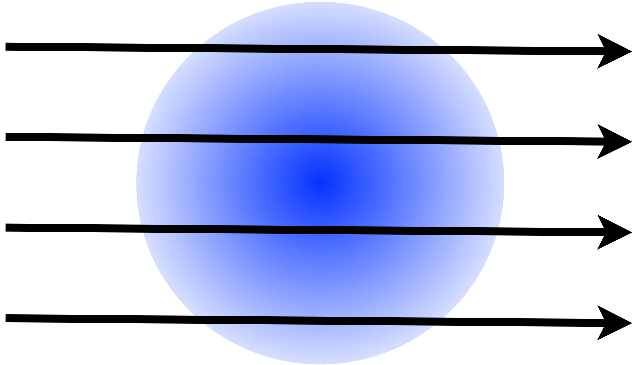
- where the notation C_{ij} is used instead of q_{ij} for collision rate coefficients,
- and the additional constraint

$$\sum_j n_j = n$$

A coupled problem, and some ways to solve this that are *not* Monte Carlo methods

A coupled problem

- The eqn of statistical equilibrium includes the average radiation field J
- In the limit that the radiation field generated by the atoms / molecules is weak, the solution is straightforward
  - optically thin limit
  - only include the strength of the CMB and any dust continuum field
  - neither depends on the level populations: the problem is *local*
- ⇒ calculate excitation based on collisions and J
- ⇒ ray-tracing gives $I_\nu(\alpha,\delta)$



A coupled problem (2)

- In the limit that the radiation field generated by the atoms / molecules is not negligible, the problem becomes coupled
  - optically thick limit
  - *J* follows from solving the RT eqn including line photons

$$n_l \left[\sum_{k<l} A_{lk} + \sum_{k\neq l} (B_{lk} J_\nu + C_{lk})\right] = \sum_{k>l} n_k A_{kl} + \sum_{k\neq l} n_k (B_{kl} J_\nu + C_{kl}).$$

iterate

&

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

$$J_\nu \equiv \frac{1}{4\pi} \int I_\nu \, d\Omega$$

$$j_\nu = \frac{h\nu_0}{4\pi} n_2 A_{21} \phi(\nu)$$

$$\alpha_\nu = \frac{h\nu_0}{4\pi} (n_1 B_{12} - n_2 B_{21}) \phi(\nu).$$

Solution methods

- In principle, one can do a *full* calculation for the excitation at *all* locations in your object, solving RT along *all* lines of sight, and iteratively obtaining a solution
- In practice, this is inpractical
- So either
  - perform this iterative calculation for a *limited set of locations* in the object and a *limited set of rays*
    - e.g., Monte Carlo methods, Accelerated Lambda Iteration

  - or use an *approximation to the long-range RT*, and only self-consistently calculate the *local* radiative coupling
    - e.g., Large Velocity Gradient / Sobolev, Escape Probability

- Many hybrid methods exist, that work well for particular situations

Simplest example

- The two simplest approximations are

  - Assume LTE
    - OK if densities are well above critical density

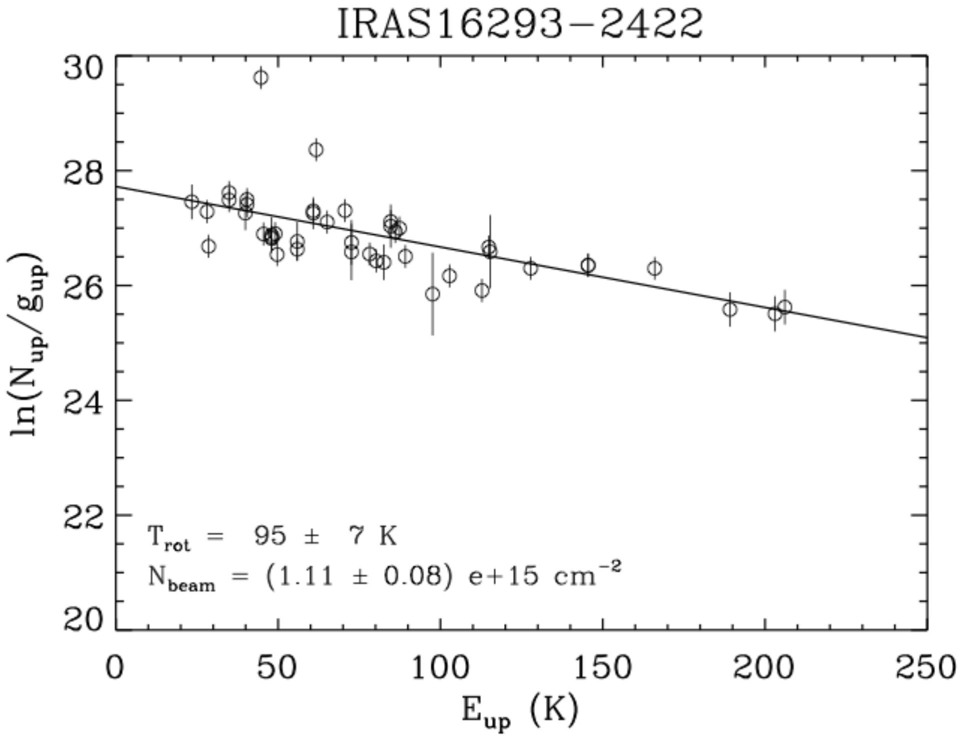
  - Assume optically thin regim
    - OK is abundance of species is very low

- In both these limits, the level populations are easily obtained, and the eqn of RT can be solved without iterations

Example: rotation diagrams

- One or both of these assumptions is (implicitely) adopted when using *rotation diagrams*
- If many lines, from different energies, of the same species are observed, plot relative strength (converted to column density) vs energy of the upper level
    - Useful for species such as CH_3OH and CH_3CN that have many transitions close together in frequency
    - Assumes optically thin lines; can make correction for (known or guessed) opacity

- In LTE, a single temperature corresponds to straight line
    - Steeper line means lower temperature
    - If not in LTE, at least gives excitation temperature (T_{rot})



Example: Escape probability

- Another simple assumption is that the radiative coupling only occurs *locally*
  - E.g., because the line photons are Doppler shifted by more than the width of the line profile function after a short distance: *Large Velocity Gradient*
  - One can calculate a probability of a photon escaping the medium: *Escape Probability*
    - fraction β radiation is trapped
    - fraction 1-β disappears to outer space
    - Given a source geometry (usually simple, like a sphere or an infinite slab), β follows from the line opacity

⇒ No need to solve RT!

- These methods often assume a homogenous medium (single density, single temperature, single abundance)
- But can be generalized to include arbitrarily complex structures

Escape probabilities

A very crude form of β in a one-dimensional case can be estimated as:

$$\beta =< e^{-\tau} >= \frac{1}{\tau} \int_0^{\tau} e^{-\tau'}\, d\tau' = \frac{1-e^{-\tau}}{\tau}.$$

In other expressions one usually expresses β in terms of the optical depth τ in the direction of the observer. It happens that the from of β for a radially expanding sphere is equal to the result above. This is called the Sobolev or large velocity gradient (LVG) approximation; see for example Elitzur (2), p. 44 for a derivation:

$$\beta = \frac{1-e^{-\tau}}{\tau}$$

For a homogeneous slab is found:

$$\beta = \frac{(1-e^{-3\tau})}{3\tau}$$

Also for a turbulent medium an escape probability has been estimated:

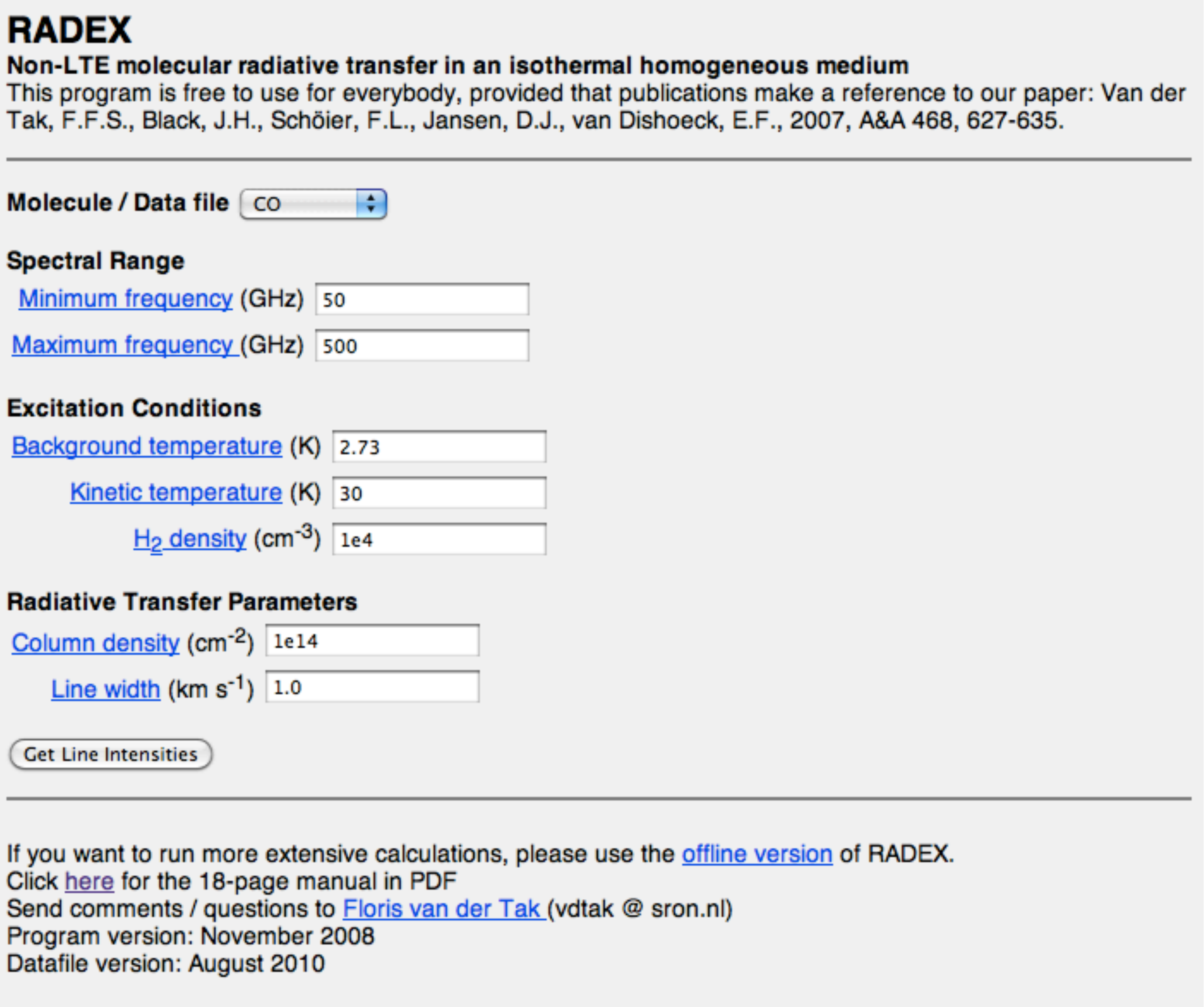
$$\beta = \frac{1}{\tau\sqrt{\pi \ln(\tau/2)}}$$

Finally for a uniform sphere, Osterbrock (6) derives

$$\beta = \frac{1.5}{\tau}[1 - \frac{2}{\tau^2} + (\frac{2}{\tau} + \frac{2}{\tau^2})e^{-\tau}].$$

RADEX

- RADEX
- http://www.sron.rug.nl/~vdtak/radex/radex.php
- Van der Tak et al. 2007



RADEX

Non-LTE molecular radiative transfer in an isothermal homogeneous medium

This program is free to use for everybody, provided that publications make a reference to our paper: Van der Tak, F.F.S., Black, J.H., Schöier, F.L., Jansen, D.J., van Dishoeck, E.F., 2007, A&A 468, 627-635.

Molecule / Data file CO

Spectral Range

Minimum frequency (GHz) 50

Maximum frequency (GHz) 500

Excitation Conditions

Background temperature (K) 2.73

Kinetic temperature (K) 30

H_2 density (cm^{-3}) 1e4

Radiative Transfer Parameters

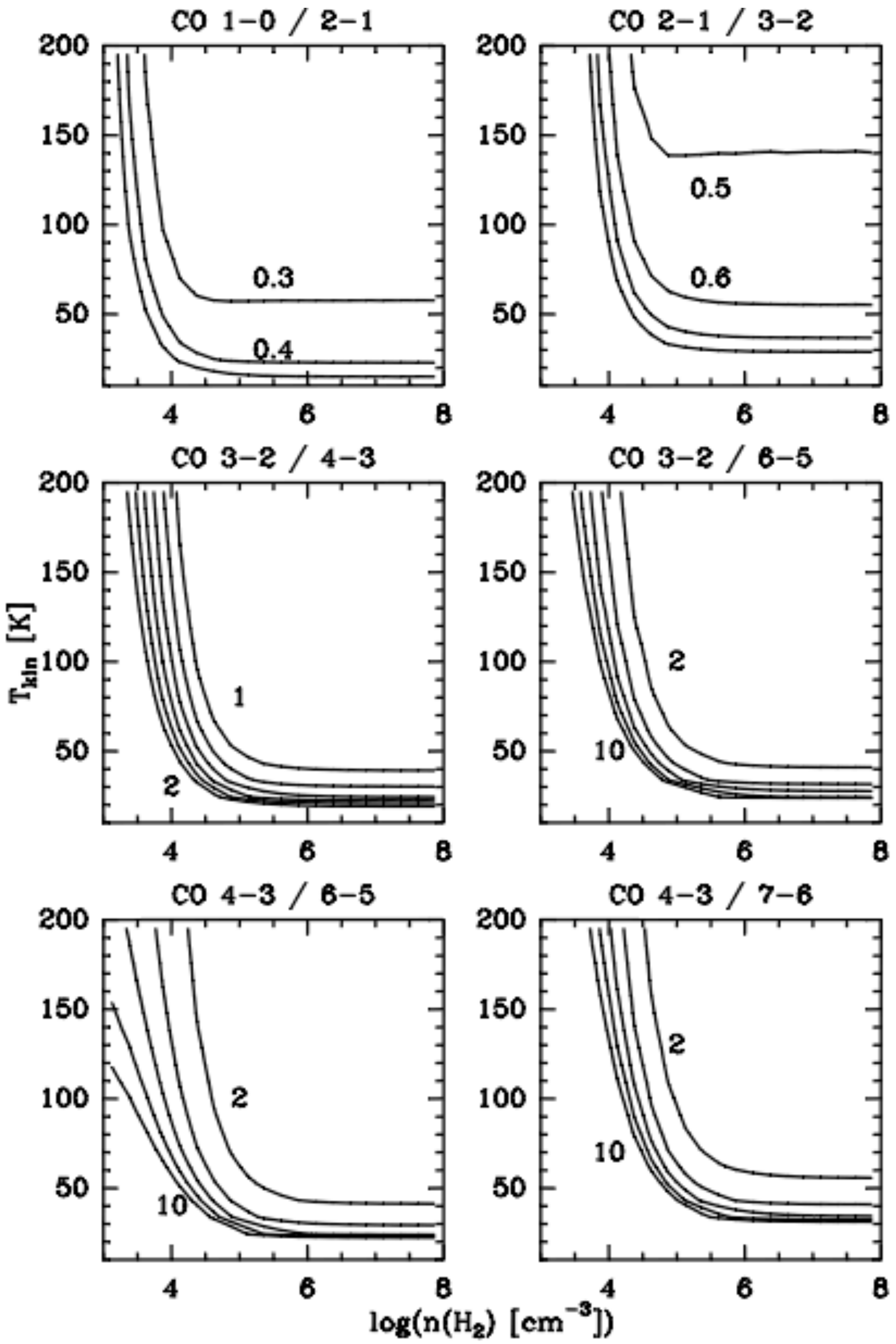
Column density (cm^{-2}) 1e14

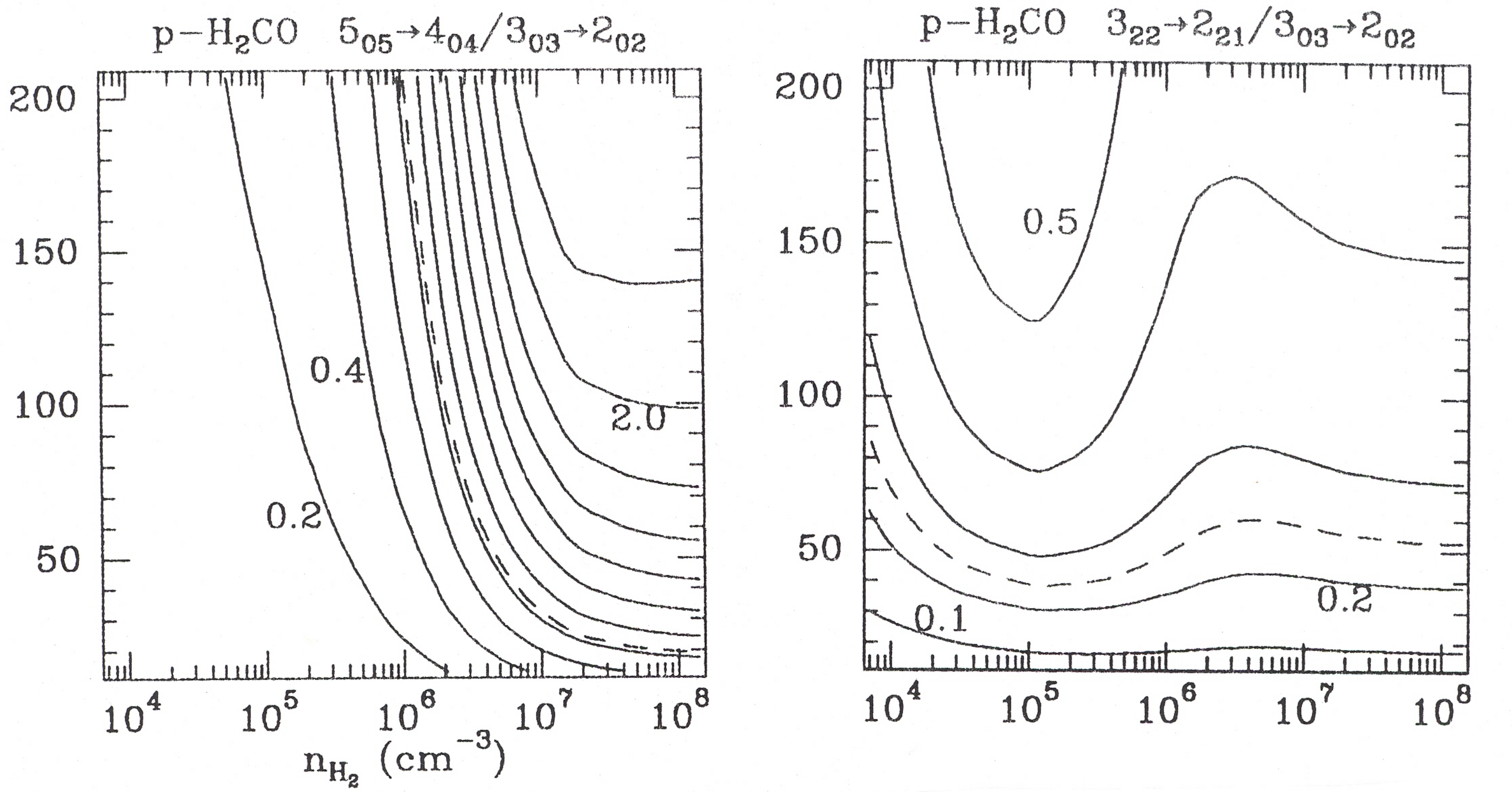
Line width (km s^{-1}) 1.0

If you want to run more extensive calculations, please use the offline version of RADEX.
Click here for the 18-page manual in PDF
Send comments / questions to Floris van der Tak (vdtak @ sron.nl)
Program version: November 2008
Datafile version: August 2010

Using line ratios

- Under these simple assumptions, theoretical plots can be made of line ratio as function of density and temperature
  - not dependent on abundance (if optically thin)
  - obtain *n* and *T* from observing just 3 lines!

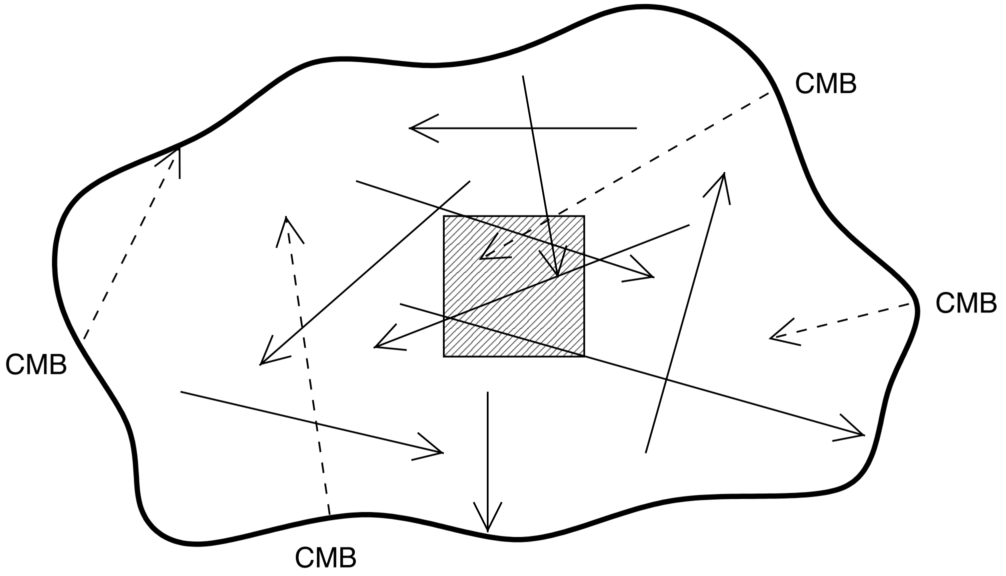




Van Dishoeck et al. 1993, 1995
Jansen et al. 1993
van der Tak et al. 2007

Example: Monte Carlo methods

- If you suspect that a local approximation like an escape probability is not good enough for your problem, you need to use an iterative method including ‘full’ sampling of the RT, or at least a sufficiently good approximation of that
  - Methods: Monte Carlo methods (RATRAN, LIME, ...); Accelerated Lambda Iteration, ...
  - Penalty: (much!) longer calculation times
  - Bonus: more accurate line *profiles*



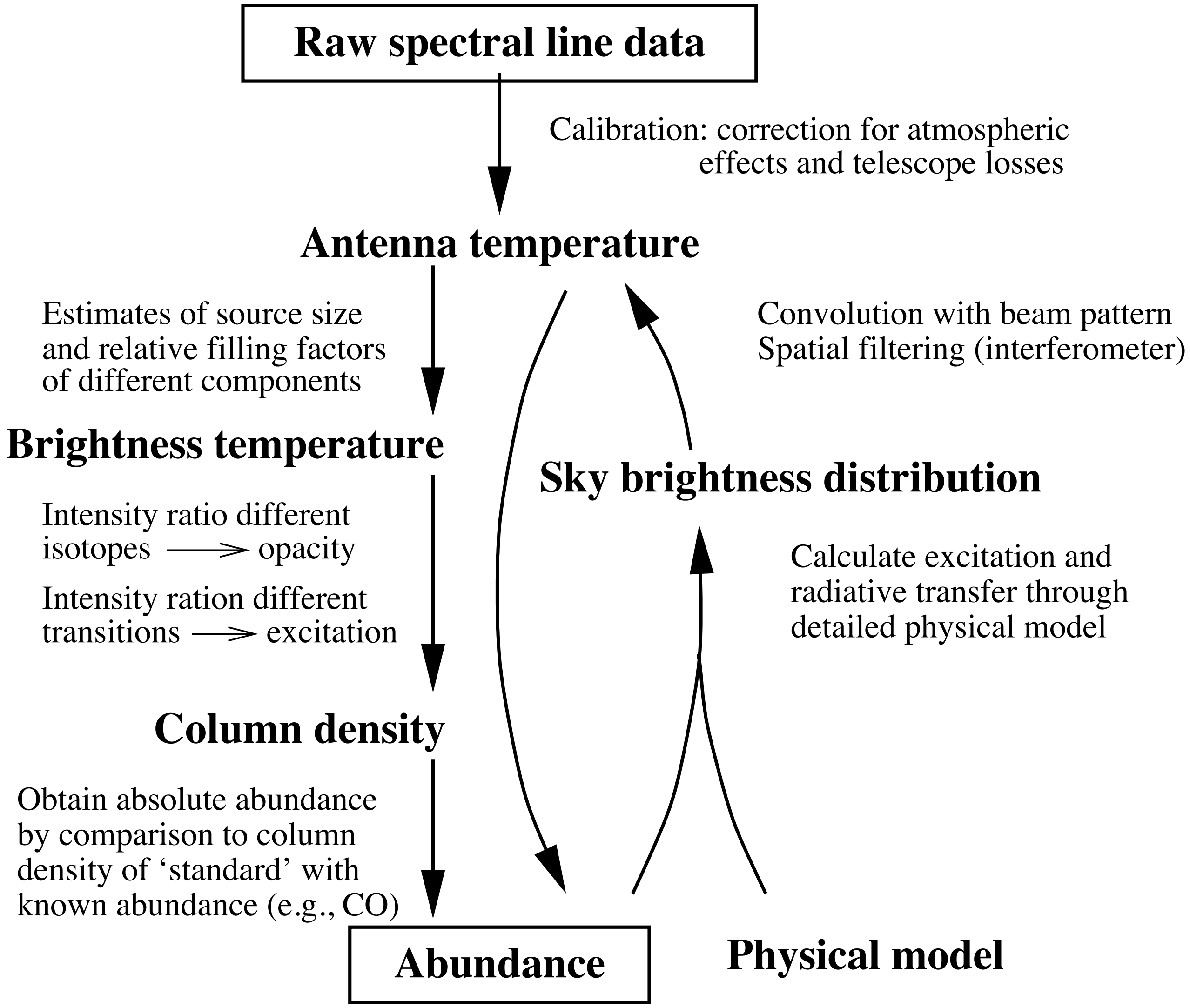
Collision rate coefficients

- *All* methods (except LTE) require the knowledge of collision rate coefficients
- Very few of these are measured in the laboratory
- They require quantum mechanical calculation, usually involing some sort of approximation
  - Often calculated for He and scaled to H_2
  - Or obtained from a very similar species, e.g., $H_2O \rightarrow H_2S$
  - May need to include different rates for ortho-H_2 and para-H_2
  - Needs to be available for sufficient range of temperatures

- Several databases collect available rates from the literature
  - basecol: basecol.obspm.fr
  - lamda: www.strw.leidenuniv.nl/~moldata

Forward vs reverse modeling

reverse



Raw spectral line data

Calibration: correction for atmospheric effects and telescope losses

Antenna temperature

Estimates of source size and relative filling factors of different components

Convolution with beam pattern
Spatial filtering (interferometer)

Brightness temperature

Sky brightness distribution

Intensity ratio different isotopes ⟶ opacity

Intensity ration different transitions ⟶ excitation

Calculate excitation and radiative transfer through detailed physical model

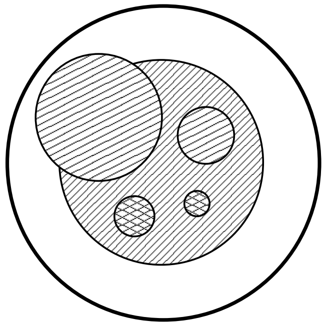
Column density

Obtain absolute abundance by comparison to column density of 'standard' with known abundance (e.g., CO)

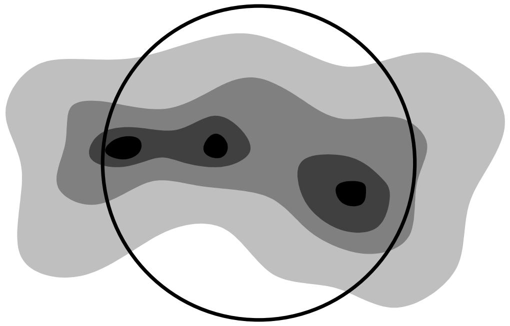
Abundance

Physical model

forward



Telescope beam



Telescope beam

GIGO

- Remember
  - your fit results are only as good as the assumptions you make!
  - Garbage In = Garbage Out

- Even when using a very accurate method to solve molecular excitation and radiative transfer, your results will be no better than the quality of your model
  - more model parameters
    - ‘better’ fit
    - ...but also better understanding?

- Sometimes / often you learn more from a simple approach !

Further reading

- van Dishoeck & Blake 1998, ARA&A 36, 317
- Tielens: The Interstellar Medium (book)
- Rybicki & Lightman: Radiative Processes in Astrophysics (book)

- RADEX: www.strw.leidenuniv.nl/~moldata/radex.html
  - http://www.strw.leidenuniv.nl/~brinch/website/lime.html

- LAMDA: www.strw.leidenuniv.nl/~moldata
  - http://www.strw.leidenuniv.nl/~brinch/website/lime.html

- RATRAN: www.strw.leidenuniv.nl/~michiel
  - http://www.strw.leidenuniv.nl/~brinch/website/lime.html

- LIME: http://www.strw.leidenuniv.nl/~brinch/website/lime.html
  - http://www.strw.leidenuniv.nl/~brinch/website/lime.html