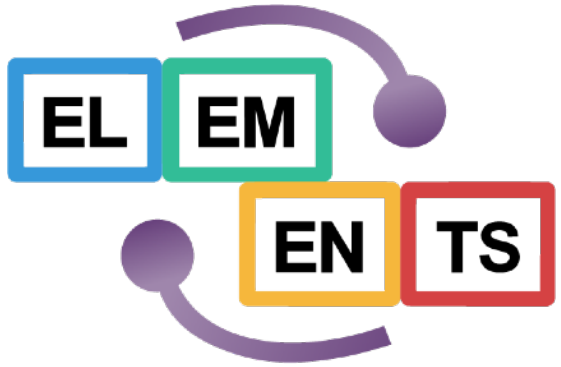


From stellar spectra to chemical abundances

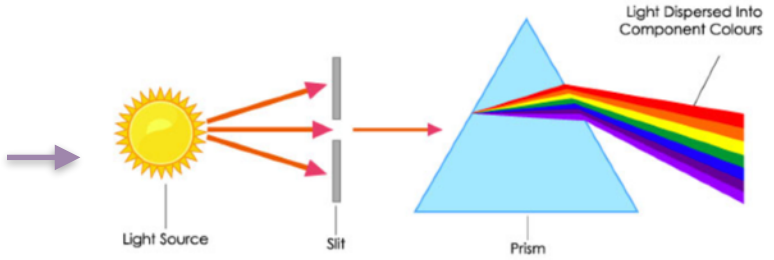
How to derive chemical abundances in 1D LTE

Linda Lombardo, EASE School, 30/07/2024

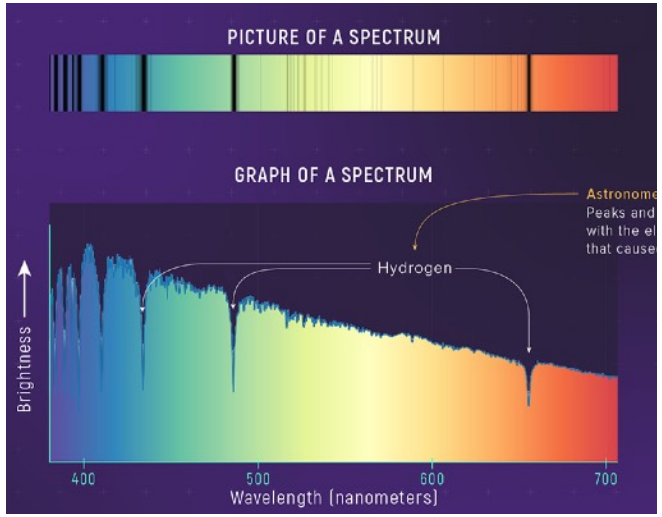
GOETHE UNIVERSITÄT FRANKFURT AM MAIN
TECHNISCHE UNIVERSITÄT DARMSTADT
JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
GSI

Stellar spectroscopy

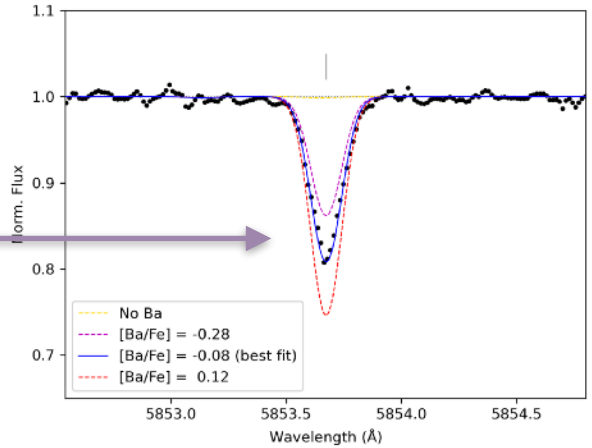
1) Observe the star with a spectrograph



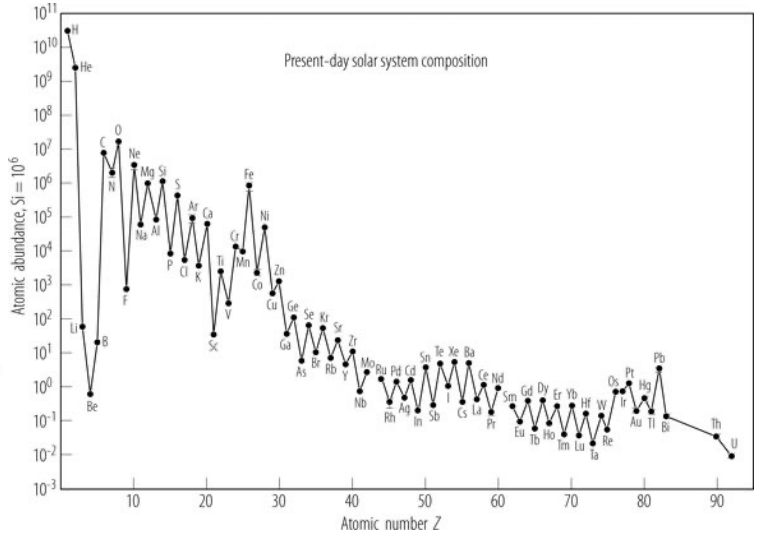
2) Reduce the data to obtain a spectrum of the star



3) Measure the absorption lines



4) Obtain the chemical composition of the star



Stellar spectroscopy

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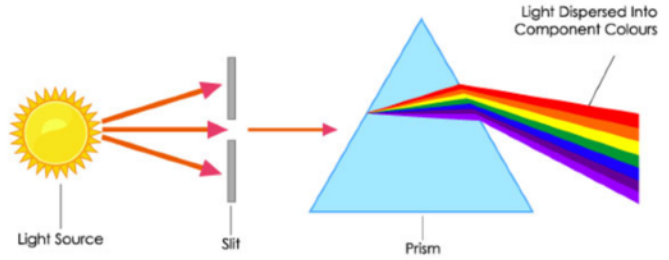

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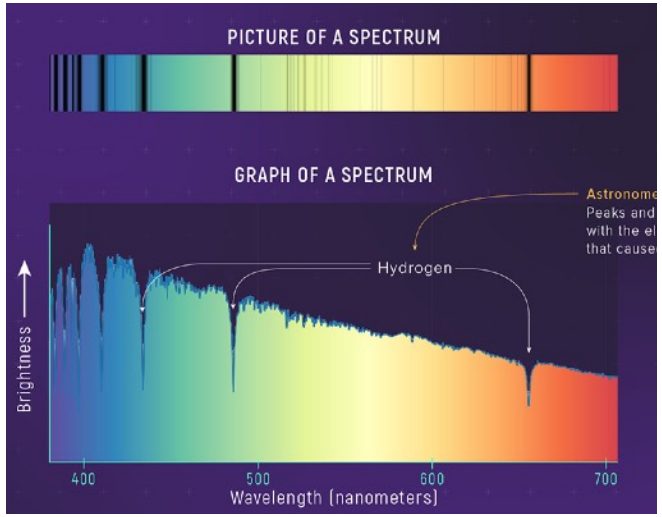

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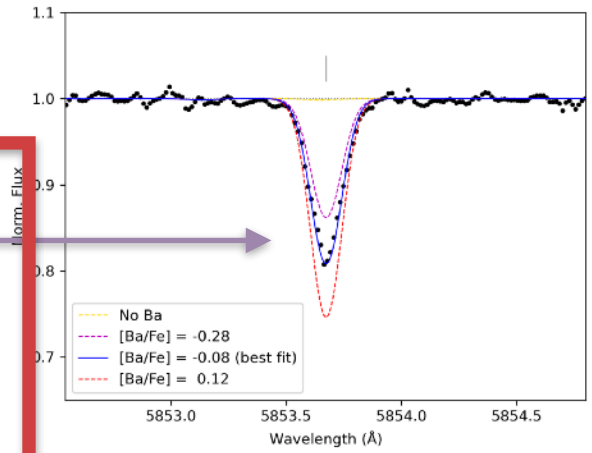

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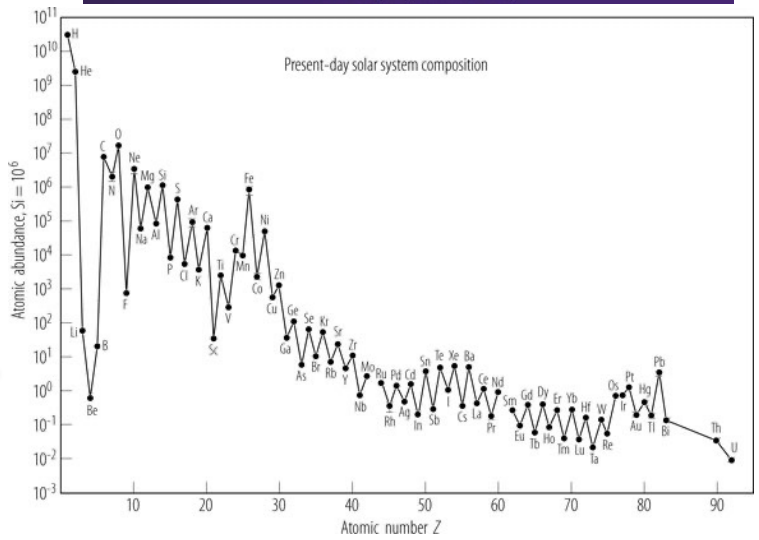


Today!

From stellar spectra to chemical abundances

Input needed for deriving chemical abundances:

- Observed stellar spectra
- Model atmosphere (e.g. ATLAS9)
- Stellar parameters (Teff, logg, [M/H], vt)
- Atomic data (energy levels, transition strengths, ionisation stage, …)
- Spectrum synthesis code (MOOG)

Steps:

- Computation (or interpolation) of a model atmosphere with appropriate stellar parameters
- Computation of synthetic stellar spectrum
- Comparison between observed and synthetic spectra

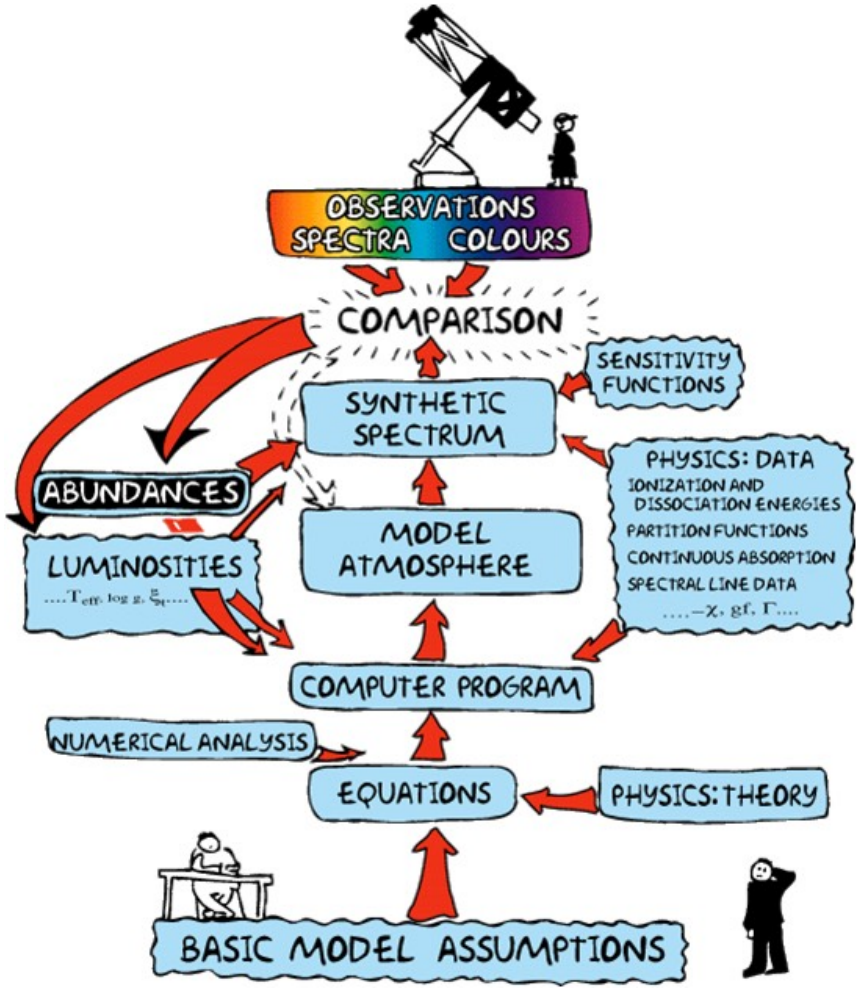


Figure by Bengt Gustafsson, Astronomical Observatory, Uppsala

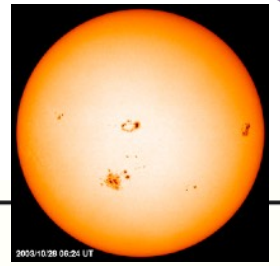
Stellar photosphere

Stellar photosphere absorbs and emits photons

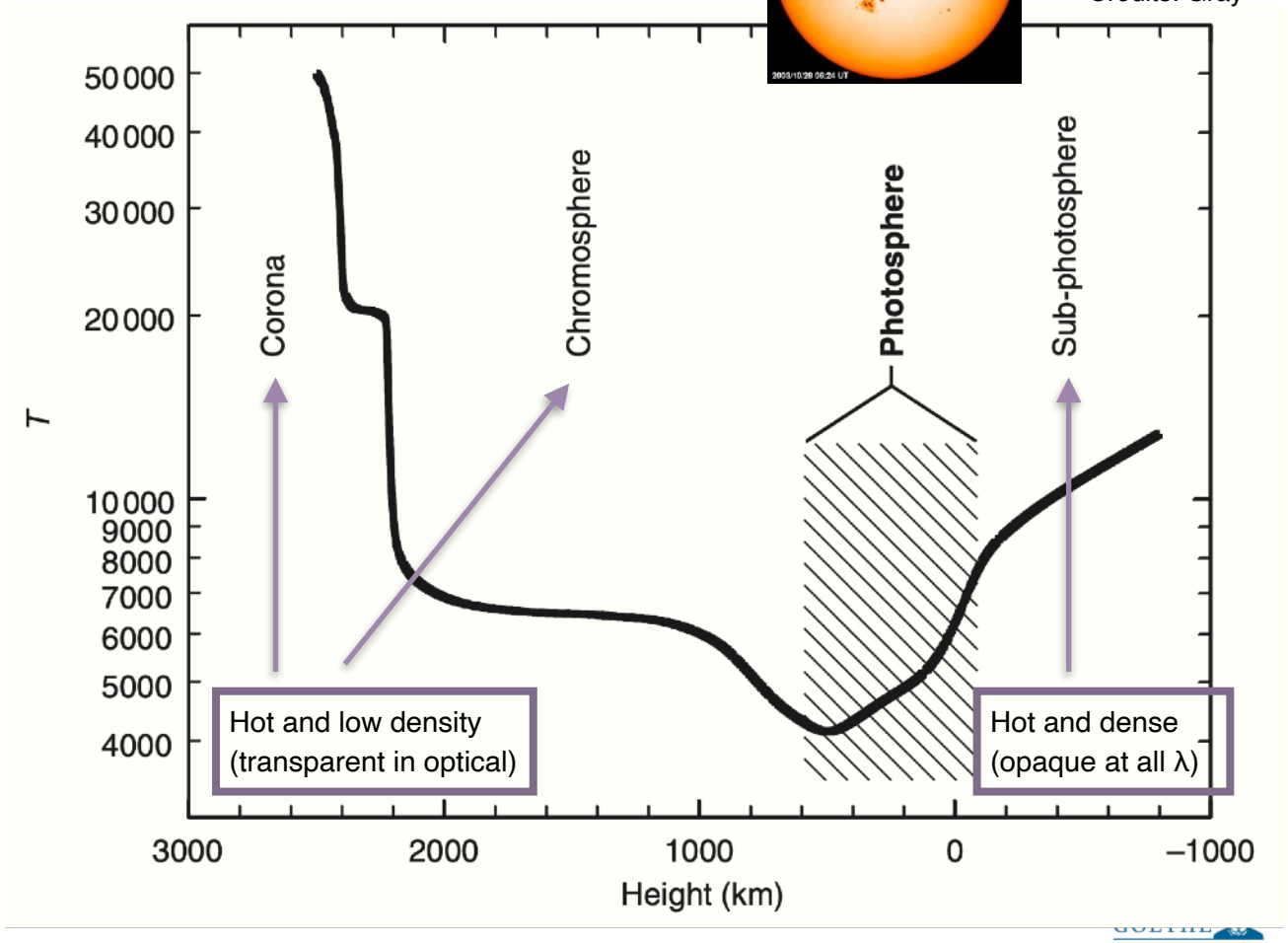
—> where visible light come from!

The properties of the stellar photosphere depends on the stellar parameters: effective temperature (Teff), surface gravity (logg), metallicity ([M/H])

SOHO/NASA



Credits: Gray



Stellar photosphere

Effective temperature: $\int_0^\infty F_\nu d\nu = \sigma T_{\text{eff}}^4$ ← Stefan-Boltzmann law!

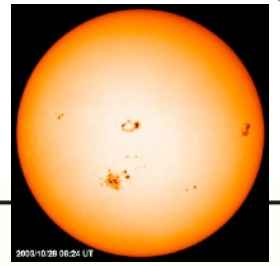
Where F_ν is the flux leaving the stellar surface

Teff: temperature of a black body having the same power output per unit area as the star

Luminosity :

$$L = 4\pi R^2 \int_0^\infty F_\nu d\nu = 4\pi R^2 \sigma T_{\text{eff}}^4$$

SOHO/NASA



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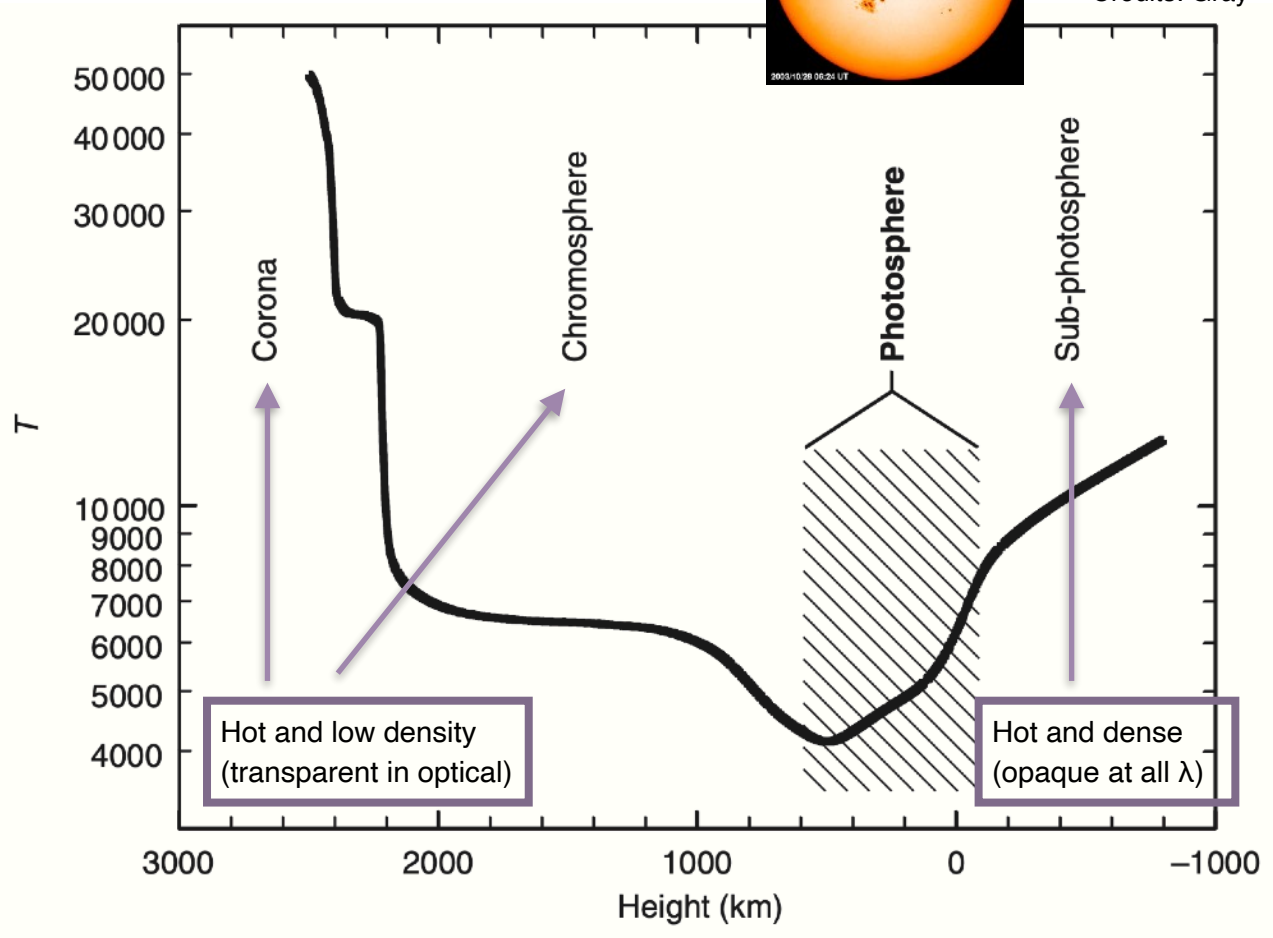


Model Atmosphere

Mathematical models that describe the physical conditions of the stellar photosphere

1D LTE model atmosphere assumptions:

- Thin relative to the stellar radius: all physical variables are function only of the depth into the photosphere → plane parallel geometry (1D)
- Hydrostatic equilibrium: pressure balances gravity, the photosphere is static → $\frac{dP}{dr} = \rho g$ with $g = \frac{GM_*}{R_*^2}$
- Radiative equilibrium: the flux of energy is constant with depth, no creation of energy within the atmosphere → $F = \sigma T_{\text{eff}}^4$
- Homogeneous layers except in the normal direction: we ignore granulation, starspots, magnetic fields, etc.
- Steady state: gas state and radiation transport are constant in time
- Atomic abundances are specified and constant

+

Each layer is in local thermodynamic equilibrium (LTE)

1D LTE model atmosphere

Assumptions:

- **Excitation equilibrium (Boltzmann eq.)**

$$\frac{N_n}{N} = \frac{g_n e^{-\chi_n/kT}}{g_1 + g_2 e^{-\chi_2/kT} + g_3 e^{-\chi_3/kT} + \cdots} = \frac{g_n}{u(T)} e^{-\chi_n/kT}.$$

N_n : number of atoms per cm^3 in *n*th level

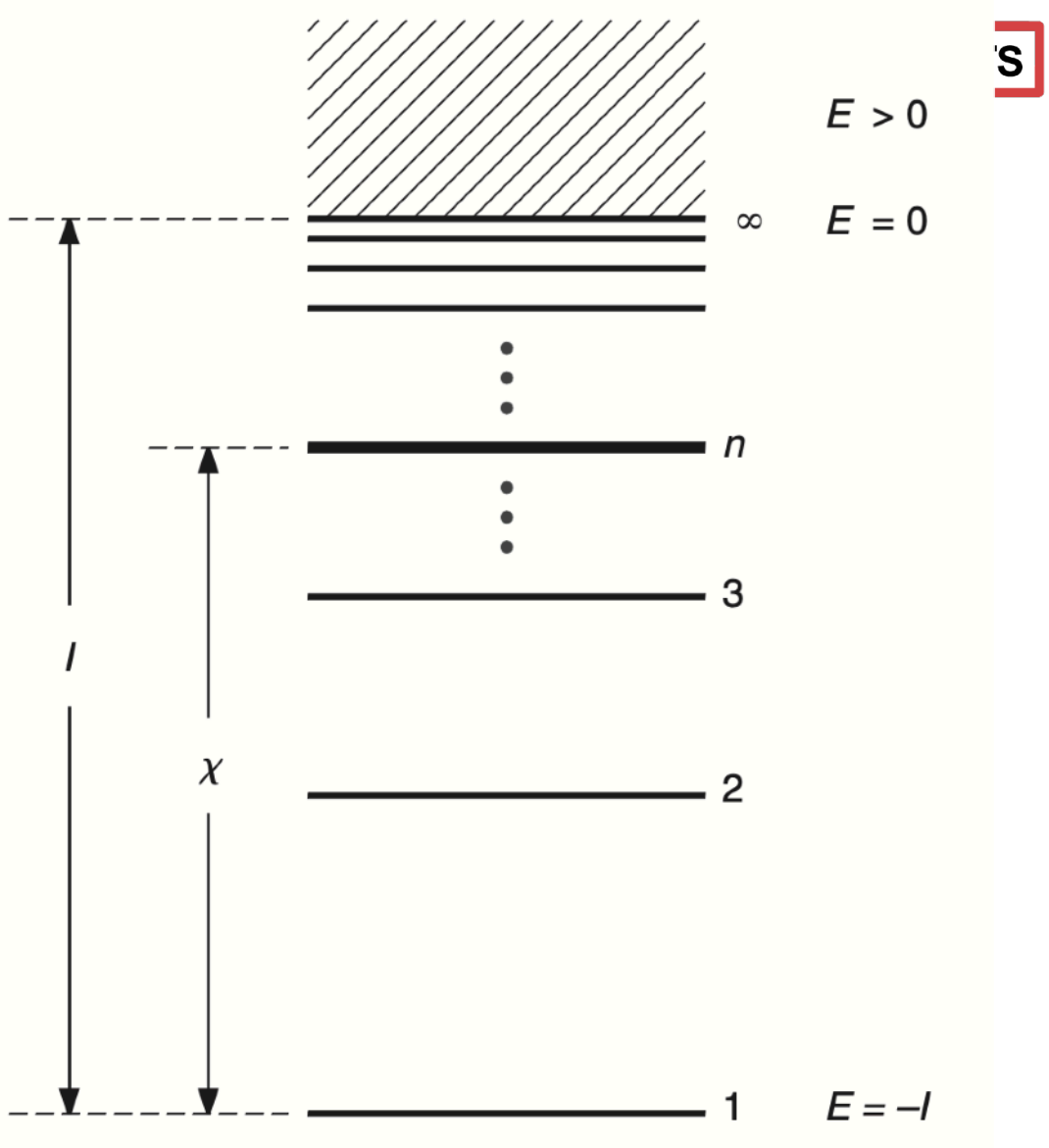
N : number of all atoms of the same species

g_n : statistical weight

χ_n : excitation potential

k : Boltzmann constant

u(T) : partition function



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1D LTE model atmosphere

Assumptions:

- **Ionisation equilibrium (Saha eq.)**

$$\frac{N_1}{N_0} = \frac{2u_1(T)}{n_e u_0(T)} \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} e^{-I/kT}$$

N_1/N_0 : ions to neutrals ratio

$u(T)_1/u(T)_0$: ionic to neutral partition functions ratio

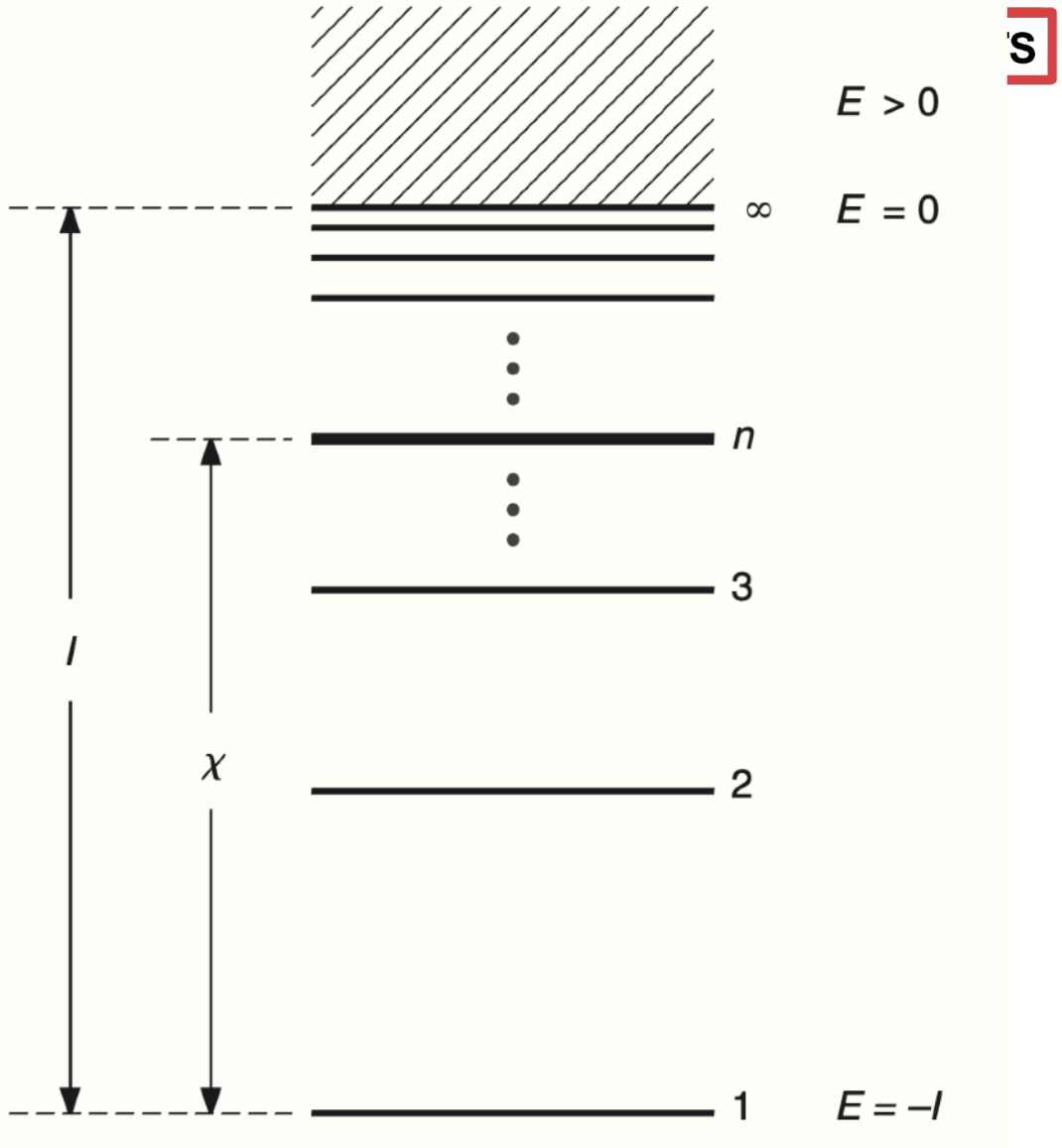
n_e : number of e- per cm^3

m_e : electron mass

I : ionisation potential

k : Boltzmann constant

h : Planck constant



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1D LTE model atmosphere

Assumptions:

- **Maxwell-Botzmann velocity distribution**

$$f(v)dv = 4\pi v^2 \left(\frac{m}{2\pi kT}\right)^{3/2} e^{mv^2/2kT} dv$$

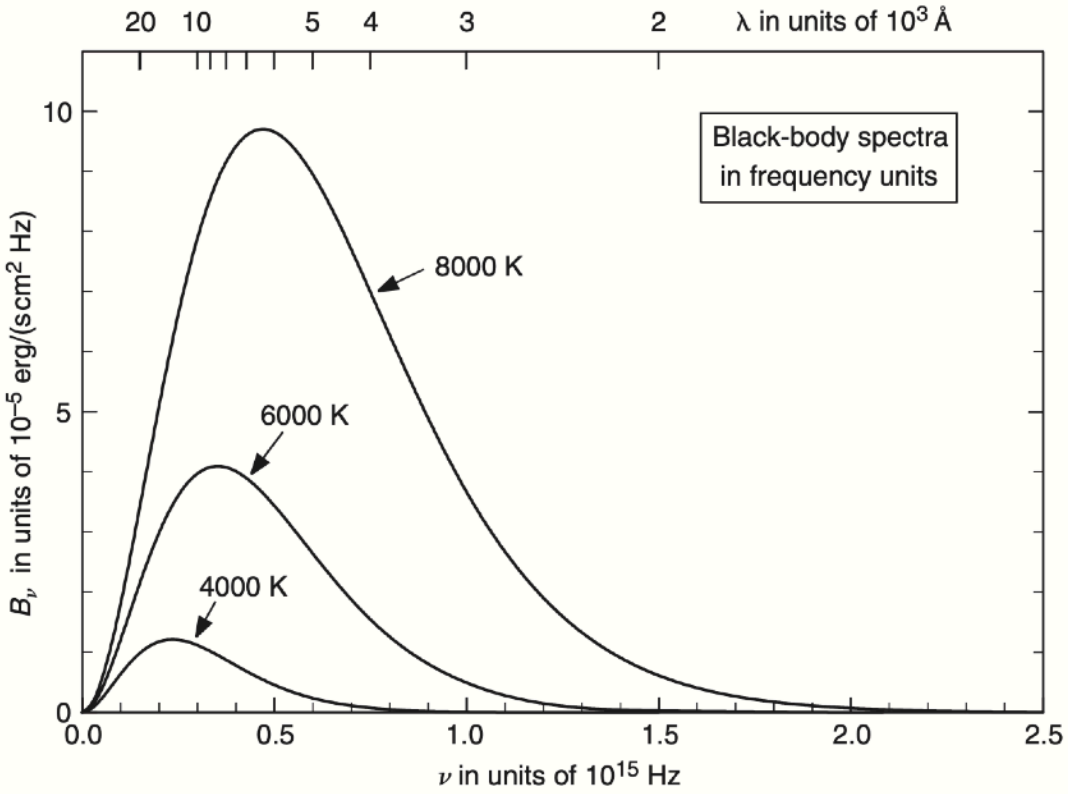
- **Source function* is Planck's law**

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

*Source function $S_\nu = \frac{j_\nu}{k_\nu}$

j_ν: emissivity (energy fraction added to the photon beam)

k_ν: opacity (energy fraction removed from the photon beam)



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1D LTE model atmosphere

Assumptions 1D LTE:

- **Excitation equilibrium (Boltzmann eq.)**
- **Ionisation equilibrium (Saha eq.)**
- **Maxwell-Botzmann velocity distribution**
- **Source function is Planck's law**

Each layer can be treated separately and described by temperature, gas pressure, e- number density, and opacity

Model computation (in few words): iterative process to find the thermodynamic parameters that describe each layer

Each layer is identified by an independent variable, usually optical depth at a certain frequency (τ_ν) or column mass density or mass depth (m)

$$\tau_\nu = \int -k_\nu dx \ , \quad m = \int \rho dx$$

E.g.

ATLAS models —> m

MARCS models —> $\tau_{Rosseland}$ (mean optical depth)

1D LTE model atmosphere

Model computation (in few words): iterative process to find the thermodynamic parameters that describe each layer

1) Temperature structure initial guess —> compute gas pressure, e- number density, and opacity for each layer

2) Solve the radiative transfer equation $\frac{dI_\nu}{d\tau_\nu} = -I_\nu + S_\nu$ at each point

3) Check that the radiative equilibrium is satisfied, i.e. find the temperature distribution for which the total flux is conserved

1D LTE model atmosphere

Example of ATLAS9 model atmosphere (Kurucz R.L. 1970)

This is the kind of models that you will use as input for MOOG spectral synthesis code (Sneden et al. 2012, version 2019)

```
KURUCZ
  4782./   1.7/   -2.5      mic = 1.8700
                72
 2.47401767E-02   3272.0 1.298E+00 2.329E+06 5.391E-06
 3.29405303E-02   3273.0 1.729E+00 2.942E+06 5.457E-06
 4.36923395E-02   3276.0 2.293E+00 3.743E+06 5.576E-06
 5.76651183E-02   3281.4 3.026E+00 4.785E+06 5.745E-06
 7.56643298E-02   3290.5 3.971E+00 6.143E+06 5.974E-06
 9.86441219E-02   3304.1 5.177E+00 7.907E+06 6.267E-06
 1.27744340E-01   3321.3 6.704E+00 1.017E+07 6.620E-06
...
 4.13280827E+02   7587.7 2.168E+04 1.674E+14 2.075E+00
 4.17833612E+02   7726.6 2.192E+04 2.035E+14 2.566E+00
 4.22770160E+02   7860.1 2.218E+04 2.440E+14 3.141E+00
 4.28121796E+02   8000.0 2.246E+04 2.932E+14 3.873E+00
 4.33967127E+02   8128.5 2.277E+04 3.455E+14 4.684E+00
       1.8700
NATOMS          0          -2.52
NMOL            0
```

In the practical lesson, you will not compute models, but you will interpolate in a pre-computed grid

Castelli's grid: https://wwwuser.oats.inaf.it/fiorella.castelli/grids.html

1D LTE model atmosphere

Example of ATLAS9 model atmosphere (Kurucz R.L. 1970)

Stellar parameters:

Teff, logg, [M/H], vt

N° of layers

```
KURUCZ
  4782./   1.7/   -2.5       mic = 1.8700
                 72
 2.47401767E-02   3272.0 1.298E+00 2.329E+06 5.391E-06
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 7.56643298E-02   3290.5 3.971E+00 6.143E+06 5.974E-06
 9.86441219E-02   3304.1 5.177E+00 7.907E+06 6.267E-06
 1.27744340E-01   3321.3 6.704E+00 1.017E+07 6.620E-06
...
```

ρx (rhox) mass depth	T temperature	P gas pressure	Ne- e- n° density	κRoss Rosseland mean opacity in mass scale

Opacity sources: continuous + lines

Continuous opacity: caused by bound-free (bf) and free-free (ff) transitions mainly of hydrogen

In cool stars: H^- (I = 0.75 eV) is the main source in the optical and near-IR spectra

Line opacity: caused by bound-bound transitions of other elements. It depends on temperature, pressure, and chemical composition

Not easy to determine: very large number of lines is needed with known atomic data

Ideally: line opacity computed at several points across each spectral line as a function of optical depth

—> **but** atomic and molecular data are often not available + very expensive in terms of computer time

Alternative: generate an **Opacity Distribution Function** for the lines —> can be used as continuous opacity in model atmosphere computation

Line formation

Model atmospheres give us the temperature and pressure as a function of (optical) depth —> we can study how the electronic transitions in atoms and molecules lead to absorption lines at characteristic wavelengths

The strength of a spectral line depends on the number of absorbers along the line of sight through the visible depths of the atmosphere. However, the atmosphere depth changes with the amount of continuous absorption —> if the continuous absorption is strong, the path length will be short and vice versa

The line strength is proportional to the ratio of line to continuous absorption coefficients:

$$\frac{F_c - F_\nu}{F_c} \propto \frac{\ell_\nu}{\kappa_\nu} = R \rightarrow \textbf{valid for weak lines}$$

where F_c and F_ν are the continuous and line fluxes

Weak lines strength vs Teff

In cool stars: $\kappa_\nu \propto T^{-5/2} P_e e^{0.75/kT}$ (H^- bound-free absorption)

For a **neutral line** of an element that is mostly ionised (**e.g. Fe I**), the fractional change of R with T is:

$$\frac{1}{R}\frac{dR}{dT} \propto \frac{\chi + 0.75 - I}{kT^2}$$ →depending on χ, neutral lines decrease with T by 10%-30% per 100 K

Lines of different χ can be used to constrain Teff (**excitation equilibrium**)→ ***xiru***: Fe I excitation equilibrium for Teff (see Arthur's talk)

For a **ionised line** of mainly ionised elements (**e.g. Fe II**), one finds low sensitivities to Teff, except those with a large χ. These become stronger with T by up to 20% per 100 K.

Weak lines strength vs logg

Ionisation equation: $\frac{N_{i+1}}{N_i} = \frac{\Phi(T)}{P_e}$

In cool stars: $P_g \propto P_e^2$ and $P_g \propto g^{2/3}$, $P_e \propto g^{1/3}$ —> pressure dependences can be translated into approximate gravity dependences

For a **neutral line** of an element that is mostly ionised (**e.g. Fe I**):

with $N_{i+1} \sim N_{tot} = \text{const}.$ —> $N_i \propto P_e$ —> $\ell_\nu \propto N_i \propto P_e$

But $\kappa_\nu \propto P_e$ (H^- bound-free absorption) —> $\ell_\nu / \kappa_\nu \sim \text{const}.$ —> **insensitive to logg**

For a **ionised line** of mainly ionised elements (**e.g. Fe II**) :

$N_i \sim N_{tot} = \text{const}.$ —> $\ell_\nu \sim \text{const}.$ —> $\ell_\nu / \kappa_\nu \propto 1/P_e \propto g^{-1/3}$ —> **sensitive to logg**

Lower pressure (logg) causes greater line strength via the continuous opacity of H^-

Combining Fe I + II abundances to constrain logg (**ionization equilibrium**) →

xiru: Fe I+II ionisation equilibrium for logg (see Arthur's talk)

Weak lines strength vs abundance

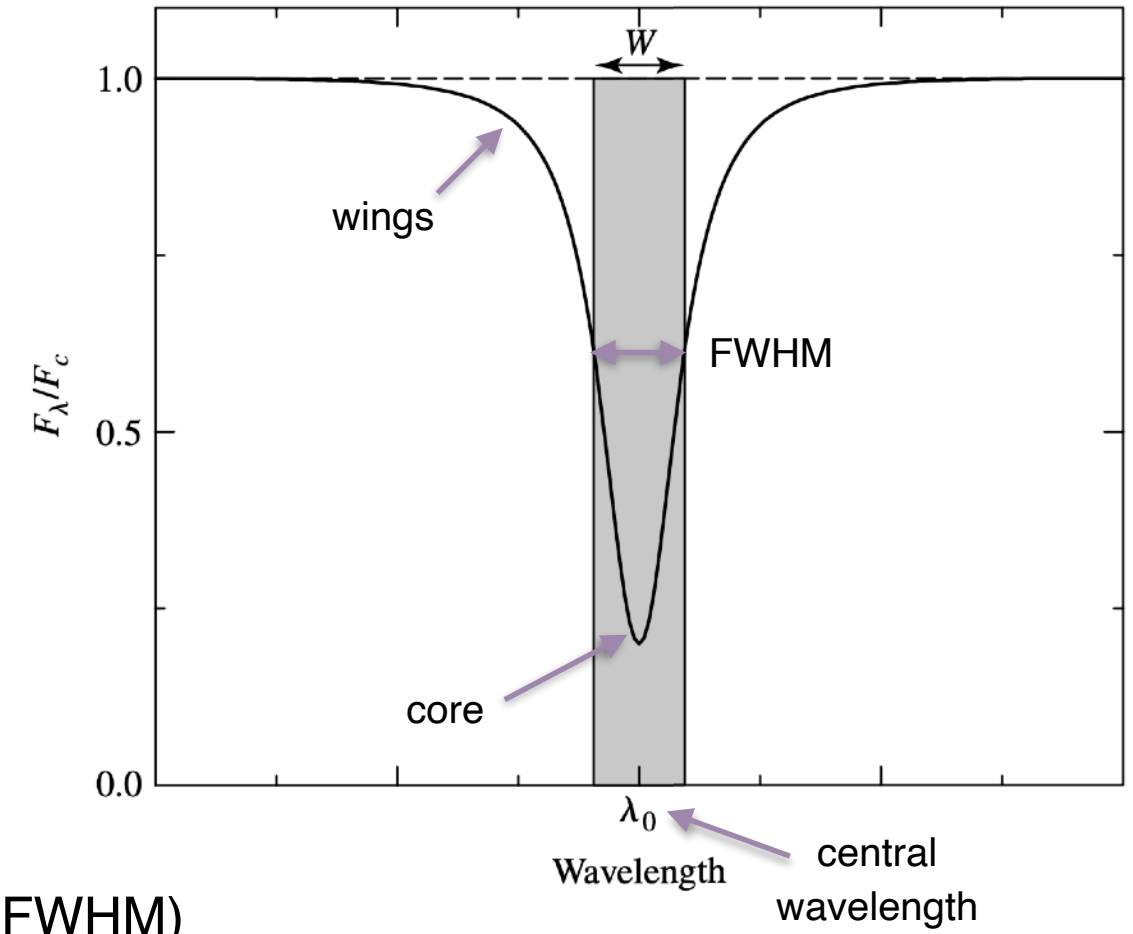
The line profile is defined by the core and the wings

$(F_c - F_\lambda)/F_c$ is called *depth* of the line

The line strength is measured in terms of equivalent width (EW)

The EW is defined as the width of a box reaching up the continuum that has the same area as the spectral line

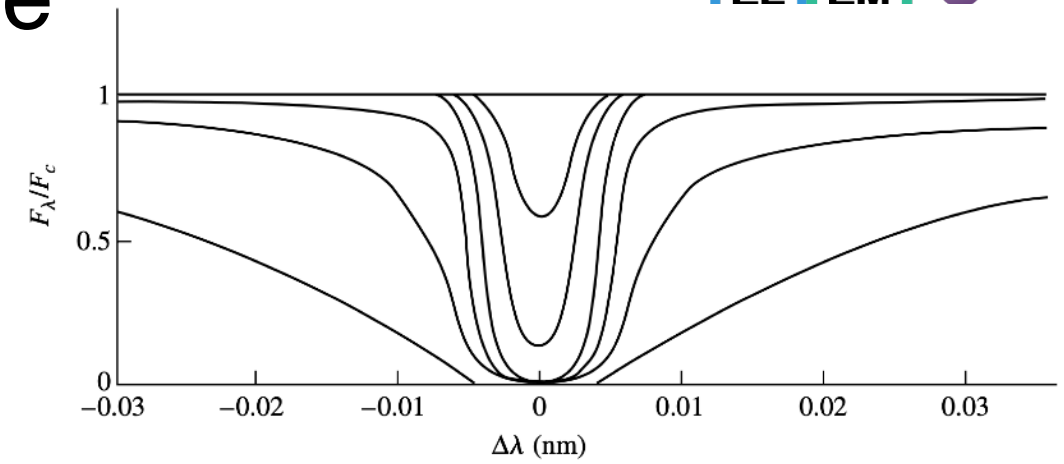
$$\text{EW} = W = \int \frac{F_c - F_\lambda}{F_c} d\lambda$$



$(F_c - F_\lambda)/(F_c - F_{\lambda_0})$ = 1/2 —> full width half maximum (FWHM)

Weak lines strength vs abundance

The equivalent width (EW) changes with the number of absorbing atoms per unit area (number density) that produce the line (N_a)



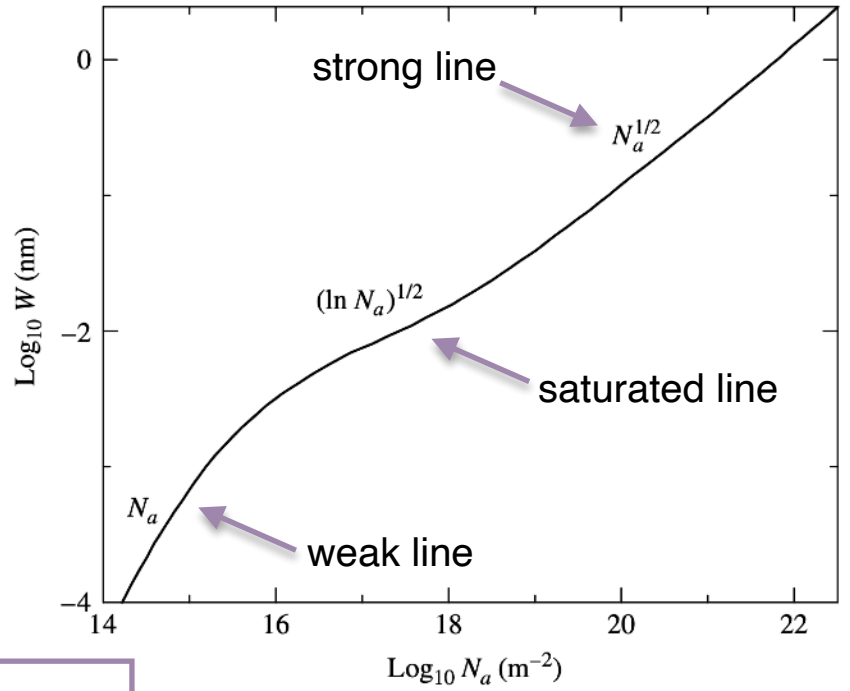
Three regimes:

1) weak lines: core dominates → $W \propto N_a$

2) saturated lines: line centre becomes optically thick, no significant change in profile → $W \propto \sqrt{\ln N_a}$

3) strong lines: line wings begin to grow → $W \propto \sqrt{N_a}$

EW + curve of growth → N_a → chemical abundance!



Weak lines are the best choice to estimate chemical abundances

Broadening

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

Microscopic:

1. natural broadening (reflecting $\Delta E\, \Delta t \geq h/2\pi$)
2. thermal (Doppler) broadening (Gaussian)
3. microturbulence vt (treated like extra thermal broadening, Gaussian)
4. (isotopic shift, hfs, Zeeman effect)
5. collision broadening (Lorentzian)→ important for strong lines

Macroscopic

1. macroturbulence
2. rotation
3. (instrumental broadening)

Microturbulence (vt or ξ)

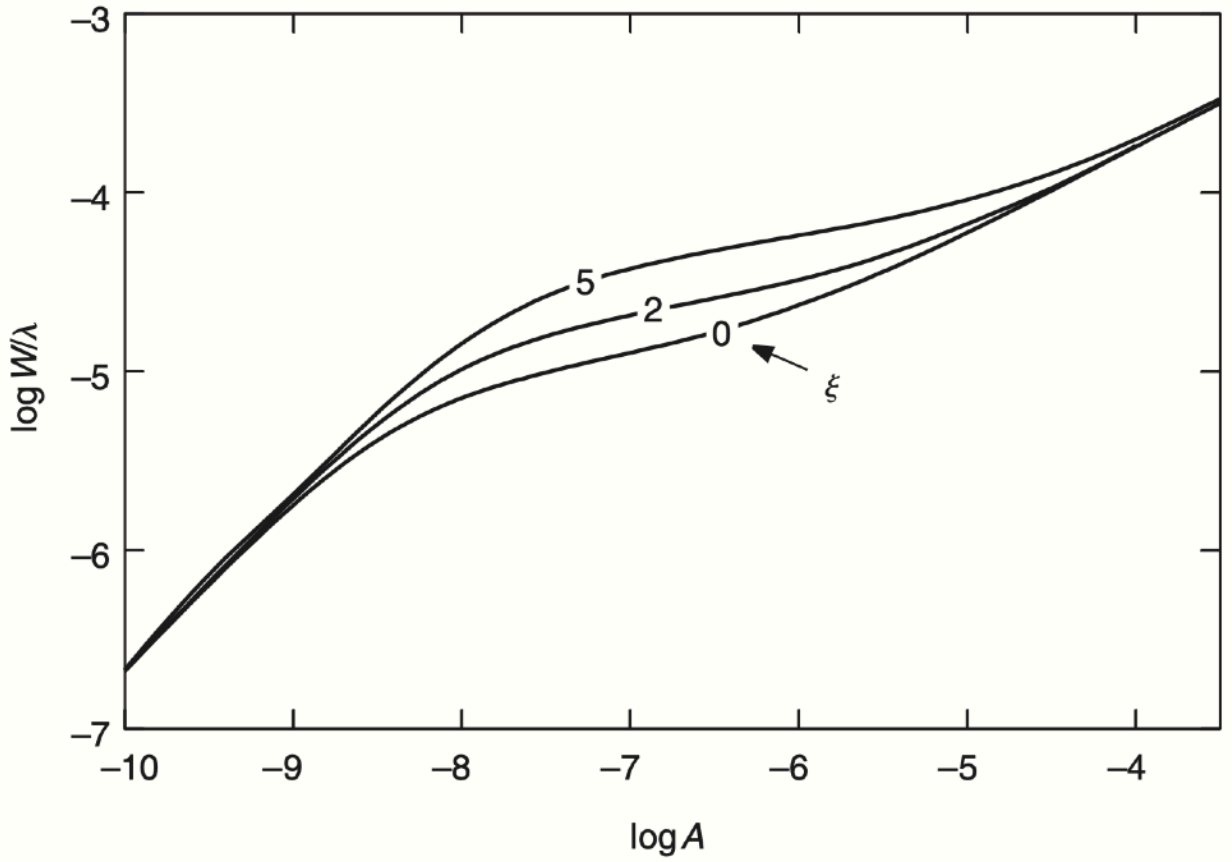
Additional broadening used as correction parameter in 1D LTE abundance analysis

Without microturbulence, lines of intermediate or high strength return too high abundances

Lines of the same element with many different strengths (EW) can be used to constrain vt

xiru: Many Fe I lines with different EW for vt (see Arthur's talk)

log(W/λ)=reduced EW



Atomic data: Line lists

To produce a realistic synthetic spectrum we need atomic and molecular line lists.

Line lists are tables that contain the parameters of the atomic transitions and molecular bands (from vibrational or rotational-vibrational molecular transitions)

The line profile (EW) depends on:

$$\log\left(\frac{w}{\lambda}\right) = \log\left[\text{constant}\,\frac{\pi e^2}{mc^2}\,\frac{N_j/N_{\mathrm{E}}}{u(T)}N_{\mathrm{H}}\right] + \log A + \log g_n f\lambda - \theta_{\mathrm{ex}}\chi - \log\kappa_\nu$$
$$= \log C + \log A + \log g_n f\lambda - \theta_{\mathrm{ex}}\chi - \log\kappa_\nu. \qquad (16.4)$$

C=constant, A=abundance, loggf=oscillator strength, χ=excitation potential, κ_ν=absorption coefficient

loggf: linked to transition probability → calculated numerically or measured in lab

Atomic data: Line lists

VALD: Vienna Atomic Line Database (https://www.astro.uu.se/valdwiki/FrontPage)

NIST: National Institute of Standards and Technology (https://physics.nist.gov/PhysRefData/ASD/lines_form.html)

Main Parameters **Spectrum** Mg I *e.g.,* Fe I *or* Na;Mg; Al *or* mg i-iii *or* 198Hg I

Search for Wavelength **Lower:** 5100 Å

Upper: 5200 Å

Output Wavelength Units: Å

Reset input | Retrieve Data | Show Graphical Options | Show Advanced Settings

Observed Wavelength Air (Å)	Rel. Int. (?)	A_{ki} (s^{-1})	log($g_i f_{ik}$)	Acc.	E_i (eV)		E_k (eV)	Lower Level Conf., Term, J	Upper Level Conf., Term, J	Type	TP Ref.	Line Ref.
5 167.3216	42	1.13e+07	−0.870	B+	2.7091049	-	5.1078270	3s3p ^{3}P° 0	3s4s ^{3}S 1		c45	L7428
5 172.6843	44	3.37e+07	−0.393	B+	2.7115919	-	5.1078270	3s3p ^{3}P° 1	3s4s ^{3}S 1		c45	L7428
5 183.6042	45	5.61e+07	−0.167	A	2.7166398	-	5.1078270	3s3p ^{3}P° 2	3s4s ^{3}S 1		c45	L7428

In the afternoon session: creating line lists with **LINEMAKE** (https://github.com/vmplacco/linemake)

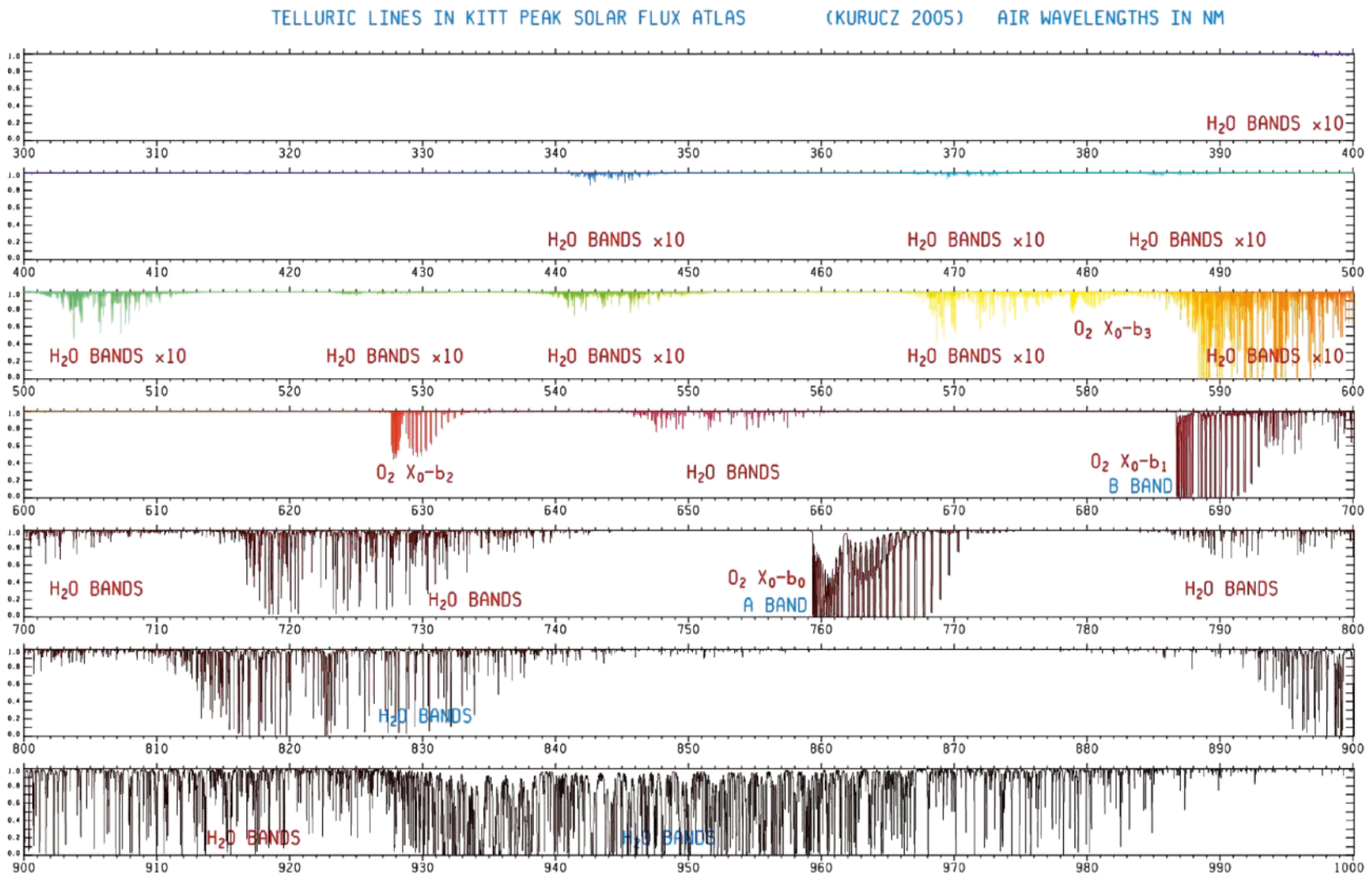
Atomic data: Telluric lines

The Earth's atmosphere produces so-called **telluric lines**

In the optical, some regions suffer from telluric absorption

In the infrared many regions have telluric absorption

Careful when deriving abundances!



Abundance nomenclature

Mass fractions: let X, Y, Z denote the mass-weighted abundances of H, He and all other elements ("metals"), respectively, normalised to unity (X + Y + Z =1)

example: X = 0.744, Y = 0.242, Z = 0.014 for the Sun

Absolute abundance : $A(X) = \log \varepsilon(X) = \log (N_X / N_H) + 12$

example: A(Fe)= log ε(Fe) = 7.50 dex (Asplund et al. 2009)

A(H) = log ε(H) = 12

When we talk about metallicity we refer to the [Fe/H] of the star

Abundance ratio: $[X/H] = A(X)_\star - A(X)_\odot = \log (N_X / N_H)_\star - \log (N_X / N_H)_\odot$

example: [Fe/H]=—1 , the star has and iron abundance 1/10 of the iron abundance in the Sun

$[Fe/H]_\odot=0$ → Sun is our reference star

Synthetic spectra

Spectrum synthesis: computation of a complete spectral interval in which all the observed lines are included

Synthetic spectrum computation (in few words):

- Given the model atmosphere and the line list, compute line opacities, continuum opacities and source functions at each depth
- Integrate the source function to obtain the surface flux or the surface intensity

This can be performed by spectrum synthesis codes like **MOOG** (see Arthur's talk)

From stellar spectra to chemical abundances

Input needed:

- **Observed stellar spectra**
- Stellar parameters (Teff, logg, vt, [M/H]) —> **Model atmosphere**
- Atomic data (energy levels, transition strengths, ionisation stage, …) —> **Line list**
- **Spectrum synthesis code** (MOOG**)**

Now we can derive abundances!

However:

- Lines may lack or have inaccurate atomic data
- Lines can be blended —> overestimated abundances (if blends are not properly taken into account)
- Lines can be subject to effect you are unaware of, e.g. hyperfine, isotopic and Zeeman splitting; 3D and NLTE effects (see Andy's talk)
- …

From stellar spectra to chemical abundances

Example of a spectrum synthesis of the Ba line at 5853 Å

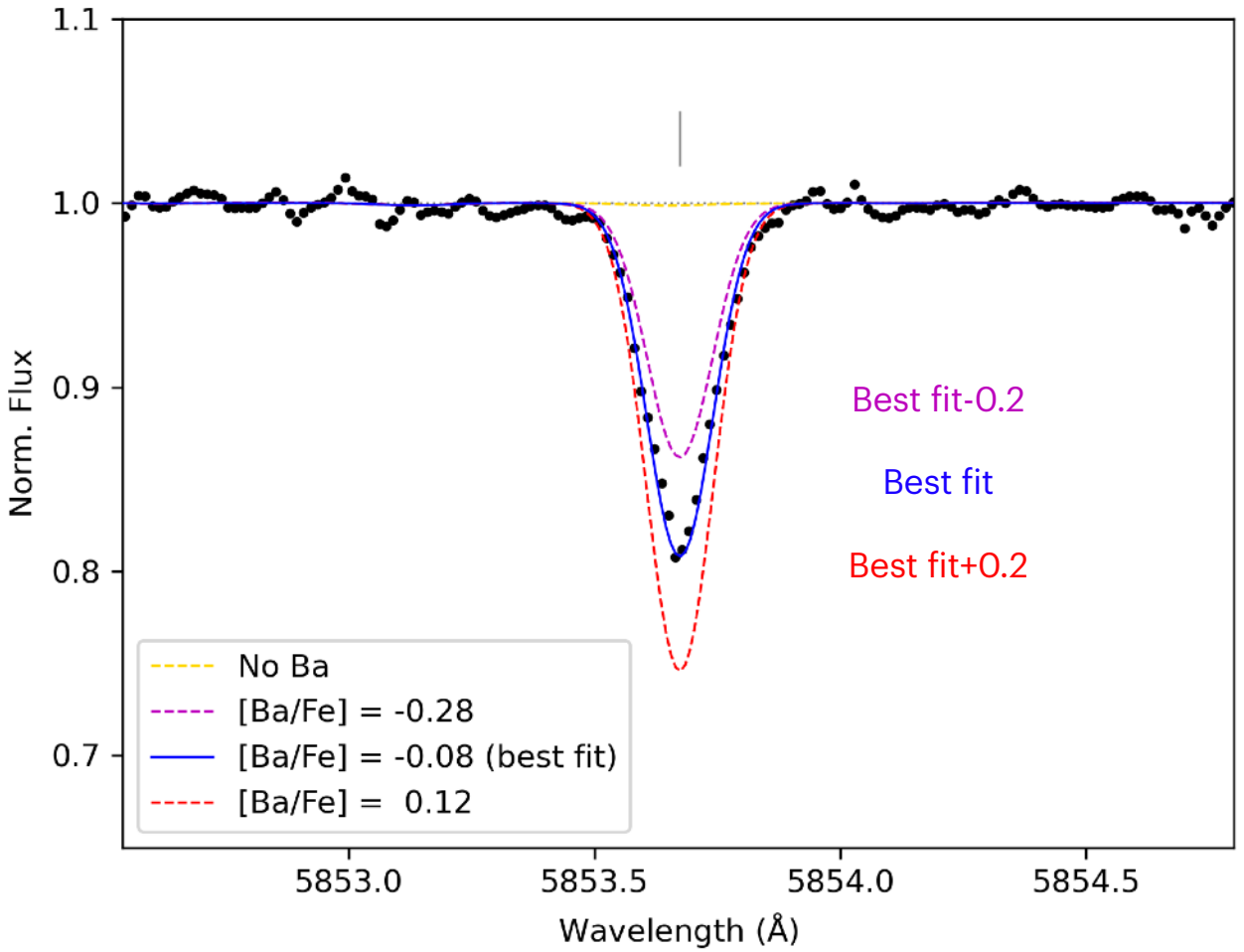
Given the proper stellar parameters and model atmosphere + line list, we can compute several synthetic spectra with different abundances

Yellow: No Ba in the synthetic spectrum

Blue: Ba abundance at which the synthetic and observed spectra coincide (best fit)

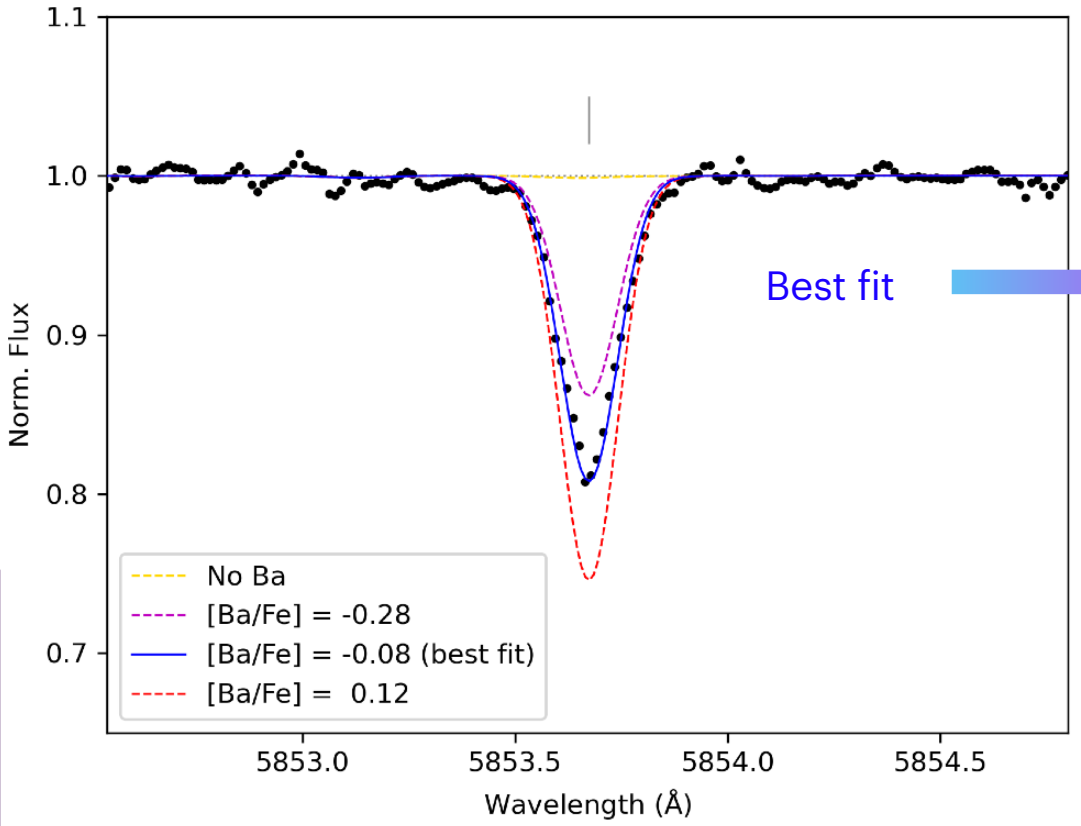
Magenta and red: increase and decrease Ba abundance by 0.2 dex to see how the line profile changes

Ba abundance is given by the synthetic spectrum that corresponds to the best fit (+ uncertainties)

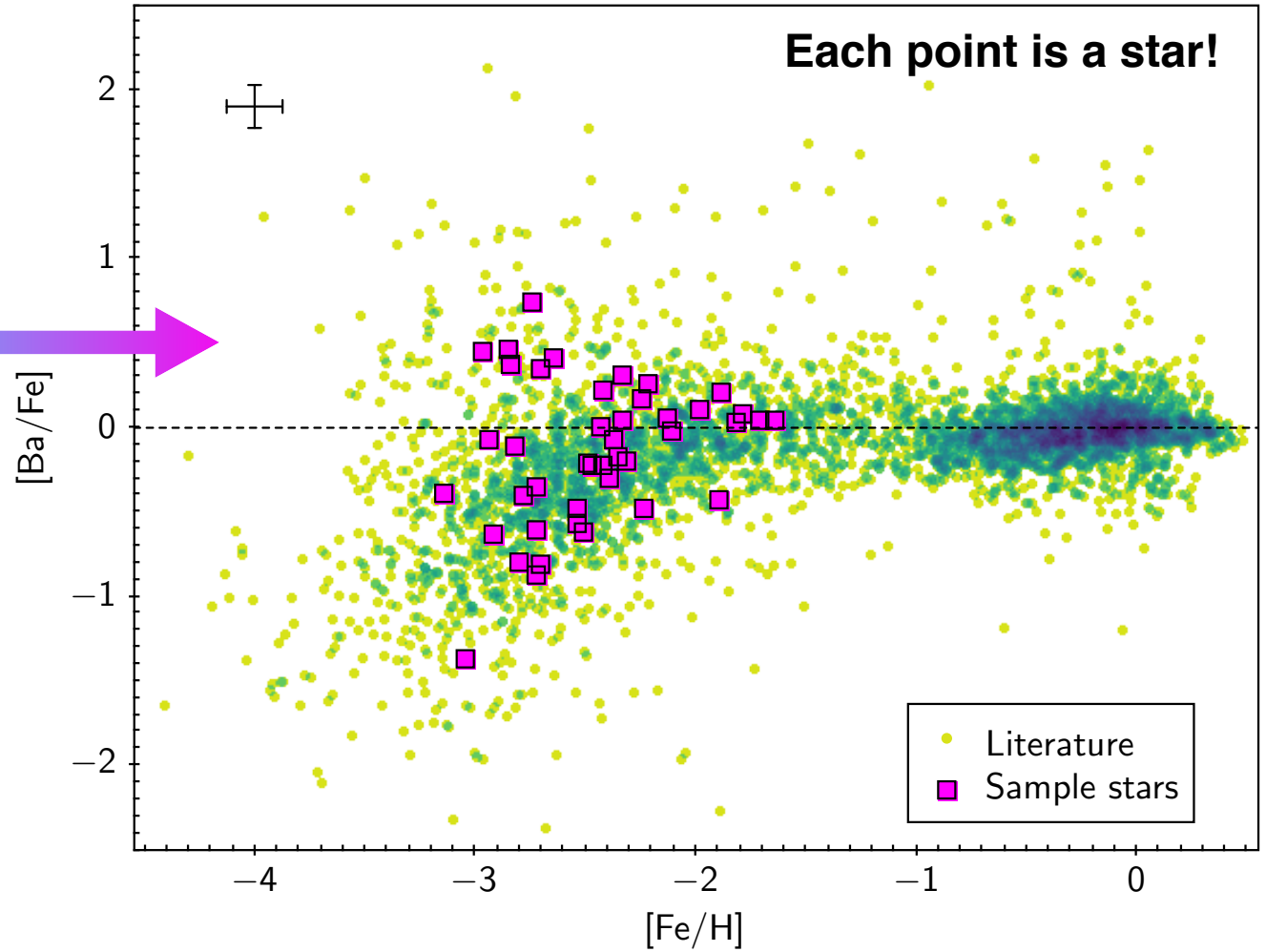


From stellar spectra to chemical abundances

For each star:



Best fit

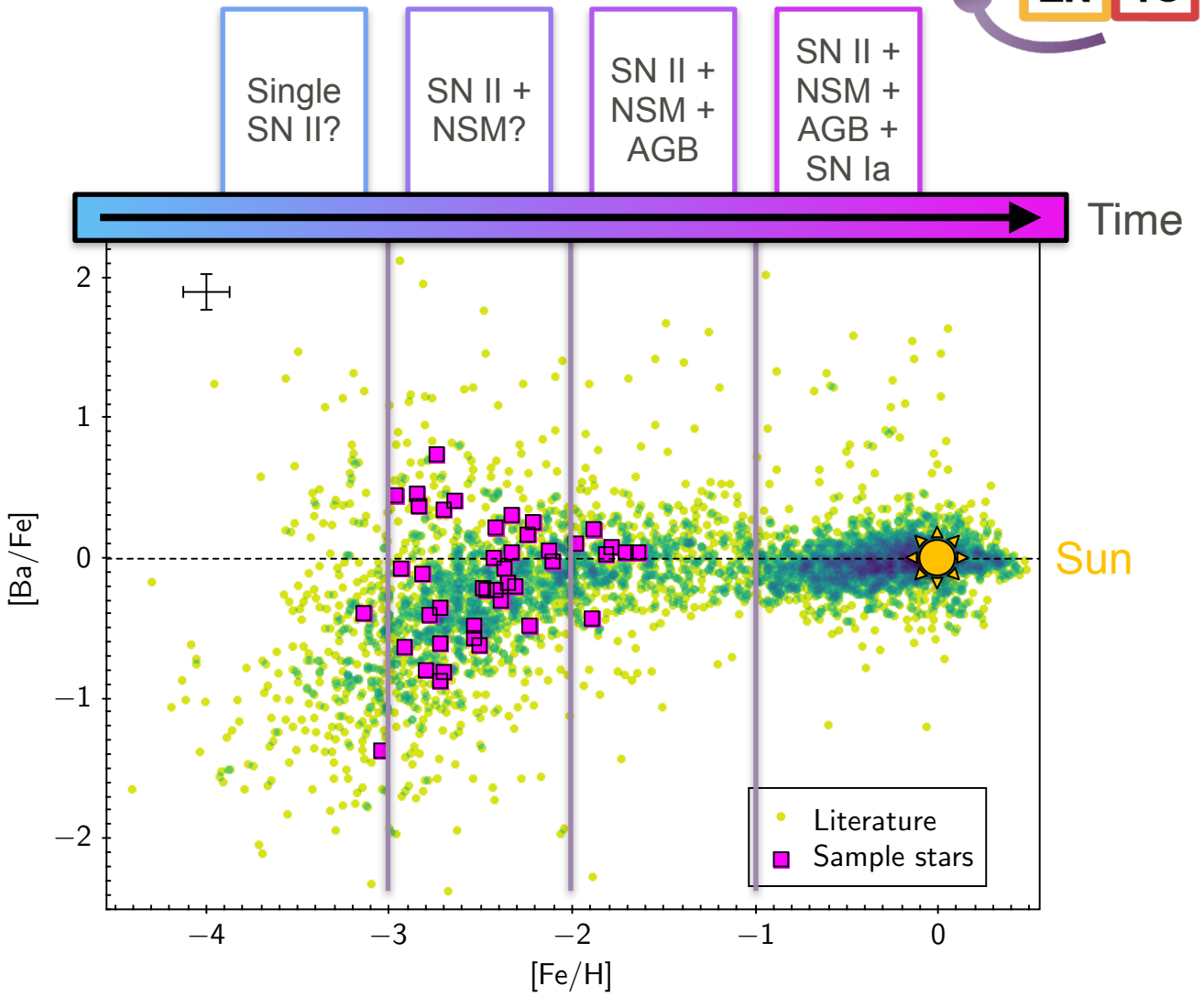


Why chemical abundances are important?

Different sites (SNe II, NSM, AGB stars, SNe Ia…) produce different elements in various amounts

Abundance ratios diagrams can tell us

- the different contributions of those sites on their respective time scales -> **we can study the Galactic Chemical Evolution (GCE)** (see Marta's talk)



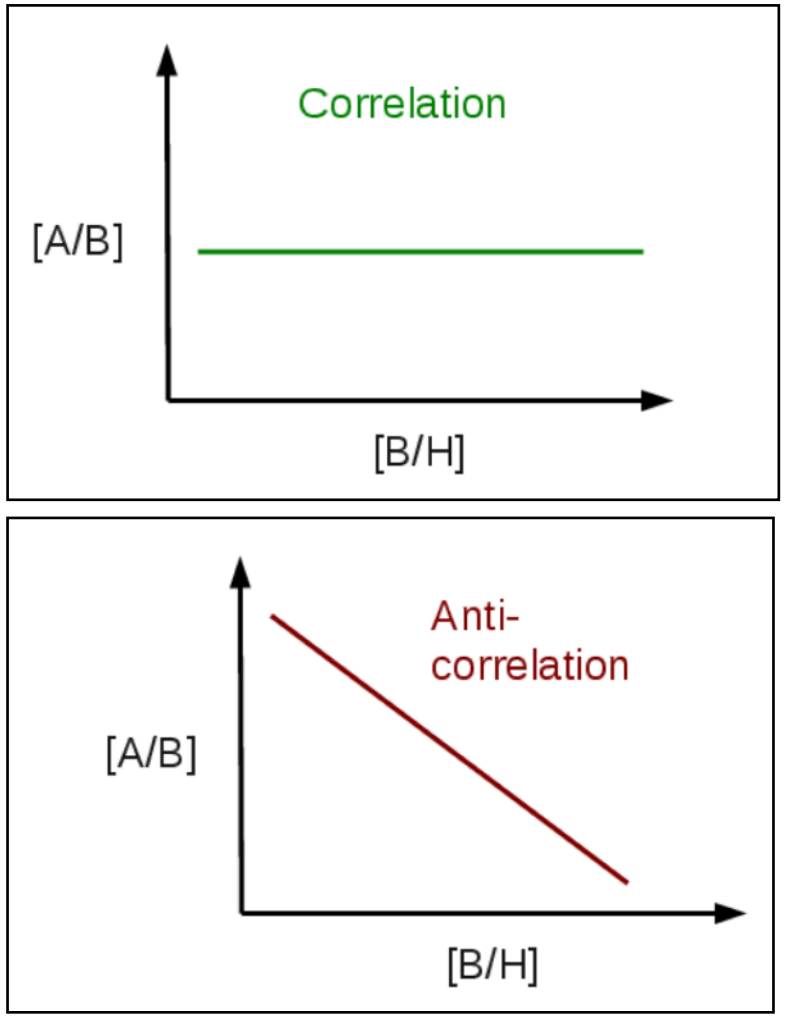
Why chemical abundances are important?

Figure from Hansen 2012

Different sites (SNe II, NSM, AGB stars, SNe Ia…) produce different elements in various amounts

Abundance ratios diagrams can tell us

- **if the elements are co-produced or not** through correlations between elements pairs



Absolute abundance: $\log_{10}\varepsilon(X)_{\star} = \log_{10}(N_X/N_H)_{\star} + 12$

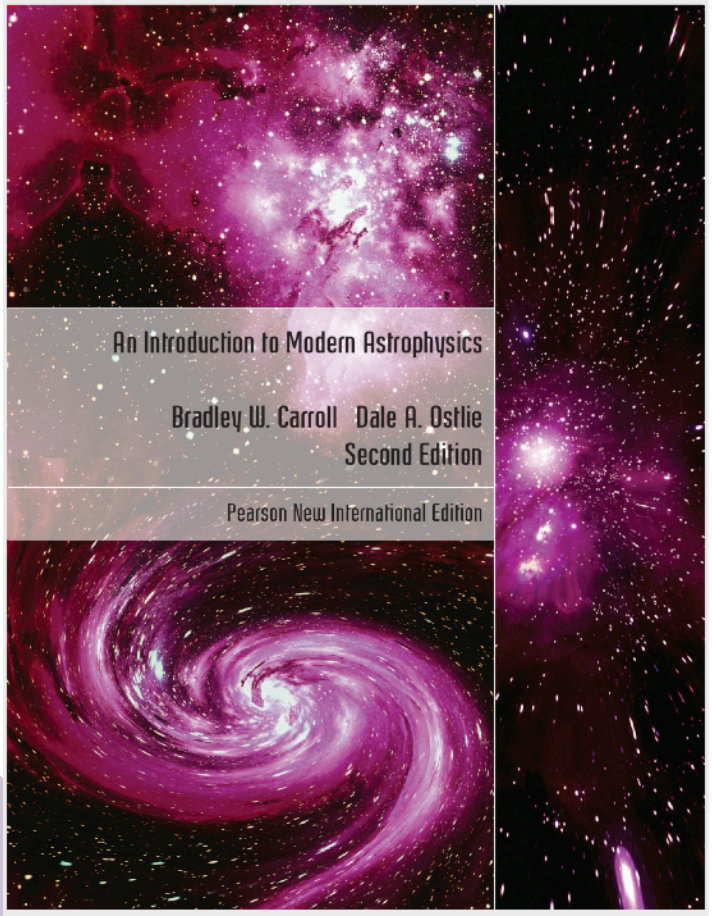
Abundance ratio: $[X/Y] = \log_{10}(N_X/N_Y)_{\star} - \log_{10}(N_X/N_Y)_{\odot}$

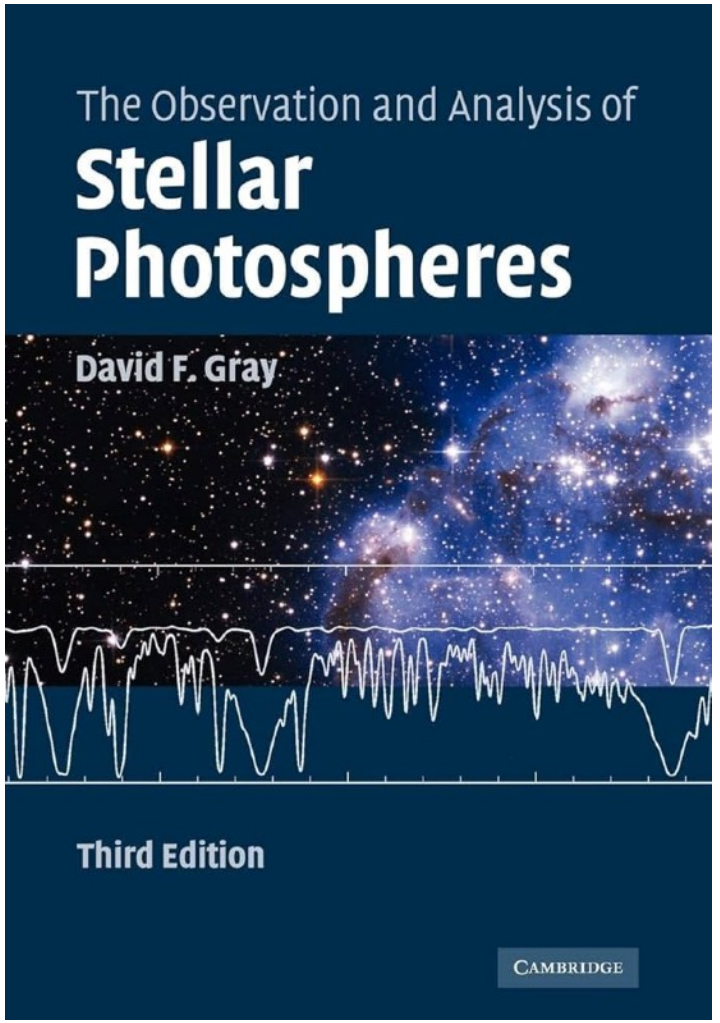
For the Sun: $[X/Y]_{\odot} = 0$

Suggested readings

"An introduction to Modern Astrophysics"

Carroll B.W. and Ostlie D.A.





"The observation and analysis of Stellar Photospheres" - Gray D.F.

Afternoon session

The art of TOPCAT (or how to deal with large catalogues and tables without python)

TOPCAT

Tool for OPerations on Catalogues And Tables

Does what you want with tables

https://www.star.bris.ac.uk/~mbt/topcat/

The art of TOPCAT

I found this nice beginner guide :

https://ui.adsabs.harvard.edu/abs/2020OJAp....3E...2P/abstract

https://arxiv.org/pdf/1905.13189v2

We will follow some of the procedures described in Sect.4

I will show you how to:

- Open files and catalogues with TOPCAT
- Crossmatch with SIMBAD and GAIA catalogues
- Make plots
- Basic queries in the Astronomical Data Query Language (ADQL)