Microphysical processes

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Absorption and emission of radiation

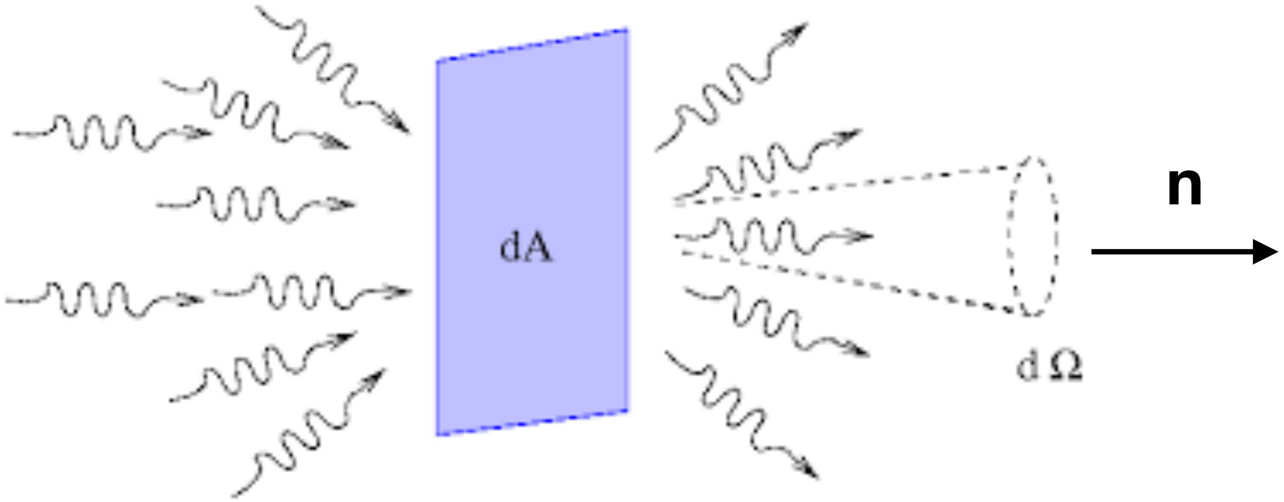
- In this lecture, we will discuss the emission and absorption of radiation by atoms and molecules

- Crucial topic in study of ISM:
  - Central to understanding radiative heating & cooling of interstellar gas
  - Vital for understanding where the radiation we observe comes from and what it tells us about the ISM

- Our starting point: how do we characterise the radiation field at a given point in space?

- For reasons that will become clear later, it is useful to work in terms of the **specific intensity**

- The specific intensity at a location **r** and in a direction **n** is the total energy per unit time per unit area per unit solid angle per unit frequency flowing in that direction



- Why this quantity?
  - Can calculate radiation energy density, photon number density etc. by integrating specific intensity
  - E.g. energy density given by:

$$u_\nu = \frac{1}{c}\int I_\nu(\Omega)d\Omega$$

  - Can’t go the other way: energy density has no information on **direction** in which photons are going
  - Specific intensity <u>conserved</u> along light rays

- Units of specific intensity:

$$[I_\nu] = \text{erg s}^{-1}\ \text{cm}^{-2}\ \text{Hz}^{-1}\ \text{sr}^{-1}$$

- Sometimes convenient to integrate over frequency if dealing with continuum processes

- For line emission/absorption, generally better to work in terms of frequency-dependent version

- Now consider two quantum states of atom: initial state i, final state f, with $E_i < E_f$

- Define the **transition rate** between these two states to be the rate of change of probability of finding atom in state f

- Transition rate caused by interaction with radiation is proportional to specific intensity:

$$W_{if} = B_{if} I_\nu(\nu_{if}),$$

- Constant of proportionality B_{if} between transition rate and specific intensity is the **Einstein coefficient of absorption**

- Note that with the definition of transition rate used here, the rate per unit volume at which transitions occur is:

$$R_{if} = W_{if} n_{i},$$

- Provided we're dealing with systems with many atoms, can ignore discrete nature of transitions and work in terms of continuous rates

- When dealing with very small numbers of atoms, may instead need to use Monte Carlo approach

- Radiation can also cause transition in opposite direction, from state f to state i
- This process is known as **stimulated emission**
- Transition rate:

$$W_{fi} = B_{fi} I_\nu(\nu_{if}),$$

- B_{fi} is the **Einstein coefficient of stimulated emission**

- If states i, f are not degenerate, then time invariance of laws of physics implies that:

$$B_{if} = B_{fi}$$

- More generally, if states have degeneracies g_i, g_f, we have:

$$g_i B_{if} = g_f B_{fi},$$

- Suppose we have a system with N_i atoms in state i, N_f atoms in state f

- System is in complete thermal equilibrium with radiation field with temperature T

- Ratio of N_f to N_i is then simply the Boltzmann distribution:

$$\frac{N_f}{N_i} = \frac{g_f}{g_i} e^{-E_{if}/kT}$$

E_{if} is the energy separation between the two states

- Even if system in equilibrium, microscopically there are many photon absorptions, emissions occurring
- Equilibrium simply implies that these are in balance
- What level population ratio do we get if stimulated emissions balance absorptions?
- Setting two transition rates equal:

$$N_i W_{if} = N_f W_{fi}.$$

yields:

$$\frac{N_f}{N_i} = \frac{B_{if}}{B_{fi}}.$$

- Second line follows because stimulated emission, absorption both have same dependence on I_ν

- Given relationship between B_{if}, B_{fi}, we therefore find:

$$\frac{N_f}{N_i} = \frac{g_f}{g_i}$$

- This is NOT the Boltzmann distribution!

- Something has clearly gone wrong here?

- Problem is our assumption that stimulated emission balances absorption

- In reality, additional emission process also acting, which we term **spontaneous emission**

- Spontaneous emission is transition from f to i with rate that is <u>independent</u> of radiation field

- Transition rate quantified by A_{fi}, the **Einstein coefficient for spontaneous emission**

- Let:

$$W_{fi}^{\mathrm{spon}} = A_{fi},$$

- Then:

$$N_i W_{if} = N_f \left(W_{fi} + W_{fi}^{\mathrm{spon}} \right).$$

and:

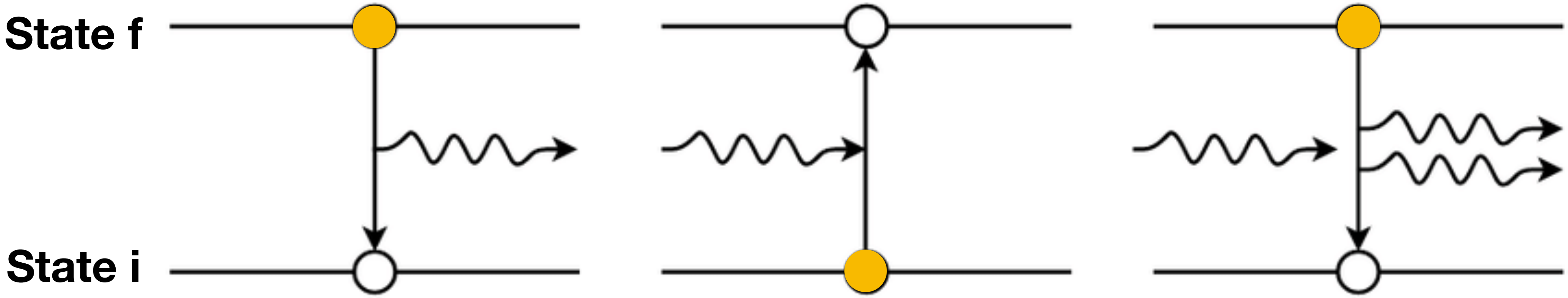
$$\begin{aligned} \frac{N_f}{N_i} &= \frac{W_{if}}{W_{fi} + W_{fi}^{\mathrm{spon}}}, \\ &= \frac{B_{if} I_\nu(\nu_{if})}{B_{fi} I_\nu(\nu_{if}) + A_{fi}}, \\ &= \frac{(g_f/g_i) I_\nu(\nu_{if})}{I_\nu(\nu_{if}) + A_{fi}/B_{fi}}, \\ &= \frac{g_f}{g_i} \frac{1}{1 + A_{fi}/\left(B_{fi} I_\nu(\nu_{if})\right)}. \end{aligned}$$

- In thermal equilibrium, specific intensity of radiation field is given by Planck function:

$$B_\nu(T) = \frac{2h\nu_{if}^3/c^2}{\exp\left(\frac{E_{if}}{kT}\right) - 1}.$$

- If $I_\nu = B_\nu$, then our expression for level population ratio yields Boltzmann distribution provided that:

$$A_{fi} = \frac{2h\nu_{if}^3}{c^2} B_{fi}.$$



Spontaneous emission

Absorption

Stimulated emission

State f

State i

A_{fi}

$B_{if} \, I_{if}$

$B_{fi} \, I_{if}$

- **Warning:** some sources define the Einstein coefficients as the constants of proportionality linking the energy density of the radiation field to the transition rates

- In that case:

$$\begin{aligned} W_{if} &= B_{if} u_\nu(\nu_{if}), \\ W_{fi} &= A_{fi} + B_{fi} u_\nu(\nu_{if}), \end{aligned}$$

with:

$$u_\nu(\nu_{if}) = \frac{4\pi}{c} I_\nu(\nu_{if}).$$

- When using this convention, A_{fi} and B_{fi} are related by:

$$A_{fi} = \frac{8\pi h\nu_{if}^3}{c^2} B_{fi}.$$

- Make sure you know which convention a given source is using!

- In two-state model, lifetime of upper state is approx:

$$t \sim A_{ul}^{-1}$$

- More generally, lifetime is given by:

$$t \sim \left(\sum_l A_{ul}\right)^{-1}$$

where we sum over all possible downwards transitions

- Value of B coefficients directly related to size of transition matrix element
- Value of A coefficient depends on this (via B) but <u>also</u> on cube of frequency — high frequency (i.e. high energy) transitions have much higher spontaneous probabilities
- Fine structure and hyperfine structure transitions are slow for two reasons:
  - Forbidden transitions, so matrix element small, B coeffs. are consequently small
  - Low energy compared to permitted transitions

- For example:
  - Lyman-α: $A_{21} = 6.3 \times 10^{8}\ \mathrm{s}^{-1}$, $E_{21} = 10.2$ eV
  - [CII] 158 μm: $A_{21} = 2.4 \times 10^{-6}\ \mathrm{s}^{-1}$, $E_{21} = 0.008$ eV
  - Einstein B coefficient for permitted Lyman-α transition is ~10^{5} times larger than for forbidden [CII] transition
  - Einstein A coefficients differ by ~10^{13}: factor of ~10^{5} from difference in B coeffs., factor of ~10^{8} from difference in energies

- Einstein coefficients describe emission, absorption by single atoms, molecules
- When we have many particles, more convenient to work in terms of bulk emission and absorption coefficients
- Consider volume with length ds, cross-sectional area dA:

Volume: dV = ds dA

- Radiation flows into one side, out the other
- How much radiation is absorbed within this volume?
- Energy absorbed per unit time in the frequency range [ν, $\nu+d\nu$] and in solid angle element $d\Omega$ by a <u>single atom</u> is:

$$de_\nu = I_\nu \, \sigma_\nu \, dt \, d\nu \, d\Omega$$

σ_ν is the absorption cross-section at frequency ν

- Total energy removed per unit time for this frequency range, solid angle is therefore:

$$dE_\nu = N\, I_\nu\, \sigma_\nu\, dt\, d\nu\, d\Omega$$

- N = total number of atoms in volume = n dV = n ds dA
- n = number density of atoms

- We can also write dE_ν in terms of change in specific intensity within volume:

$$dE_\nu = -dI_\nu\, dA\, dt\, d\nu\, d\Omega$$

- Equating these yields:

$$dI_\nu = -n\, I_\nu\, \sigma_\nu\, ds$$

- We can also write this in terms of an absorption coefficient $\alpha_\nu = n\, \sigma_\nu$

$$dI_\nu = -\alpha_\nu\, I_\nu\, ds$$

- In the absence of emission, the specific intensity therefore satisfies the following transfer equation:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -\alpha_\nu I_\nu.$$

- We now introduce the **optical depth** element:

$$\mathrm{d}\tau_\nu = \alpha_\nu \mathrm{d}s,$$

- and total optical depth:

$$\tau_\nu = \int_0^L \alpha_\nu(s)\mathrm{d}s,$$

- We can therefore write the formal solution of the transfer equation as:

$$I_\nu(\tau_\nu) = I_{\nu,0} e^{-\tau_\nu}.$$

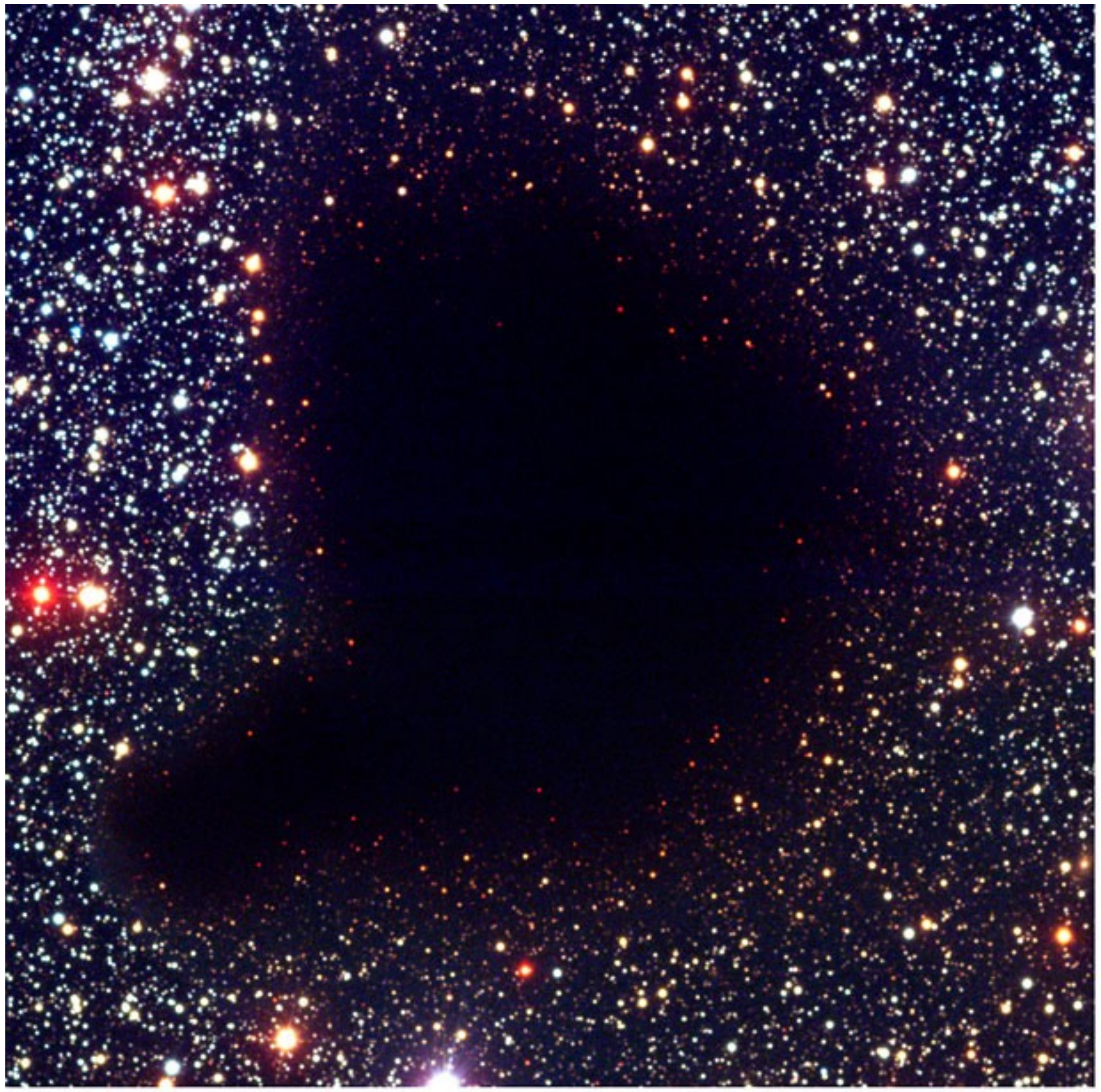
- I_ν decreases exponentially with increasing optical depth

- If $\tau_\nu < 1$, line of sight is **optically thin**

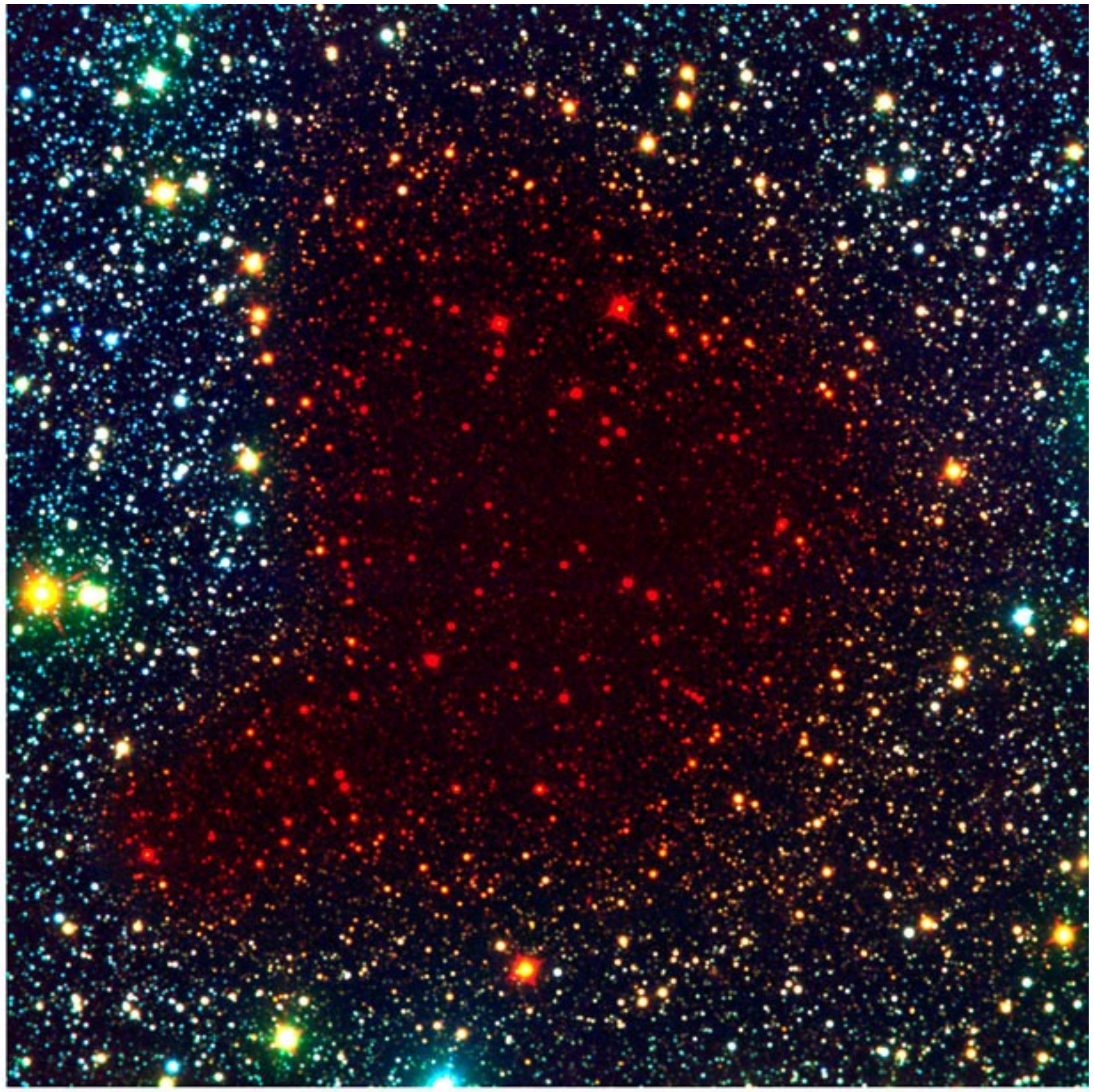
- If $\tau_\nu > 1$, line of sight is **optically thick**

- Since optical depth depends on frequency, whether or not a particular line of sight is optically thick also depends on frequency

- Terrestrial example: clouds are optically thick in the visible, but optically thin at radio wavelengths



B, V, I



B, I, K

Credit: ESO

- Value of absorption coefficient depends on density, hence varies widely in gas of different densities

- Sometime convenient to suppress this density dependence

- We therefore define the opacity κ_ν as:

$$\kappa_\nu = \frac{\alpha_\nu}{\rho}.$$

- Optical depth is related to opacity via:

$$\tau_\nu = \int_0^\infty \rho \kappa_\nu \mathrm{d}s.$$

- Still need to determine how to express σ_ν, α_ν as functions of the Einstein coefficients

- For single atom, rate at which photons are absorbed in a transition l → u is simply:

$$W_{lu} = B_{lu} J_\nu(\nu_{lu}),$$

- Here, J_ν is the **mean specific intensity**:

$$J_\nu = \frac{1}{4\pi} \int I_\nu(\Omega) \mathrm{d}\Omega.$$

(Note that this is simply the angle-average of the specific intensity I)

- This expression for W_{lu} assumes that only photons with <u>exactly</u> the right energy can cause the transition l → u

- In reality, photons with energies close to transition energy have some probability of causing transition

- To account for this, we write W_{lu} in the more general form:

$$W_{lu} = \int_0^\infty B_{lu} J_\nu \phi_\nu \mathrm{d}\nu,$$

- ϕ_ν is the line profile function, normalised so that its integral over all frequencies equals 1

- For photons in the frequency range ν, ν + dν, the rate per atom at which energy is absorbed is therefore:

$$P_{lu} = B_{lu} J_\nu h\nu \phi_\nu \mathrm{d}\nu.$$

- The total energy absorbed within our volume dV during a period dt within solid angle element dΩ is then:

$$\mathrm{d}E_\nu = \frac{1}{4\pi} n_l B_{lu} I_\nu(\Omega) h\nu \phi_\nu \, \mathrm{d}\nu \, \mathrm{d}V \, \mathrm{d}t \, \mathrm{d}\Omega,$$

- Comparison with our previous expression for $\mathrm{d}E_\nu$ then shows us that:

$$\alpha_\nu = \frac{h\nu}{4\pi} n_l B_{lu} \phi_\nu.$$

- What about emission?

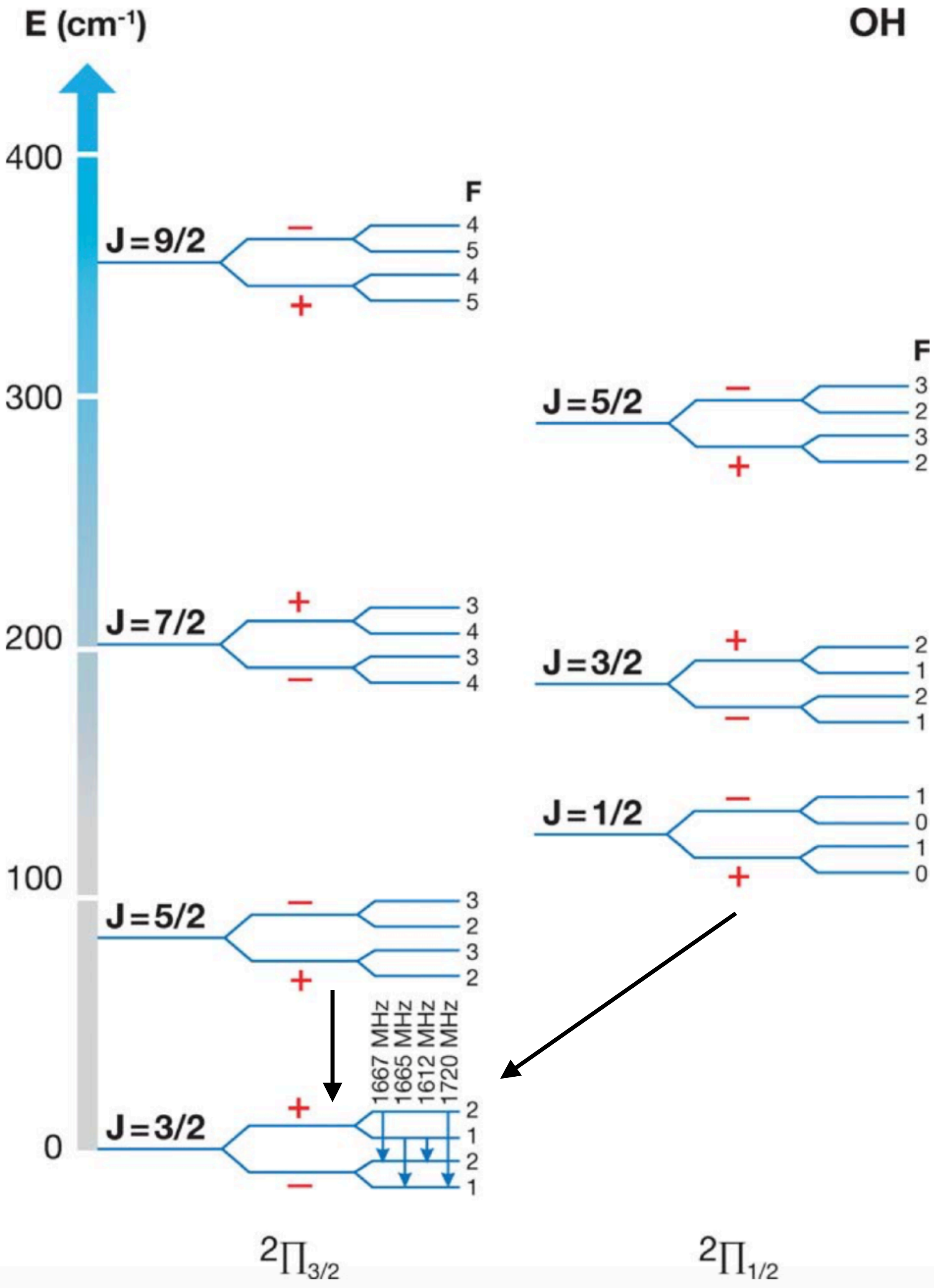
- Stimulated emission is typically treated as if it were negative absorption:

$$\alpha_\nu = \frac{h\nu}{4\pi}\left(n_l B_{lu} - n_u B_{ul}\right)\phi_\nu.$$

- The stimulated emission term is unimportant when $n_u \ll n_l$ but can be significant if $n_u \sim n_l$

- If we have a **population inversion**, so that $n_u > (g_u/g_l)\, n_l$, then the absorption coefficient becomes negative

- Negative absorption implies negative optical depth
- Incident flux exponentially amplified!
- This is operating principle behind the **laser**
- Natural lasers don't occur in the ISM, but we do find the equivalent behaviour in the microwave regime: the **maser**


E (cm⁻¹)
OH
400
300
200
100
0
J=9/2
J=7/2
J=5/2
J=3/2
F
4
5
4
5
3
4
3
4
3
2
3
2
2
1
2
1
−
+
1667 MHz
1665 MHz
1612 MHz
1720 MHz
J=5/2
J=3/2
J=1/2
F
3
2
3
2
2
1
2
1
1
0
1
0
$^2\Pi_{3/2}$
$^2\Pi_{1/2}$

Lo (2005)

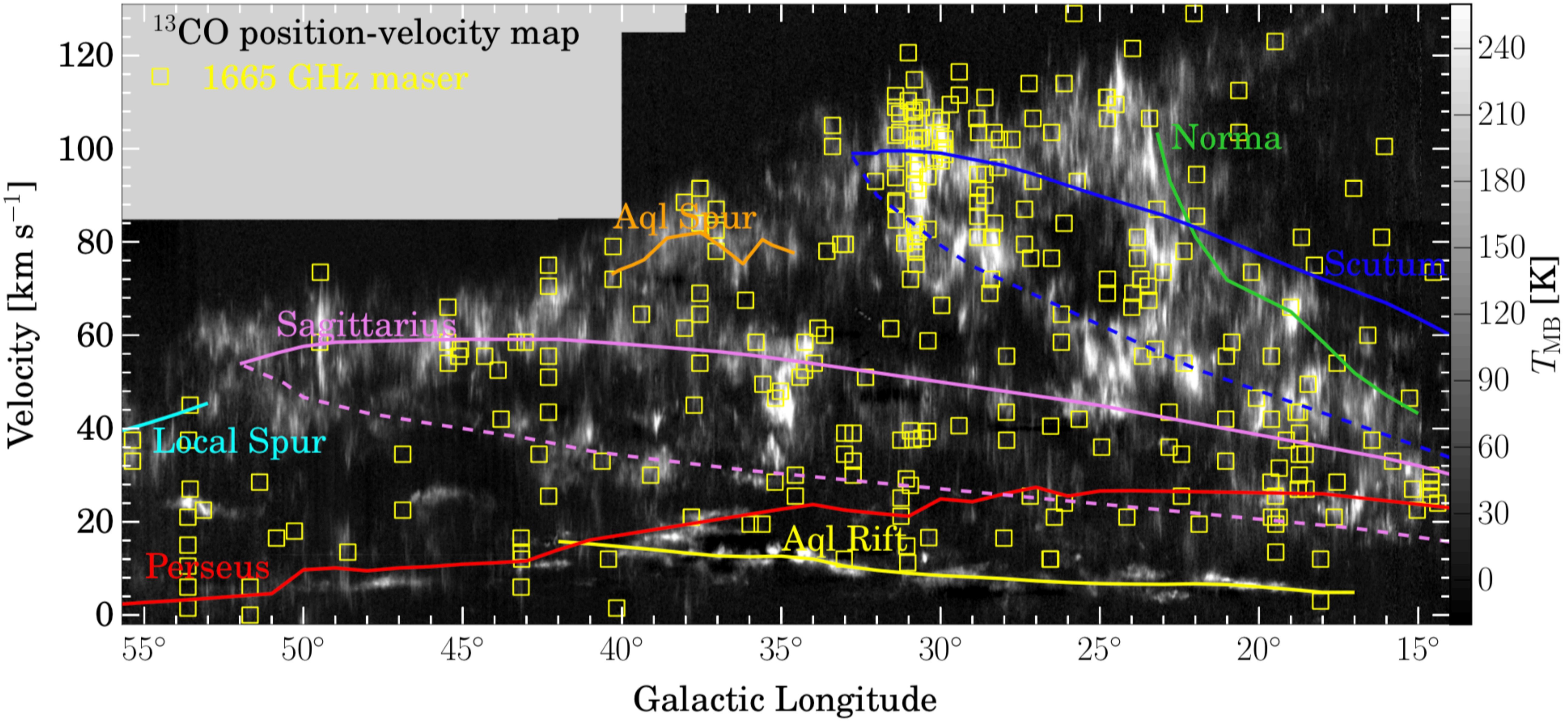
- Electronic ground state of OH has non-zero electron orbital angular momentum

- Split by **Lambda doubling**: reflection symmetric state (+) has slightly larger energy than antisymmetric state (-)

- Each state has hyperfine structure, so 4 possible hyperfine transitions

- Transition rates very small, so population inversion can occur if + state “pumped” by radiative decay from excited state with different J

- Result is four possible maser lines, with frequencies 1612, 1665, 1667 and 1720 MHz



Beuther et al (2019)

- For spontaneous emission, define an **emission coefficient** analogous to absorption coefficient:

$$\mathrm{d}E_{\nu,\mathrm{emiss}}(\Omega) = j_\nu(\Omega)\,\mathrm{d}\nu\,\mathrm{d}V\,\mathrm{d}t\,\mathrm{d}\Omega.$$

- j_ν = energy emitted per unit time per unit frequency per unit volume and per unit solid angle

- Related to Einstein A coefficient via:

$$j_\nu = n_u A_{ul} \frac{h\nu}{4\pi} \phi_\nu,$$

- Change in specific intensity over distance ds due to emission is simply $dI_\nu = j_\nu\,ds$

- Accounting for both emission and absorption therefore yields the **radiative transfer equation**:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = j_\nu - \alpha_\nu I_\nu.$$

- This has the solution:

$$I_\nu(L) = I_{\nu,0}e^{-\tau_{\nu,L}} + \int_0^L j_\nu e^{-\tau_\nu(s)}\,\mathrm{d}s,$$

with:

$$\tau_{\nu,s} = \int_0^s \alpha_\nu(s')\,\mathrm{d}s',$$

- To solve this, we need to know how α_ν, j_ν vary as a function of location

- These quantities are not independent, as we now show

- Consider a mix of radiation and matter in total thermal equilibrium. In that case, the radiation field is simply:

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

- If the system is isothermal, then I_ν is constant and hence:

$$j_\nu - \alpha_\nu B_\nu(T) = 0.$$

- Therefore, in thermal equilibrium:

$$\frac{j_\nu}{\alpha_\nu} = B_\nu(T).$$

This is **Kirchhoff’s law**

- We have derived this assuming total thermal equilibrium
- <u>However</u>: left-hand side can be written in terms of Einstein coefficients and level populations — doesn’t depend on properties of radiation field!
- Kirchhoff’s law holds if level populations have thermal equilibrium values, i.e. system is in **local thermodynamic equilibrium (LTE)**

- For a medium in LTE, but which is not isothermal, we can write the transfer equation as

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = \alpha_\nu(s)\left[B_\nu(T(s)) - I_\nu(s)\right],$$

- Effect of absorption, emission is to drive I_ν toward local value of Planck function

- What about systems that are not in LTE?

- Define a quantity known as the **source function**:

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

- In LTE, $S_\nu = B_\nu$

- More generally:

$$S_\nu = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}}.$$

- In terms of the source function:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = \alpha_\nu(s)\left[S_\nu(s) - I_\nu(s)\right].$$

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = S_\nu - I_\nu.$$

- If source function doesn’t vary (or varies slowly):

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

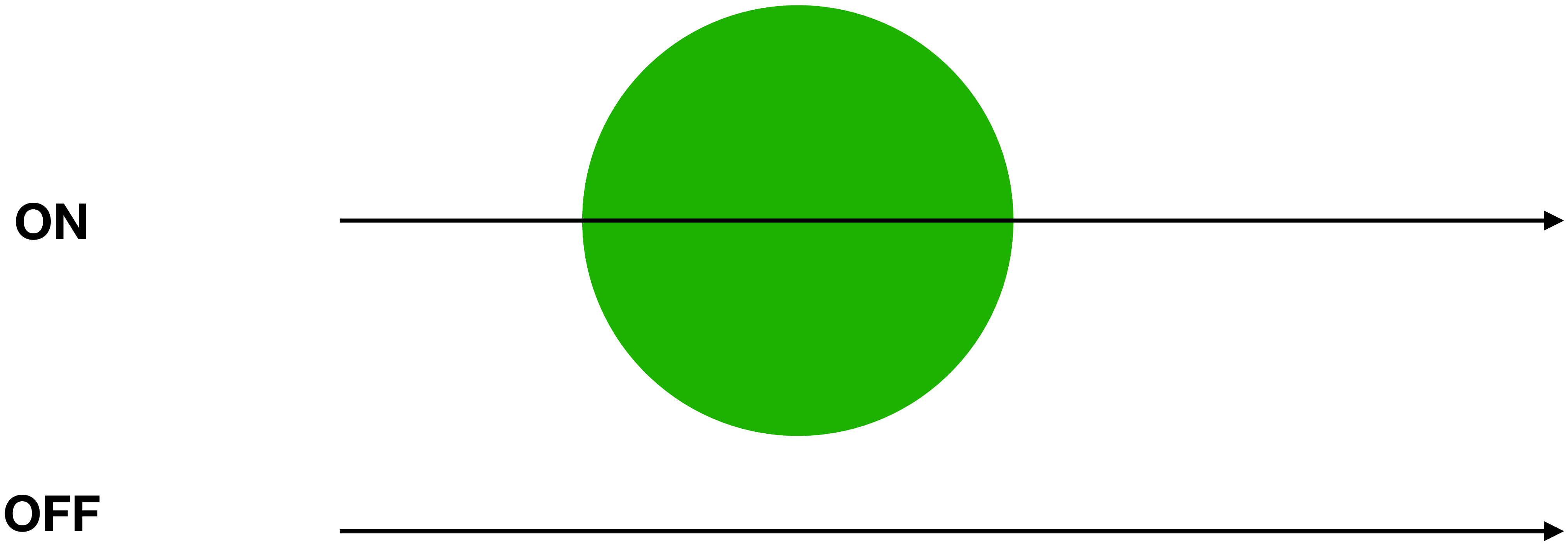
- For low optical depth (τ << 1):

$$I_\nu \simeq \tau_\nu S_\nu + I_{\nu,0}$$

- If background weak/absent ($I_{\nu,0}$ ~ 0), then:

$$I_\nu \simeq \tau_\nu S_\nu$$

- If background strong but smooth, can get same result by background subtraction



ON

OFF

On: $I_\nu \simeq \tau_\nu S_\nu + I_{\nu,0}$

Off: $I_\nu \simeq I_{\nu,0}$

On - Off: $I_\nu \simeq \tau_\nu S_\nu$

- In these conditions (optically thin line, weak or smooth background), background-subtracted intensity is proportional to optical depth

- Since optical depth is proportional to column density, it follows that <u>intensity is proportional to column density</u>

- If background not smooth but spatial variation can be modelled accurately, can get same result by subtracting modelled background

- If background not smooth and <u>cannot</u> be easily modelled, then line can’t be robustly detected

- Finally, if line is optically thick (τ >> 1), then:

$$I_\nu \simeq S_\nu,$$

- For optically thick emission, line strength depends only on source function, independent of optical depth

- Optically thick lines provide no information on column density of emitted/absorber

Line profiles

- Spectral lines have finite width, described by line profile function
- Two main reasons for this that are relevant for ISM:
  - Natural broadening
  - Doppler broadening
- In stars, pressure broadening also important, but not at typical ISM densities

- **Natural broadening** is a consequence of Uncertainty Principle

- Excited atomic/molecular states have finite lifetimes; e.g. for a two-level atom:

$$\Delta t = A_{ul}^{-1}$$

- Uncertainty principle tells us that:

$$\Delta E \Delta t \geq \hbar.$$

- Therefore minimum uncertainty in line energy:

$$\Delta E = A_{ul}\hbar,$$

- Energy uncertainty corresponds to frequency uncertainty:

$$\Delta\nu = \frac{A_{ul}}{2\pi}.$$

- Can be shown that this source of uncertainty leads to a **Lorentzian** line profile:

$$\phi_\nu = \frac{\Gamma/\left(4\pi^2\right)}{(\nu-\nu_0)^2 + \left[\Gamma/(4\pi)\right]^2},$$

$$\Gamma = \sum_{l<u} A_{ul}.$$

- **Doppler broadening** (a.k.a. **thermal broadening**) occurs because of thermal motion of particles

- Consider some fluid element composed of many emitting particles, with some distribution of thermal motions

- Choose frame of reference in which centre of mass of fluid element is at rest (i.e. no bulk motion)

- Individual particles remain in motion in this frame because of their thermal velocities

- Some will move away from us (redshift), some towards us (blueshift)

- Suppose each emitter produces photons in some narrow range of energies that we can approximate with δ function

- Then, collective emission from large number of atoms will have a frequency distribution:

$$\phi_\nu = \int_{-\infty}^{\infty} f(v)\delta\left(\nu - \nu_0\left\{1 - \frac{v}{c}\right\}\right)\,\mathrm{d}v,$$

  Here, f(v) is the velocity distribution function

- For a Maxwell-Boltzmann distribution, this yields:

$$\phi_\nu = \frac{1}{\sqrt{\pi}\Delta\nu_{\mathrm{D}}} e^{-(\Delta\nu/\Delta\nu_{\mathrm{D}})^2},$$

- **Doppler width** of line:

$$\Delta\nu_{\mathrm{D}} = b(\nu_0/c)$$

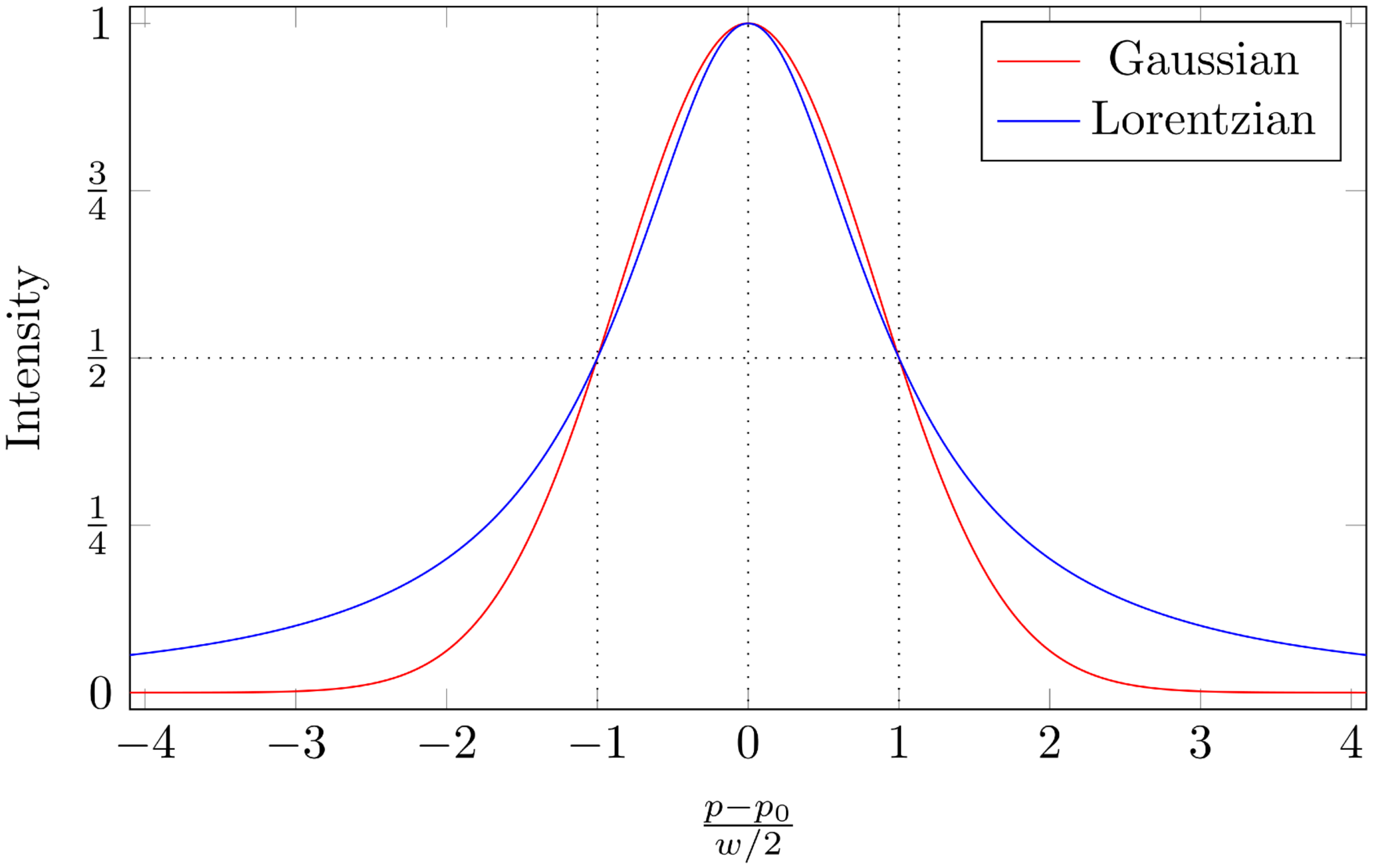
- b is the Doppler broadening parameter:

$$b^2 = 2kT/m$$

- If gas has small-scale turbulence (“microturbulence”), this can be generalized to:

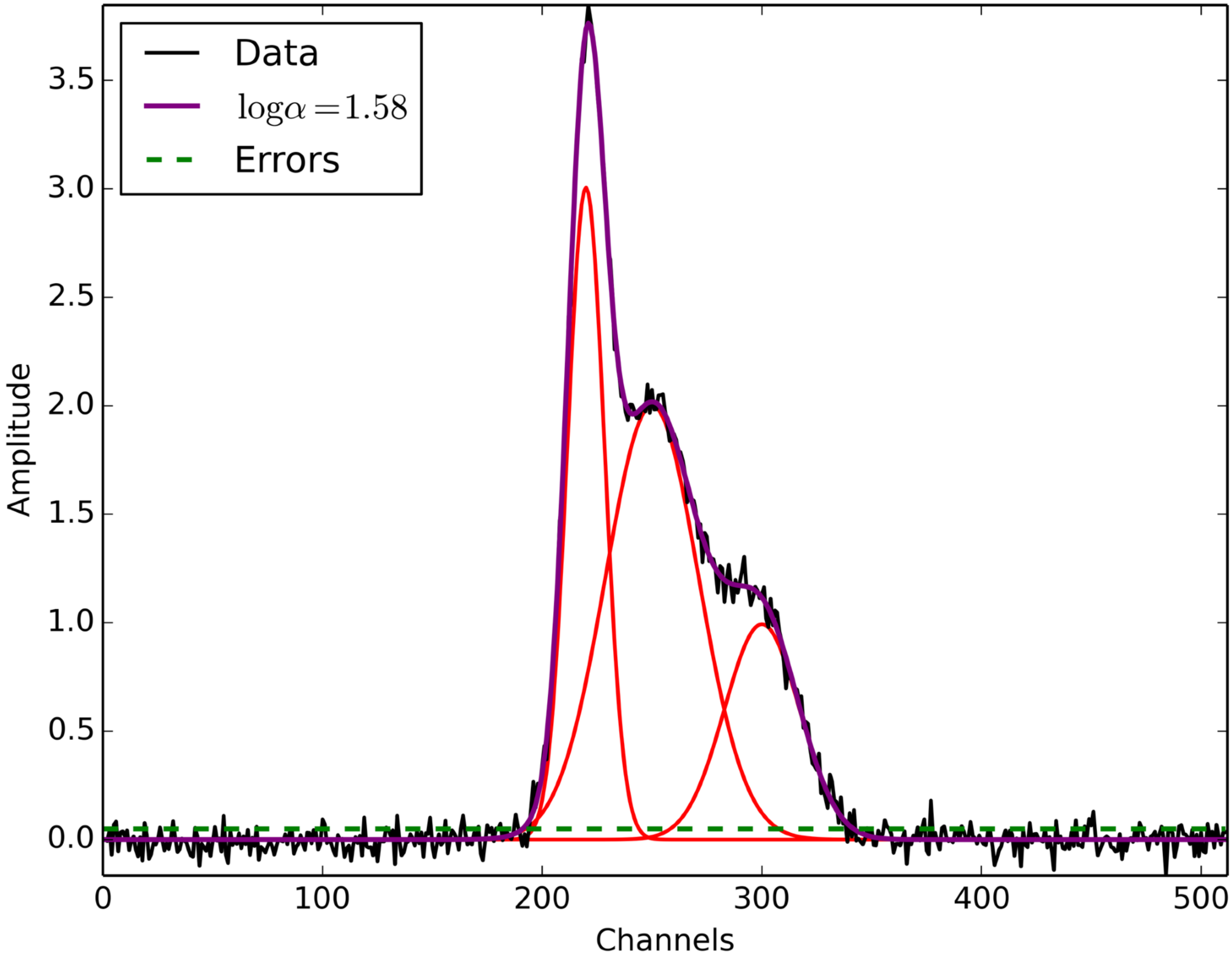
$$b^2 = 2kT/m + 2\sigma_{\mathrm{mt}}^2$$

- In general, Doppler width >> natural width
- Close to line centre, Doppler broadening dominates
- BUT: Doppler broadening creates Gaussian profile, falls off exponentially far from line centre
- Lorentzian profile falls off as $(\Delta\nu)^{-2}$ far from line centre — dominates in wings of line

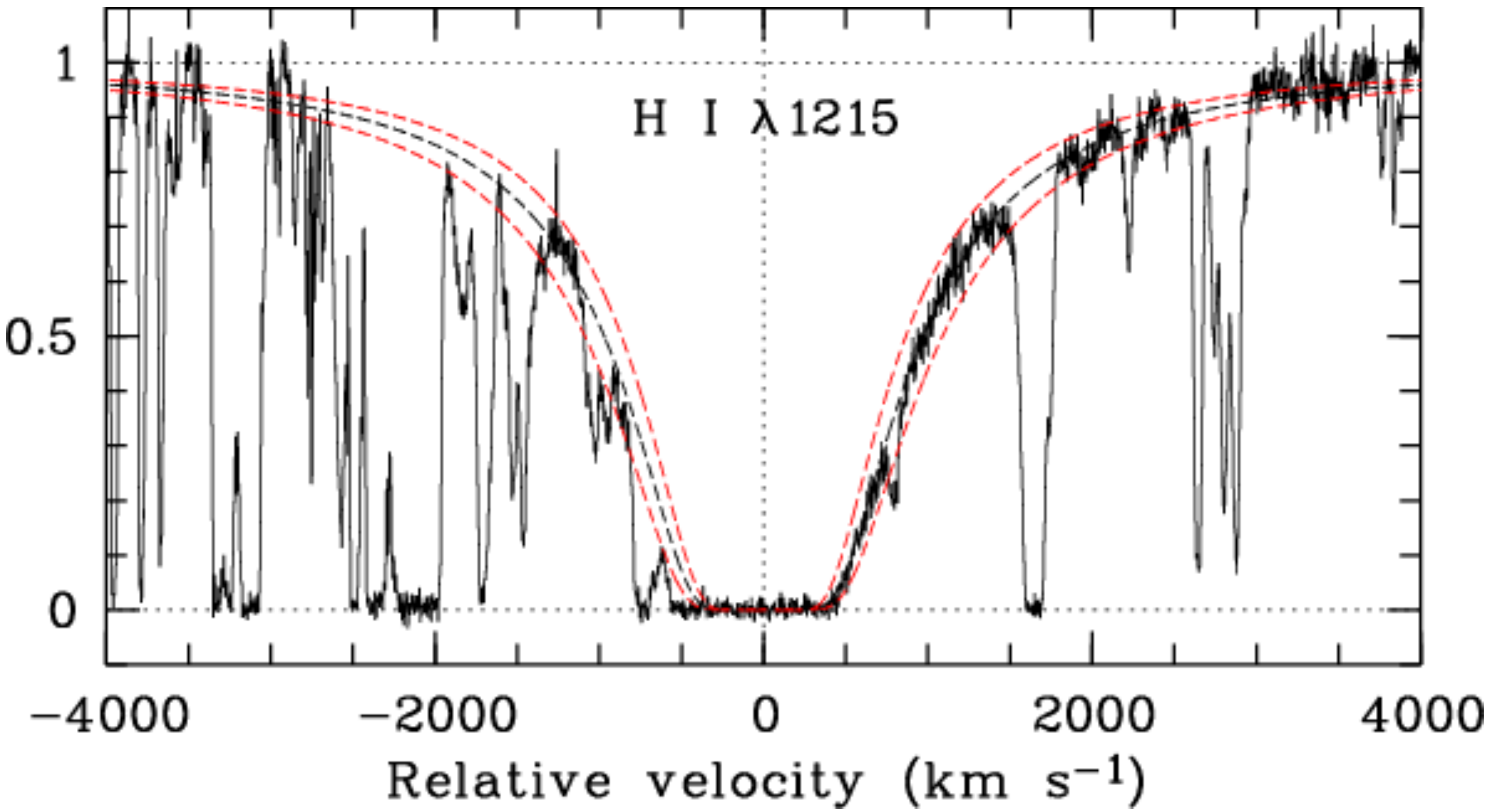


Note: Lines in this example have same height, FWHM;
in general, however, Gaussian profile has much larger FWHM

Credit: Wikipedia

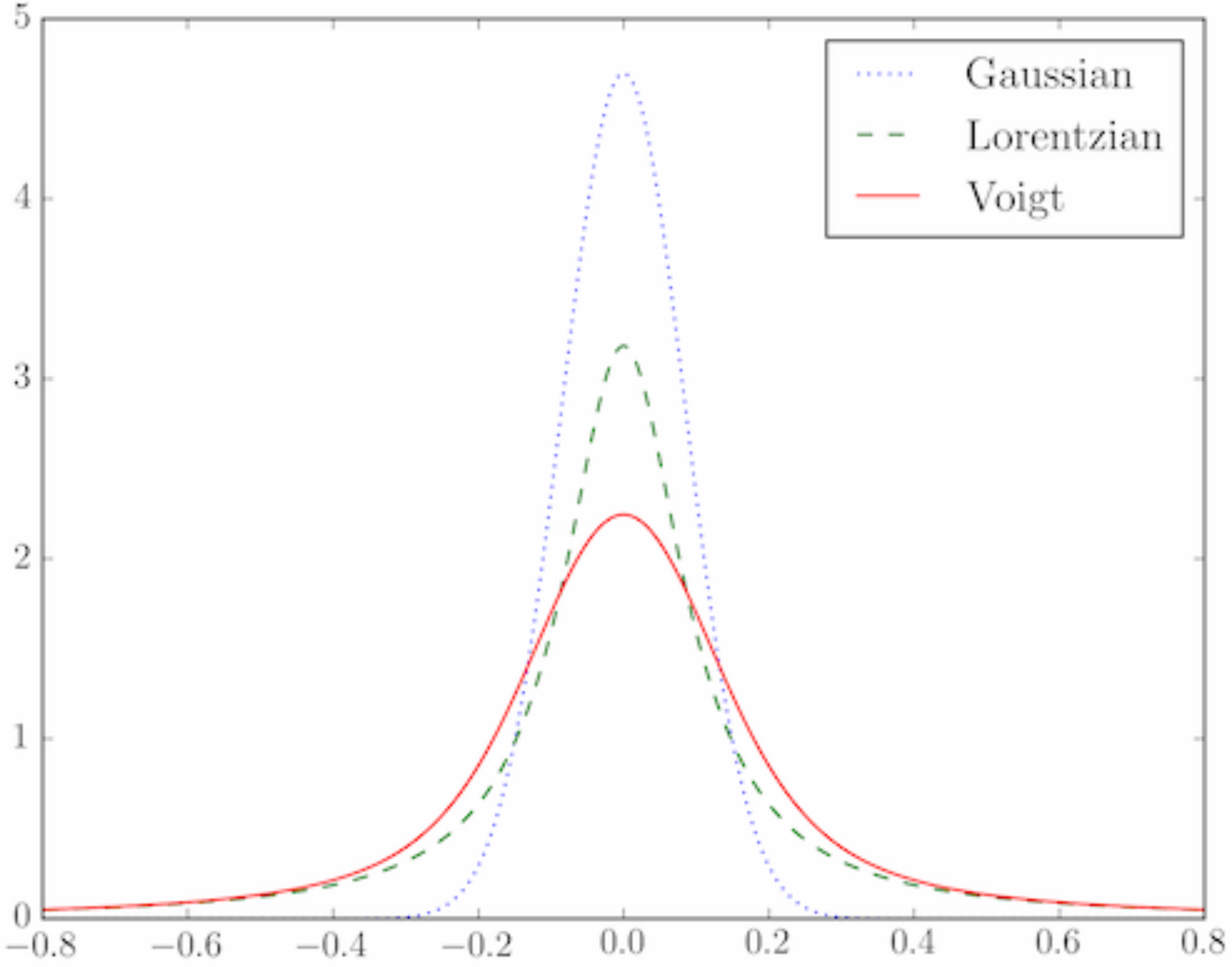


Credit: GaussPy team



Noterdaeme et al (2007)

- Most general line profile is convolution of Gaussian, Lorentzian profiles — the Voigt profile



Hill (2020)

Summary

- Useful to characterise radiation field in terms of its specific intensity I_v
- When dealing with radiation in discrete spectral lines, three key processes:
    - Spontaneous emission (A_{ji})
    - Stimulated emission (B_{ji} I_{ji})
    - Absorption (B_{ij} I_{ij})
- Can write down expressions for emission, absorption coefficients in terms of Einstein coefficients (A_{ji}, B_{ji}, B_{ij})

- Size of B coefficients depends on strength of transition (i.e. whether allowed or forbidden, size of dipole moment)

- Size of A coefficient depends on size of B coefficients plus also ν_{ij}^3 — high frequency transitions have large A's

- Source function S_ν:
    - Ratio of emission and absorption coefficients
    - In LTE, equal to Planck function
    - In optically thick gas, $I_\nu \rightarrow S_\nu$ as radiation propagates through the gas

- Spectral line shapes described by the line profile function

- In ISM, two main types of broadening:
  - Doppler broadening (random thermal motions)
  - Natural broadening (consequence of HUP)

- Doppler broadening yields Gaussian profile

- Natural broadening yields Lorentz profile

- Convolution of both = Voigt profile