Spectral lines

(172)⁾

EQUIVALENT WIDTH FWHM FWZI

Spectral Lines

173

(e.g. 2D echelle image of optical Solar spectrum)



Continuous Energy Distribution



Spectra of stars, clusters, galaxies...

175

Spectral lines and continuum energy distributions provide temperatures and metallicity of individual stars, plus ages of clusters & galaxies (since the highest mass stars are visually the brightest).



Spectral Lines



Impact of Spectral Resolution



Line depth

177

We now turn from the continuous energy distribution to the line spectrum.

Relative intensity r_{λ} (not very common term, usually applied to emission lines):

$$r_{\lambda} = \frac{F_{\lambda}}{F_c}$$

The line depth R_{λ} :

$$R_{\lambda} = \frac{F_c - F_{\lambda}}{F_c} = 1 - \frac{F_{\lambda}}{F_c}$$

The largest $R_{\lambda,0}$ the central line depth



Equivalent Width

178

• The total area in a spectral line divided by the continuum flux F_c is called the line equivalent width, i.e. an integral over a line depth R_{λ}

$$W_{\lambda} = \int \frac{F_c - F_{\lambda}}{F_c} d\lambda = \int R_{\lambda} d\lambda$$

- The division by the continuum flux means that this is a measurement of the flux in units of the continuum the equivalent width is identical to a rectangular line of width W_{λ} .
- EW of absorption lines is positive, emission lines have negative EWs, and are measured in Ångströms (at optical wavelengths).



FWHM and FWZI

• Other measures of the line width are the Full Width at Half Maximum (FWHM), the distance between the half line depth from blue to red, i.e. $(\Delta\lambda)_{1/2}$, and the Full Width at Zero Intensity (FWZI),



Line core and the wings

- We denote optically (thin) thick lines as those in which the line core is (not) saturated, i.e. reaching zero intensity. In reality, zero intensity is only reached for lines in non-LTE.
- The region close to the centre of the spectral line is referred to as the line core, whilst the wings sweep up the local continuum.



Example: Solar spectrum

	λ	Element	W(Å)	Name
	4920.51	Fe I	0.43	
	4957.61	Fe I	0.45	
	5167.33	Mg I	0.65	b₄
	5172.70	Mg I	1.26	\mathbf{b}_2
	5183.62	Mg I	1.58	b,
	5232.95	Fe I	0.35	
	5269.55	Fe I	0.41	
	5324.19	Fe I	0.32	
	5238.05	Fe I	0.38	
	5528.42	Mg I	0.29	
ſ	5889.97	Na I	0.63	D_2
l	5895.94	Na I	0.56	D_1
	6122.23	Ca I	0.22	
	6162.18	Ca I	0.22	
	6562.81	H_{α}	4.02	С
	6867.19	O_2	tell	B
	7593.70	O ₂	tell	Α
	8194.84	Na I	0.30	
	8498.06	Ca II	1.46	
	8542.14	Ca II	3.67	
	8662.17	Ca II	2.60	
	8688.64	Fe I	0.27	
	8736.04	Mg I	0.29	



Strong spectral lines in the Solar spectrum typically have equivalent widths $W_{\lambda} \approx 1$ Å, such as the Na I D lines in the yellow. In other stars, line equivalent widths can reach tens or even hundreds of Angstroms. EWs are by definition measured relative to the continuum strength, unlike line fluxes.

Formation of absorption lines

----- (182)

• We obtained earlier that the emergent flux from the stellar surface is π times the Source function at an optical depth of 2/3: $F_{\lambda}(0) = \pi S_{\lambda}(\tau_{\lambda} = 2/3) = \pi B_{\lambda}(T(\tau_{\lambda} = 2/3))$

- In spectral lines, the opacity is much larger, thus we see much higher layers at these wavelengths. These layers have a lower temperature and so B_{λ} is smaller, leading to a smaller F_{λ} in the line than F_{c} , the continuum flux in the neighbourhood of the line.
- In the following few lectures, we will study theory of line formation.

Spectral line formation

183



Bound-Bound (free-free) transitions

There are 3 basic kinds of line processes associated with bound-bound transitions of atoms or ions:

- 1. **Direct Absorption**, in which the absorbed photon induces a bound electron to go into a higher energy level.
- 2. **Spontaneous Emission**, in which an electron in a higher energy level spontaneously decays to lower level, emitting the energy difference as a photon.
- 3. Stimulated Emission, in which an incoming photon induces an electron in a higher energy level to decay to a lower level, emitting in effect a second photon that is nearly identical in energy (and even phase) to the original photon.

The probability that the atom will emit (or absorb) its quantum of energy is described by Einstein probability coefficients, written as B_{ij} , A_{ji} , and B_{ji} .



Spontaneous emission

Absorption

Stimulated emission

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.

Spontaneous emission

Consider an upper level u and a lower level l separated by an energy hv.

- The probability that the atom will spontaneously emit its quantum of energy within a time dt and in a solid angle $d\omega$ is $A_{ul} dt d\omega$.
- The proportionality constant, A_{ul}, is the Einstein probability coefficient for spontaneous emission [s⁻¹].
- Occurs independently of the radiation field.
- Emits **isotropically**.

For H α , A_{32} =4.4×10⁷ s⁻¹. If at time t_0 =0 there are $N_u(0)$ atoms in level u, then at time t the population is $N_u(t)=N_u(0)\exp(-A_{ul} t)$. Lifetime = $1/A_{ul}$





Consider an upper level u and a lower level l, separated by an energy hv.

- Photons with energies *close* to hv cause transitions from levels *l* to *u*.
- The probability per unit time for this process will evidently be proportional to the mean intensity J_{v} at the frequency v.
- $B_{lu}J$: transition probability of absorption per unit time.
- The proportionality constant B_{lu} is one of the Einstein B-coefficients.



Stimulated emission

Planck's law does **not** follow from considering only spontaneous emission and absorption. Must also include stimulated emission, which like absorption is proportional to the mean intensity *J*.

- The system goes from an upper level *u* to a lower level *l* stimulated by the presence of a radiation field (*hv* corresponding to the energy difference between levels *u* and *l*).
- The energy of the emitted photon is the same as of the incoming photon (also direction and phase are the same).
- $B_{ul}J$: transition probability of stimulated emission per unit time.
- The proportionality constant B_{ul} is a second Einstein *B*-coefficient.
- The process of stimulated emission is sometimes referred to as a process of *negative absorption*.
- Stimulated emission occurs into the **same** state (frequency, direction, polarization) as the photon that stimulated the emission.



Stimulated emission

Relation between Einstein coefficients

180

Einstein's Coefficients are not independent. To find a relation between them, let's assume strict Thermodynamic Equilibrium (TE), and, for simplicity, adopt a 2-level approximation.

In TE, each process is in equilibrium with its inverse, i.e., within one line there is no netto destruction or creation of photons (detailed balance)

$$n_1 B_{12} J_{\nu} = n_2 A_{21} + n_2 B_{21} J_{\nu}$$

Transitions $1 \rightarrow 2$ equal to $2 \rightarrow 1$ n₁, n₂: number density of e⁻ in levels 1,2

Thermodynamic equilibrium: Boltzmann, $J = B_v(T)$

$$y = \frac{A_{21}/B_{21}}{\left(\frac{n_1}{n_2}\right)\left(\frac{B_{12}}{B_{21}}\right) - 1}$$

$$\frac{n_1}{n_2} = \frac{g_1}{g_2} e^{h v_{21}/kT}$$





Comparison with Planck blackbody radiation:

$$B_{\nu}(T) = \frac{A_{21}}{B_{21}} \left(\frac{g_1 B_{12}}{g_2 B_{21}} e^{\frac{h\nu_{21}}{kT}} - 1 \right)^{-1} = \frac{2h\nu_{21}^3}{c^2} \left(e^{\frac{h\nu_{21}}{kT}} - 1 \right)^{-1}$$

$$\frac{A_{21}}{B_{21}} = \frac{2hv_{21}^3}{c^2} \rightarrow A_{21} = B_{21}\frac{2hv_{21}^3}{c^2}$$
$$\frac{g_1B_{12}}{g_2B_{21}} = 1 \rightarrow g_1B_{12} = g_2B_{21}$$

Einstein coefficients

· 191'

Thus, if one of the Einstein Coefficients is known then two other can be calculated.

Important: The Einstein's coefficients are **atomic constants**. Although the above relations were derived under the conditions of TE, these relations hold in any non-TE state.

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

$$n_1 B_{12} J_{\nu} - n_2 B_{21} J_{\nu} = n_1 B_{12} J_{\nu} \left(1 - \frac{n_2 B_{21}}{n_1 B_{12}} \right) = n_1 B_{12} J_{\nu} \left(1 - \frac{g_1 n_2}{g_2 n_1} \right)$$

Thus, to take into account negative absorption (stimulated emission), one must multiply the number of absorbed photons by

$$\left(1 - e^{-hv_{12}/kT}\right)$$
 (we already did it before)

Comparison of induced and spontaneous emission

Home work:

• When (at what temperatures, wavelengths) is spontaneous or induced emission stronger?

Assume LTE (blackbody)

Lifetime of atom in excited state

In the absence of collisions and of any other transitions than the *ul* one, the mean lifetime of particles in state *u* is Lifetime = $1/A_{ul}$

If at time $t_0=0$ there are $N_u(0)$ atoms in level *u*, then at time *t* the population is

----- ((193)) -----

 $N_u(t) = N_u(0)e^{-A_{ul}t}.$

Typical value of A_{ii} is 10⁷- 10⁸ s⁻¹ (for H α , A_{32} =4.4×10⁷ s⁻¹), so lifetime is ~10⁻⁸ s.

However, not all transitions are allowed, some are strictly forbidden! In practice, strictly forbidden means very low probability of occurrence → Metastable states at which a lifetime is much longer than of the ordinary excited states but shorter than of the ground state.

Lifetimes at metastable states can reach several hours and even longer!

Forbidden line transitions are noted by placing square brackets around the atomic species in question, e.g. [O III] or [S II]. A semi-forbidden line, designated with a single square bracket, such as C III], occurs where the transition probability is about a thousand times higher than for a forbidden line.

Einstein A-coefficients for Hydrogen

(194)

i k	1	2	3	4	5	6	7
2 3 4 5 6 7 8	$\begin{array}{r} 4,67\cdot 10^{3} \\ 5,54\cdot 10^{7} \\ 1,27\cdot 10^{7} \\ 4,10\cdot 10^{6} \\ 1,64\cdot 10^{6} \\ 7,53\cdot 10^{5} \\ 3,85\cdot 10^{5} \end{array}$	$\begin{array}{r}$		$\begin{array}{c}\\\\ 2,68 \cdot 10^{6}\\ 7,67 \cdot 10^{5}\\ 3,03 \cdot 10^{5}\\ 1,42 \cdot 10^{5} \end{array}$	$ \begin{array}{c}$		 2,26.10 ⁵

Spectral line formation

195

EINSTEIN COEFFICIENTS LINE PROFILES: NATURAL BROADENING BROADENING OF SPECTRAL LINES NATURAL LINE BROADENING THERMAL (DOPPLER) BROADENING CONVOLUTION OF DIFFERENT BROADENING PROCESSES PRESSURE BROADENING INGIS-TELLER RELATION ROTATIONAL AND INSTRUMENTAL BROADENING



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

Energy levels are **not** infinitely sharp. An unavoidable source of broadening is due to the Heisenberg uncertainty principle:

dE dt ~ $h/2\pi$

dt being the timescale of decay (finite lifetime of energy levels).

In each spectral line, photons of different frequencies (but close to central frequency v_0) can be absorbed.

Let us call $\varphi(\nu)$ the probability that the transition occurs by emitting or absorbing a photon with energy $h\nu$ (emission or absorption line, $\int \varphi(\nu) d\nu \equiv 1$).

This natural broadening has the form of a Lorentzian function.

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 $\omega_0 = 2\pi v_0$.
- The scattering cross-section for a *classical oscillator* can be written as

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

where the classical damping constant $\gamma = 2e^2 \omega_0^2 / 3m_e c^3 = (8\pi^2 e^2 / 3m_e c^3) v_0^2$

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

Lorentz function (1)

------ (198) ------



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

Note that γ defines the width of the line.



Lorentz function (2)

200

The Lorentz function

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

is sharply peaked around $v = v_0$ with a maximum of $\varphi(v_0) = A/(\gamma/4\pi)^2$.

To find the full-width at half maximum (FWHM) we find the value of v_1 at which the function is $\frac{1}{2}$ its maximum, i.e. $\varphi(v_1)=1/2 \varphi(v_0)$ and then solve for the FWHM = $\Delta v_{1/2}=2(v_1-v_0)$:

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

we obtain $|\nu_1 - \nu_0| = (\gamma/4\pi)$

 $\Delta v_{1/2} = 2(|v_1 - v_0|) = \gamma/2\pi$

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

Classical electron radius



Oscillator Strength

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

----- (202) ------

$$\sigma_{total} = \int_{0}^{\infty} \sigma_{\nu} d\nu = \frac{e^2}{m_e c} \int_{0}^{\infty} \frac{\gamma/4\pi}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} d\nu = \frac{\pi e^2}{m_e c}$$

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

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

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:

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

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 an H α photon and make a transition to the n=3 orbit, than it is to absorb an H β photon and jump to the n=4 orbit. For **forbidden** lines, $f_{ij} \ll 1$.

λ (Å)	Line	$f_{ m lu}$	$g_{ m low}$	${g_{ m up}}$
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	Ηα	0.64	8	18
4861.3	Ηβ	0.12	8	32
4340.5	Ηγ	0.04	8	50

Spectral line formation

(204

EINSTEIN COEFFICIENTS LINE PROFILES: NATURAL BROADENING **BROADENING OF SPECTRAL LINES: THERMAL (DOPPLER) BROADENING** CONVOLUTION OF DIFFERENT BROADENING PROCESSES PRESSURE BROADENING INGIS-TELLER RELATION ROTATIONAL AND INSTRUMENTAL BROADENING

Broadening of spectral lines

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

- 1. Natural broadening
- 2. Thermal broadening $\sqrt{}$
- Microturbulence (treated like extra thermal broadening)
- 4. Collisions (important for strong lines)
- 5. Isotopic shift, hyperfine splitting (hfs) Zeeman effect
- 6. Macroturbulence
- 7. Rotation

microscopic

nacro

8. Instrumental broadening



Natural Line Broadening (1)

As just noticed above, 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 .

$$\left. \begin{array}{c} \Delta E \Delta t = h/2\pi \\ E = hv = h\omega/2\pi \end{array} \right\} \Rightarrow \Delta \omega \Delta t = 1$$

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_{ii} for spontaneous emission.

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

• 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:

 $\frac{dN}{N} = \frac{1}{\sqrt{\pi}} e^{-(v_r/v_{th})^2} \frac{dv_r}{v_{th}}$

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

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

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



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

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

substituting
$$v_r = \frac{v - v_0}{v_0} c$$
 and $\Delta v_D = \frac{v_0}{c} v_{th} = \frac{v_0}{c} \sqrt{\frac{2kT}{m}}$ (the Doppler width)

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

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

Again, the maximum is at v_0 .

Temperature dependency: $\Delta v_{\text{th}} \sim \sqrt{T}$

Doppler broadening (FWHM)

• We can again obtain the line FWHM via $v=v_1$ where

 $\phi(v_1)=1/2\phi(v_0)$ and then solve for the FWHM = $\Delta v_{1/2}=2(v_1-v_0)$

- 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, $\Delta \nu_{1/2} = 2(\nu_1 - \nu_0) = 2\Delta \nu_D \sqrt{\ln 2} = 1.67 \Delta \nu_D = 2.139 \times 10^{12} \sqrt{(T/\mu)} / \lambda_0 (\text{\AA}) \text{ Hz}$

(*µ* is the atomic mass)

• In wavelength units
$$\Delta \lambda_{1/2} = \frac{\lambda_0^2}{c} \Delta \nu_{1/2} = 7.1 \times 10^{-7} \lambda_0 (\text{\AA}) \sqrt{(T/\mu)} \text{\AA}$$

Doppler broadening (example)

(211))

• For the Sun, with $T \sim 6000$ K at H α :

 $\Delta \nu_{1/2} = 2.139 \times 10^{12} \sqrt{(T/\mu)} / \lambda_0 (\text{\AA}) =$

i.e. in wavelength units $\Delta \lambda_{1/2} = \frac{\lambda_0^2}{c} \Delta \nu_{1/2} = 7.1 \times 10^{-7} \lambda_0 (\text{\AA}) \sqrt{(T/\mu)} \text{\AA} =$



Doppler broadening (example)

----- (212) -

• For the Sun, with $T \sim 6000$ K at H α :

 $\Delta v_{1/2} = 2.139 \times 10^{12} \sqrt{(T/\mu)} / \lambda_0(\text{\AA}) = 2.139 \times 10^{12} \sqrt{6000/1)} / 6563 = 25.2 \text{ GHz}$

i.e. in wavelength units $\Delta \lambda_{1/2} = \frac{\lambda_0^2}{c} \Delta \nu_{1/2} = \frac{(6563 \times 10^{-8})^2}{3 \times 10^8} 25.2 \times 10^9 = 0.36 \text{ Å}$

or velocity units:
$$\Delta v_{1/2} = c \frac{\Delta \lambda_{1/2}}{\lambda_0} = 3 \times 10^5 \text{ km/s} \frac{0.36}{6562} = 16.5 \text{ km/s}$$

- 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.