

# Interstellar Medium (ISM)

Week 5

2025 March 31 (Monday), 2PM

updated on 03/30, 12:08

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## [3] Line Broadening Mechanisms

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- ***Atomic levels are not infinitely sharp***, nor are the lines connecting them.
  - (1) Doppler (Thermal) Broadening
  - (2) Natural Broadening
  - (3) Collisional Broadening
  - (4) Thermal Doppler + Natural Broadening
- **[1] Doppler (Thermal) Broadening**
  - The simplest mechanism for line broadening in the Doppler effect. An atom is in thermal motion, so that the frequency of emission or absorption in its own frame corresponds to a different frequency for an observer.
  - Each atom has its own Doppler shift, so that the net effect is to spread the line out, but not to change its total strength.
  - The change in frequency associated with an atom with velocity component  $v_z$  along the photon propagation direction (say,  $z$  axis) is, to lowest order in  $v_z/c$ , given by

$$\nu - \nu_0 = \nu_0 \frac{v_z}{c}$$

Recall Doppler shift:  $\left[ \frac{\nu}{\nu_0} = \frac{1}{\gamma(1 - \beta \cos \theta)} \rightarrow \nu \approx \nu_0 (1 + \beta \cos \theta) \rightarrow \nu - \nu_0 = \frac{\nu_0 v_z}{c} \right]$

- Here,  $\nu_0$  is the rest-frame frequency.

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- We need to consider the velocity distribution of atoms. The number of atoms having velocities in the range  $(v_z, v_z + dv_z)$  is proportional to

$$f(v_z)dv_z = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mv_z^2}{2kT}\right) dv_z \quad \text{Here, } m = \text{mass of the atom}$$

- From the Doppler shift formula, we have

$$v_z = \frac{c(\nu - \nu_0)}{\nu_0} \rightarrow dv_z = \frac{cd\nu}{\nu_0}$$

- Therefore, the strength of the emission is proportional to

$$\exp\left(-\frac{mv_z^2}{2kT}\right) dv_z \propto \exp\left[-\frac{mc^2(\nu - \nu_0)^2}{2\nu_0^2 kT}\right] d\nu$$

- Then, the normalized profile function is

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

where

$\Delta\nu_D = \frac{\nu_0}{c} v_{\text{th}}$  is the Doppler width.

$v_{\text{th}} = \sqrt{\frac{2kT}{m}}$  is the thermal velocity.

$$\left( v_{\text{rms}} = \sqrt{\frac{kT}{m}} \right)$$

- Numerical value of the velocity broadening is

$$v_{\text{th}} = \left( \frac{2k_{\text{B}}T}{m} \right)^{1/2} = 1.3 \text{ km s}^{-1} \left( \frac{T}{100 \text{ K}} \right)^{1/2} \left( \frac{m}{m_{\text{H}}} \right)^{-1/2}$$

- In addition to thermal motions, there can be turbulent velocities associated with macroscopic velocity fields. The turbulent motions are accounted for by an effective Doppler width.

$$\Delta\nu_{\text{D}} = \nu_0 \frac{b}{c}$$

$$b \equiv (v_{\text{th}}^2 + v_{\text{turb}}^2)^{1/2}$$

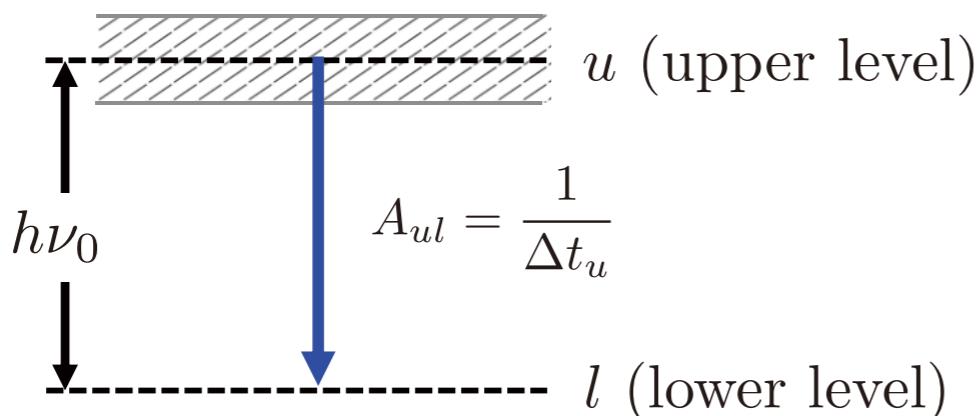
where  $v_{\text{turb}}$  is  $\sqrt{2}$  times a root-mean-square measure of the turbulent velocities. This assumes that the turbulent velocities also have a Gaussian distribution.

The convolution of two Gaussian functions with the widths (standard deviations)  $\sigma_1$  and  $\sigma_2$  is a Gaussian function with the width of  $\sigma$ , given by:  $\sigma = \sqrt{\sigma_1^2 + \sigma_2^2}$

## • [2] Natural Broadening

- The intrinsic line width of a line is due to ***the Heisenberg uncertainty principle***. If an energy level  $u$  has a lifetime  $\Delta t$ , then uncertainty (spread) in energy  $\Delta E$  must be  $\Delta E \sim \hbar/\Delta t$  ( $\hbar = h/2\pi$ ), and the resulting spread in the frequency of emitted photons is  $\Delta\nu = \Delta E/h$ .

### (1) Line width due to the uncertainty principle:



$A_{ul}$  = decay rate  
= decay probability per unit time, Einstein A coefficient.

$\Delta E_u$  = uncertainty in energy of  $u$

$\Delta t_u$  = the uncertainty in time of occupation of  $u$

$\Delta\nu_u$  = spread in frequency

$$= \Delta E_u/h = 1/(2\pi\Delta t_u) = A_{ul}/(2\pi)$$



### (2) Line width of the Lorentz function:

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

In terms of the line width  $\Delta\nu$ , the normalized Lorentz profile can be rewritten as

$$\phi_\nu = \frac{1}{2\pi} \frac{\Delta\nu/2}{(\nu - \nu_0)^2 + (\Delta\nu/2)^2}$$

Hence, the FWHM of the Lorentz function:  $\Delta\nu_u = \gamma/2\pi$



Comparing (1) and (2), we find that  
 $\gamma$  is equivalent to the Einstein A-coefficient., i.e.,  $\gamma = A_{ul}$ .

# Classical Physical Meaning

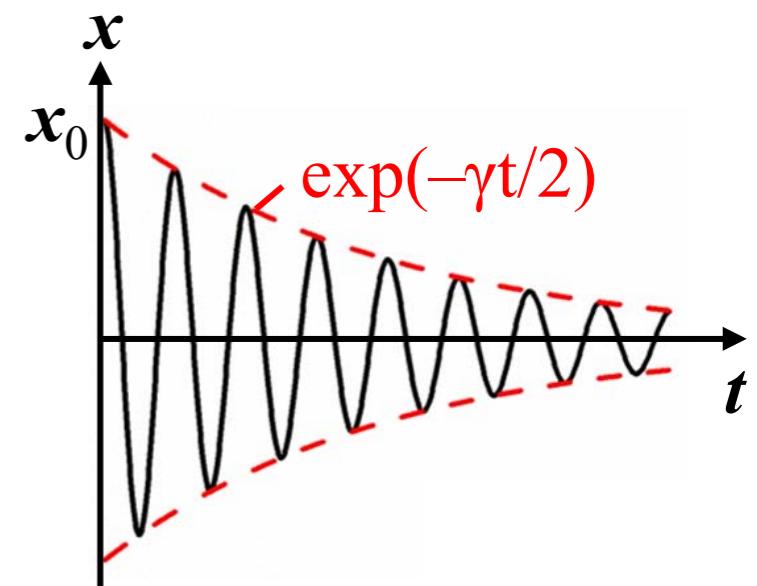
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Suppose that the electric field is of the form  $e^{-\gamma t/2}$  and then the energy decays proportional to  $e^{-\gamma t}$ .

We then have an emitted spectrum determined by the decaying sinusoid type of electric field.

Its Fourier transform (spectral profile) is a Lorentz (or natural, or Cauchy) profile:

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



# Semiclassical (Weisskopf-Woolley) Picture of Quantum Levels

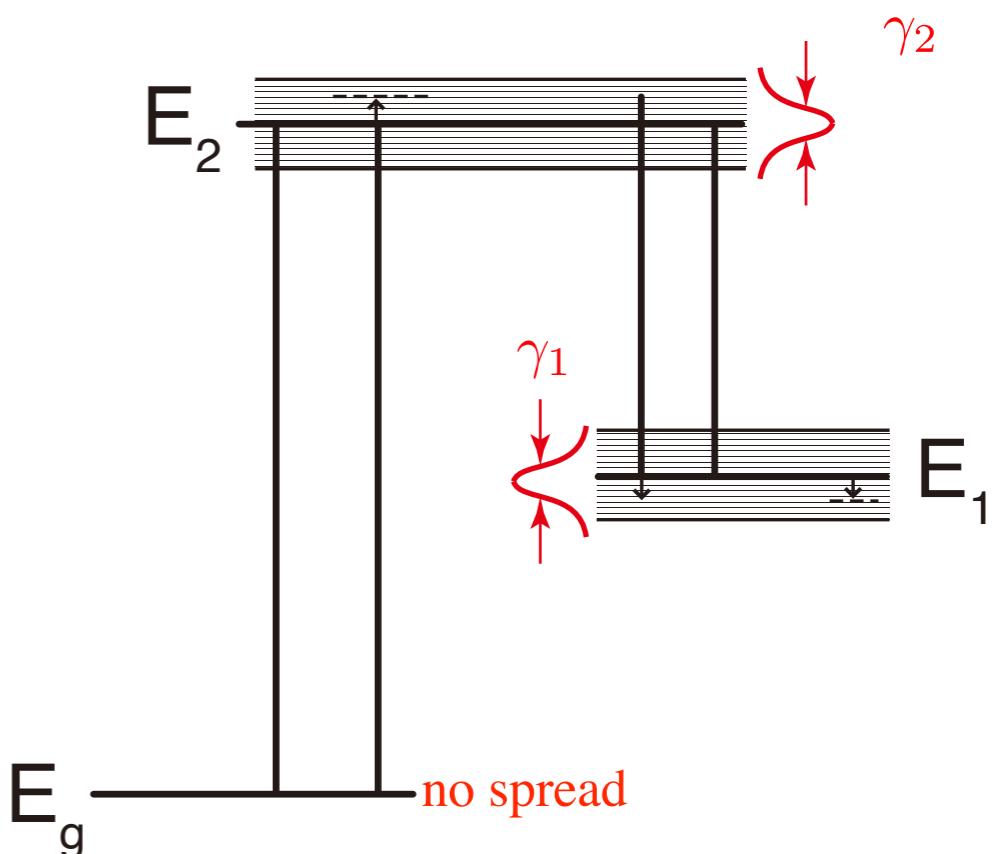
- In the semiclassical picture, each level is viewed as a continuous distribution of sublevels with energies close to the energy of the level ( $E_n$ ).

The distribution of sublevels are explained by the Heisenberg Uncertainty Principle. The level has a lifetime  $\Delta t = 1/A$  ( $A$  = Einstein A coefficient) and a spread in energy about  $\Delta E \approx \hbar/\Delta t = \hbar A$ .

$$\Delta E \Delta t \approx \hbar$$

The ground level has no spread in energy

because  $\Delta t = \infty$ .



The atom is in a definite sublevel of some level.

A transition in a spectral line is considered to be an **instantaneous transition** between a definite sublevel of an initial level to a definite sublevel of a final level.

- The energy spread of sublevels is described by a Lorentzian profile with the damping parameter of  $\gamma = A$ .*
- This picture implies that the emission line profile is the same as the absorption line profile.*

- The intrinsic line width is  $\gamma = A_{ul}$ .
  - This means **forbidden lines are intrinsically narrower than permitted lines.**
  - For instance, the permitted Ly $\alpha$  line has  $A_{ul}/\nu_{ul} \sim 3 \times 10^{-7}$ , while the forbidden [OIII] 5007Å has a tiny width  $A_{ul}/\nu_{ul} \sim 3 \times 10^{-17}$ .
  - The intrinsic line width of [O III] 5007Å is equivalent to the Doppler broadening of

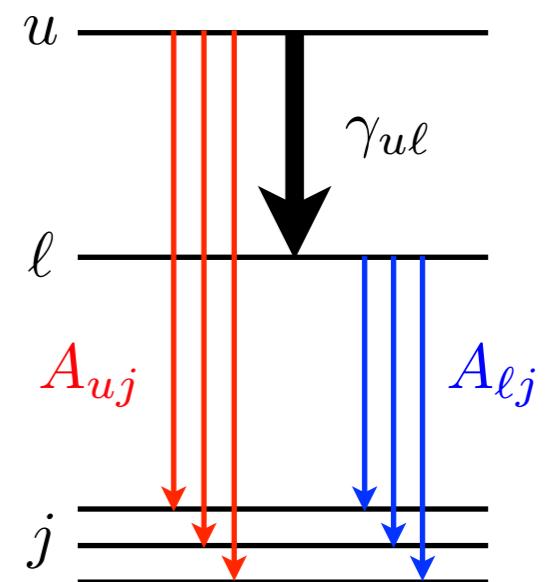
$$\Delta\nu_D = \nu_{ul} \frac{\Delta v}{c} \rightarrow \Delta v \sim 3 \times 10^{-17} c \sim 10 \text{ nm s}^{-1} \sim 30 \text{ cm yr}^{-1}$$

$$\Delta\nu_D \approx A_{ul}$$

- For a multiple-level absorber, the upper and lower can both be broadened by transitions to other levels.

$$\gamma_{ul} = \sum_{E_j < E_u} A_{uj} + \sum_{E_j < E_\ell} A_{\ell j}$$

- For Ly $\alpha$  ( $n = 1-2$ ),  $\gamma_{ul} = A_{21} = 6.3 \times 10^8 \text{ s}^{-1}$   
 $\Delta\nu/\nu = (\gamma/2\pi)/(c/\lambda) \sim 4 \times 10^{-8}$
- For H $\alpha$  ( $n = 2-3$ ),  $\gamma_{ul} = A_{32} + A_{31} + A_{21} = 8.9 \times 10^8 \text{ s}^{-1}$   
 $\Delta\nu/\nu \sim 3 \times 10^{-7}$

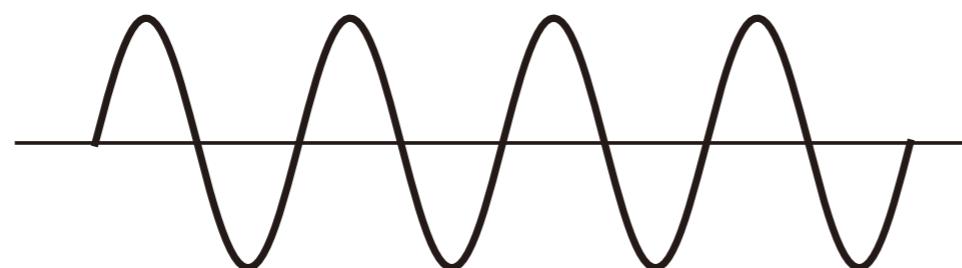


Convolution of two Lorentzian functions are a Lorentz function with  $\gamma = \gamma_1 + \gamma_2$ .

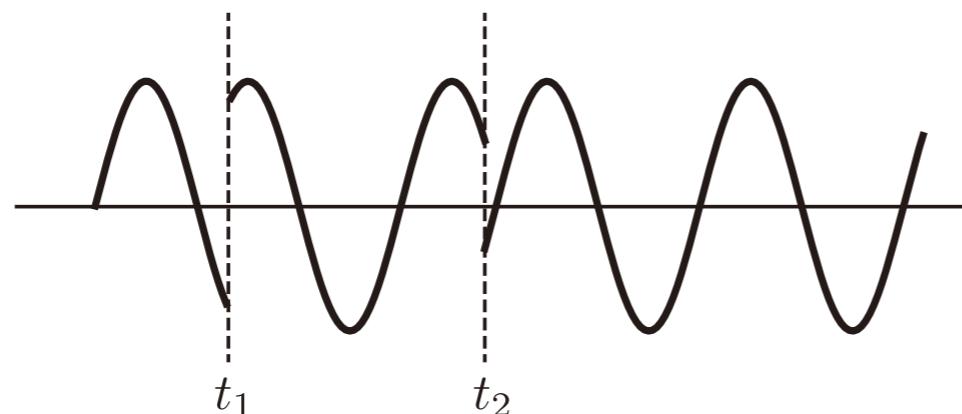
### • [3] Collisional Broadening (or Pressure Broadening)

- The Lorentz profile applies even to certain types of collisional broadening mechanisms.
- If the atom suffers “*elastic*” collisions with other particles while it is emitting, the phase of the emitted radiation can be altered suddenly. ***If the phase changes completely randomly at the collision times, then information about the emitting frequencies is lost.***
- If the collisions occur with frequency  $\nu_{\text{col}}$ , that is, each atom experiences  $\nu_{\text{col}}$  collisions per unit time on the average, then the profile is

$$\phi_\nu = \frac{\Gamma/4\pi^2}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2} \quad \text{where} \quad \Gamma = \gamma + 2\nu_{\text{col}}$$



purely sinusoidal



random phase interruptions  
by atomic collisions

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## • [4] Voigt profile : Thermal + Natural broadening

- Atoms shows both a Lorentz profile plus the Doppler effect. In this case, we can write the profile as an average of the Lorentz profile over the various velocity states of the atom. Let's assume that the photon propagates along the  $z$ -axis.

Change of variables for the Maxwell distribution:  $v_{\text{th}} \equiv \sqrt{\frac{2kT}{m}}$ ,  $y \equiv \frac{v_z}{v_{\text{th}}}$

$$f_{v_z} = \frac{1}{\pi^{1/2} (2kT/m)^{1/2}} \exp(-mv_z^2/2kT) \longrightarrow f_y = \frac{1}{\pi^{1/2}} \exp(-y^2)$$

To interact with an atom with velocity  $v_z$ , the photon central frequency should be  $\nu_0 + \nu_0(v_z/c)$ . Then, the Lorentz profile at the frequency  $\nu' = \nu - [\nu_0 + \nu_0(v_z/c)] = (\nu - \nu_0) - \nu_0(v_{\text{th}}/c)y$  is supposed to be multiplied with the Maxwell distribution.

Change of variables for the Lorentz function:  $\phi_y^L = \phi_\nu^L \left| \frac{d\nu}{dy} \right| = \phi_\nu^L \times \left( \nu_0 \frac{v_{\text{th}}}{c} \right)$

Let  $\Delta\nu_D \equiv \nu_0 \frac{v_{\text{th}}}{c}$ ,  $u \equiv \frac{\nu - \nu_0}{\Delta\nu_D} = \frac{\nu - \nu_0}{\nu_0} \frac{c}{v_{\text{th}}}$ ,  $a = \frac{\Gamma/4\pi}{\Delta\nu_D}$

$$\begin{aligned} \phi(\nu) &= \int_{-\infty}^{\infty} \phi_y^L f_y dy \\ &= \int_{-\infty}^{\infty} \left( \nu_0 \frac{v_{\text{th}}}{c} \right) \frac{\Gamma/4\pi^2}{[(\nu - \nu_0) - \nu_0(v_{\text{th}}/c)y]^2 + (\Gamma/4\pi)^2} \left( \frac{1}{\pi^{1/2}} \right) \exp(-y^2) dy \\ &= \frac{a}{\pi^{3/2} \Delta\nu_D} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(u - y)^2 + a^2} dy \end{aligned}$$

- The profile can be written using the Voigt function.

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} H(u, a)$$

Here,  $a$  is a ratio of the intrinsic broadening to the thermal broadening.

$u$  is a measure of how far you are from the line center, in units of thermal broadening parameter.

In terms of Doppler velocity,  $u$  can be expressed as

$$u = \frac{\nu - \nu_0}{\Delta\nu_D} = \frac{\nu - \nu_0}{\nu_0} \frac{c}{v_{\text{th}}}$$

In the velocity term,

$$u = \frac{v}{v_{\text{th}}}, \text{ where } v = \frac{\nu - \nu_0}{\nu_0} c$$

**Voigt-Hjerting function:**

$$H(u, a) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{(u - y)^2 + a^2}$$

$$a \equiv \frac{\Gamma}{4\pi\Delta\nu_D}$$

$$u \equiv \frac{\nu - \nu_0}{\Delta\nu_D}$$

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

Including the turbulent motion,

$$\Delta\nu_D = \nu_0 \frac{v_{\text{th}}}{c} \rightarrow \Delta\nu_D = \nu_0 \frac{b}{c} = \frac{b}{\lambda_0}$$

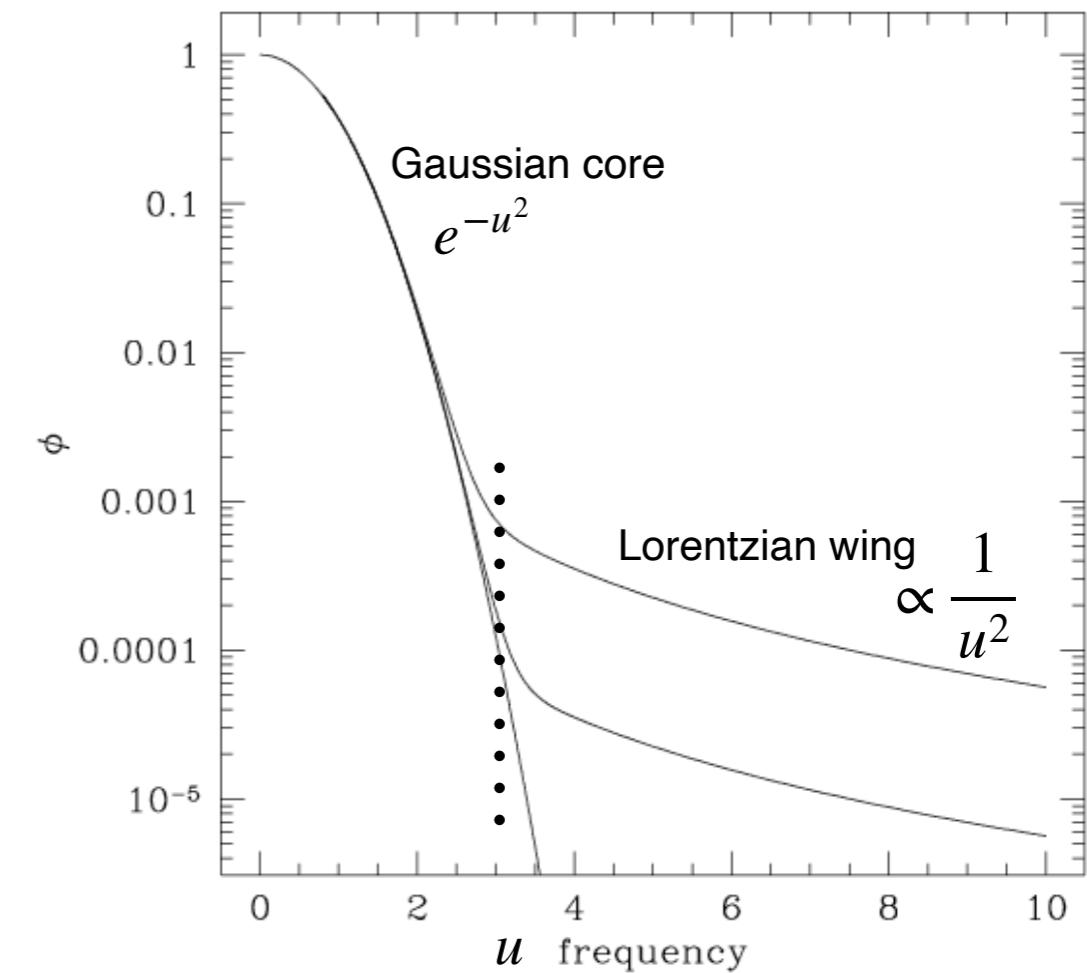
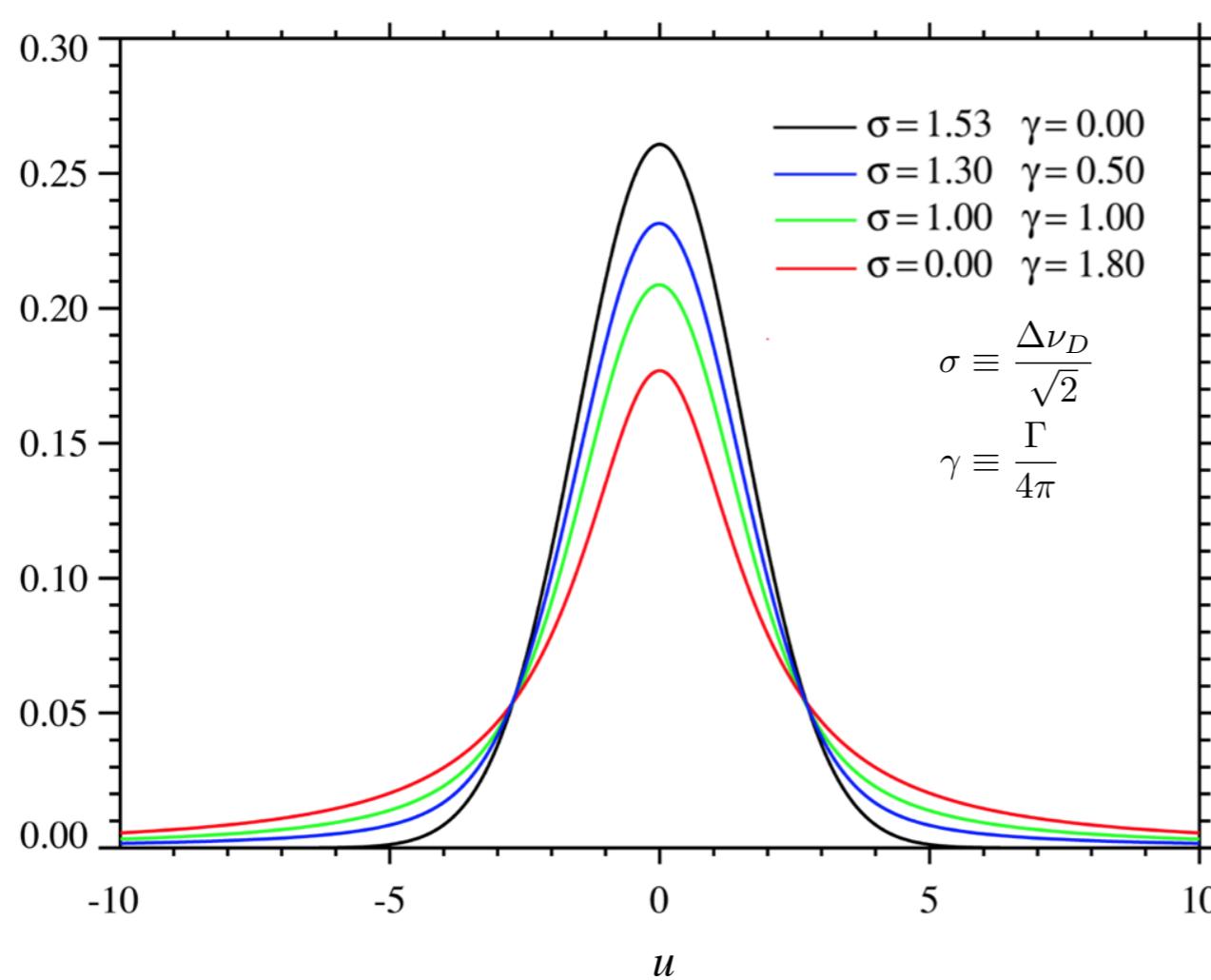
where  $b = \sqrt{v_{\text{th}}^2 + v_{\text{turb}}^2}$ ,  $v_{\text{th}} = \sqrt{\frac{2kT}{m}}$ ,  $v_{\text{turb}} = \sqrt{2}\sigma_{\text{turb}}^{\text{rms}}$

$$u = \frac{v}{b}$$

# Properties of Voigt Function

- For small  $a$ , the “core” of the line is dominated by the Gaussian (Doppler) profile, whereas the “wings” are dominated by the Lorentz profile.

$$H(u, a) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{(u - y)^2 + a^2}$$



- In most cases,  $a \ll 1$ . For Ly $\alpha$  at  $T = 10^4$  K,  $a \sim 0.005$ .

- Line center:

$$H(0, a) = \exp(a^2) \operatorname{Erfc}(a) \approx 1 - \frac{2}{\sqrt{\pi}}a + a^2 - \mathcal{O}(a^3)$$

- Taylor series expansion of the Voigt function :

$$H(u, a) \equiv \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{(u - y)^2 + a^2}$$

- Near the line center ( $u \rightarrow 0$ ), the contribution to the integral is dominated by  $y = u$ . Therefore,

$$H(u, a) \simeq \frac{a}{\pi} e^{-u^2} \int_{-\infty}^{\infty} \frac{dy}{y^2 + a^2} = e^{-u^2}$$

which is known as the Doppler core.

- In the line wings away from the core ( $u \gg 1$ ), the integral is dominated by  $y \sim 0$  because of the rapidly decreasing function in the numerator.

$$H(u, a) \simeq \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2} dy}{u^2} = \frac{a}{\pi} \frac{\sqrt{\pi}}{u^2} = \frac{a}{\sqrt{\pi} u^2}$$

- In summary, we obtain the Voigt function in a Taylor series expansion around  $a = 0$ .

$$H(u, a) \approx H(u, 0) + a \left. \frac{dH}{da} \right|_{a=0} \approx e^{-u^2} + a \frac{1}{\sqrt{\pi} u^2}$$

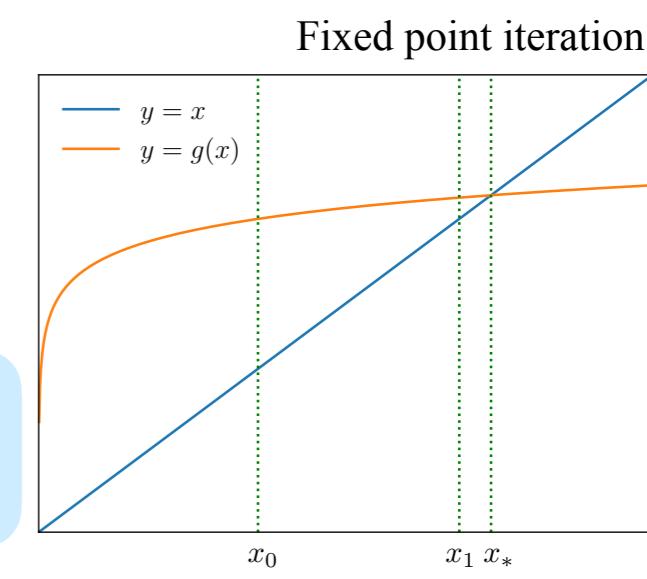
- The first term represents the Gaussian core, provided by the thermal broadening, and the second term represents the Lorentzian damping wing.
- Transition from Doppler core to damping wing can be found by solving:

$$e^{u^2} = \frac{\sqrt{\pi}}{a} u^2 \rightarrow u^2 = \ln\left(\frac{\sqrt{\pi}}{a}\right) + \ln u^2$$

- The solution for this transcendental equation for Ly $\alpha$  is

$$u^2 \approx 10.31 + \ln \left[ \left( \frac{6.265 \times 10^8 \text{ s}^{-1}}{\gamma_{ul}} \right) \left( \frac{1215.67 \text{ \AA}}{\lambda_{ul}} \right) \left( \frac{b}{10 \text{ km s}^{-1}} \right) \right]$$

$b = 13 \text{ km s}^{-1} (T/10^4 \text{ K})^{1/2}$  for hydrogen



provided that the quantity in square brackets is not very large or very small. The damping wing for  $|u| \gtrsim 3.2$  or velocity shifts  $|v| \gtrsim 3.2 (b/10 \text{ km s}^{-1})$ .

# Atomic Processes related to Line emission

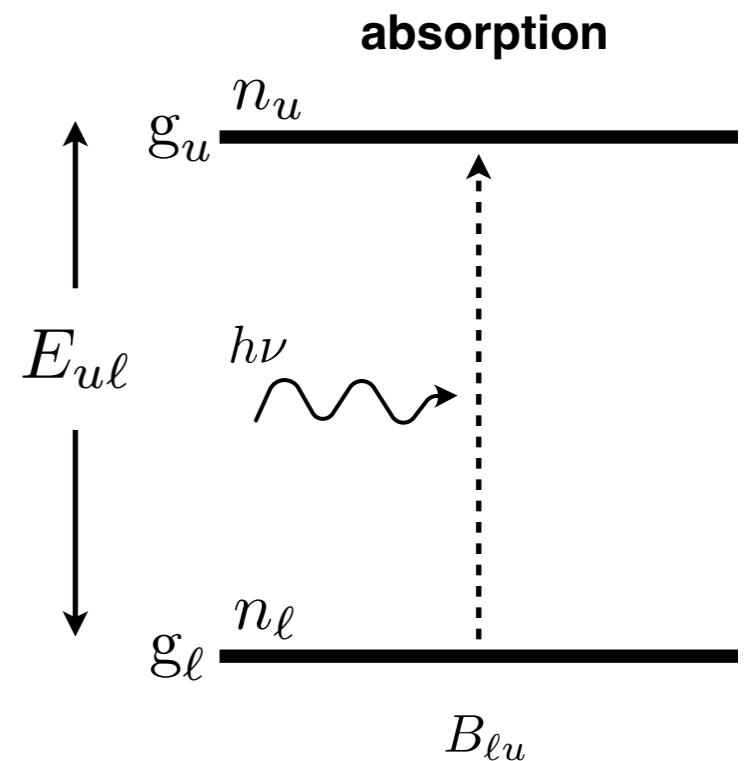
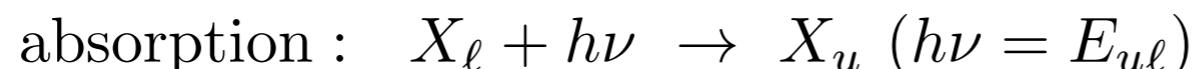
- **Excitation and de-excitation (Transition)**
  - ▶ Radiative excitation (photoexcitation; photoabsorption)
  - ▶ Radiative de-excitation (spontaneous emission and stimulated emission)
  - ▶ Collisional excitation
  - ▶ Collisional de-excitation
- **Emission Line**
  - ▶ Collisionally-excited emission lines
  - ▶ Recombination lines (recombination following photoionization or collisional ionization)
- **Ionization**
  - ▶ Photoionization and Auger-ionization
  - ▶ Collisional Ionization (Direct ionization and Excitation-autoionization)
- **Recombination**
  - ▶ Radiative recombination  $\Leftrightarrow$  Photoionization
  - ▶ Dielectronic Recombination (not dielectric!)
  - ▶ Three-body recombination  $\Leftrightarrow$  Direct collisional ionization
- **Charge exchange**

# Radiative Excitation and De-excitation (Absorption and Emission)

- Three Radiative Transitions and Einstein Coefficients

- **Absorption:**

- If an absorber (atom, ion, molecule, or dust grain)  $X$  is in a lower level  $\ell$  and there is radiation present with photons having an energy equal to  $E_{u\ell}$ . The absorber can absorb a photon and undergo an upward transition.



- The rate per volume at which the absorbers absorb photons will be proportional to both the energy density  $u_\nu$  of photons of the appropriate energy and the number density  $n_\ell$  of absorbers in the lower level  $\ell$ .

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} = - \left( \frac{dn_\ell}{dt} \right)_{\ell \rightarrow u} = n_\ell B_{\ell u} u_\nu$$

- The proportionality constant  $B_{\ell u}$  is the **Einstein B coefficient** for the upward transition  $\ell \rightarrow u$ .

- **Emission:**

- ▶ An absorber X in an excited level  $u$  can decay to a lower level  $\ell$  with emission of a photon. There are two ways this can happen:

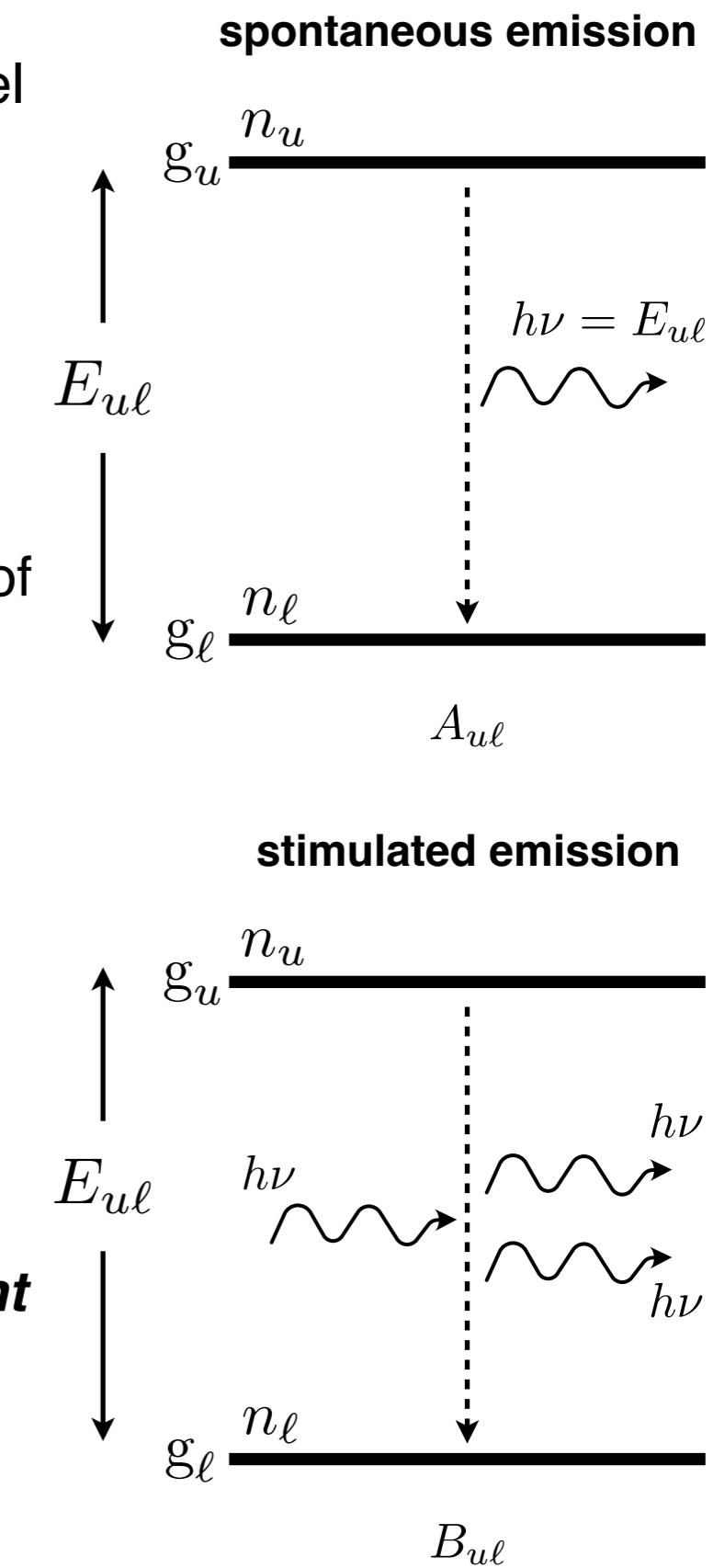
spontaneous emission :  $X_u \rightarrow X_\ell + h\nu$  ( $h\nu = E_{u\ell}$ )

stimulated emission :  $X_u + h\nu \rightarrow X_\ell + 2h\nu$  ( $h\nu = E_{u\ell}$ )

- ▶ **Spontaneous emission** is a random process, independent of the presence of a radiation field.
- ▶ **Stimulated emission** occurs if photons of the identical frequency, polarization, and direction of propagation are already present, and the rate of stimulated emission is proportional to the energy density  $u_\nu$  of these photons.

$$\left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell} = - \left( \frac{dn_u}{dt} \right)_{u \rightarrow \ell} = n_u (A_{u\ell} + B_{u\ell} u_\nu)$$

- ▶ The probability per unit time  $A_{u\ell}$  is the **Einstein A coefficient** for spontaneous transition. The coefficient  $B_{u\ell}$  is the **Einstein B coefficient** for the downward transition  $u \rightarrow \ell$ .



# Relations between the Einstein coefficients

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- The three Einstein coefficients are not mutually independent.
- ***In thermal equilibrium***, the radiation field becomes the “blackbody” radiation field and the two levels must be populated according to the Boltzmann distribution.

$$(u_\nu)_{\text{TE}} = \frac{4\pi}{c} B_\nu(T) = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/k_B T} - 1}$$

$$\left( \frac{n_u}{n_\ell} \right)_{\text{TE}} = \frac{g_u}{g_\ell} e^{-E_{u\ell}/k_B T} \quad \text{Here, } E_{u\ell} = h\nu.$$

- The net rate of change of level  $u$  should be equal to zero, in TE.

$$\begin{aligned} \frac{dn_u}{dt} &= \left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} + \left( \frac{dn_u}{dt} \right)_{u \rightarrow \ell} \\ &= n_\ell B_{\ell u} u_\nu - n_u (A_{u\ell} + B_{u\ell} u_\nu) \\ &= 0 \end{aligned}$$

$$n_\ell B_{\ell u} u_\nu - n_u (A_{u\ell} + B_{u\ell} u_\nu) = 0$$

$$(n_\ell B_{\ell u} - n_u B_{u\ell}) u_\nu = n_u A_{u\ell}$$

$$\begin{aligned} u_\nu &= \frac{n_u A_{u\ell}}{n_\ell B_{\ell u} - n_u B_{u\ell}} \\ &= \frac{(n_u A_{u\ell}) / (n_\ell B_{\ell u})}{1 - (n_u B_{u\ell}) / (n_\ell B_{\ell u})} \\ &= \frac{(g_u/g_\ell) e^{-h\nu/kT} (A_{u\ell}/B_{\ell u})}{1 - (g_u/g_\ell) e^{-h\nu/kT} (B_{u\ell}/B_{\ell u})} \quad \leftarrow \quad \frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} e^{-h\nu_{u\ell}/kT_{\text{exc}}} \\ &= \frac{(g_u/g_\ell) (A_{u\ell}/B_{\ell u})}{e^{h\nu/kT} - (g_u/g_\ell) (B_{u\ell}/B_{\ell u})} \end{aligned}$$

Comparing the above eq. with Planck function,

$$u_\nu = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1}$$

we can immediately recognize that the following relations should be satisfied.

$$(g_u/g_\ell) (A_{u\ell}/B_{\ell u}) = \frac{8\pi h\nu^3}{c^3}$$

$$(g_u/g_\ell) (B_{u\ell}/B_{\ell u}) = 1$$

**Therefore, only one coefficient is independent.**

[Note] If there is no stimulated emission ( $B_{u\ell} = 0$ ), the only way to make the left eq. consistent with the Planck function is to assume  $h\nu/kT \gg 1$  (Wien's regime). Therefore, the stimulated emission is negligible in the Wien's regime. In other words, the stimulated emission term is required in the Rayleigh-Jean regime.

In summary, we obtained the following relations between the Einstein coefficients.

$$A_{u\ell} = \frac{8\pi h\nu^3}{c^3} B_{u\ell}$$

$$B_{\ell u} = \frac{g_u}{g_\ell} B_{u\ell}$$

$$B_{u\ell} = \frac{c^3}{8\pi h\nu^3} A_{u\ell}$$

$$B_{\ell u} = \frac{g_u}{g_\ell} \frac{c^3}{8\pi h\nu^3} A_{u\ell}$$

- We note the Einstein coefficients are intrinsic properties of the absorbing material, irrelevant to the assumption of TE. Hence, **the relations between the Einstein coefficients should hold in any condition.**
- Using the relation, we can rewrite the downward and upward transition rates:

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} = n_\ell \frac{g_u}{g_\ell} \frac{c^3}{8\pi h\nu^3} A_{u\ell} u_\nu \quad \left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell} = n_u A_{u\ell} \left( 1 + \frac{c^3}{8\pi h\nu^3} u_\nu \right)$$

- It is helpful to use a dimensionless quantity, the photon occupation number:

$$n_\gamma \equiv \frac{c^2}{2h\nu^3} I_\nu \quad \xrightarrow{\text{averaging over directions}} \quad \langle n_\gamma \rangle = \frac{c^2}{2h\nu^3} J_\nu = \frac{c^3}{8\pi h\nu^3} u_\nu$$

- Then, the above transition rates are simplified:

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} = n_\ell \frac{g_u}{g_\ell} A_{u\ell} \langle n_\gamma \rangle \quad \left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell} = n_u A_{u\ell} (1 + \langle n_\gamma \rangle)$$

- The photon occupation number determines the relative importance of stimulated and spontaneous emission: stimulated emission is important only when  $\langle n_\gamma \rangle \gg 1$ .

# Absorption and Emission Coefficients in terms of Einstein coefficients

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- The Einstein coefficients are useful means of analyzing absorption and emission processes. However, we often find it even more useful to use cross section because **the cross section has a natural geometric meaning.**
- (pure) Absorption cross section:**

- The number density of photons per unit frequency interval is  $u_\nu/h\nu$ . Let  $\sigma_{\ell u}(\nu)$  be the cross section for absorption of photons for the transition  $\ell \rightarrow u$ . Then, the absorption rate is

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} = n_\ell \int d\nu \sigma_{\ell u}(\nu) c \frac{u_\nu}{h\nu} \approx n_\ell u_\nu \frac{c}{h\nu_{ul}} \int d\nu \sigma_{\ell u}(\nu)$$

- Here, we assumed that  $u_\nu/h\nu$  do not vary appreciably over the profile of the cross section. Therefore, we derive a simple relation between the absorption cross section and the Einstein B coefficient:

$$\int d\nu \sigma_{\ell u}(\nu) = \frac{h\nu_{ul}}{c} B_{\ell u} = \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{ul}^2} A_{ul}$$

- If the cross section has a normalized profile of  $\phi_\nu$ , we can write the absorption cross section as follows:

$$\sigma_{\ell u}(\nu) = \frac{h\nu_{ul}}{c} B_{\ell u} \phi_\nu = \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{ul}^2} A_{ul} \phi_\nu \quad \text{with} \quad \int \phi_\nu d\nu = 1$$

- **(effective) Absorption Coefficient**

- We note that the stimulated emission is proportional to the energy density of ambient radiation field. In the radiative transfer equation, it is convenient to include the stimulated emission term in the absorption coefficient as a negative absorption.

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} - \left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell}^{\text{stimulated}} = n_\ell B_{\ell u} u_\nu - n_u B_{u \ell} u_\nu$$

$$= n_\ell B_{\ell u} u_\nu - n_u \left( \frac{g_\ell}{g_u} B_{\ell u} \right) u_\nu$$

- Therefore, we may define the cross section for stimulated emission and the net (effective) absorption coefficient as follows:

$$\sigma_{u\ell} = \frac{g_\ell}{g_u} \sigma_{\ell u}$$

$$\kappa_\nu = n_\ell \sigma_{\ell u} - n_u \sigma_{u\ell}$$

$$= n_\ell \sigma_{\ell u} \left( 1 - \frac{n_u/n_\ell}{g_u/g_\ell} \right)$$

pure absorption coefficient

- Using the definition of the excitation temperature, we can rewrite them:

$$\kappa_\nu = n_\ell \sigma_{\ell u} \left[ 1 - \exp \left( -\frac{h\nu_{u\ell}}{k_B T_{\text{exc}}} \right) \right] \quad \text{or} \quad \sigma_\nu^{\text{eff}} = \sigma_{\ell u} \left[ 1 - \exp \left( -\frac{h\nu_{u\ell}}{k_B T_{\text{exc}}} \right) \right]$$

---

- **Emission coefficient (Emissivity)**

- The emissivity is defined as the power radiated per unit frequency per unit solid angle per unit volume.
- The line emissivity can be expressed in terms of the spontaneous downward transition rate:

$$4\pi \int d\nu j_\nu = h\nu_{u\ell} \left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell}^{\text{spontaneous}}$$

- Comparing with the definition of the Einstein A coefficient, we obtain:
- $$\int d\nu j_\nu = n_u \frac{A_{u\ell}}{4\pi} h\nu_{u\ell}$$
- If the emission line has a normalized profile of  $\phi_\nu$ , we can write the emissivity as follows:

$$j_\nu = n_u \frac{A_{u\ell}}{4\pi} h\nu_{u\ell} \phi_\nu \quad \text{with} \quad \int d\nu \phi_\nu = 1$$

- 
- The correction factor for the stimulated emission in absorption coefficient:

- For Ly $\alpha$  line,

$$h\nu_{u\ell} = 10.2 \text{ eV} \rightarrow 1 - \exp\left(-\frac{h\nu_{u\ell}}{k_B T_{\text{exc}}}\right) = 1 - \exp\left(-\frac{1.1837 \times 10^5 \text{ K}}{T_{\text{exc}}}\right)$$

$$\simeq 1 \quad \text{for } T_{\text{exc}} \approx T_{\text{gas}} < 1 \times 10^5 \text{ K}$$

- ▶ The stimulated emission is negligible.

- For 21 cm line,

$$h\nu_{u\ell} = 6 \mu\text{eV} \rightarrow 1 - \exp\left(-\frac{h\nu_{u\ell}}{k_B T_{\text{exc}}}\right) = 1 - \exp\left(-\frac{0.068 \text{ K}}{T_{\text{exc}}}\right)$$

$$\simeq \frac{0.068 \text{ K}}{T_{\text{exc}}} \ll 1 \quad \text{for } T_{\text{exc}} \approx T_{\text{gas}} \sim 100 \text{ K}$$

- ▶ The correction for stimulated emission is very important. **We, therefore, need to take into account the stimulated emission in dealing with the 21 cm line.**

- Two limiting cases:

- At radio and sub-mm frequencies, the upper levels are often appreciably populated, and it is important to include both spontaneous and stimulated emission.
- When we consider propagation of optical, UV, or X-ray radiation in cold ISM, the upper levels of atoms and ions usually have negligible populations, and stimulated emission can be neglected.

# Generalized Kirchhoff's Law

---

- **Source Function:**

$$\begin{aligned}
 S_\nu &= \frac{j_\nu}{\alpha_\nu} \\
 &= \frac{(1/4\pi)n_u A_{ul} h\nu_{ul} \phi_\nu^{\text{emiss}}}{n_\ell \sigma_{\ell u}^{\text{eff}}(\nu)} \\
 &= \frac{n_u \frac{A_{ul}}{4\pi} h\nu_{ul} \phi_\nu^{\text{emiss}}}{n_\ell \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{ul}^2} A_{ul} \phi_\nu^{\text{abs}} [1 - \exp(-h\nu_{ul}/k_B T_{\text{exc}})]} \quad \leftarrow \frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp(-h\nu_{ul}/k_B T_{\text{exc}}) \\
 &= \frac{2h\nu_{ul}^3}{c^2} \frac{1}{\exp(h\nu_{ul}/k_B T_{\text{exc}}) - 1} \quad \leftarrow \phi_\nu^{\text{emiss}} = \phi_\nu^{\text{abs}}
 \end{aligned}$$

- This is called the **generalized Kirchhoff's law**.
- **The intrinsic profiles for absorption and emission should be the same.**
  - ▶ The source function should approach the Planck function in LTE ( $T_{\text{exc}} = T_{\text{kinetic}}$ ). For this to be true, the intrinsic profile of emission line should be the same as that of absorption line.
  - ▶ We can show that the intrinsic emission and absorption profiles are, indeed, the same, using a semi-classical model for an atom.

# Oscillator Strength

- In the previous slides, we characterized the absorption cross section by the Einstein A coefficient. Equivalently, we can express the cross section in terms of the oscillator strength for the absorption transition  $\ell \rightarrow u$ , defined by the relation:

$$\int \sigma_{\ell u}(\nu) d\nu = \frac{\pi e^2}{m_e c} f_{\ell u} \quad \rightarrow \quad \boxed{\sigma_{\ell u}(\nu) = \frac{\pi e^2}{m_e c} f_{\ell u} \phi_\nu}$$

- Here, the factor  $\frac{\pi e^2}{m_e c} = 0.02654 \text{ cm}^2 \text{ Hz}$  is the cross-section, integrated over the line profile, for a classical oscillator model.
- The oscillator strength is the factor which corrects the classical result. The quantum mechanical process can be interpreted as being due to a (fractional) number  $f$  of equivalent classical electron oscillators of the same frequency.
- The Einstein A coefficient is related to the absorption oscillator strength of the upward transition by

$$A_{u\ell} = \frac{8\pi^2 e^2 \nu_{u\ell}^2}{m_e c^3} \frac{g_\ell}{g_u} f_{\ell u} = \left( \frac{0.8167 \text{ cm}}{\lambda_{u\ell}} \right)^2 \frac{g_\ell}{g_u} f_{\ell u} [\text{s}^{-1}]$$

- For 21.1 cm line,  $g_u = 3$ ,  $g_\ell = 1$  ( $g_F = 2F + 1$ )

$$A_{u\ell} = 2.88 \times 10^{-15} [\text{s}^{-1}] = (11 \text{ Myr})^{-1} \quad f_{\ell u} = 5.75 \times 10^{-12}$$

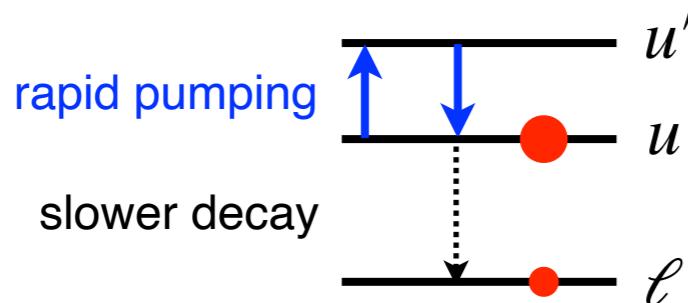
- For Ly $\alpha$  (1215.67 Å) line,  $g_u = 3$ ,  $g_\ell = 1$  ( $g_L = 2L + 1$ )

$$A_{u\ell} = 6.265 \times 10^8 [\text{s}^{-1}] \quad f_{\ell u} = 0.4164 \quad \text{for } 1^2S_{1/2} \rightarrow 2^2P$$

$f_{\ell u} = 0.27760$  for  ${}^2S_{1/2} \rightarrow {}^2P_{3/2}$   
 $= 0.13881$  for  ${}^2S_{1/2} \rightarrow {}^2P_{1/2}$

# Maser Lines

- Population inversion
  - Under some conditions, a process may act to “pump” an excited state  $u$  by either collisional or radiative excitation of a higher level  $u'$  that then decays to populate level  $u$ . If this pumping process is rapid enough (relative to the processes that depopulate  $u$ ), it may be possible for the relative level populations between  $u$  and  $\ell$  to satisfy the inequality (also to have a negative excitation temperature).



$$n_u > \frac{g_u}{g_\ell} n_\ell \quad \rightarrow \quad T_{\text{exc},u\ell} < 0.$$

- When this population inversion occurs, stimulated emission is stronger than pure absorption, and ***the radiation is amplified as it propagates***. Then, the effective absorption coefficient, optical depth, and attenuation factor are

$$\kappa_\nu = \sigma_{\ell u} \left( 1 - \frac{n_u/g_u}{n_\ell/g_\ell} \right) < 0, \quad \tau_\nu = \int \kappa_\nu ds < 0, \quad e^{-\tau_\nu} > 1$$

- Maser
  - Such population inversion have been observed for microwave transitions of H I, OH, H<sub>2</sub>O, and SiO, and hence we speak of ***maser (microwave amplification by stimulated emission of radiation)*** emission.

- 
- Observational properties
    - If  $|k_B T_{\text{exc}, u\ell}| \gg h\nu$ , the RT equation becomes
$$\begin{aligned}T_A &= T_A(0)e^{-\tau_\nu} + T_{\text{exc}}(1 - e^{-\tau_\nu}) \\&= (T_A(0) + |T_{\text{exc}}|)e^{|\tau_\nu|} - |T_{\text{exc}}|\end{aligned}$$
    - The factor  $e^{|\tau_\nu|}$  is in some cases very large - some OH and H<sub>2</sub>O masers have been observed to have  $T_A > 10^{11}$  K.
    - We note that
      - ▶  $e^{|\tau_\nu|}$  is more strongly peaked on the sky than  $|\tau_\nu|$  - the angular size of the maser is less than the actual transverse dimension of the maser region.
      - ▶  $e^{|\tau_\nu|}$  is more strongly in  $\nu$  than  $|\tau_\nu|$  - the maser line is narrower than the actual velocity distribution of the maser species.
    - Some maser can be very bright, allowing the use of interferometry, as well as observations of sources at large distances.
      - ▶ This has enabled measurements of proper motion of maser spots in star-forming regions of the Milky Way, as well as in material orbiting a supermassive black hole in the spiral galaxy NGC 4258 (Hernstein et al. 1999).

# Collisional Excitation & De-excitation

- **Collisional Rate (Two Level Atom)**

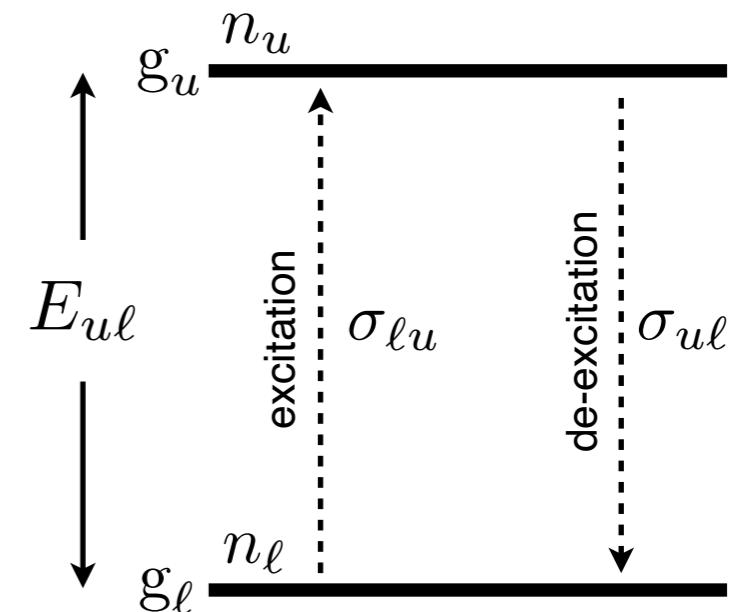
- ▶ The cross section  $\sigma_{\ell u}$  for collisional excitation from a lower level  $\ell$  to an upper level  $u$  is, in general, inversely proportional to the impact energy (or  $v^2$ ) above the energy threshold  $E_{ul}$  and is zero below.
- ▶ The collisional cross section can be expressed in the following form using a dimensionless quantity called the **collision strength**  $\Omega_{\ell u}$ :

$$\begin{aligned}\sigma_{\ell u}(v) &= (\pi a_0^2) \left( \frac{hR_H}{\frac{1}{2}m_e v^2} \right) \frac{\Omega_{\ell u}}{g_\ell} \text{ cm}^2 \quad \text{for } \frac{1}{2}m_e v^2 > E_{ul} \\ &= \frac{h^2}{4\pi m_e^2 v^2} \frac{\Omega_{\ell u}}{g_\ell}\end{aligned}$$

or  $\sigma_{\ell u}(E) = \frac{h^2}{8\pi m_e E} \frac{\Omega_{\ell u}}{g_\ell} \quad \left( E = \frac{1}{2}m_e v^2 \right)$

where,  $a_0 = \frac{\hbar^2}{m_e e^2} = 5.12 \times 10^{13}$  cm, Bohr radius

$$R_H = \frac{m_e e^4}{4\pi \hbar^3} = 109,737 \text{ cm}^{-1}, \text{ Rydberg constant} \quad \left( \hbar = \frac{h}{2\pi} \right)$$



- ▶ The collision strength  $\Omega_{\ell u}$  is a function of electron velocity (or energy) but is often approximately constant near the threshold. Here,  $g_\ell$  and  $g_u$  are the statistical weights of the lower and upper levels, respectively.

- Advantage of using the collision strength is that (1) it removes the primary energy dependence for most atomic transitions and (2) they have the symmetry between the upper and the lower states.

**The principle of detailed balance** states that ***in thermodynamic equilibrium each microscopic process is balanced by its inverse.***

$$n_e n_\ell v_\ell \sigma_{\ell u}(v_\ell) f(v_\ell) dv_\ell = n_e n_u v_u \sigma_{u\ell}(v_u) f(v_u) dv_u$$

Here,  $v_\ell$  and  $v_u$  are related by  $\frac{1}{2}m_e v_\ell^2 = \frac{1}{2}m_e v_u^2 + E_{u\ell}$ , and  $f(v)$  is a Maxwell velocity distribution of electrons. Using the Boltzmann equation of thermodynamic equilibrium,

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

we derive the following relation between the cross-sections for excitation and de-excitation are

$$g_\ell v_\ell^2 \sigma_{\ell u}(v_\ell) = g_u v_u^2 \sigma_{u\ell}(v_u) \quad \text{Here, } \frac{1}{2}m_e v_\ell^2 = \frac{1}{2}m_e v_u^2 + E_{u\ell} \rightarrow g_\ell \cdot (E + E_{u\ell}) \cdot \sigma_{\ell u}(E + E_{u\ell}) = g_u \cdot E \cdot \sigma_{u\ell}(E)$$

and the symmetry of the collision strength between levels. where  $E = \frac{1}{2}m_e v_u^2$

$$\Omega_{\ell u} = \Omega_{u\ell}$$

more precisely  $\Omega_{\ell u}(E + E_{u\ell}) = \Omega_{u\ell}(E)$

These two relations were derived in the TE condition. However, ***the cross-sections are independent on the assumptions, and thus the above relations should be always satisfied.***

► Collisional excitation and de-excitation rates

The ***collisional de-excitation rate per unit volume per unit time, which is thermally averaged,*** is

$$\left( \frac{dn_\ell}{dt} \right)_{u \rightarrow \ell} = n_e n_u \int_0^\infty v \sigma_{u\ell}(v) f(v) dv \\ = n_e n_u k_{u\ell} \quad [\text{cm}^{-3} \text{ s}^{-1}]$$

$$k_{u\ell} \equiv \langle \sigma v \rangle_{u \rightarrow \ell}$$

$$k_{u\ell} = \int_0^\infty v \sigma_{u\ell}(v) f(v) dv \\ = \left( \frac{2\pi\hbar^4}{k_B m_e^3} \right)^{1/2} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_u} \\ = \frac{8.62942 \times 10^{-6}}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_u} \quad [\text{cm}^3 \text{ s}^{-1}],$$

**effective collision strength:**

$$\langle \Omega_{u\ell} \rangle \equiv \int_0^\infty \Omega_{u\ell}(E) e^{-E/k_B T} d(E/k_B T)$$

and the ***collisional excitation rate per unit volume per unit time*** is

$$\left( \frac{dn_u}{dt} \right)_{\ell \rightarrow u} = n_e n_\ell k_{\ell u}$$

$$k_{\ell u} \equiv \langle \sigma v \rangle_{\ell \rightarrow u}$$

$$k_{\ell u} = \int_{v_{\min}}^\infty v \sigma_{\ell u}(v) f(v) dv \quad \text{Here, } \frac{1}{2} m_e v_{\min}^2 = E_{u\ell} \\ = \left( \frac{2\pi\hbar^4}{k_B m_e^3} \right)^{1/2} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{k_B T}\right)$$

Here,  $k_{\ell u}$  and  $k_{u\ell}$  are the **collisional rate coefficient for excitation and de-excitation** coefficients in units of  $\text{cm}^3 \text{ s}^{-1}$ , respectively. We also note that ***the rate coefficients for collisional excitation and de-excitation are related by***

$$k_{\ell u} = \frac{g_u}{g_\ell} k_{u\ell} \exp\left(-\frac{E_{u\ell}}{k_B T}\right)$$

$$\langle \sigma v \rangle_{\ell \rightarrow u} = \frac{g_u}{g_\ell} \langle \sigma v \rangle_{u \rightarrow \ell} \exp\left(-\frac{E_{u\ell}}{k_B T}\right)$$

# Sum rule for collision strengths

---

- Quantum mechanical sum rule for collision strengths for the case where one term consists of a singlet ( $S = 0$  or  $L = 0$ ) and the second consists of a multiplet: the collision strength of each fine structure level  $J$  is related to the total collision strength of the multiplet by

$$\Omega_{(SLJ, S'L'J')} = \frac{(2J' + 1)}{(2S' + 1)(2L' + 1)} \Omega_{(SL, S'L')}$$

Here,  $(2J' + 1)$  is the statistical weight of an individual level in the multiplet, and  $(2S' + 1)(2L' + 1)$  is the statistical weight of the multiplet term.

We can regard the collision strength of the term as “shared” amongst these levels in proportion to the statistical weights of the individual levels ( $g_J = 2J + 1$ ).

- The flux ratio between the lines in a multiplet is proportional to the ratio of their collision strengths, in a low density medium.*** Then, the flux ratio is determined by the ratio of their statistical weights.

- C-like ions ( $1s^2 2s^2 2p^2 \rightarrow 1s^2 2s^2 2p^2$ ) forbidden or inter combination transitions.

ground states (triplet) -  ${}^3P_0 : {}^3P_1 : {}^3P_2 = 1 : 3 : 5$

excited states (singlets) -  ${}^1D_2, {}^1S_1$

- Li-like ions ( $1s^2 2s^1 \rightarrow 1s^2 2p^1$ ) resonance transitions

ground state (singlet) -  ${}^2S_{1/2}$

excited states (doublet) -  ${}^2P_{3/2} : {}^2P_{1/2} = 2 : 1$

# Collisionally-Excited Emission Line

---

- Emission line flux

- In the low density limit, the collisional rate between atoms and electrons is much slower than the (spontaneous) radiative de-excitation rate of the excited level. Thus, we can balance the collisional feeding into level  $u$  by the rate of radiative transition back down to level  $\ell$ . The level population is determined by

$$n_e n_\ell k_{\ell u} = A_{u\ell} n_u$$

$$\frac{n_u}{n_\ell} = \frac{n_e k_{\ell u}}{A_{u\ell}}$$

$$= \frac{n_e}{A_{u\ell}} \beta \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} T^{-1/2} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

where  $A_{u\ell}$  is the Einstein coefficient for spontaneous emission. The line emissivity is given by

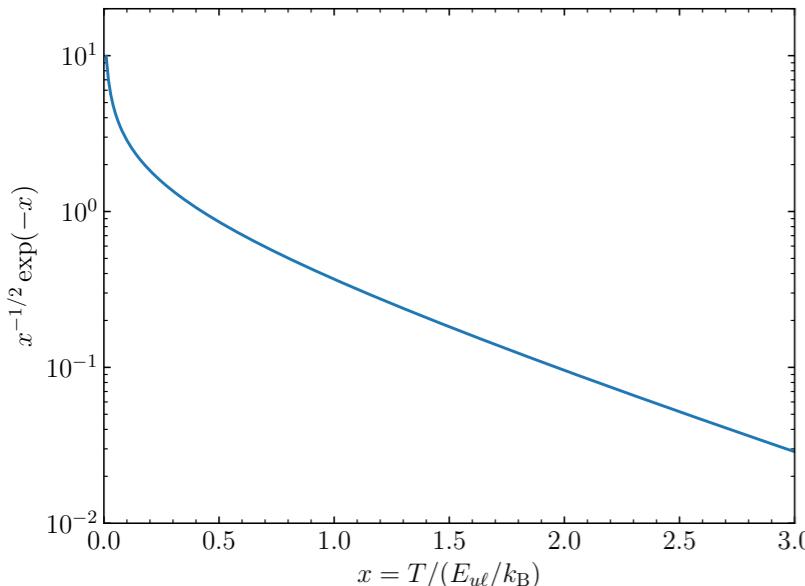
$$4\pi j_{u\ell} = E_{u\ell} A_{u\ell} n_u = E_{u\ell} n_e n_\ell k_{\ell u}$$

$$= n_e n_\ell E_{u\ell} \frac{8.62942 \times 10^{-6}}{T^{1/2}} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right) \text{ [erg cm}^{-3} \text{ s}^{-1}\text{]}$$

$$\simeq \beta \chi n_e^2 E_{u\ell} T^{-1/2} \frac{\langle \Omega_{u\ell} \rangle}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

Here,  $\beta = \left(\frac{2\pi\hbar^4}{km_e^2}\right)^{1/2} = 8.62942 \times 10^{-6}$

$$\chi = n_\ell/n_e$$



For low temperature, the exponential term dominates because few electrons have energy above the threshold for collisional excitation, so that the line rapidly fades with decreasing temperature.

At high temperature, the  $T^{-1/2}$  term controls the cooling rate, so the line fades slowly with increasing temperature.

- ▶ In **high-density limit**, the level population are set by the Boltzmann equilibrium, and the line emissivity is

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} \exp\left(-\frac{E_{u\ell}}{kT}\right)$$

$$\begin{aligned} 4\pi j_{u\ell} &= E_{\ell u} A_{u\ell} n_u \\ &= n_\ell E_{\ell u} A_{u\ell} \frac{g_u}{g_\ell} \exp\left(-\frac{E_{\ell u}}{kT}\right) \\ &\simeq \chi n_e E_{\ell u} A_{u\ell} \frac{g_u}{g_\ell} \exp\left(-\frac{E_{\ell u}}{kT}\right) \\ &\rightarrow n_\ell E_{\ell u} A_{u\ell} \frac{g_u}{g_\ell} \quad \text{as } kT \gg E_{\ell u} \end{aligned}$$

Here, the line flux scales as  $n_e$  rather than  $n_e^2$ , but the line flux tends to be a constant value at high temperature.

- ▶ **Critical density** is defined as the density where the radiative depopulation rate matches the collisional de-excitation for the excited state.

$$A_{u\ell} n_u = n_e n_u k_{u\ell}$$

$$n_{\text{crit}} = \frac{A_{u\ell}}{k_{u\ell}}$$

$$\begin{aligned} \rightarrow n_{\text{crit}} &= A_{u\ell} \frac{g_u}{\beta \langle \Omega_{u\ell} \rangle} T^{1/2} \\ &= 1.2 \times 10^3 \frac{A_{u\ell}}{10^{-4} \text{ s}^{-1}} \frac{g_u}{\langle \Omega_{u\ell} \rangle} \left( \frac{T}{10^4 \text{ K}} \right)^{1/2} [\text{cm}^{-3}] \end{aligned}$$

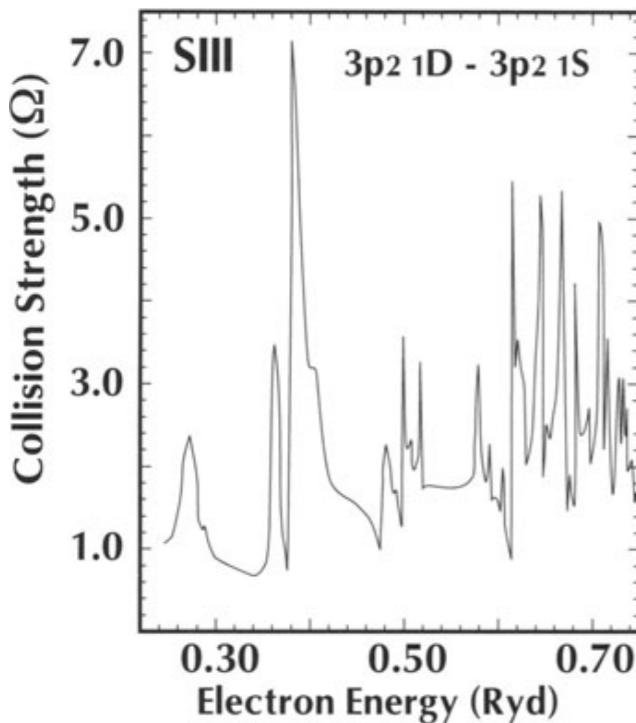
- ▶ At densities higher than the critical density, collisional de-excitation becomes significant, and the forbidden lines will be weaker as the density increases.

*At around the critical density, the “line emissivity vs density” plotted in log-log scale changes slope from +2 to +1.*

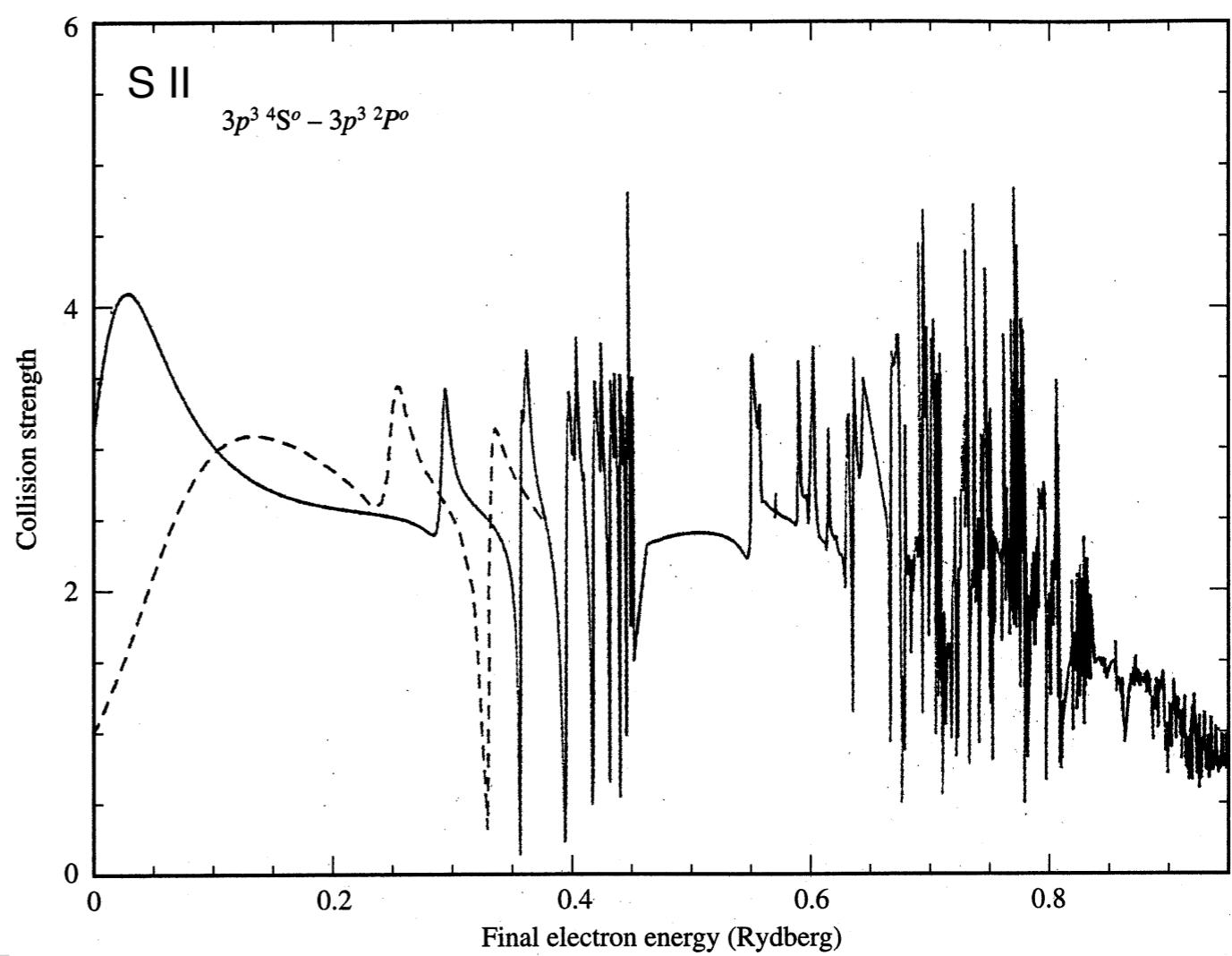
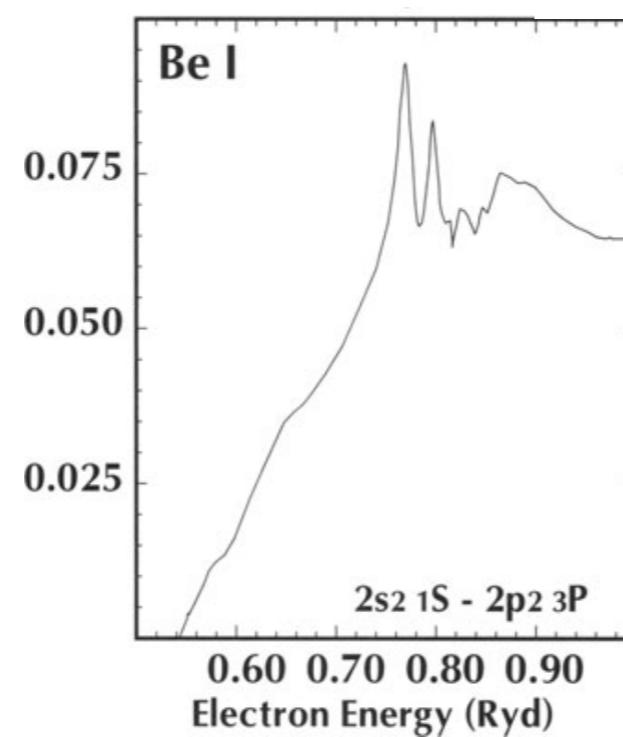
- Collision Strength

- Quantum mechanical calculations show that (1) the resonance structure in the collision strengths is important and (2) the collision strength increases with energy for neutral species.

Tayal (1996)



Badnell (1999)



The **effective collision strength**, which is thermally averaged, has a value in a range of

$$\langle \Omega_{ul} \rangle = \int_0^{\infty} \Omega_{ul}(E) e^{-E/k_B T} d(E/k_B T)$$

$$10^{-2} < \langle \Omega_{ul} \rangle < 10$$

See Table F.1 to F.5 in [Draine]

- As can be seen in the Tables and the formula, collisional de-excitation is negligible for resonance and most forbidden lines in the ISM.

Ion	$\ell$	u			$n_{H,\text{crit}}(u)$	
			$E_\ell/k$ (K)	$E_u/k$ (K)	$\lambda_{u\ell}$ ( $\mu\text{m}$ )	$T = 100 \text{ K}$ ( $\text{cm}^{-3}$ )
C II	$^2\text{P}_{1/2}^o$	$^2\text{P}_{3/2}^o$	0	91.21	157.74	$2.0 \times 10^3$
CI	$^3\text{P}_0$	$^3\text{P}_1$	0	23.60	609.7	620
	$^3\text{P}_1$	$^3\text{P}_2$	23.60	62.44	370.37	720
O I	$^3\text{P}_2$	$^3\text{P}_1$	0	227.71	63.185	$2.5 \times 10^5$
	$^3\text{P}_1$	$^3\text{P}_0$	227.71	326.57	145.53	$8.4 \times 10^3$
Si II	$^2\text{P}_{1/2}^o$	$^2\text{P}_{3/2}^o$	0	413.28	34.814	$1.0 \times 10^5$
Si I	$^3\text{P}_0$	$^3\text{P}_1$	0	110.95	129.68	$4.8 \times 10^4$
	$^3\text{P}_1$	$^3\text{P}_2$	110.95	321.07	68.473	$9.9 \times 10^4$
						$1.5 \times 10^3$

Table 17.1 in [Draine]

- However, it is not true for the 21 cm hyperfine structure line of hydrogen.
  - The critical density for 21cm line is
 
$$n_{\text{crit}} \sim 10^{-3} (T/100 \text{ K})^{-1/2} [\text{cm}^{-3}]$$

$$A_{u\ell} = 2.88 \times 10^{-15} [\text{s}^{-1}]$$
  - The hyperfine levels are thus essentially in collisional equilibrium in the CNM.

The collisional strengths and other atomic data are available in the CHIANTI atomic database (<https://www.chiantidatabase.org/>).

Ion	Transition l-u	$\lambda$ $\mu\text{m}$	$A_{ul}$ $\text{s}^{-1}$	$\Omega_{ul}$	$n_{\text{crit}}$ $\text{cm}^{-3}$
C I	$^3\text{P}_0 - ^3\text{P}_1$	609.1354	$7.93 \times 10^{-8}$	–	(500)
	$^3\text{P}_1 - ^3\text{P}_2$	370.4151	$2.65 \times 10^{-7}$	–	(3000)
C II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	157.741	$2.4 \times 10^{-6}$	1.80	47 (3000)
N II	$^3\text{P}_0 - ^3\text{P}_1$	205.3	$2.07 \times 10^{-6}$	0.41	41
	$^3\text{P}_1 - ^3\text{P}_2$	121.889	$7.46 \times 10^{-6}$	1.38	256
	$^3\text{P}_2 - ^1\text{D}_2$	0.65834	$2.73 \times 10^{-3}$	2.99	7700
	$^3\text{P}_1 - ^1\text{D}_2$	0.65481	$9.20 \times 10^{-4}$	2.99	7700
N III	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	57.317	$4.8 \times 10^{-5}$	1.2	1880
O I	$^3\text{P}_2 - ^3\text{P}_1$	63.184	$8.95 \times 10^{-5}$	–	$2.3 \times 10^4 (5 \times 10^5)$
	$^3\text{P}_1 - ^3\text{P}_0$	145.525	$1.7 \times 10^{-5}$	–	$3400 (1 \times 10^5)$
	$^3\text{P}_2 - ^1\text{D}_2$	0.63003	$6.3 \times 10^{-3}$	–	$1.8 \times 10^6$
O II	$^4\text{S}_{3/2} - ^2\text{D}_{5/2}$	0.37288	$3.6 \times 10^{-5}$	0.88	1160
	$^4\text{S}_{3/2} - ^2\text{D}_{3/2}$	0.37260	$1.8 \times 10^{-4}$	0.59	3890
O III	$^3\text{P}_0 - ^3\text{P}_1$	88.356	$2.62 \times 10^{-5}$	0.39	461
	$^3\text{P}_1 - ^3\text{P}_2$	51.815	$9.76 \times 10^{-5}$	0.95	3250
	$^3\text{P}_2 - ^1\text{D}_2$	0.50069	$1.81 \times 10^{-2}$	2.50	$6.4 \times 10^5$
	$^3\text{P}_1 - ^1\text{D}_2$	0.49589	$6.21 \times 10^{-3}$	2.50	$6.4 \times 10^5$
	$^1\text{D}_2 - ^1\text{S}_0$	0.43632	1.70	0.40	$2.4 \times 10^7$
Ne II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	12.8136	$8.6 \times 10^{-3}$	0.37	$5.9 \times 10^5$
Ne III	$^3\text{P}_2 - ^3\text{P}_1$	15.5551	$3.1 \times 10^{-2}$	0.60	$1.27 \times 10^5$
	$^3\text{P}_1 - ^3\text{P}_0$	36.0135	$5.2 \times 10^{-3}$	0.21	$1.82 \times 10^4$
Si II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	34.8152	$2.17 \times 10^{-4}$	7.7	$(3.4 \times 10^5)$
S II	$^4\text{S}_{3/2} - ^2\text{D}_{5/2}$	0.67164	$2.60 \times 10^{-4}$	4.7	1240
	$^4\text{S}_{3/2} - ^2\text{D}_{3/2}$	0.67308	$8.82 \times 10^{-4}$	3.1	3270
S III	$^3\text{P}_0 - ^3\text{P}_1$	33.4810	$4.72 \times 10^{-4}$	4.0	1780
	$^3\text{P}_1 - ^3\text{P}_2$	18.7130	$2.07 \times 10^{-3}$	7.9	$1.4 \times 10^4$
S IV	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	10.5105	$7.1 \times 10^{-3}$	8.5	$5.0 \times 10^4$
Ar II	$^2\text{P}_{1/2} - ^2\text{P}_{3/2}$	6.9853	$5.3 \times 10^{-2}$	2.9	$1.72 \times 10^6$
Ar III	$^3\text{P}_2 - ^3\text{P}_1$	8.9914	$3.08 \times 10^{-2}$	3.1	$2.75 \times 10^5$
	$^3\text{P}_1 - ^3\text{P}_0$	21.8293	$5.17 \times 10^{-3}$	1.3	$3.0 \times 10^4$
Fe II	$^6\text{D}_{7/2} - ^6\text{D}_{5/2}$	35.3491	$1.57 \times 10^{-3}$	–	$(3.3 \times 10^6)$
	$^6\text{D}_{9/2} - ^6\text{D}_{7/2}$	25.9882	$2.13 \times 10^{-3}$	–	$(2.2 \times 10^6)$

# Overall Properties of the Cold Neutral Medium (CNM)

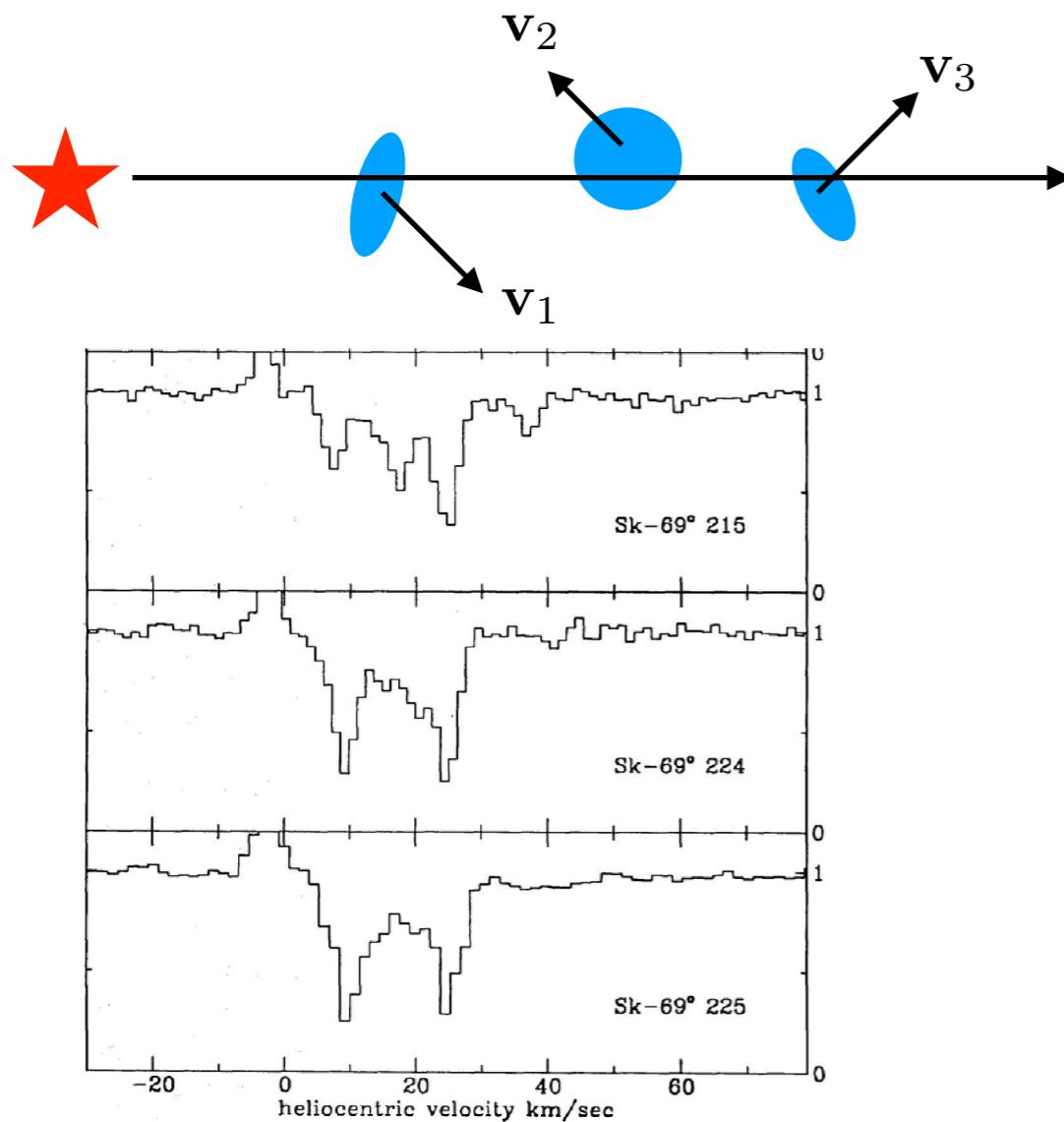
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- Overall properties of the CNM
  - Temperature  $T \sim 100 \text{ K}$
  - Mean kinetic energy per particle  $\langle E \rangle = (3/2)kT \sim 0.013 \text{ eV}$
  - Number density
    - ▶  $n_{\text{atom}} \sim 30 \text{ cm}^{-3}$  for atoms
    - ▶  $n_e \sim 0.04 \text{ cm}^{-3}$  for free electrons
  - Thermal velocity
    - ▶  $v_{\text{th}}(\text{H}) \sim 1.6 \text{ km s}^{-1}$  for hydrogen atoms
    - ▶  $v_{\text{th}}(e) \sim 67 \text{ km s}^{-1}$  for free electrons
  - Mean free path
    - ▶  $\lambda_{\text{mfp}}(\text{HH}) \sim 0.74 \text{ AU}$  for atom-atom collisions
    - ▶  $\lambda_{\text{mfp}}(e\text{H}) \sim 1700 \text{ AU}$  for atom-electron collisions
    - ▶  $\lambda_{\text{mfp}}(ee) \sim 1.9 \times 10^{-3} \text{ AU}$  for electron-electron collisions
  - Collisional time scale
    - ▶  $t_{\text{coll}}(\text{HH}) \sim 2.2 \text{ yr}$  for atom-atom collisions
    - ▶  $t_{\text{coll}}(e\text{H}) \sim 120 \text{ yr}$  for atom-electron collisions
    - ▶  $t_{\text{coll}}(ee) \sim 1.2 \text{ hr}$  for electron-electron collision

See [reference - collisional time scale.pdf](#)  
for the detailed calculations of the numerical values

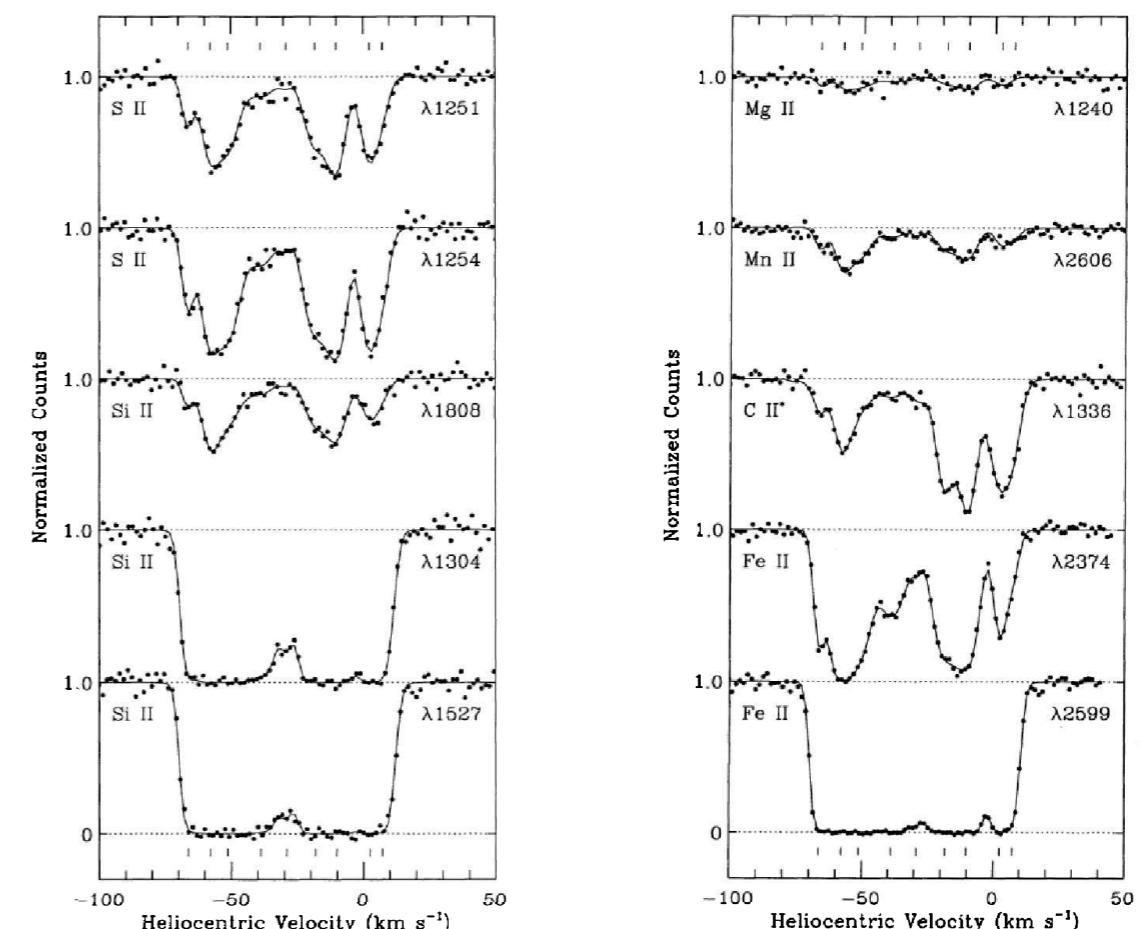
# Observations of Absorption Lines Toward the CNM

- The CNM gives rise to a number of absorption features in the spectra of hot background stars (and quasars).
  - The most prominent absorption lines at visible wavelengths are Ca II K and H lines at  $\lambda = 3933, 3968 \text{ \AA}$ , and Na I D<sub>1</sub> and D<sub>2</sub> doublet lines at  $\lambda = 5890, 5896 \text{ \AA}$ .



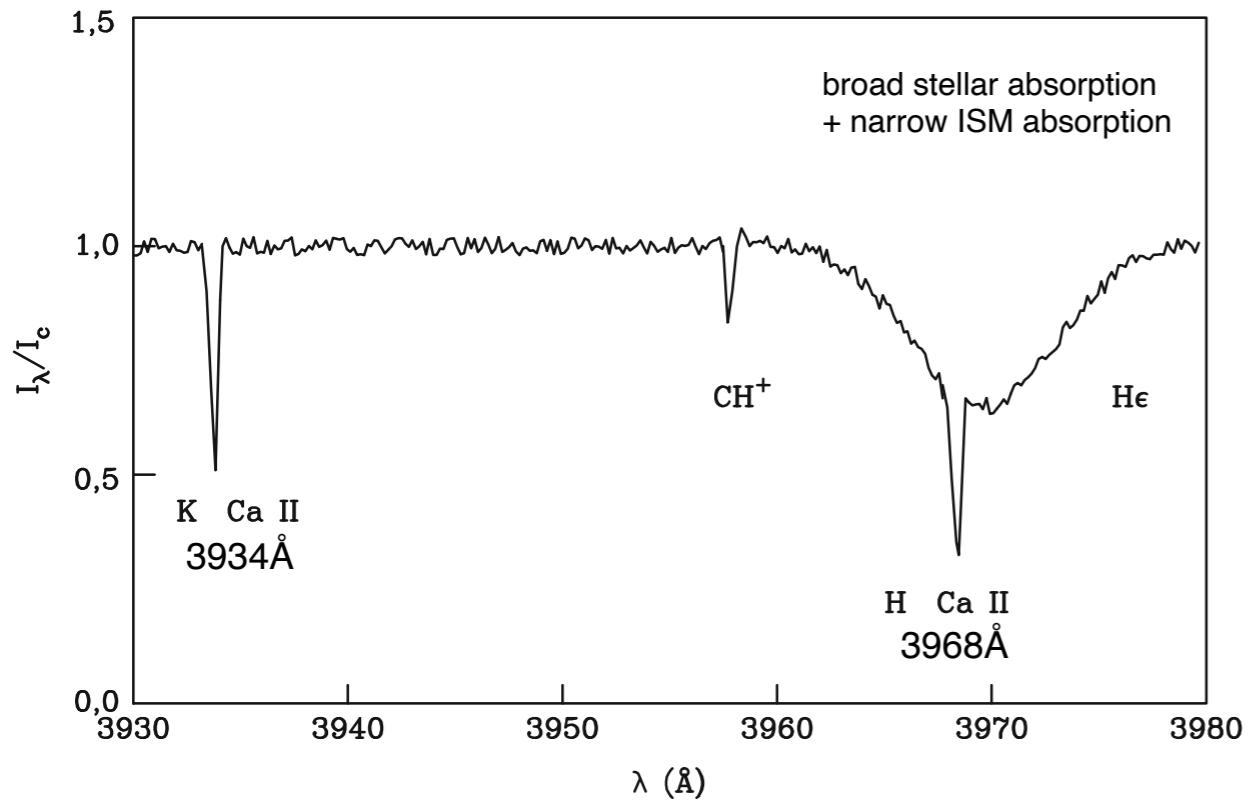
Na I D<sub>2</sub> interstellar absorption line seen along 3 lines of sight to stars in LMC (Molaro et al. 1993)

[Note] The cold gas is  $\sim 100$  pc away from Earth, meaning that 5 arcmin corresponds to  $\sim 0.15$  pc.



UV interstellar absorption lines toward an O-type star HD93521. (Spitzer & Fitzpatrick 1993)

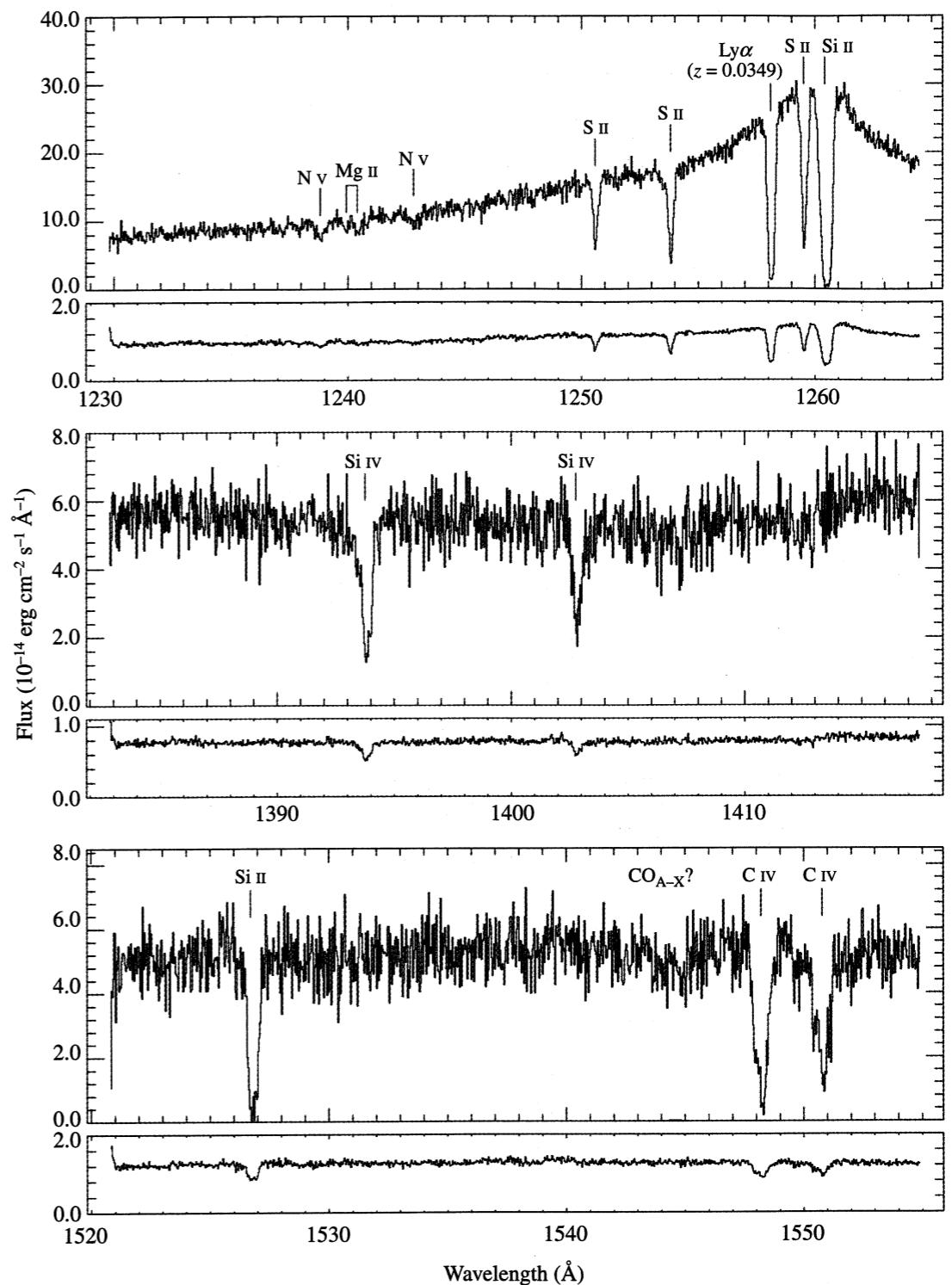
[Note] (1) multiple velocity components and (2) line saturation on Si II and Fe II.  
The multiple velocities are due primarily to the differential rotation of our galaxy. (clouds at different distances)



Interstellar absorption lines in the spectrum of  $\zeta$  Oph (O9.5V).

Note that the Ca II H line occurs inside the He hydrogen line, which is much broader and of stellar origin.

Figure 4.6 in Astrophysics of the Interstellar Medium [Maciel]



Interstellar absorption lines toward the Seyfert 1 galaxy ESO 141-055.

Figure 5.5 in Physics and Chemistry of the Interstellar Medium [Kwok]

- The alkali metals (Li, K, and Na) and alkaline earth metals (Ca) produce absorption lines at visible wavelengths ( $4000 \text{ \AA} < \lambda < 7300 \text{ \AA}$ ,  $1.7 \text{ eV} < E < 3.1 \text{ eV}$ ); these elements have loosely bound outer electrons.
- Most other elements produce UV absorption lines ( $\lambda < 4000 \text{ \AA}$ ,  $E > 3.1 \text{ eV}$ ).
  - Therefore, the study of the CNM was extensively made by the launch of orbiting UV telescopes (Copernicus, IUE, etc).
  - In particular, Ly $\alpha$  ( $\lambda = 1215.67 \text{ \AA}$ ;  $E = 10.2 \text{ eV}$ ) from hydrogen.
- Interstellar absorption lines at visible wavelengths were also found from neutral atoms such as Ca I, K I, Li I, ions such as Ti II, and diatomic molecules such as CH, NH, CN, CH<sup>+</sup> and C<sub>2</sub>.
  - [Note] The first discovery of interstellar molecules was made by the detection of CH absorption at  $\lambda \sim 4300$  (4315) $\text{\AA}$  (Swings & Rosenfeld 1937, ApJ), not at radio wavelengths.
  - CH, NH, and CN are referred to as “**radicals**”, in chemistry, meaning molecules that contain at least one unpaired electron. They quickly combine with one another, or with single atoms in laboratory. But, in the low density of the ISM, they have long lifetimes.

- 
- The composition and excitation of interstellar gas can be studied using absorption lines that appear in the spectra of background stars (or other sources).
  - The interstellar lines are typically narrow compared to spectral features produced by absorption in stellar photospheres, and in practice can be readily distinguished.
    - For instance, consider the Fraunhofer lines in the Sun's spectrum. The Ca H and K lines, with equivalent widths of 14Å and 19Å respectively, are the strongest absorption lines. The Na I D<sub>1</sub> and D<sub>2</sub> lines have equivalent widths of 0.6Å and 0.8Å.
    - On the other hand, for many interstellar lines, the equivalent width is sufficiently small that the mÅ is a convenient unit.
  - It is normally possible to detect absorption only by the ground state (and perhaps the excited fine-structure levels of the ground electronic state) - the populations in the excited electronic states are too small to be detected in absorption.
  - The widths of absorption lines are usually determined by Doppler broadening, with line widths of a few km s<sup>-1</sup> (or  $\Delta\lambda/\lambda \approx 10^{-5}$ ) - often observed in cool clouds.
  - Absorption lines (and emission lines) contains a lots of information about number density, temperature, chemical abundances, ionization states, and excitation states.
  - However, interpreting the information requires understanding the ways in which light interacts with baryonic matter, radiative transfer.
  - **We need to know the line profile to analyze absorption lines.**

# Optical Depth

- The optical depth in an absorption line can be written

$$\tau_\nu = \frac{\pi e^2}{m_e c} f_{\ell u} \left( 1 - \frac{n_u/g_u}{n_\ell/g_\ell} \right) N_\ell \phi_\nu \simeq \frac{\pi e^2}{m_e c} f_{\ell u} N_\ell \phi_\nu$$

Here,  $N_\ell \equiv \int n_\ell ds$  is the column density of the absorbers.

The line profile is given by  $\phi_\nu = \frac{1}{\Delta\nu_D \sqrt{\pi}} H(u, a)$ , and its value at the line center is

$$\begin{aligned} \phi_\nu(\nu = \nu_{\ell u}) &= \frac{1}{\nu_{\ell u}(b/c)\sqrt{\pi}} H(0, a) & u &= \frac{\nu - \nu_{\ell u}}{\Delta\nu_D} = \frac{\nu - \nu_{u\ell}}{\nu_{\ell u}(b/c)} \\ &\approx \frac{1}{\nu_{\ell u}(b/c)\sqrt{\pi}} & &= \frac{v}{b} \quad \left( v = \frac{\nu - \nu_{\ell u}}{\nu_{\ell u}} c, b = \sqrt{2}v_{\text{rms}} = \sqrt{\frac{2k_B T}{m}} \right) \end{aligned}$$

The correction factor for stimulated emission is negligible for the optical lines. Then, dropping the correction factor, the optical depth can be written

$$\tau_\nu = \tau_0 H(u, a) \quad \text{Here, } \tau_0 \text{ is the optical depth at the line center.}$$

$$\tau_0 = \frac{\sqrt{\pi}e^2}{m_e c} f_{\ell u} \frac{\lambda_{\ell u}}{b} N_\ell$$

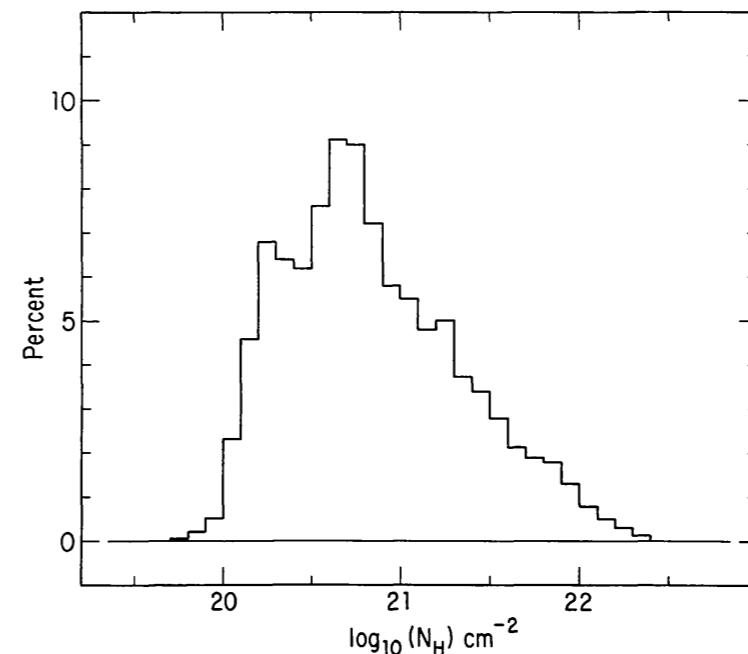
- The central optical depth for Ly $\alpha$  is

$$\tau_0 = 0.7580 \left( \frac{N_\ell}{10^{13} \text{ cm}^{-2}} \right) \left( \frac{f_{\ell u}}{0.4164} \right) \left( \frac{\lambda_{\ell u}}{1215.67 \text{ \AA}} \right) \left( \frac{10 \text{ km s}^{-1}}{b} \right)$$

- In the WNM, Ly $\alpha$  will be optically thin ( $\tau_0 < 1$ ) when  $N_\ell < 10^{13} \text{ cm}^{-2}$  and optically thick ( $\tau_0 > 1$ ) when  $N_\ell > 10^{13} \text{ cm}^{-2}$ .
- In the CNM, Ly $\alpha$  will be optically thin when  $N_\ell < 10^{12} \text{ cm}^{-2}$  and optically thick when  $N_\ell > 10^{12} \text{ cm}^{-2}$  (because  $b \approx 1 \text{ km s}^{-1}$ ).
- In Milky Way, the total column density of hydrogen atom is  $N_\ell \sim 10^{20} - 10^{22} \text{ cm}^{-2}$ .

The percentage of the sky covered by H I at a given  $N_{\text{H}}$ .

Figure 4 in Dickey & Lockman (1990, ARA&A)



- As a reference, the column density of the Earth's atmosphere, looking upward from sea level, is  $N \sim 2 \times 10^{25} \text{ cm}^{-2}$ .

# Absorption Line Shapes

- Lyman  $\alpha$  absorption line profiles for  $b = 10 \text{ km s}^{-1}$

$$F_\nu/F_\nu(0) = e^{-\tau_0 H(u,a)}$$

- When  $\tau_0 < 1$ ,  $F_\nu/F_\nu(0) \approx 1 - \tau_\nu$  and thus the shape of an absorption line resembles the upside-down Voight function.
- When  $\tau_0 \gg 1$ , the absorption line saturates at its center and becomes increasingly “box-shaped.”

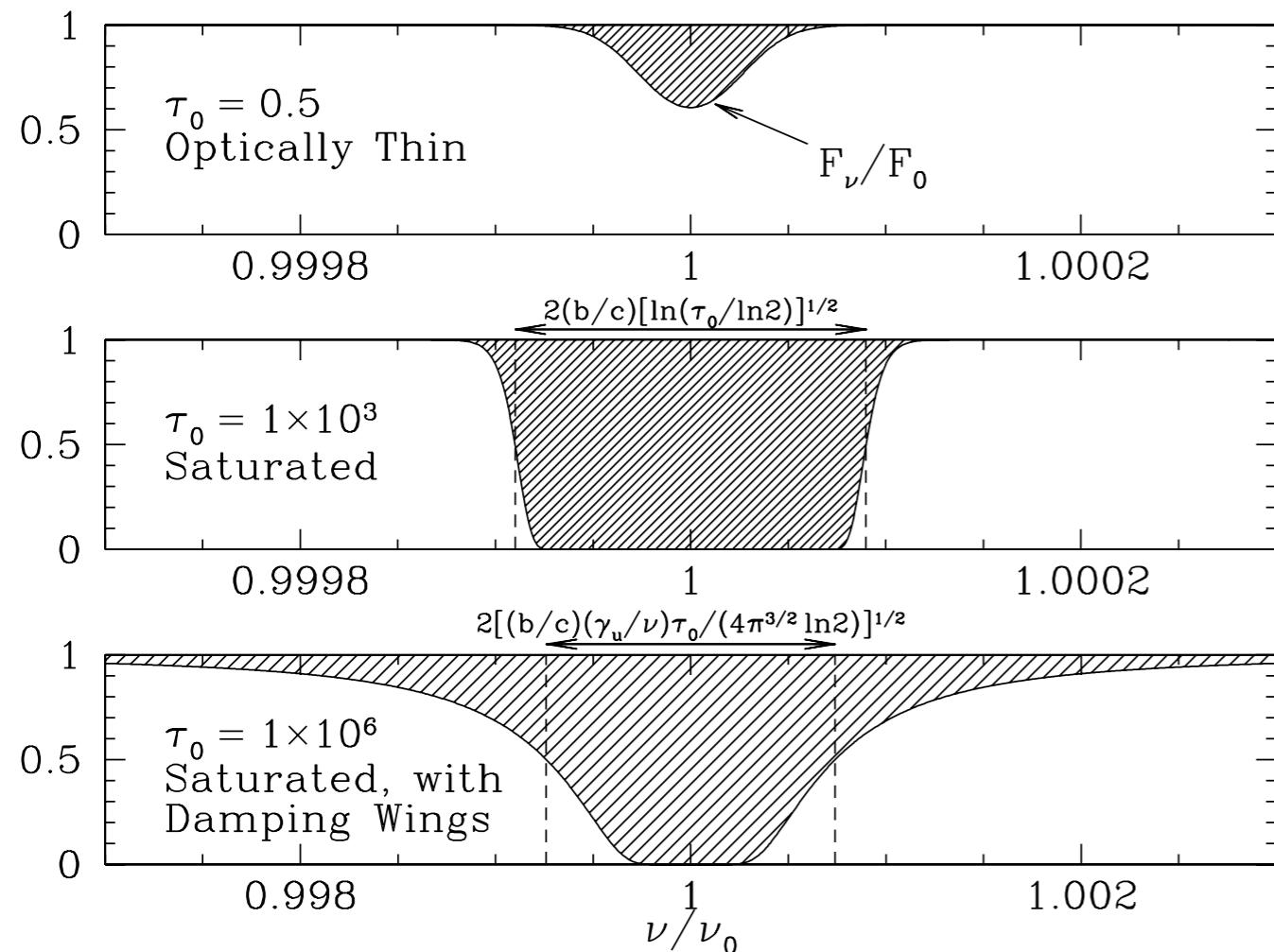
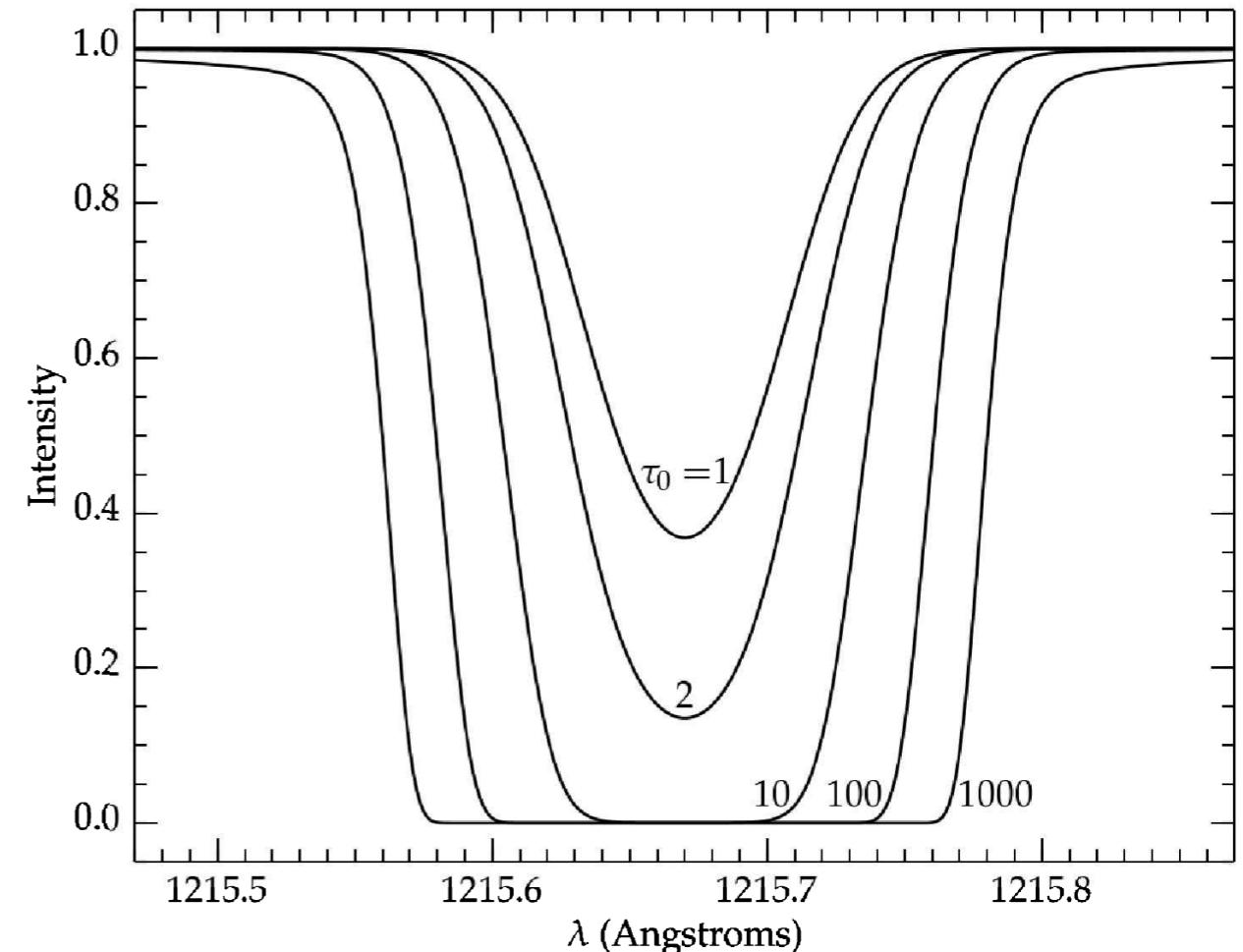


Figure 9.1 in [Draine]

Note the different abscissa in the lowest panel.



Lyman  $\alpha$  absorption lines for  $b = 10 \text{ km s}^{-1}$ .

Figure 2.6 in [Ryden]

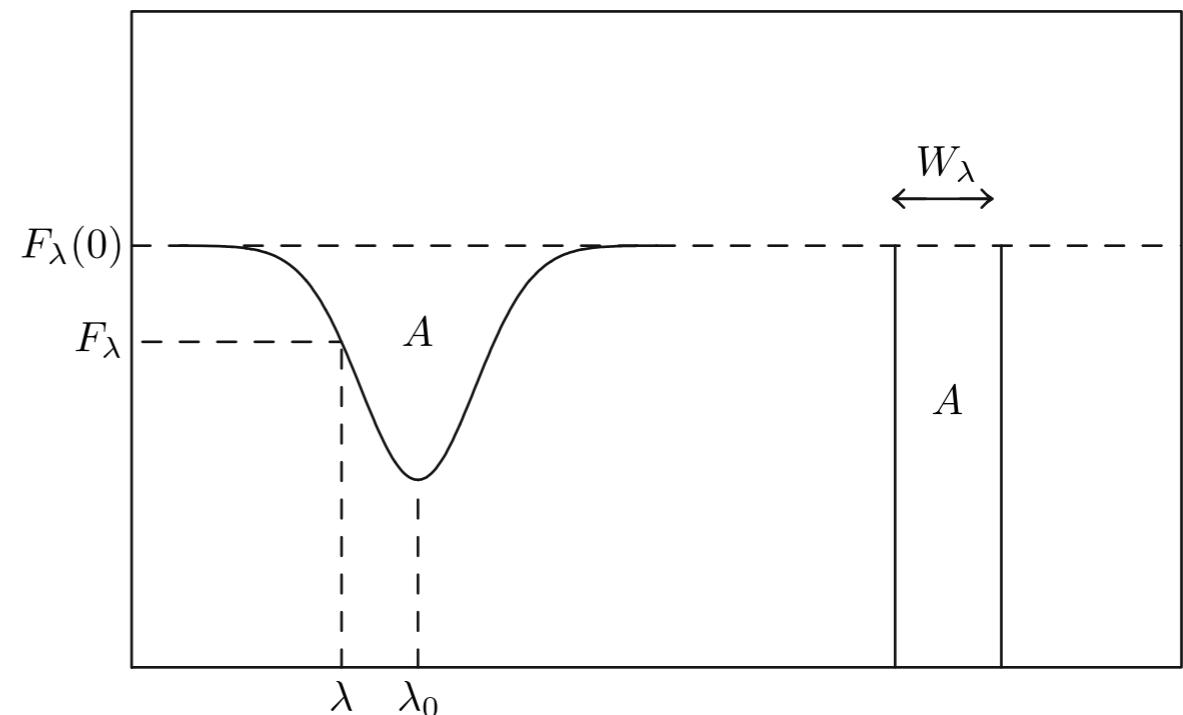
# Equivalent Width & Curve of growth

- ***Equivalent width***

- The spectrograph often lacks the spectral resolution to resolve the profiles of narrow lines, but can measure the total amount of “missing power” resulting from a narrow absorption line.
- *The equivalent width is a measure of the strength of an absorption line, in terms of “missing power” in the unresolved absorption line.*

A diagram illustrating the absorption of radiation. A blue rectangle represents the initial flux density  $F_\nu(0)$ . An arrow points from  $F_\nu(0)$  to  $F_\nu(s)$ , representing the flux density after passing through a medium. Below the diagram is the equation:

$$F_\nu = F_\nu(0)e^{-\tau_\nu}$$



- ***Curve of growth***

- The curve of growth refers to the numerical relation between the observed equivalent width and the underlying optical depth (or the column density) of the absorber.

# Equivalent Width

- Suppose that we measure the energy flux density  $F_\nu$  using an aperture of solid angle  $\Delta\Omega$ . Then, we obtain the flux density at the observer:

$$F_\nu = F_\nu(0)e^{-\tau_\nu} + B_\nu(T_{\text{exc}})\Delta\Omega(1 - e^{-\tau_\nu})$$

Here,  $F_\nu(0)$  is the flux density of the background light source.

- At optical frequencies and in the neutral medium, nearly all atoms are in their ground state. Thus, we normally have  $n_u/n_\ell \ll 1$  and  $B_\nu(T_{\text{exc}})\Delta\Omega \ll F_\nu(0)$ . Then, we can neglect the emission from the ISM.

$$\frac{h\nu}{k_B T_{\text{exc}}} = \frac{6000}{\lambda} \frac{2.4 \times 10^4 \text{ K}}{T_{\text{exc}}} \gg 1$$

$$F_\nu = F_\nu(0)e^{-\tau_\nu}$$

- If the background spectrum is smooth, we can define the **dimensionless equivalent width** and the **wavelength equivalent width** as follows:

$$W \equiv \int \frac{d\nu}{\nu_0} \left[ 1 - \frac{F_\nu}{F_\nu(0)} \right] = \int \frac{d\nu}{\nu_0} (1 - e^{-\tau_\nu})$$

$$W_\lambda \equiv \int d\lambda (1 - e^{-\tau_\lambda}) \approx \lambda_0 W$$

- The equivalent width is the width of a straight-sided, perfectly black absorption line that has the same integrated flux deficit as the actual absorption line.

# Overall Shape of the Curve of Growth

## **The Curve of Growth**

= the relation between optical depth at line center and equivalent width

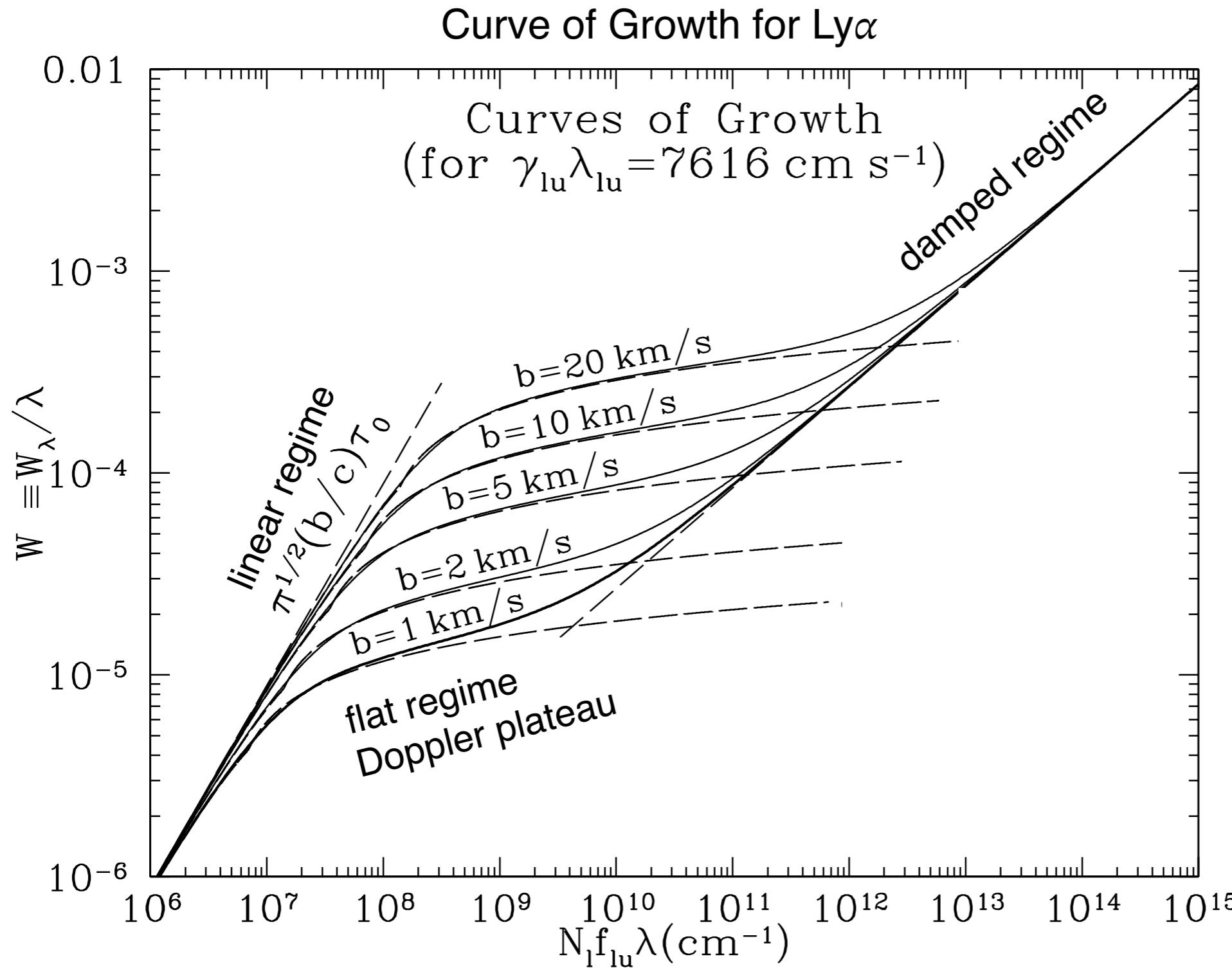


Figure 9.2 in [Draine]

# Homework (due date: 04/14)

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## [Q5] Voigt profile

- We want to derive an approximate formula for the transition point from the Gaussian core to the Lorentz wing, which is defined by

$$u^2 = \ln(\sqrt{\pi}/a) + \ln u^2 \quad \text{or} \quad x = \ln(\sqrt{\pi}/a) + \ln x, \text{ where } x \equiv u^2$$

The above equation can be expressed in the form:

$$x = g(x) \text{ where } g(x) = \ln x + \ln(\sqrt{\pi}/a)$$

This equation can be solved using “**Fixed Point Iteration Method.**” Starting from any initial point  $x_0$ , the following recursive process gives an approximate solution of the equation.

$$x_{n+1} = g(x_n)$$

- (2) Calculate  $a = \Gamma/(4\pi\nu_D)$  for Ly $\alpha$  and  $b = 10 \text{ km s}^{-1}$ , which is appropriate for Ly $\alpha$  in the warm neutral medium (WNM) with  $T \sim 10000 \text{ K}$ . Note that  $\Gamma = \gamma_{u\ell} = 6.265 \times 10^8 \text{ s}^{-1}$  and  $\lambda_{u\ell} = 1215.67 \text{ \AA}$ .

- 
- (2) Plot two graphs,  $f(x) = x$  and  $g(x) = \ln(x) + \ln\left(\sqrt{\pi}/a\right)$ .
- (3) By looking at the two graphs, choose an approximate solution of  $x = g(x)$ . In other words, choose an approximate value where  $y = x$  and  $y = g(x)$  intersect.

Let this approximate solution be  $x_0$ , and then find the numerical solution of  $x = g(x)$  using the fixed point iteration method, as follows:

$$x_1 = g(x_0)$$

$$x_2 = g(x_1)$$

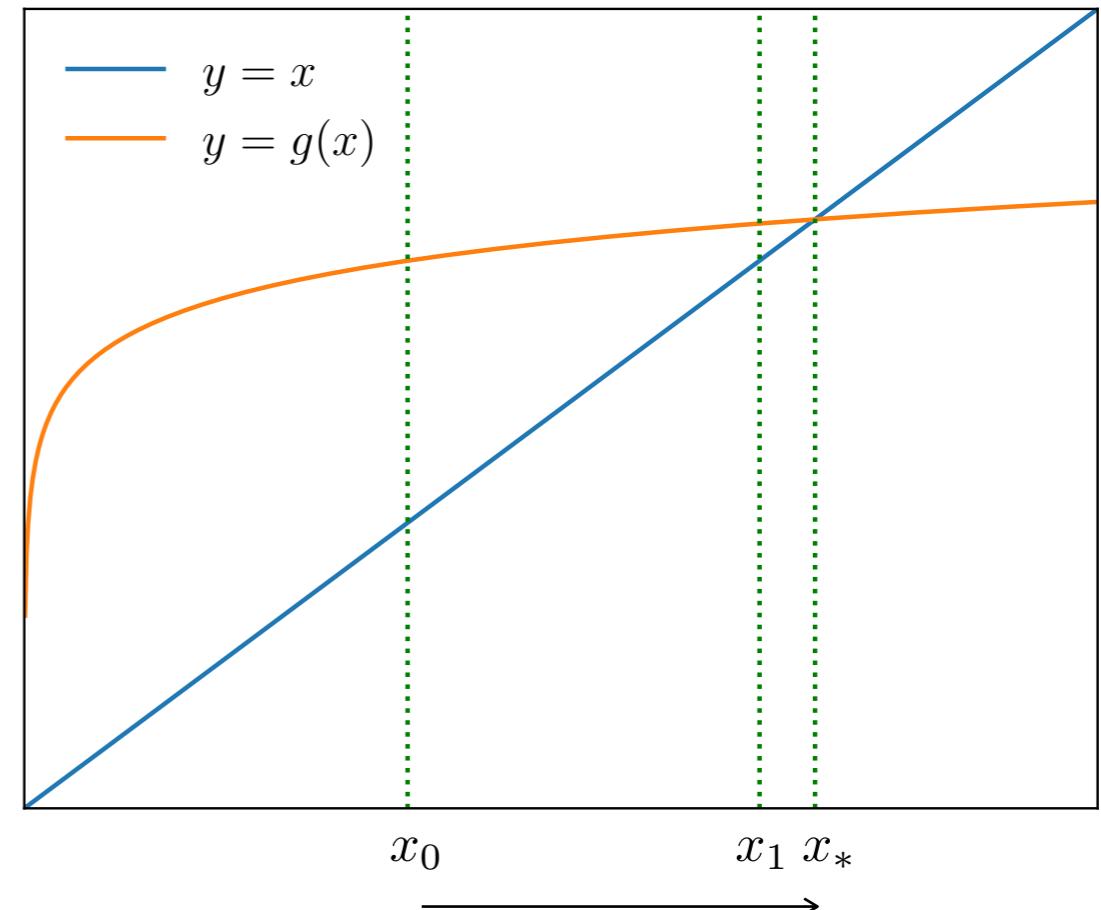
$$x_3 = g(x_2)$$

...

Denote the solution as  $x_*$ .

$$x_* = x_n \text{ as } n \rightarrow \infty$$

What is the value of  $x_*$  that you have found?



- (4) Let's denote the width parameter  $a$  for Ly $\alpha$  and  $b = 10 \text{ km s}^{-1}$  as  $a_*$ . This means that

$$x_* = \ln x_* + \ln(\sqrt{\pi}/a_*)$$

Now, for any parameter  $a$  which is slightly different from  $a_*$ , you may express the constant term in  $g(x)$  as follows:

$$\ln(\sqrt{\pi}/a) = \ln(a_*/a) + \ln(\sqrt{\pi}/a_*)$$

To find the solution for  $a \neq a_*$  (but, still close to  $a_*$ , i.e.,  $a \approx a_*$ ), choose an initial guess for this case as  $x_0 = x_*$ .

Show that the solution for any  $a$  can be expressed, after a single iteration, as follow:

$$x_1 = x_* + \ln(a_*/a)$$

Insert numerical values into the above equation, and confirm that your solution is equivalent with or the same as the results in this lecture note and Eq. (6.42) in Draine's book.

- (5) Compare your solution with Eq. (2.39) in Ryden's book (our textbook). Does the equation in Ryden's book is equivalent with that of yours?