Stellar Atmospheres
Lecture 14

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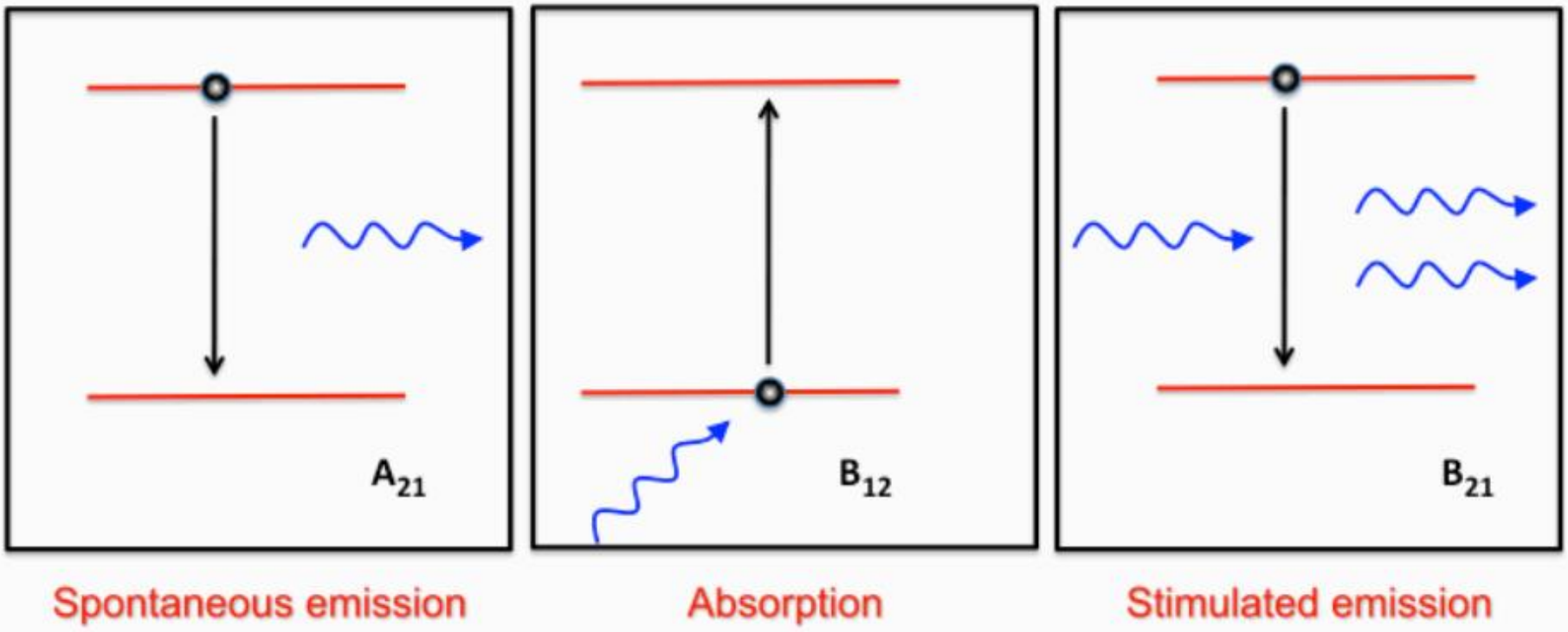
Spectral line formation

EINSTEIN COEFFICIENTS
LINE ABSORPTION COEFFICIENT
NATURAL LINE WIDTH
NATURAL BROADENING
DOPPLER BROADENING

Einstein coefficients



Einstein coefficients concern the probability that a particle spontaneously emits a photon, the probability to absorb a photon, and the probability to emit a photon under the influence of another incoming photon. Einstein's coefficients are valid for all radiation fields.

Relation between Einstein coefficients

$$\frac{A_{21}}{B_{21}} = \frac{2h\nu_{21}^3}{c^2} \quad \rightarrow \quad A_{21} = B_{21}\frac{2h\nu_{21}^3}{c^2}$$

$$\frac{g_1 B_{12}}{g_2 B_{21}} = 1 \quad \rightarrow \quad g_1 B_{12} = g_2 B_{21}$$

Comparison of induced and spontaneous emission

There was Home work:

- When (temperatures, wavelengths) is spontaneous or induced emission stronger?

  Assume LTE (blackbody)

Induced and Spontaneous emission

When is spontaneous emission stronger?

Total amount of emitted photons per unit time at a given frequency is

Spontaneous emission: $\eta_{sp} = n_2 A_{21}$

Stimulated emission: $\eta_{st} = n_2 B_{21} J_\nu$

$$\frac{\eta_{sp}}{\eta_{st}} = \frac{n_2 A_{21}}{n_2 B_{21} J} = \frac{2h\nu_{21}^3}{c^2 J}$$

TE: blackbody, $J = B_\nu(T)$

$$B_\nu(T) = \frac{2h\nu_{21}^3}{c^2}\left(e^{\frac{h\nu_{21}}{kT}} - 1\right)^{-1}$$

$$\frac{\eta_{sp}}{\eta_{st}} = e^{\frac{h\nu_{21}}{kT}} - 1$$

$$e^{\frac{h\nu_{21}}{kT}} = 2 \quad \Rightarrow \quad h\nu_{21} = kT \ln 2 \quad \Rightarrow \quad \lambda_* = \frac{hc}{kT \ln 2} = \frac{2.076 \times 10^8}{T}\,\text{Å}$$

At wavelengths shorter than λ_* spontaneous emission is dominant

T=5777K → $\lambda_* \approx 41000$ Å $\lambda_* = 6563$ Å → T≈31600K $\lambda_* = 4340$Å → T≈48000K

Line profiles

All the spectral lines are not monochromatic but have a finite width and a particular profile. Width and shape of a line depend directly in atomic transitions and plasma environment

In each spectral line, photons of different frequencies (but close to central frequency ν_0) can be absorbed. Let us call **φ(ν)** the probability that the transition occurs by emitting or absorbing a photon with energy $h\nu$
(emission or absorption line, $\int \varphi(\nu)d\nu \equiv 1$).

Natural Line Width

- A spectral line of an atom is formed by a transition of electron between two energy levels, whose difference yields the frequency of the line.
- The bound-bound absorption problem is analogous to the mechanical system of a damped, driven harmonic oscillator.
- In the classical picture of an atom, we can consider the electron as being bound to the atom. Any force trying to remove it will be counteracted by an opposing force. If a force were to pull on the electron and then let go, it would oscillate with eigenfrequencies $\omega_0 = 2\pi\nu_0$.
- The scattering cross-section for a *classical oscillator* can be written as

$$\sigma = \frac{8\pi}{3}\frac{e^4}{m_e^2 c^4}\left[\frac{\omega^4}{(\omega^2 - \omega_0^2)^2 + \gamma^2\omega^2}\right] \qquad \omega = 2\pi\nu$$

where the classical damping constant $\gamma = 2e^2\omega_0^2 / 3m_e c^3 = (8\pi^2 e^2 / 3m_e c^3)\nu_0^2$

- This is the **Lorentz function** which is sharply peaked around $\omega = \omega_0$.

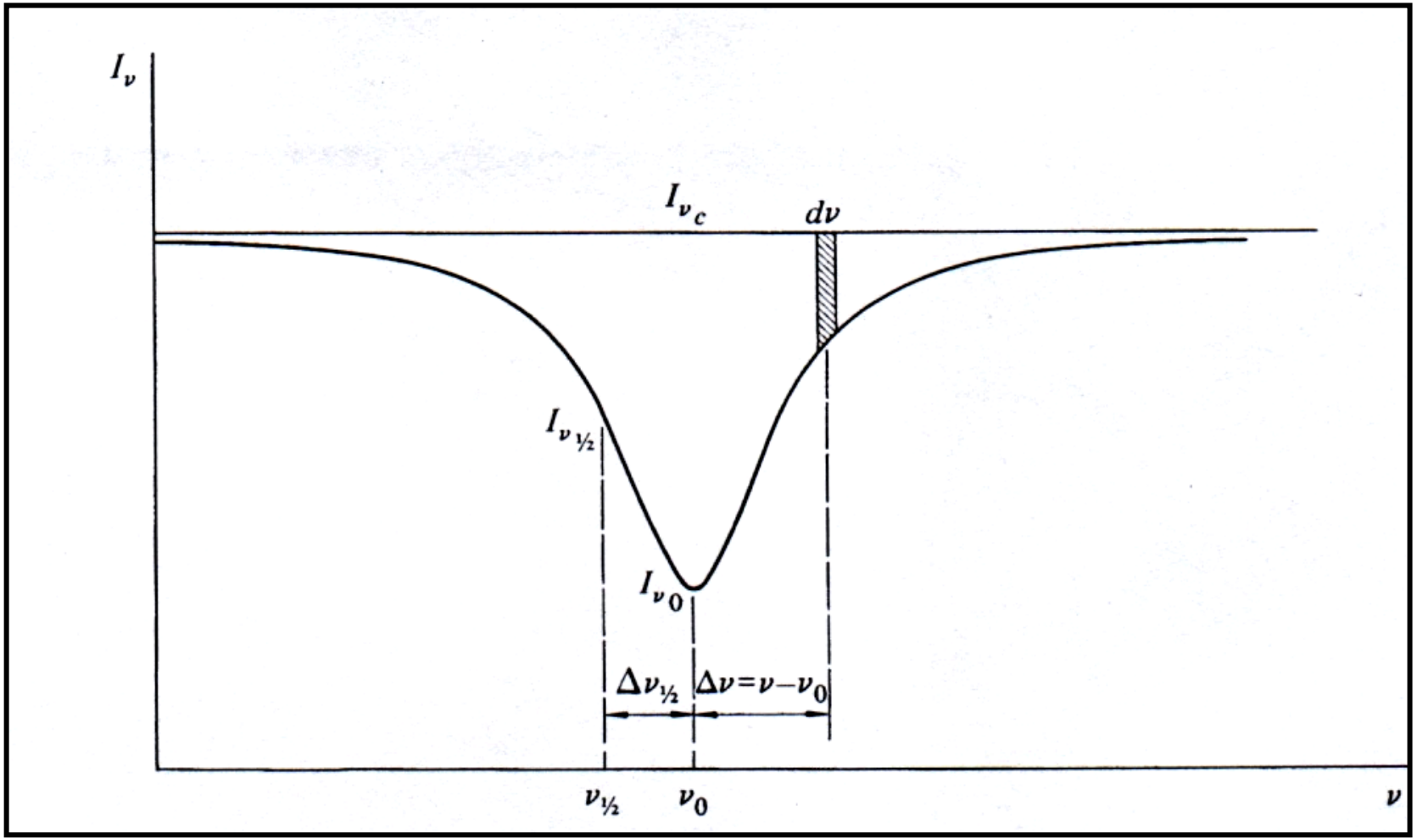
Lorentz function (1)

$$\sigma_\nu = \frac{8\pi}{3}\frac{e^4}{m_e^2 c^4}\left[\frac{\omega^4}{(\omega^2-\omega_0^2)^2+\gamma^2\omega^2}\right] \qquad \omega=2\pi\nu \quad \gamma = \frac{8\pi^2 e^2}{3m_e^2 c^3}\nu_0^2$$

$$\sigma_\nu = \frac{e^2}{m_e c}\left[\frac{\gamma/4\pi}{(\nu^2-\nu_0^2)^2+(\gamma/4\pi)^2}\right]$$

Note that γ defines the width of the line.

The Classical Damping Line Profile



Lorentz function (2)

The Lorentz function $\phi(\nu) = \left[\dfrac{A}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \right]$

is sharply peaked around $\nu = \nu_0$ with a maximum of $\phi(\nu_0) = A/(\gamma/4\pi)^2$.

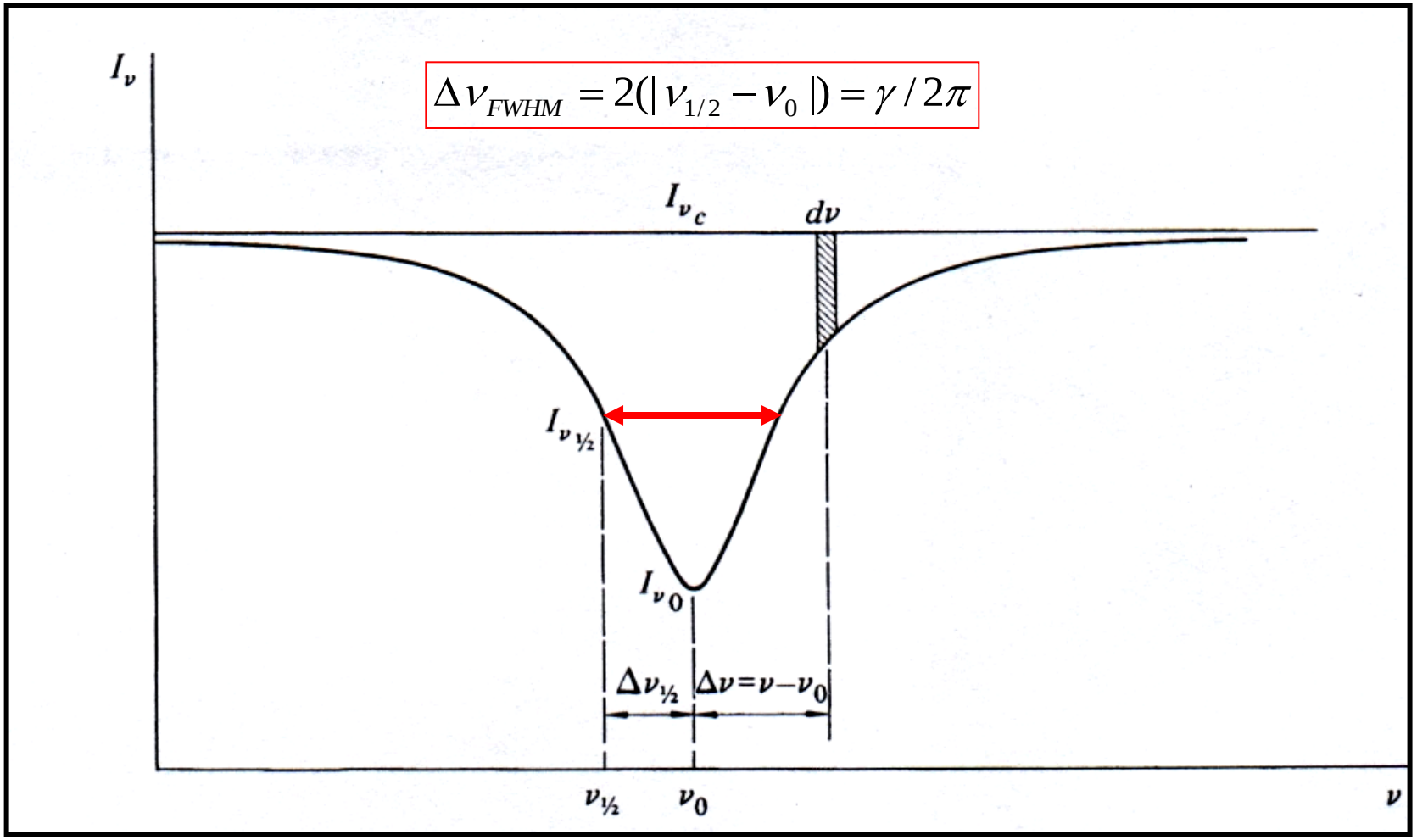
To find the full-width at half maximum (FWHM) we find the value of ν_1 at which the function is ½ its maximum, i.e. $\phi(\nu_1) = 1/2\,\phi(\nu_0)$ and then solve for the FWHM $= \Delta\nu_{1/2} = 2(\nu_1 - \nu_0)$

$$\frac{1}{2}\frac{A}{(\gamma/4\pi)^2} = \left[\frac{A}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \right] \qquad (\nu - \nu_0)^2 + (\gamma/4\pi)^2 = 2(\gamma/4\pi)^2$$

we obtain $|\nu_1 - \nu_0| = (\gamma/4\pi) \qquad \Delta\nu_{1/2} = 2(|\nu_1 - \nu_0|) = \gamma/2\pi$

i.e. $$(\Delta\lambda)_{1/2} = \frac{\lambda_0^2}{c}(\Delta\nu)_{1/2} = \frac{\lambda_0^2}{c}\frac{\gamma}{2\pi} = \frac{4\pi e^2}{3mc^2} = \frac{4\pi}{3} r_e = 0.00012 \text{ Å}$$

FWHM


$\Delta\nu_{FWHM} = 2(|\nu_{1/2} - \nu_0|) = \gamma / 2\pi$
I_ν
$I_{\nu c}$
$d\nu$
$I_{\nu ½}$
$I_{\nu 0}$
$\Delta\nu_{½}$
$\Delta\nu = \nu - \nu_0$
$\nu_{½}$
ν_0
ν

Oscillator Strength

We obtain the "integrated line scattering cross-section" by integrating over all frequencies

$$\sigma_{Tot} = \int_0^\infty \sigma_\nu d\nu = \frac{e^2}{m_e c} \int_0^\infty \frac{\gamma/4\pi}{(\nu-\nu_0)^2 + (\gamma/4\pi)^2} d\nu = \frac{\pi e^2}{m_e c}$$

This **classical** result predicts a **unique** scattering relation for **all** transitions.

The **quantum-mechanical** treatment shows that line scattering cross-sections may in fact **differ** greatly. The customary way of writing this result is via

$$\sigma_{Tot} = \frac{\pi e^2}{m_e c} f_{ij}$$

where f_{ij} is the (dimensionless) **oscillator strength** of the transition.

Obtained from lab measurements, the Solar spectrum or quantum mechanical calculations (e.g. Opacity Project), f_{ij} and Einstein A coefficient are related via:

$$A_{ij} = \frac{6.67 \times 10^{15}}{\lambda_{ij}^2 (\text{Å})} \frac{g_i}{g_j} f_{ij}$$

f_{ij} for Lyman and Balmer lines

Only for the strongest transitions does f_{ij} approach unity. An electron in the n=2 orbit of H is about 5 times more likely to absorb a Hα photon and make a transition to the n=3 orbit, than it is to absorb a Hβ photon and jump to the n=4 orbit.
For **forbidden** lines, f_{ij} «1.

λ (Å)	Line	f_{lu}	g_{low}	g_{up}
1215.7	Ly α	0.41	2	8
1025.7	Ly β	0.07	2	18
972.5	Ly γ	0.03	2	32
6562.8	H α	0.64	8	18
4861.3	H β	0.12	8	32
4340.5	H γ	0.04	8	50

Broadening of spectral lines

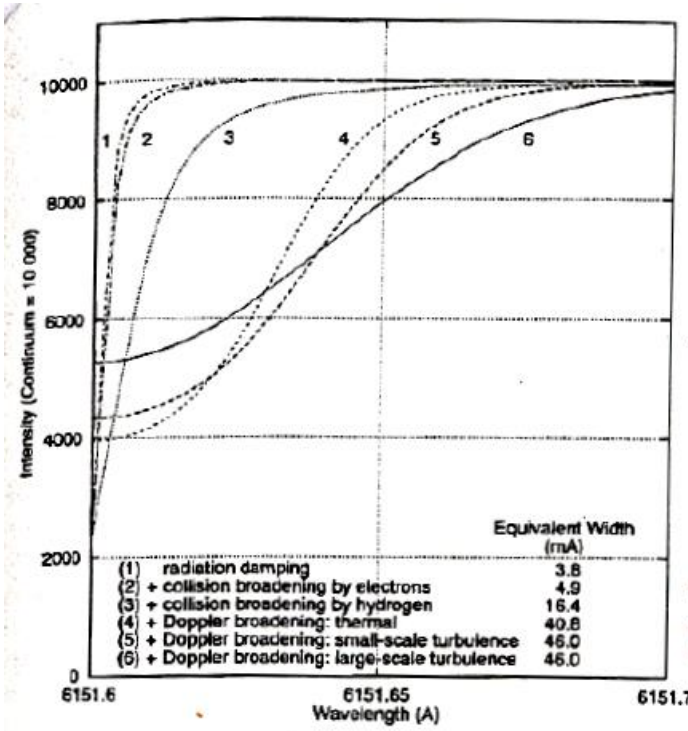
There are numerous broadening mechanisms which influence the apparent shape of spectral lines:

microscopic

1. Natural broadening
2. Thermal broadening
3. Microturbulence
   (treated like extra thermal broadening)
4. Collisions (important for strong lines)
5. Isotopic shift, *hfs*, Zeeman effect

macro

6. Macroturbulence
7. Rotation
8. Instrumental broadening



Holweger 1996

Natural Line Broadening (1)

Energy levels of atoms are intrinsically broadened due to the **Heisenberg uncertainty principle**. A decaying state *j* does not have a perfectly defined energy E_j, but rather a superposition of states spread around E_j.

$$\left.\begin{aligned} \Delta E \Delta t &= h/2\pi \\ E &= h\nu = h\omega/2\pi \end{aligned}\right\} \Rightarrow \Delta\omega\Delta t = 1$$

The longer the atom is in a state (dt high), the more precisely its energy can be measured (dE low).

A large transition probability leads to a short life in the state (low dt) and a large energy uncertainty (high dE).

Thus, the spectral lines are broadened. This type of broadening is called **natural broadening**.

Natural Line Broadening (2)

- The resulting absorption coefficients have the same form as the classical case, except that the classical damping coefficient γ is replaced by Γ, the Quantum Mechanical damping constant, the sum of all transition probabilities A_{ij} for spontaneous emission.

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

- ϕ is the natural or Lorentz profile with FWHM (as before)

$$\Delta\lambda_{1/2} = \frac{\lambda_0^2}{c}\Delta\nu_{1/2} = \frac{\lambda_0^2}{c}\frac{\Gamma}{2\pi} \approx f_{ij} \times 7 \times 10^{-4}\ \text{Å}$$

- Still very small, since f is at most of order unity!
  Clearly other line broadening mechanisms should dominate.

Thermal (Doppler) broadening

- The light emitting atoms in a stellar atmosphere are not at rest, but have a thermal motion → Maxwellian velocity distribution.

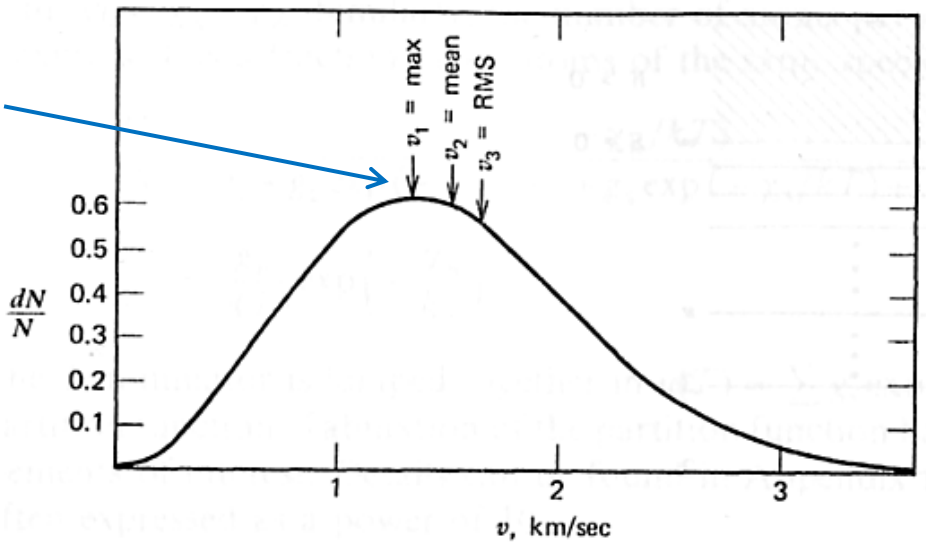
- Because the particles produce Doppler shifts, the line of sight velocities have a distribution that is an important special case for spectroscopy:

$$\frac{dN}{N} = \frac{1}{\sqrt{\pi}} e^{-(u_r/u_{th})^2} \frac{du_r}{u_{th}}$$

where u_r is the radial (line of sight) velocity component, and u_{th} is the most probable velocity $u_{th} = \sqrt{2kT/m}$

- The frequency (wavelength) shift (linear Doppler effect) is related to u_r :

$$\frac{\Delta\lambda}{\lambda_0} = \frac{\Delta\nu}{\nu_0} = \frac{u_r}{c}$$



Doppler broadening

- The distribution of $\Delta\lambda$ or $\Delta\nu$ values gives us the shape of the absorption coefficient.
- Integrating the Maxwell distribution over all velocities, we obtain

$$\phi(\nu) = \frac{\nu_0}{c\sqrt{\pi}\Delta\nu_D} \exp[-(\nu-\nu_0)^2/\Delta\nu_D^2]$$

substituting $u_r = \frac{\nu-\nu_0}{\nu_0}c$ and $\Delta\nu_D = \frac{\nu_0}{c}u_{th} = \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}}$ (the Doppler width)

- With $\int_0^\infty \phi(\nu) = 1$, we obtain the Gaussian line profile in terms of the Doppler width :

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

Again, the maximum is at ν_0. Temperature dependency $\Delta\nu_{\text{th}} \sim \sqrt{T}$

Doppler broadening (FWHM)

- We can again obtain the line FWHM via $\nu=\nu_1$ where

  $\phi(\nu_1)=1/2\phi(\nu_0)$ and then solve for the FWHM $=\Delta\nu_{1/2}=2(\nu_1-\nu_0)$

- This implies that $2=\exp[(\nu_1-\nu_0)^2/\Delta\nu_D^2]$ or $(\nu_1-\nu_0)^2=\Delta\nu_D^2\ln 2$

- Finally,

$$\Delta\nu_{1/2}=2(\nu_1-\nu_0)=2\Delta\nu_D\sqrt{\ln 2}=1.67\Delta\nu_D=2.139\times10^{12}\sqrt{(T/\mu)}/\lambda_0(\text{Å})\ \text{Hz}$$

(μ is the atomic mass)

- In wavelength units $\Delta\lambda_{1/2}=\dfrac{\lambda_0^2}{c}\Delta\nu_{1/2}=7.1\times10^{-7}\lambda_0(\text{Å})\sqrt{(T/\mu)}$ Å

Doppler broadening (example)

- For the Sun, with T~6000K at Hα:

$$\Delta\nu_{1/2} = 2.139\times10^{12}\sqrt{(T/\mu)}/\lambda_0(\text{Å}) = 2.139\times10^{12}\sqrt{6000/1)}/6563 = 25.2\ \text{GHz}$$

i.e. in wavelength units

$$\Delta\lambda_{1/2} = \frac{\lambda_0^2}{c}\Delta\nu_{1/2} = \frac{(6563\times10^{-8})^2}{3\times10^8}25.2\times10^9 = 0.36\ \text{Å}$$

or velocity units:

$$\Delta u_{1/2} = c\frac{\Delta\lambda_{1/2}}{\lambda_0} = 3\times10^5\ \text{km/s}\,\frac{0.36}{6562} = 16.5\ \text{km/s}$$

- This is much larger than the natural damping width of the line (10^{-4} Å), but still relatively small relative to some pressure broadening mechanisms (will discuss later).
- The atomic mass dependence in the denominator implies smaller line widths for metallic lines, e.g. a factor of $(56)^{1/2}$ smaller for iron lines having wavelengths close to Hα

Pressure broadening

- The orbitals of an atom can be perturbed in a collision with a neutral atom (collisional broadening) or encounter with the electric field of an ion (pressure broadening).
- The change in energy induced by the collision is a function of the separation r between the absorber and perturbing particle, and can be approximated by a power law of the form $\Delta E \sim Constant\ x\ r^n$ where n is an integer, such that the change in frequency is $\Delta\nu = \Delta E/h = C_n r^{-n}$

Pressure broadening (2)

$$\Delta\nu = \frac{C_n}{r^n}$$

n =	name	interaction of
2	linear Stark effect	hydrogen-like ions + p, e
3	resonance broadening	neutral atoms with each other, H+H
4	quadratic Stark effect	ions + e, p
6	van der Waals broadening	metals + H

Two approximations exist – impact broadening for n>2 (n=3 resonance, n=4 quadratic Stark, n=6, van der Waals) and a quasi-static approximation (i.e. surrounding particles are nearly at rest; for linear Stark broadening, n=2).

Direct collisions?

- Collisions in the gas de-excite atoms before they naturally decay, (shortening its lifetime).
- The resulting line profile is Lorenzian (as with natural broadening) with a width of $\nu_{1/2}=1/(\pi t)$ where t is the time between collisions.
- The number of collisions (per second) is the number of perturbers in the volume swept out by the atom, i.e. $N\sigma v$. Since $\frac{1}{2} mv^2=3/2\ kT$, the time between collisions is

$$t \approx 1/(N\sigma\sqrt{3kT/m})$$

- So, the FWHM in terms of pressure ($P=NkT$) is:

$$\Delta\nu_{1/2}(Hz) = P\sigma/\pi\sqrt{3/kTm} = 3.6\times10^{19}\,P\sigma/\sqrt{mT/m_H}$$

- For the Sun (T=5800K, $P=10^5$ dyne/cm^2),
  H atom *direct* collisions ($\sigma=\pi a_0^2=8\text{x}10^{-17}$ cm^2) cause

$$\Delta\nu_{1/2} = 3.6\cdot10^{24}\times10^4\times8\cdot10^{-21}/\sqrt{1\times5800} = 4MHz$$

  i.e. less than the natural width

Impact broadening

- Nevertheless, the impact approximation can be used for some broadening mechanisms, which are important since atoms can interact without direct collision.

  We will discuss these mechanisms in more detail later.