Interstellar Medium (ISM)

Week 5
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[3] Line Broadening Mechanisms

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

  - Here, ν_0 is the rest-frame frequency.

- 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

$$f(v_z)dv_z = \left(\frac{m}{2\pi kT}\right)^{1/2} \exp\left(-\frac{mv_z^2}{2kT}\right) dv_z$$

Here, m = mass of the atom

- From the Doppler shift formula, we have

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

- 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

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

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

$$\boxed{\begin{array}{l} \Delta\nu_D = \dfrac{\nu_0}{c} v_{\rm th} \text{ is the Doppler width.} \\ \\ v_{\rm th} = \sqrt{\dfrac{2kT}{m}} \text{ is the thermal velocity.} \end{array}}$$

- Numerical value of the velocity broadening is

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

- 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.

$$\boxed{\begin{aligned}\Delta\nu_{\rm D} &= \nu_0\frac{b}{c} \\ b &\equiv \left(v_{\rm th}^2 + v_{\rm turb}^2\right)^{1/2}\end{aligned}}$$

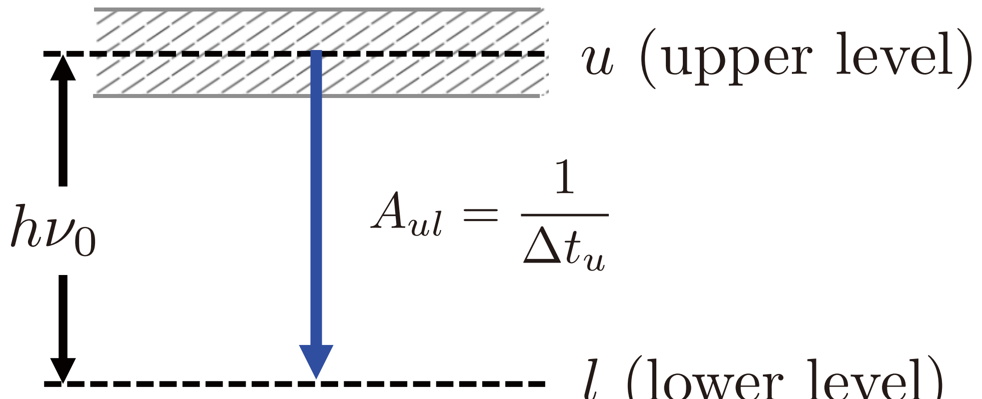
where $v_{\rm turb}$ is $\sqrt{2}$ times a root-mean-square measure of the turbulent velocities. This assumes that the turbulent velocities also have a Gaussian distribution.

The convolution of two Gaussian functions with the widths (standard deviations) σ_1 and σ_2 is a Gaussian function with the width of σ, 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 Δt, then uncertainty (spread) in energy ΔE 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

$$\Delta\nu_u = \text{spread in frequency}$$
$$= \Delta E_u/h = 1/(2\pi\Delta t_u) = A_{ul}/(2\pi) \longrightarrow$$

(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

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

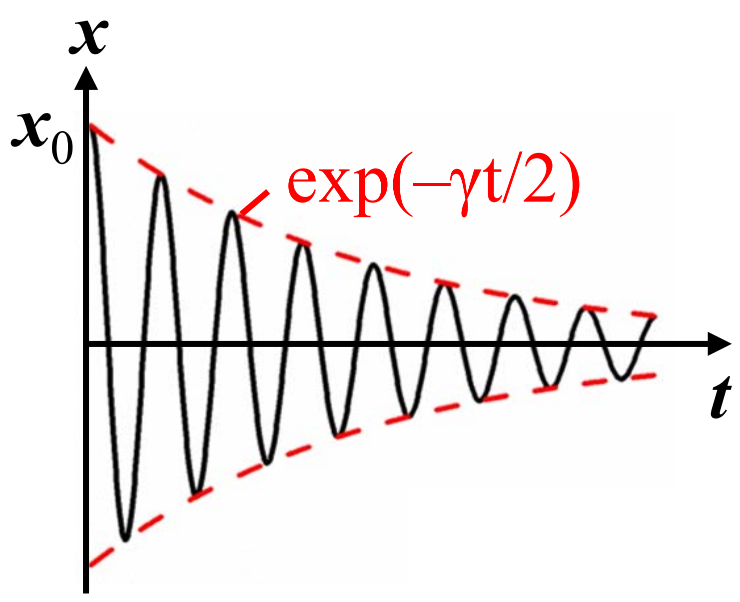
Hence, the FWHM of the Lorentz function: $\Delta\nu_u = \gamma/2\pi$

↓

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

Classical Physical Meaning

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).

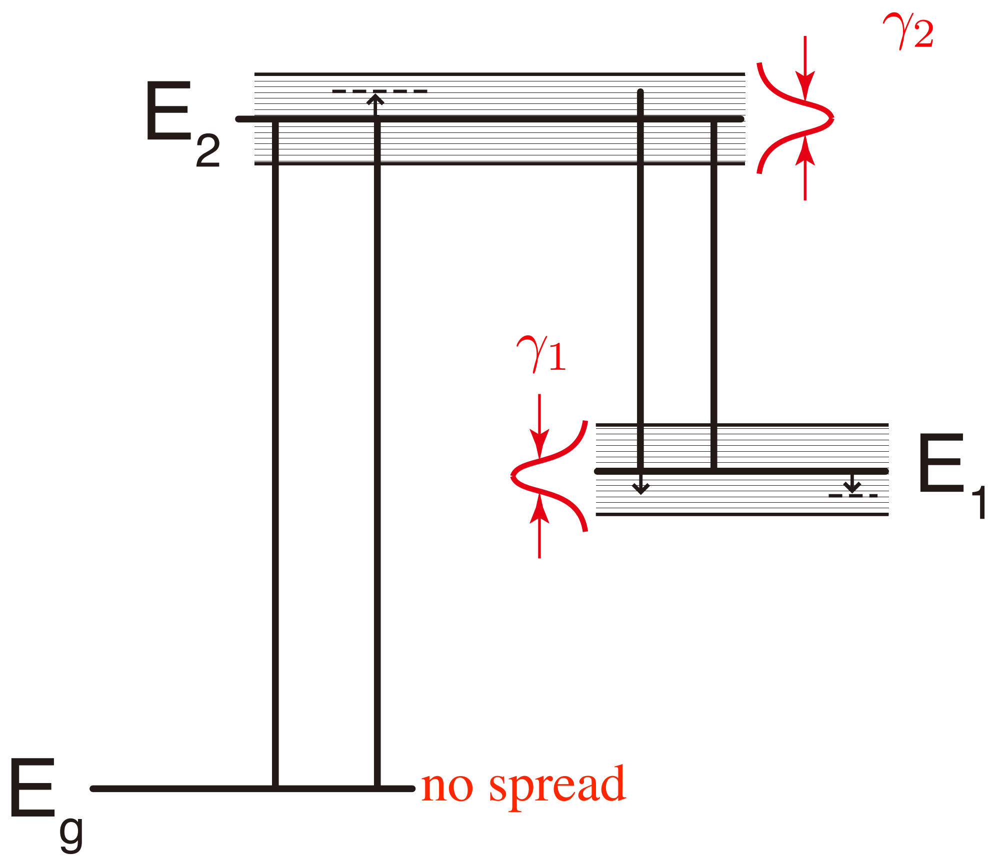
  The distribution of sublevels are explained by the Heisenberg Uncertainty Principle. The level has a lifetime $\Delta t = 1/A$ (A = Einstein A coefficient) and a spread in energy about $\Delta E \approx \hbar/\Delta t = \hbar A$.

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

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.

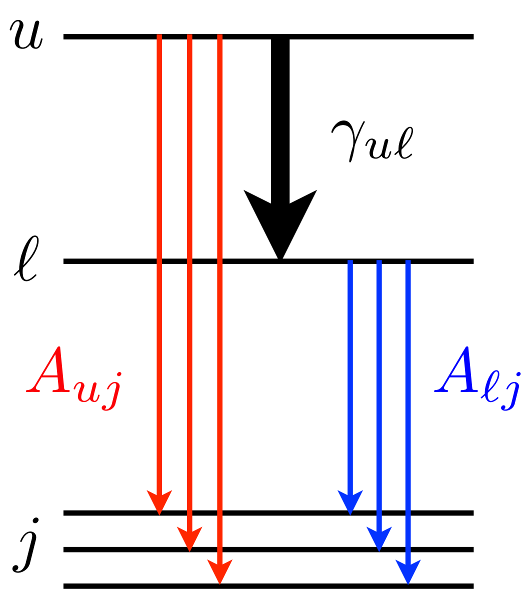
- *The energy spread of sublevels is described by a Lorentzian profile with the damping parameter of* $\gamma = A$*.*
- *This picture implies that the emission line profile is the same as the absorption line profile.*

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

$$\begin{aligned}\Delta\nu_{\rm D} &= \nu_{u\ell}\frac{\Delta v}{c} \\ \Delta\nu_{\rm D} &\approx A_{u\ell}\end{aligned} \quad \longrightarrow \quad \Delta v \sim 3 \times 10^{-17} c \sim 10\,{\rm nm\,s^{-1}} \sim 30\,{\rm cm\,yr^{-1}}$$

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

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



  - For Lyα (n = 1-2), $\gamma_{u\ell} = A_{21} = 6.3 \times 10^{8}\,{\rm s^{-1}}$

$$\Delta\nu/\nu = (\gamma/2\pi)/(c/\lambda) \sim 4 \times 10^{-8}$$

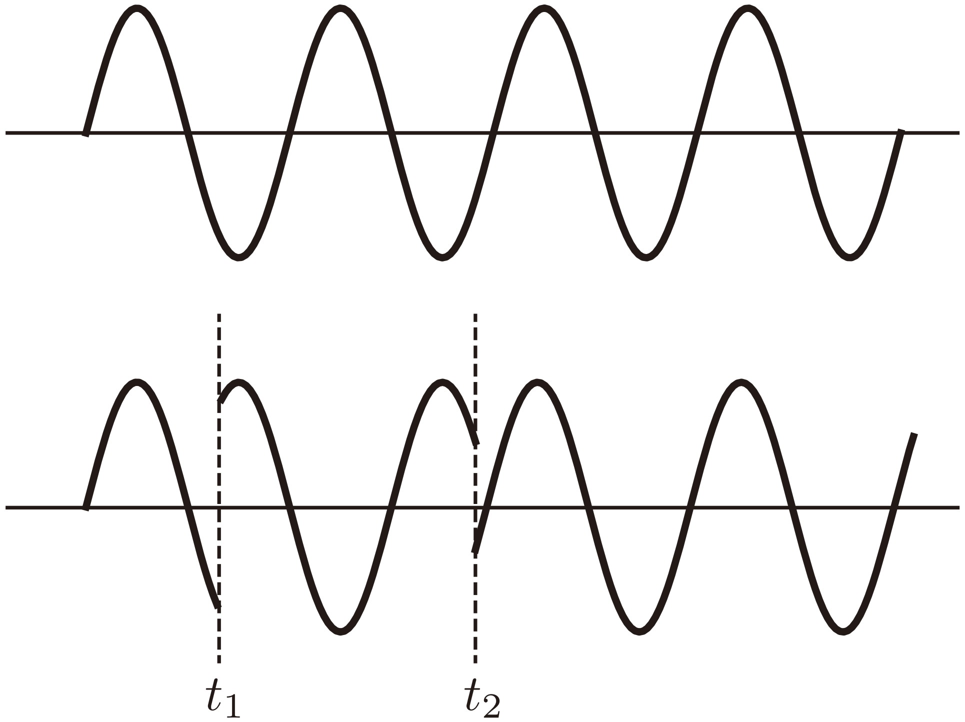
  - For Hα (n = 2-3), $\gamma_{u\ell} = A_{32} + A_{31} + A_{21} = 8.9 \times 10^{8}\,{\rm s^{-1}}$

$$\Delta\nu/\nu \sim 3 \times 10^{-7}$$

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 $\nu_{\rm col}$, that is, each atom experiences $\nu_{\rm col}$ collisions per unit time on the average, then the profile is

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



purely sinusoidal

random phase interruptions by atomic collisions

For derivation of the above formula, see Problem 10.7 of Radiative Processes in Astrophysics [Rybiki & Lightman], Chap. 11 of Atomic Spectroscopy and Radiative Processes [Degl'Innocenti], and Chap 8.3 in Theory of Stellar Atmospheres [Hubeny & Mihalas]

- **[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: $v_{\rm th} \equiv \sqrt{\dfrac{2kT}{m}},\ y \equiv \dfrac{v_z}{v_{\rm th}}$

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

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 $\nu' = \nu - [\nu_0 + \nu_0(v_z/c)] = (\nu - \nu_0) - \nu_0(v_{\rm th}/c)y$ is supposed to be multiplied with the Maxwell distribution.

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

Let $\Delta\nu_{\rm D} \equiv \nu_0 \dfrac{v_{\rm th}}{c},\ u \equiv \dfrac{\nu - \nu_0}{\Delta\nu_{\rm D}} = \dfrac{\nu-\nu_0}{\nu_0}\dfrac{c}{v_{\rm th}},\ a = \dfrac{\Gamma/4\pi}{\Delta\nu_{\rm D}}$

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

- The profile can be written using the Voigt function.

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

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

$$u = \frac{\nu - \nu_0}{\Delta\nu_{\mathrm{D}}} = \frac{\nu - \nu_0}{\nu_0}\frac{c}{v_{\mathrm{th}}}$$

In the velocity term,

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

Voigt-Hjerting function:

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

$$a \equiv \frac{\Gamma}{4\pi\Delta\nu_{\mathrm{D}}}$$

$$u \equiv \frac{\nu - \nu_0}{\Delta\nu_{\mathrm{D}}}$$

$$\Delta\nu_{\mathrm{D}} = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}}$$

Including the turbulent motion,

$$\Delta\nu_{\mathrm{D}} = \nu_0 \frac{v_{\mathrm{th}}}{c} \ \rightarrow \ \Delta\nu_{\mathrm{D}} = \nu_0 \frac{b}{c} = \frac{b}{\lambda_0}$$

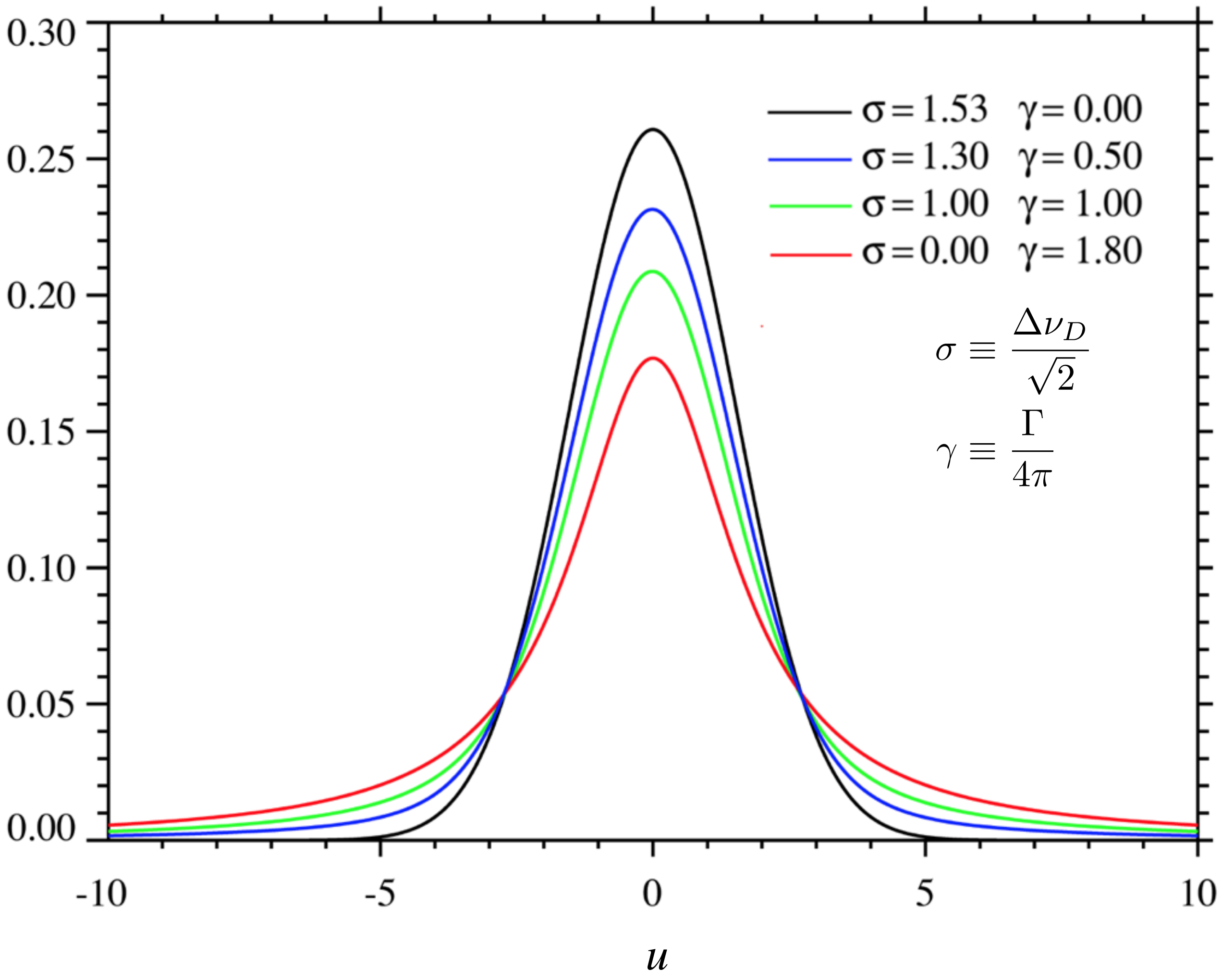
$$\text{where } b = \sqrt{v_{\mathrm{th}}^2 + v_{\mathrm{turb}}^2}, \ v_{\mathrm{th}} = \sqrt{\frac{2kT}{m}}, \ v_{\mathrm{turb}} = \sqrt{2}\sigma_{\mathrm{turb}}^{\mathrm{rms}}$$

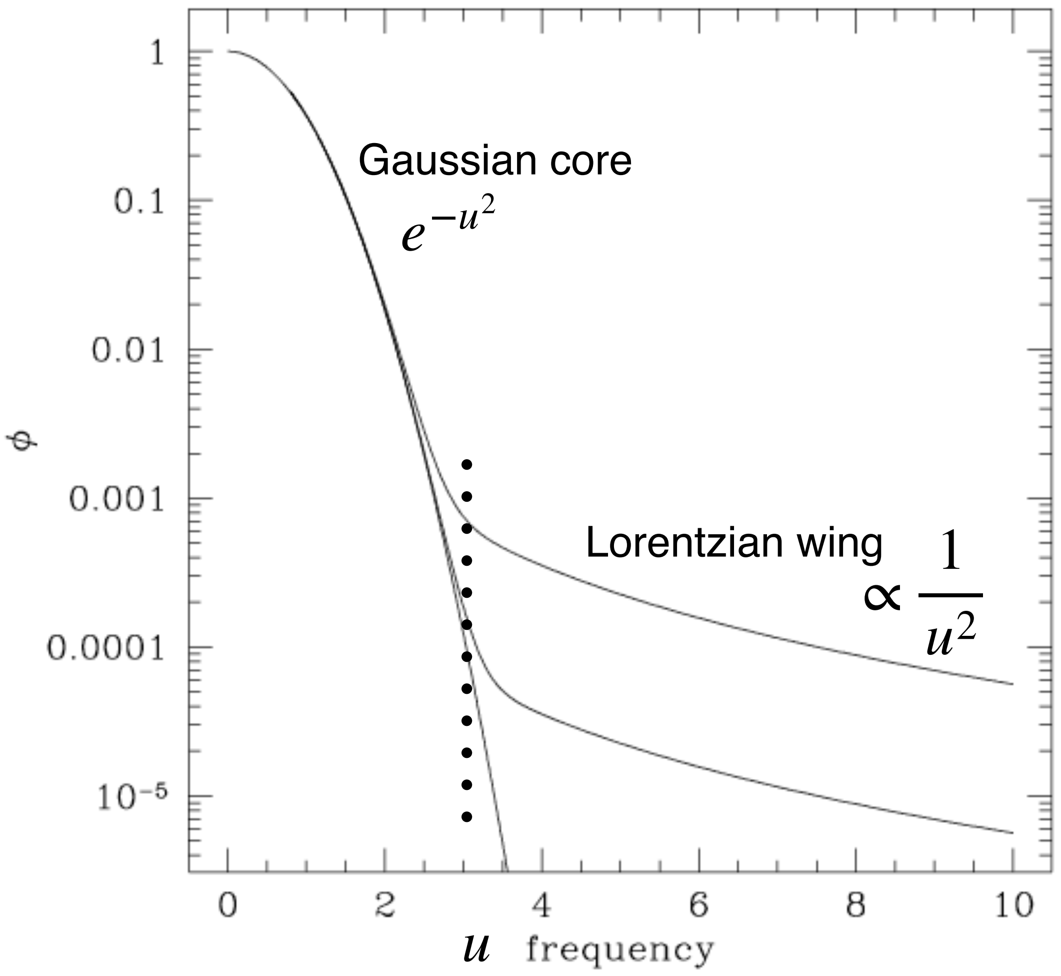
$$u = \frac{v}{b}$$

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 Lyα at T = 10^4 K, $a \sim 0.005$.

- Line center:

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

- 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 $a = 0$.

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

  - 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:

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

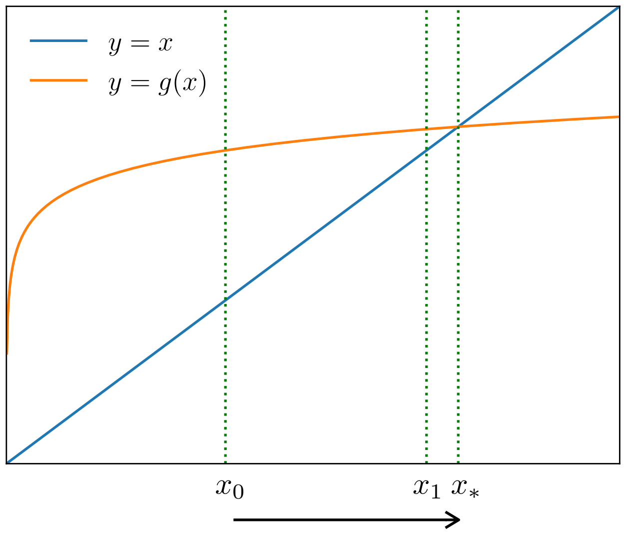
  - The solution for this transcendental equation for Lyα is

$$u^2 \approx 10.31 + \ln\left[\left(\frac{6.265\times10^8\,\mathrm{s^{-1}}}{\gamma_{u\ell}}\right)\left(\frac{1215.67\,\mathrm{\AA}}{\lambda_{u\ell}}\right)\left(\frac{b}{10\,\mathrm{km\,s^{-1}}}\right)\right]$$

$b = 13\,\mathrm{km\,s^{-1}}\,(T/10^4\,\mathrm{K})^{1/2}$ 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 $|v| \gtrsim 3.2\,(b/10\,\mathrm{km\,s^{-1}})$.

Fixed point iteration



Atomic Processes related to Line emission

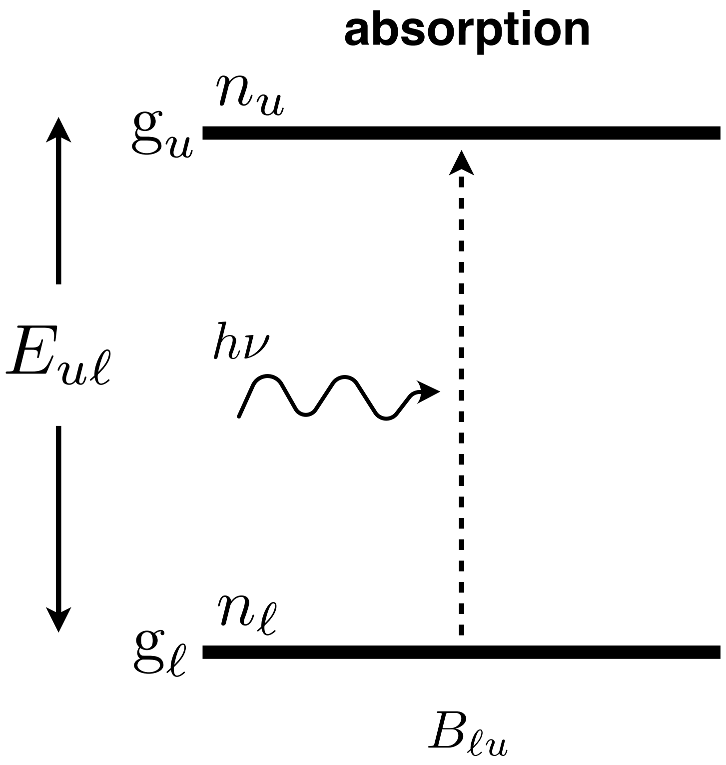
- **Excitation and de-excitation (Transition)**
    - Radiative excitation (photoexcitation; photoabsorption)
    - Radiative de-excitation (spontaneous emission and stimulated emission)
    - Collisional excitation
    - Collisional de-excitation

- **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 <=> Photoionization
    - Dielectronic Recombination (not dielectric!)
    - Three-body recombination <=> 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 ℓ 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.



$$\text{absorption}: \quad X_\ell + h\nu \ \rightarrow \ X_u \ (h\nu = E_{u\ell})$$

    - The rate per volume at which the absorbers absorb photons will be proportional to both the energy density u_ν of photons of the appropriate energy and the number density n_ℓ of absorbers in the lower level ℓ.

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

    - 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 ℓ with emission of a photon. There are two ways this can happen:

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

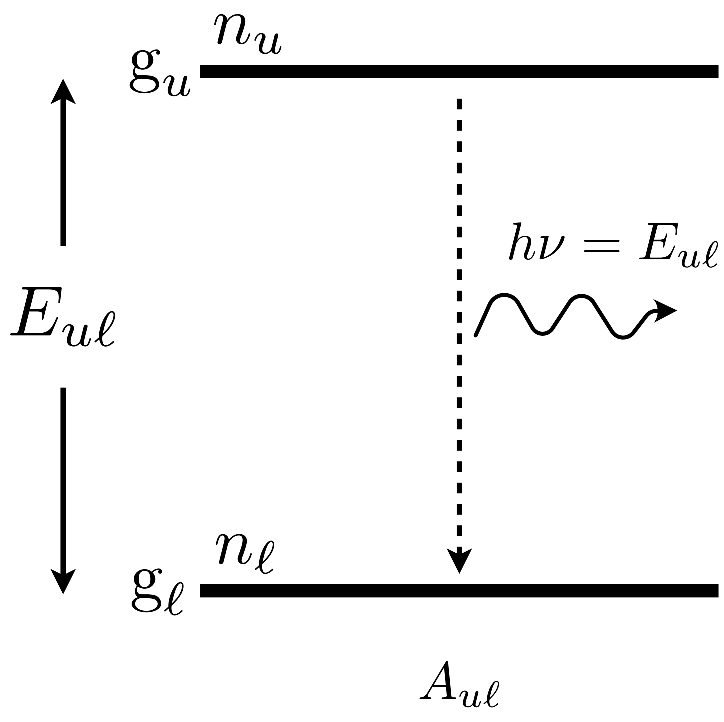
$$\text{stimulated emission}: \quad X_u + h\nu \;\rightarrow\; X_\ell + 2h\nu \quad (h\nu = E_{u\ell})$$

  - ***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_ν of these photons.

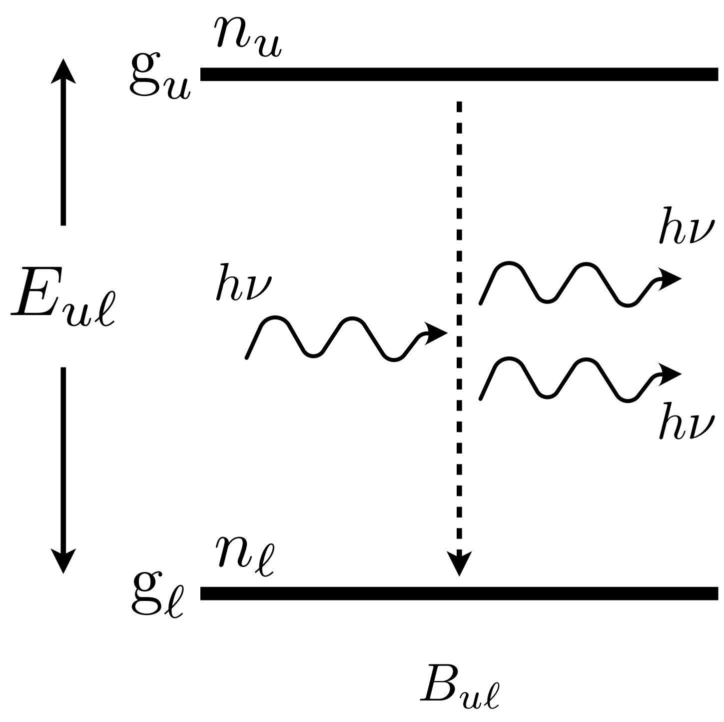
$$\left(\frac{dn_\ell}{dt}\right)_{u\rightarrow\ell} = -\left(\frac{dn_u}{dt}\right)_{u\rightarrow\ell} = n_u\left(A_{u\ell} + B_{u\ell}u_\nu\right)$$

  - 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 $u \rightarrow \ell$.

spontaneous emission



stimulated emission



Relations between the Einstein coefficients

- 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.

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

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

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

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

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

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

$$\begin{aligned} u_\nu &= \frac{n_u A_{u\ell}}{n_\ell B_{\ell u} - n_u B_{u\ell}} \\ &= \frac{\left(n_u A_{u\ell}\right) / \left(n_\ell B_{\ell u}\right)}{1 - \left(n_u B_{u\ell}\right) / \left(n_\ell B_{\ell u}\right)} \\ &= \frac{\left(\mathrm{g}_u/\mathrm{g}_\ell\right) e^{-h\nu/kT} \left(A_{u\ell}/B_{\ell u}\right)}{1 - \left(\mathrm{g}_u/\mathrm{g}_\ell\right) e^{-h\nu/kT} \left(B_{u\ell}/B_{\ell u}\right)} \quad \leftarrow \quad \frac{n_u}{n_\ell} = \frac{\mathrm{g}_u}{\mathrm{g}_\ell} e^{-h\nu_{u\ell}/kT_{\rm exc}} \\ &= \frac{\left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(A_{u\ell}/B_{\ell u}\right)}{e^{h\nu/kT} - \left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(B_{u\ell}/B_{\ell u}\right)} \end{aligned}$$

[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.

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.

$$\left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(A_{u\ell}/B_{\ell u}\right) = \frac{8\pi h\nu^3}{c^3}$$

$$\left(\mathrm{g}_u/\mathrm{g}_\ell\right) \left(B_{u\ell}/B_{\ell u}\right) = 1$$

Therefore, only one coefficient is independent.

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

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

$$B_{\ell u} = \frac{\mathrm{g}_u}{\mathrm{g}_\ell} B_{u\ell} \qquad B_{\ell u} = \frac{\mathrm{g}_u}{\mathrm{g}_\ell} \frac{c^3}{8\pi h\nu^3} A_{u\ell}$$

- 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:

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

  - 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:

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

  - 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

- 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

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

  - 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:

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

  - If the cross section has a normalized profile of ϕ_ν, we can write the absorption cross section as follows:

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

(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.

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

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

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

pure absorption coefficient

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

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

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

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

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

or

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

- ***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:

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

  - 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 ϕ_ν, we can write the emissivity as follows:

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

- The correction factor for the stimulated emission in absorption coefficient:
  - For Lyα line,

$$h\nu_{u\ell} = 10.2\,\mathrm{eV} \quad \rightarrow \quad 1 - \exp\left(-\frac{h\nu_{u\ell}}{k_{\mathrm{B}}T_{\mathrm{exc}}}\right) = 1 - \exp\left(-\frac{1.1837\times10^{5}\,\mathrm{K}}{T_{\mathrm{exc}}}\right)$$
$$\simeq 1 \quad \text{for } T_{\mathrm{exc}} \approx T_{\mathrm{gas}} < 1\times10^{5}\,\mathrm{K}$$

    - ‣ The stimulated emission is negligible.
  - For 21 cm line,

$$h\nu_{u\ell} = 6\,\mu\mathrm{eV} \quad \rightarrow \quad 1 - \exp\left(-\frac{h\nu_{u\ell}}{k_{\mathrm{B}}T_{\mathrm{exc}}}\right) = 1 - \exp\left(-\frac{0.068\,\mathrm{K}}{T_{\mathrm{exc}}}\right)$$
$$\simeq \frac{0.068\,\mathrm{K}}{T_{\mathrm{exc}}} \ll 1 \quad \text{for } T_{\mathrm{exc}} \approx T_{\mathrm{gas}} \sim 100\,\mathrm{K}$$

    - ‣ 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***:

$$
\begin{aligned}
S_\nu &= \frac{j_\nu}{\alpha_\nu} \\
&= \frac{(1/4\pi) n_u A_{u\ell} h\nu_{u\ell} \phi_\nu^{\rm emiss}}{n_\ell \sigma_{\ell u}^{\rm eff}(\nu)} \\
&= \frac{n_u \frac{A_{u\ell}}{4\pi} h\nu_{u\ell} \phi_\nu^{\rm emiss}}{n_\ell \frac{g_u}{g_\ell} \frac{c^2}{8\pi\nu_{u\ell}^2} A_{u\ell} \phi_\nu^{\rm abs} \left[1 - \exp\left(-h\nu_{u\ell}/k_{\rm B}T_{\rm exc}\right)\right]} && \leftarrow \frac{n_u}{n_\ell} = \frac{{\rm g}_u}{{\rm g}_\ell} \exp\left(-h\nu_{u\ell}/k_{\rm B}T_{\rm exc}\right) \\
&= \frac{2h\nu_{u\ell}^3}{c^2} \frac{1}{\exp\left(h\nu_{u\ell}/k_{\rm B}T_{\rm exc}\right) - 1} && \leftarrow \phi_\nu^{\rm emiss} = \phi_\nu^{\rm abs}
\end{aligned}
$$

- This is called the ***generalized Kirchhoff's law***.
- **The intrinsic profiles for absorption and emission should are the same**.
  - The source function should approach the Planck function in LTE ($T_{\rm exc} = T_{\rm kinetic}$). 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 $\frac{\pi e^2}{m_e c} = 0.02654 \ \mathrm{cm^2\,Hz}$ 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

$$\boxed{A_{u\ell} = \frac{8\pi^2 e^2 \nu_{u\ell}^2}{m_e c^3} \frac{\mathrm{g}_\ell}{\mathrm{g}_u} f_{\ell u} = \left(\frac{0.8167\,\mathrm{cm}}{\lambda_{u\ell}} \right)^2 \frac{\mathrm{g}_\ell}{\mathrm{g}_u} f_{\ell u} \ [\mathrm{s}^{-1}]}$$

  - For 21.1 cm line, $\mathrm{g}_u = 3, \ g_\ell = 1 \ (g_F = 2F + 1)$

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

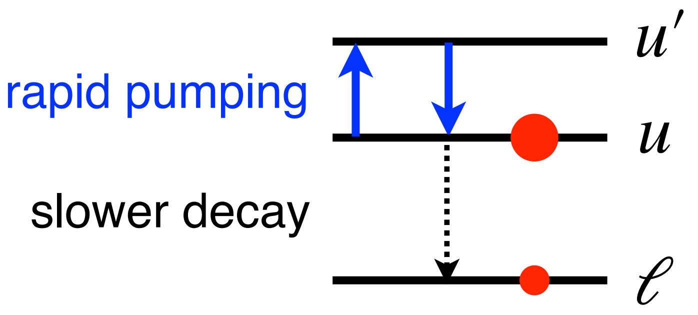
  - For Lyα (1215.67Å) line, $\mathrm{g}_u = 3, \ g_\ell = 1 \ (g_L = 2L + 1)$

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

$$\begin{aligned} f_{\ell u} &= 0.27760 \text{ for } {}^2S_{1/2} \rightarrow {}^2P_{3/2} \\ &= 0.13881 \text{ for } {}^2S_{1/2} \rightarrow {}^2P_{1/2} \end{aligned}$$

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 ℓ to satisfy the inequality (also to have a negative excitation temperature).



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

-
    - 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_2O, and SiO, and hence we speak of ***maser (microwave amplification by stimulated emission of radiation)*** emission.

- Observational properties
  - If $|k_\mathrm{B} T_{\mathrm{exc,u}\ell}| \gg h\nu$, the RT equation becomes

$$\begin{aligned} T_A &= T_A(0) e^{-\tau_\nu} + T_\mathrm{exc}\left(1 - e^{-\tau_\nu}\right) \\ &= \left(T_A(0) + |T_\mathrm{exc}|\right) e^{|\tau_\nu|} - |T_\mathrm{exc}| \end{aligned}$$

  - The factor $e^{|\tau_\nu|}$ is in some cases very large - some OH and H_2O masers have been observed to have $T_A > 10^{11}\,\mathrm{K}$.
  - 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 masing region.
    - ‣ $e^{|\tau_\nu|}$ is more strongly in ν than $|\tau_\nu|$ - the maser line is narrower than the actual velocity distribution of the masing 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

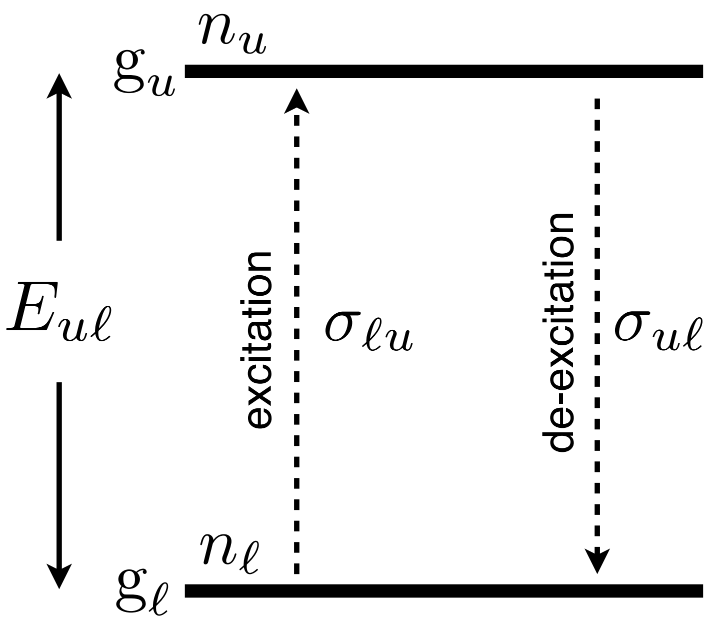
- **Collisional Rate (Two Level Atom)**
  - The cross section $\sigma_{\ell u}$ for collisional excitation from a lower level ℓ to an upper level u is, in general, inversely proportional to the impact energy (or v^2) above the energy threshold $E_{u\ell}$ and is zero below.
  - The collisional cross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

$$\boxed{\begin{aligned}\sigma_{\ell u}(v) &= (\pi a_0^2)\left(\frac{hR_{\rm H}}{\frac{1}{2}m_e v^2}\right)\frac{\Omega_{\ell u}}{{\rm g}_\ell}\quad {\rm cm}^2 \quad {\rm for}\quad \frac{1}{2}m_e v^2 > E_{u\ell} \\ &= \frac{h^2}{4\pi m_e^2 v^2}\frac{\Omega_{\ell u}}{{\rm g}_\ell}\end{aligned}}$$

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

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

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



  - The collision strength $\Omega_{\ell u}$ is a function of electron velocity (or energy) but is often approximately constant near the threshold. Here, g_ℓ 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_ℓ 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

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

where $E = \frac{1}{2}m_e v_u^2$

and the symmetry of the collision strength between levels.

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

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

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

$$\begin{aligned} k_{u\ell} &= \int_0^\infty v\sigma_{u\ell}(v) f(v) dv \\ &= \left(\frac{2\pi\hbar^4}{k_\mathrm{B} m_e^3}\right)^{1/2} T^{-1/2} \frac{\langle\Omega_{u\ell}\rangle}{g_u} \\ &= \frac{8.62942\times10^{-6}}{T^{1/2}} \frac{\langle\Omega_{u\ell}\rangle}{g_u} \quad [\mathrm{cm}^3\ \mathrm{s}^{-1}], \end{aligned}$$

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

effective collision strength:

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

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

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

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

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

Here, $k_{\ell u}$ and $k_{u\ell}$ are the **collisional rate coefficient for excitation and de-excitation** coefficients in units of cm³ s⁻¹, respectively. We also note that ***the rate coefficients for collisional excitation and de-excitation are related by***

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

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

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

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

  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) - $^2P_{3/2} : {}^2P_{1/2} = 2 : 1$

Homework (due date: 04/14)

[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

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

The above equation can be expressed in the form:

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

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.

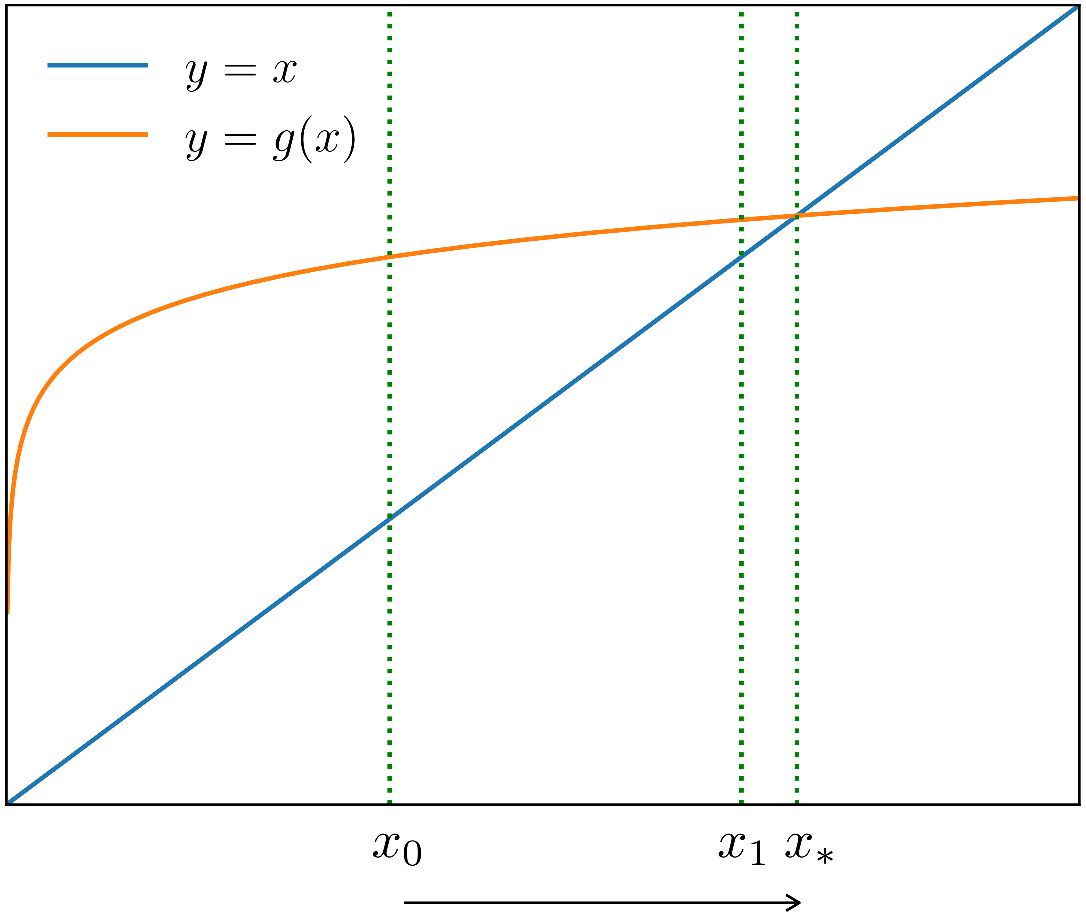
$$\boxed{x_{n+1} = g(x_n)}$$

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

(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:



$$\begin{aligned} x_1 &= g(x_0) \\ x_2 &= g(x_1) \\ x_3 &= g(x_2) \\ &\ldots \end{aligned}$$

Denote the solution as x_*.

$$x_* = x_{\mathrm{n}} \quad \text{as } n \to \infty$$

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

---

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

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

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

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

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:

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

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?