

# Classical Spectroscopy and Chemical Composition Analyses Chris Sneden, University of Texas at Austin



http://precisionspectroscopy.yolasite.com/

# Uses: from extracting some basic information out of low resolution and/or low S/N spectra



Uses: to diving into the details for precise chemical compositions of individual stars



properly accounting for

yes, that's why their line shapes look weird

making more precise Ni I abundances by recognizing isotopic substructure



does it happen to all Ni I lines? Why or why not? applying ordinary abundance techniques to binary stellar specrtra



how to do this so that the results are physically reasonable

# the power of high-res spectroscopy

- effective temperature T<sub>eff</sub>: Boltzmann eq., photometry+calibrations
  - actually inferred from an "excitation" temperature
- surface gravity log(g): Saha eq., line depth ratios, parallax+photometry
  - Saha means ionization temperature; is this physically real
- microturbulent velocity  $\xi_t$  or  $v_{turb}, \ line strengths$ 
  - remember  $\xi_t$  that is a single parameter describing complex "extra" motions
- metallicity: [Fe/H], [M/H], or something similar & vague
  - vague is the fault of authors
- abundance ratios: [X/Fe]
  - again, how are the ratios formed?
- isotopic ratios: <sup>12</sup>C/<sup>13</sup>C, (<sup>25</sup>Mg, <sup>26</sup>Mg)/<sup>24</sup>Mg, <sup>6</sup>Li/<sup>7</sup>Li, <sup>16</sup>O/<sup>17</sup>O, ...
- velocities: systemic radial, rotational, orbital, oscillational, macroturbulent
- magnetic fields, star spot analysis

# My research: to use stellar spectra to help decode stellar nucleosynthesis



The "holy grail": to understand how our Galaxy produced the solar chemical composition



Sneden et al. 2008

- $[A/B] = \log_{10}(N_A/N_B)_{star} \log_{10}(N_A/N_B)_{Sun}$ where N is an elemental number density
- $\log \epsilon(A) = \log_{10}(N_A/N_H) + 12.0$  (spectroscopy)
- $\log N(A) = \log_{10}(N_A/N_{Si}) + 6.0$  (meteorites)
- Metallicity 
   → [Fe/H] (sometimes labeled [M/H]
- Most metal-rich? [Fe/H] ~ +0.5 (proven)
- Most metal-poor? [Fe/H] ~ -5.5 (e.g., Aoki et al. 2006)
- Metallicity labels:
- metal-poor: [Fe/H] ≤ -2
- very metal-poor: [Fe/H] ≤ -2
- extremely metal-poor:  $[Fe/H] \le -3$
- NATURE paper metal-poor:  $[Fe/H] \le -6 \text{ or } -7 \text{ or } \dots$
- WATCH OUT! [] quantities have ASSUMPTIONS about solar values

# George Wallerstein 1930-2021



distinguished creator of modern high-resolution stellar spectroscopy

#### Wallerstein had metallicities conquered long ago

"Certainly, at this time, no apology is needed for a curve-of-growth analysis, no matter how crude" Helfer+ 1959

4.0

γ∕m 907-

5.0

-2

HR483 = HD10307

- I

 $\Delta \Theta_{exc} = -.025$ 



Wallerstein 1962

0

 $LOG \eta_{\pm} - 1.9$ 

+1

# invention of the bracket!

#### Helfer, Wallerstein, Greenstein 1959, ApJ, 129, 700

with the same pattern of scatter of points duplicated. Evidently, the problem of representing the true continuum by the measured continuum is more acute in the M41 star than in the other three, again reflecting a real difference between the atmospheres of the two groups of stars.

The analytical procedure used is straightforward. Let

$$[X] \equiv \log\left[\frac{X_*}{X_{\odot}}\right], \qquad (3)$$

where X is any physical quantity. From the vertical shift between the theoretical and observed curve of growth, [V] is determined, where V is the atmospheric velocity parameter. The experimental uncertainty in log V is about  $\pm 0.1$ ; a value of log  $V_{\odot} = 0.23$ 

 $[A/B] = \log_{10}(N_A/N_B)_{star} - \log_{10}(N_A/N_B)_{Sun}$ where N is an elemental number density

inspired by another George:



George Preston, alive and publishing today

#### ABUNDANCES IN G DWARFS. VI. A SURVEY OF FIELD STARS\*

GEORGE WALLERSTEIN

Berkeley Astronomical Department, University of California Received July 31, 1961; revised September 12, 1961

1962ApJS....6..407W

0

+.50

0

-.50



alpha enhancements at low metallicity



[Fe/H]

-1.50

-2.00

-1.00

#### Did Wallerstein almost discover the thick disk?



with a sample of 300 stars instead of 30?

### How much have we really progressed since Wallerstein+ 1962?



# And we have all the observational/analytical advantages now

<u>QUANTITY</u>	WALLERSTEIN ERA	TODAY
telescopes	0.7-2m	3-10m
detectors	photographic plates	CCDs, other electronic
wavelength coverage	0.4-0.9μm	0.2-5µm
analysis approach	strictly differential W.R.T. $\odot$	mostly absolute
atmosphere	single "reversing layer"	50-100 layer
radiative transfer	local thermodynamic eq. (LTE)	non-LTE in many cases
atomic line inputs	EW's, excitation energies (χ)	EW's, χ's, gf's, hyperfine,
molecular line inputs	almost nothing	good data for many diatomics
transition probabilities	few, and poorly known	good and growing all the timei
analytical efficiency	one boring star at a time	almost too easy now???

#### spectral line analysis: reminder of the basics

R. J. Rutten, "Radiative Transfer in Stellar Atmospheres": http://www.staff.science.uu.nl/~rutte101/

$$dI_{\nu} \equiv -\alpha_{\nu} I_{\nu} ds \qquad (2.19)$$

with  $\alpha_{\nu} = \sigma_{\nu} n$  the monochromatic linear extinction coefficient (units cm<sup>-1</sup>), or the monochromatic volume extinction coefficient when interpreted as cross-section per unit volume (cm<sup>2</sup> cm<sup>-3</sup> = cm<sup>-1</sup>). The definition per gram is:

 $S_{\nu}$ 

$$dI_{\nu} \equiv -\kappa_{\nu}\rho I_{\nu} ds \qquad (2.20)$$

$$\eta_{\nu} \equiv \alpha_{\nu}^{l}/\alpha_{\nu}^{c}$$

$$\equiv j_{\nu}/\alpha_{\nu} \qquad S_{\nu}^{\text{tot}} = \frac{\sum j_{\nu}}{\sum \alpha_{\nu}} \qquad S_{\nu}^{\text{tot}} = \frac{j_{\nu}^{c} + j_{\nu}^{l}}{\alpha_{\nu}^{c} + \alpha_{\nu}^{l}} = \frac{S_{\nu}^{c} + \eta_{\nu}S_{\nu}^{l}}{1 + \eta_{\nu}}$$

$$\mu \frac{\mathrm{d}I_{\nu}}{\mathrm{d}\tau_{\nu}} = I_{\nu} - S_{\nu}. \longrightarrow I_{\nu}^{+}(\tau_{\nu}, \mu) = + \int_{\tau_{\nu}}^{\infty} S_{\nu}(t_{\nu}) \,\mathrm{e}^{-(t_{\nu} - \tau_{\nu})/\mu} \,\mathrm{d}t_{\nu}/\mu$$
$$I_{\nu}^{-}(\tau_{\nu}, \mu) = + \int_{0}^{\tau_{\nu}} S_{\nu}(t_{\nu}) \,\mathrm{e}^{-(t_{\nu} - \tau_{\nu})/\mu} \,\mathrm{d}t_{\nu}/|\mu|.$$

$$\begin{split} J_{\nu}(\tau_{\nu}) &\equiv \frac{1}{2} \int_{-1}^{+1} I_{\nu}(\tau_{\nu}, \mu) \, \mathrm{d}\mu \\ &= \frac{1}{2} \int_{\tau_{\nu}}^{\infty} S_{\nu}(t_{\nu}) \, E_{1}(t_{\nu} - \tau_{\nu}) \, \mathrm{d}t_{\nu} + \frac{1}{2} \int_{0}^{\tau_{\nu}} S_{\nu}(t_{\nu}) \, E_{1}(\tau_{\nu} - t_{\nu}) \, \mathrm{d}t_{\nu} \\ &= \frac{1}{2} \int_{0}^{\infty} S_{\nu}(t_{\nu}) \, E_{1}(|t_{\nu} - \tau_{\nu}|) \, \mathrm{d}t_{\nu}, \end{split}$$

$$\begin{aligned} \mathcal{F}_{\nu}(\tau_{\nu}) &= \mathcal{F}_{\nu}^{+}(\tau_{\nu}) - \mathcal{F}_{\nu}^{-}(\tau_{\nu}) \\ &= 2\pi \int_{0}^{1} \mu I_{\nu}(\tau_{\nu}) \, \mathrm{d}\mu - 2\pi \int_{0}^{-1} \mu I_{\nu}(\tau_{\nu}) \, \mathrm{d}\mu \\ &= 2\pi \int_{\tau_{\nu}}^{\infty} S_{\nu}(t_{\nu}) \, E_{2}(t_{\nu} - \tau_{\nu}) \, \mathrm{d}t_{\nu} - 2\pi \int_{0}^{\tau_{\nu}} S_{\nu}(t_{\nu}) \, E_{2}(\tau_{\nu} - t_{\nu}) \, \mathrm{d}t_{\nu} \end{aligned}$$

$$I_{\nu}^{+}(0,\mu) = \int_{0}^{\infty} S_{\nu}(\tau_{\nu}) e^{-\tau_{\nu}/\mu} d\tau_{\nu}/\mu$$
$$\mathcal{F}_{\nu}^{+}(0) = 2\pi \int_{0}^{\infty} S_{\nu}(\tau_{\nu}) E_{2}(\tau_{\nu}) d\tau_{\nu}$$

$$\alpha_{\nu_0}^l \equiv \int_0^\infty \alpha_{\nu}^l \, \mathrm{d}\nu = \frac{h\nu_0}{4\pi} \, \left( n_l B_{lu} - n_u B_{ul} \right) \tag{2.64}$$

using  $\int h\nu \varphi(\nu - \nu_0) d\nu = h\nu_0$  and  $\int h\nu \chi(\nu - \nu_0) d\nu = h\nu_0$  assuming the profile to be symmetric or sufficiently narrow<sup>9</sup>. Throughout these lecture notes, the subscript  $\nu_0$  denotes summation over the line profile<sup>10</sup> and identifies the particular bound-bound transition. The coefficients  $\alpha_{\nu}^l$  and  $\alpha_{\nu_0}^l$  are rewritten with population departure coefficients in (2.108)–(2.115) on page 34. The monochromatic line extinction coefficient per particle, in these lecture notes always without correction for induced emission, is:

$$\sigma_{\nu}^{l} = \frac{h\nu}{4\pi} B_{lu} \varphi(\nu - \nu_{0}). \tag{2.65}$$

The total line extinction coefficient per particle is

$$\sigma_{\nu_0}^l \equiv \int_0^\infty \sigma_{\nu}^l \, \mathrm{d}\nu = \frac{h\nu_0}{4\pi} B_{lu} = \frac{\pi e^2}{m_e c} f_{lu} = 0.02654 \, f_{lu} \, \mathrm{cm}^2 \, \mathrm{Hz}.$$
(2.66)  
$$A_{ul} = 6.67 \times 10^{13} \frac{g_l}{g_u} \, \frac{f_{lu}}{\lambda^2} \, \mathrm{s}^{-1}$$

<sup>11</sup>Direct computation of gf-values is fairly straightforward for hydrogen and hydrogen-like ions but less so for more complex atomic, ionic or molecular configurations. Chapter 10 of Rybicki and Lightman (1979) presents the hydrogen computation and contains a table of HI gf-values on page 281. Extensive tabulations of experimentally measured transition probabilities used to come in thick volumes produced by the US National Bureau of Standards (*e.g.*, Corliss and Bozman 1962) but better values now result from large-scale computations and become available on the web, *e.g.*, http://vizier.u-strasbg.fr/OP.html (Opacity Project), http://wwwsolar.nrl.navy.mil/chianti.html (CHIANTI database)

**Source function.** The monochromatic line source function expressed in Einstein coefficients is

$$S_{\nu}^{l} \equiv j_{\nu}^{l} / \alpha_{\nu}^{l} = \frac{n_{u} A_{ul} \psi(\nu - \nu_{0})}{n_{l} B_{lu} \varphi(\nu - \nu_{0}) - n_{u} B_{ul} \chi(\nu - \nu_{0})}$$
(2.71)

or, using the Einstein relations (2.60)

$$S_{\nu}^{l} = \frac{\frac{A_{ul}}{B_{ul}}\frac{\psi}{\varphi}}{\frac{n_{l}}{n_{u}}\frac{B_{lu}}{B_{ul}} - \frac{\chi}{\varphi}} = \frac{2h\nu^{3}}{c^{2}}\frac{\psi/\varphi}{\frac{g_{u}n_{l}}{g_{l}n_{u}} - \frac{\chi}{\varphi}}.$$
(2.72)

every process takes a fresh sample of the probability distribution, without "memory" for any preceding process, so that  $\varphi(\nu - \nu_0) = \psi(\nu - \nu_0) = \chi(\nu - \nu_0)$ . The line source function then simplifies to

$$S_{\nu_0}^l = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} = \frac{2h\nu_0^3}{c^2} \frac{1}{\frac{g_u n_l}{g_l n_u} - 1}.$$
(2.73)

The index 0 to  $S_{\nu_0}^l$  signifies that the complete-redistribution version of the line source function is frequency-independent<sup>12</sup>. The line source function simplifies yet further to to  $S_{\nu_0}^l = B_{\nu_0}$  when the population ratio  $n_l/n_u$  in (2.73) obeys the Boltzmann distribution (2.86) on page 29 as it does in LTE.

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



Line extinction. The LTE line extinction coefficient is:

$$\left[\alpha_{\nu}^{l}\right]_{\rm LTE} = \frac{\pi e^{2}}{m_{\rm e}c} n_{l}^{\rm LTE} f_{lu} \varphi(\nu - \nu_{0}) \left[1 - e^{-h\nu_{0}/kT}\right]$$
(2.98)

with  $n_l^{\text{LTE}} \equiv [n_l]_{\text{LTE}}$  given by the Saha-Boltzmann distributions for the local kinetic temperature  $T_{\text{e}}$ . The classical oscillator strength  $f_{lu}$  is defined by (2.66) on page 23. It is often combined with the lower-level statistical weight  $g_l$  (which sits in  $n_l^{\text{LTE}}$  through (2.86)) into the so-called gf-value measuring transition probability.

No stellar abundance can be better than the input transition probabilities (gf-value) and the derived T<sub>eff</sub>, log(g)

#### where can I find all the answers?

#### for the real experts

Ivan Hubeny & Dimitri Mihalas

#### THEORY OF STELLAR ATMOSPHERES

An Introduction to Astrophysical Non-equilibrium Quantitative Spectroscopic Analysis



"The most authoritative synthesis of the quantitative spectroscopic analysis of stellar atmospheres"

#### for the rest of us

# The Observation and Analysis of Stellar Photospheres



"Each chapter contains exercises, and useful real star data and primary references can be found throughout." The simplest spectroscopic approach: equivalent width (W or EW) analyses; essentially a Boltzmann-Saha argument



#### **SOME** equivalent width codes:



[ascl:1011.002] DAOSPEC: An Automatic Code for Measuring Equivalent Widths in Highresolution Stellar Spectra

Stetson, P. B.; Pancino, E.

[ascl:1105.002] PACCE: Perl Algorithm to Compute Continuum and Equivalent Widths Riffel, Rogério; Borges Vale, Tibério

[ascl:1105.002] PACCE: Perl Algorithm to Compute Continuum and Equivalent Widths Riffel, Rogério; Borges Vale, Tibério

[asc1:1205.009] ARES: Automatic Routine for line Equivalent widths in stellar Spectra Sousa, Sérgio G.

[ascl:1502.023] ROBOSPECT: Width fitting program

Waters, Christopher Z.; Hollek, Julie K.

### and there are others, such as:



# Understanding a high-res spectrum becomes an exercise in Boltzmann-Saha statistical physics



The resonance Na I D lines get stronger with decreasing temperature because

(a) Na becomes less ionized

(b) Na I has more electrons falling to the ground state

(c) the H<sup>-</sup> continuous opacity decreases (fewer free electrons to make H<sup>-</sup>

The effect is less for the Ni I line because

(a) yes, Ni becomes less ionized but electrons are leaving the Ni I 2.0 eV state

(b) ionization energy for Ni I is 7.6 eV, much larger than for Na I (5.1 eV)

- therefore, the rush back to neutral species is slower for Ni

# the Teff alterations of Balmer lines are obvious even at low spectral resolution

The curves are idealized HY profiles, but the effect is seen in all H I lines



profiles of HY for A0 stars and warmer

profiles of HY for cooler stars; why is the EW drop much more severe than for stars hotter than A0?

this clarifies the "Saha" ionization effect. Gray's text is very valuable for this discussion The following four cases are of interest:

- 1. weak line of a neutral species with the element mostly neutral,
- 2. weak line of a neutral species with the element mostly ionized,
- 3. weak line of an ion with the element mostly neutral, and
- 4. weak line of an ion with the element mostly ionized.

#### Gray's text

## the Saha gravity (pressure) effect



#### Again, see Gray's text for the elegant explanation of these statements

- 1. Weak lines formed by any ion or atom where most of the element is in the next higher ionization stage are insensitive to pressure changes.
- 2. Weak lines formed by any ion or atom where most of the element is in that same ionization stage are pressure sensitive. Lower pressure causes greater line strength.
- 3. Weak lines formed by any ion or atom where most of the element is in the next lower ionization stage are very pressure sensitive. Lower pressure enhances the lines.

$$\left[\frac{N_{r+1}}{N_r}\right]_{\rm LTE} = \frac{1}{N_{\rm e}} \, \frac{2 \, U_{r+1}}{U_r} \left(\frac{2\pi m_{\rm e} kT}{h^2}\right)^{3/2} \, {\rm e}^{-\chi_r/kT}$$

Gray's text

# Something very illuminating that we have lost: curve-of-growth analyses



### In brief, here are curve-of-growth cartoons

A = elemental abundance, or some other quantity that makes the EW of a line change



Hey! Pay attention to this simple statement on "saturated" lines

#### General COG comments

- COG analyses mostly are rarely done today
  - they mostly require EWs of unblended lines
- But they should be consulted for physical insight:
  - what fraction of lines of a species are on the linear part of the COG?
    - often depends on spectrum quality (resolution, S/N)
  - do you really believe EW measurements of log(RW) > -6.0
    - or EW = 4 mÅ @ 4000Å; you should ask for "proof"
  - how much do the COG flat part lines dominate the abundances
    - rule of thumb: flat part lines have log(RW) > -5.0
      - or EW > 40mÅ @ 4000Å; most folks think that these are weak!
      - these have coupling between abundance and microturbulence
  - Beware of cool-star analyses ... K stars and cooler
    - I dare you to find unblended, weak lines in K-M stars
  - lines on the COG damping part can yield reliable abundances
    - but you must have good control on line damping parameters
- remember: COGs are REAL and describe actual EW responses to changing parameters



Now on to more difficult spectrum syntheses, in order to explain all the inputs needed to succeed



But how practically does determine any abundance? Example: the holmium abundance from 4045.5Å Ho II; this needs spectrum synthesis



### desired result: holmium from 4045.5Å Ho II

Line identifications begin with *Moore, Charlotte E.; Minnaert, M. G. J.; Houtgast, J.* 1966, The solar spectrum 2935 A to 8770 A, NBS Monograph



### We start by synthesizing the Sun



How do we make a line list that we can believe?

### Requirement for chemical composition analyses

#### A grid of model stellar photospheres:

- Kurucz ATLAS: <u>http://kurucz.harvard.edu/grids.html</u>
- Gustafsson MARCS: <u>marcs.astro.uu.se/</u>
- Hauschildt NEXTGEN: <u>http://hobbes.hs.uni-hamburg.de/PAPERS/NextGen/ms.html</u>

#### Typical model atmosphere computation output:

TEFE 3500, GRAVITY 0.00000 LTF TITLE SDSC GRID [+0.0] VTURB 0.0 KM/S L/H 1.25 CONVECTION ON 1.25 TURBULENCE OFF 0.00 0.00 0.00 0.00 ABUNDANCE SCALE 1.00000 ABUNDANCE CHANGE 1 0.91100 2 0.08900 READ DECK6 72 RHOX, T, P, XNE, ABROSS, ACCRAD, VTURB 1.92081317F-02 2162.9 1.918F-02 3.953F+05 6.942F-06 1.304F-03 0.000F+00 2.55242080E-02 2185.4 2.549E-02 5.259E+05 7.141E-06 1.219E-03 0.000E+00 3.37376143F-02 2204.8.3.370F-02.6.928F+05.7.301F-06.1.118F-03.0.000F+00 4.44603299E-02 2223.3 4.441E-02 9.084E+05 7.451E-06 1.024E-03 0.000E+00 5.84449198F-02 2243.2 5.838F-02 1.191F+06 7.631F-06 9.457F-04 0.000F+00 7.66163984E-02 2264.8 7.653E-02 1.561E+06 7.847E-06 8.769E-04 0.000E+00 1.00122149E-01 2288.2 1.000E-01 2.047E+06 8.106E-06 8.122E-04 0.000E+00 1.30562972E-01 2308.0 1.304E-01 2.662E+06 8.320E-06 7.329E-04 0.000E+00 1.70060206E-01 2328.6 1.699E-01 3.462E+06 8.564E-06 6.653E-04 0.000E+00

### Requirement for chemical composition analyses

#### Line analysis code:

- Kurucz WIDTH: <u>http://kurucz.harvard.edu/programs/WIDTH/</u>
- Kurucz SYNTHE: <u>http://kurucz.harvard.edu/programs/SYNTHE/</u>
- Hubeny TLUSTY: <u>http://nova.astro.umd.edu/</u>
- Plez TURBOSPECTRUM: <u>http://www.graal.univ-montp2.fr/hosted/plez/</u>
- Sneden MOOG: <u>http://www.as.utexas.edu/~chris/moog.html</u>
- Other personal programs not generally available to public

#### WHICH CODE TO USE? WHO CARES! KEEP FOCUSED ON WHAT YOU WANT TO ACCOMPLISH

These codes all have tradeoffs between convenience, speed, and sophistication of basic physics:

- Allowance for scattering in continuum opacities & source functions
- LTE or "better"
- How much atomic/molecular information comes with code
- Plane-parallel or spherical geometry
- User friendliness
- Common-sense outputs that help user avoid stupidities

### Requirement for chemical composition analyses: "reliable" model atmosphere parameters

Effective temperature T<sub>eff</sub>: colors and/or spectral line data Colors: usually B-V, V-I, V-K, J-K Calibrated with "infrared flux method"

As described in Paper I the method is based on the insensitivity to  $T_e$  of the surface flux,  $F_{S, \lambda_0}$ , from the star at an infrared wavelength  $\lambda_0$ . In the first stage of the method this flux is calculated using a model stellar atmosphere, and is combined with a measured absolute flux at the Earth,  $F_{E, \lambda_0}$ , to give  $\theta$  for the star through the expression (1)

$$\theta = 2 \sqrt{\frac{F_{\rm E, \lambda_0}}{F_{\rm S, \lambda_0}}}.$$
(1)

The resulting value of  $\theta$  is correct to 7 per cent, supposing that the measured infrared flux is correct to 10 per cent, and  $T_e$  is known to about 5 per cent. In the second stage of the method, the additional use of a measurement of the total integrated flux from the star at the Earth,

$$\mathcal{F}_{\rm E} = \int_0^\infty F_{\rm E,\,\lambda} \, d\lambda$$

gives accurate values for both  $\theta$  and  $T_{\rm e}$ .

#### Infrared flux method

The method is described concisely and formally by equations (2) and (3) that give the observed integrated flux  $\mathscr{F}_{\rm E}$  and the observed monochromatic flux  $F_{\rm E, \lambda_0}$  in terms of the variables  $T_{\rm e}$  and  $\theta$ . In equation (3), the dependence of the stellar surface flux on the model atmosphere is expressed by the function  $\phi(T_{\rm e}, g, \lambda_0)$  where g is the surface gravity.

$$\mathscr{F}_{\rm E} = \int_0^\infty F_{\rm E,\,\lambda} \, d\lambda = \frac{\theta^2}{4} \, \sigma T_{\rm e}^4 \tag{2}$$

$$F_{\mathrm{E},\,\lambda_{0}} = \frac{\theta^{2}}{4} \times F_{\mathrm{S},\,\lambda_{0}} = \frac{\theta^{2}}{4} \times \phi(T_{\mathrm{e}},g,\lambda_{0}). \tag{3}$$

The method described in Paper I is simply a means of deriving the pair of values ( $\theta$ ,  $T_e$ ) which simultaneously satisfy these equations. The nature of this formal solution is shown in

Blackwell et al. 1979



"The small gradient of line 3, and therefore the sharpness of the intersection, is due to the weak dependence of flux on temperature in the infrared. The selection of an infrared wavelength is therefore essential to the success of the method."

- calculations made for  $\lambda$  = 3.45  $\mu$ m
### Application of IR flux method



 $-0.5 < [Fe/H] \le +0.5$  (filled circles),  $-1.5 < [Fe/H] \le -0.5$  (open circles),  $-2.5 < [Fe/H] \le -1.5$  (squares), and [Fe/H]  $\le -2.5$  (triangles). The lines corresponding to our calibration for [Fe/H] = 0.0 (solid line), -1.0 (dotted line), and -2.0 (dashed line) are also shown.

#### Which are much better than these metallicitydependent correlations with B-V



Ramirez & Melendez 2005

Requirement for chemical composition analyses: "reliable" model atmosphere parameters Surface gravity log g: cluster, physical, and/or spectral line data Clusters, for example (conversion to L/L<sub>o</sub> still not trivial



#### Gravity, continued

Surface gravity log g: cluster, physical, and/or spectral line data Cluster and/or physical:



## The High-Res spectroscopic approach

Measure some EWs, put them and line parameters in some analysis code, and out comes some abundances

T<sub>eff</sub> from Boltzmann argument: want no trend with excitation energy



In practice, only Fe I lines have the excitation range necessary **SO! How would YOU change the assumed T<sub>eff</sub> to fix the slope?** 

## The High-Res spectroscopic approach Microturbulent velocity argument: want no trend with line strength



What's the cure for this slope? What are the difficulties in assuming that  $v_{micro}$  is the problem here?

### macro- and micro-turbulence



producing spectral broadening from adding up all of these cells in a whole-disk spectrum



### macro- and micro-turbulence



The microturbulent velocity is defined as the microscale non-thermal component of the gas velocity in the region of spectral line formation. Convection is the mechanism believed to be responsible for the observed turbulent velocity field, both in low mass stars and massive stars. When examined by a spectroscope, the velocity of the convective gas along the line of sight produces Doppler shifts in the absorption bands. It is the distribution of these velocities along the line of sight that produces the microturbulence broadening

The strength of the microturbulence (symbolized by  $\xi$ , in units of km s–1) can be determined by comparing the broadening of strong lines versus weak lines.

### macro- and micro-turbulence and rotation





# the good news: rotational line profiles are not Gaussian

the complex news: lines can be broadened through effects from: thermal microturbulence macroturbulence rotation instrumental slit function The High-Res spectroscopic approach Gravity (Saha) argument: want same abundances from neutral & ionized lines of same element



All OK here, how would you change log g if the abundance from Fe II was say 0.2 dex larger?

### Requirement for chemical composition analyses: synthetic spectrum line lists (or lists of lines for EW analysis) must be developed

- Ideal: high-quality laboratory data for all transitions
  - Wavelengths (!), excitation energies, transition probabilities
  - damping constants, partition functions
  - Hyperfine structures, isotopic wavelength shifts
- Reality: many transitions have little or no lab data
  - Very few lab atomic/molecular physicists
    - Wisconsin, Liege, Lund, London
  - This work is of little interests to most physicists
- Typically start with "semi-empirical" line lists
- Iteration of lists with high-quality spectra of a couple of stars
  - Sun, Arcturus, maybe Procyon
  - Adjustment of wavelengths & transition probabilities
  - Guessing at relative contributions to blended features
  - Adding fake lines!
    - Declared as Fe I,  $\chi$ = 3.5 eV, log (gf) set to match observed line

#### University of Wisconsin laboratory atomic transition efforts directly support stellar spectroscopy





# Application of the lab transition data to stellar spectra: where do the strongest lines occur?

"strength" =  $\log(\epsilon g f) - \theta \chi$ where  $\theta = 5040/T$ 

This is a RELATIVE strength that works well when comparing lines of a single species, OR comparing lines of DOMINANT species of different elements

the plot here does the strength estimates for the solar spectrum

this makes it relatively easy to identify useful lines



## A good summary site for lab atomic data

) NET www.nist.gov/pml/data/asd.cfm



NIST Home > PML > Physical Reference Data > Atomic Spectra Database

Version History & Citation Information | Disclaimer

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# NIST ATOMIC SPECTRA DATABASE

#### Version 4

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:



Spectral lines and associated energy levels displayed in wavelength order with all selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayed where available.

Levels

Energy levels of a particular atom or ion displayed in order of energy above the ground state.

#### (these are often gf's that are "normalized" in some way)

#### NIST ASD Team

Principal Developers (Currently Active): Yu. Ralchenko, A. Kramida, and J. Reader

Data Compilers (Currently Active): A. Kramida, E.B. Saloman, J.E. Sansonetti, J.J. Curry, J.R. Fuhr, L. Podobedova, and W.L. Wiese

## NIST entries for Fe I near 4045Å: 6 lines

Observed Wavelength Air (Å)	Ritz Wavelength Air (Å)	Rel. Int. (7)	A <sub>ki</sub> (s <sup>-1</sup> )	log(g <sub>i</sub> f <sub>ik</sub> )	Acc.	<i>E<sub>i</sub></i> (eV)	<i>E<sub>k</sub></i> (eV)
	4 043.88486	m				2.7275443	- 5.7926458
4 043.8964	4 043.89713	2690	8.69e+06	-0.826	D+	3.2409689	- 6.3060611
4 043.9767	4 043.97712	660				3.2409689	- 6.3060005
4 044.4906	4 044.4920	166				4.1033735	- 7.1680148
4 044.5444	4 044.5449	398				3.2671124	- 6.3317137
4 044.6089	4 044.60883	6800	8.17e+06	-1.221	в	2.8315910	- 5.8961438
4 045.1116	4 045.1122	510				4.2604530	- 7.3246244
4 045.5936	4 045.59336	3470	7.39e+06	-0.896	С	3.2111892	- 6.2749962
4 045.8122	4 045.81193	1000000	8.62e+07	0.280	Α	1.4848643	- 4.5485058
4 046.0620	4 046.06181	1620	6.85e+06	-1.297	C+	3.2657059	- 6.3291582
4 047.3037	4 047.3025	288	2.15e+05	-2.800	С	2.2786045	- 5.3411178

Acc. = their estimated accuracies for lab values; be wary of "C" and worse

# But my line list has 30 Fe I lines; they come from semi-empirical line databases

#### Robert L. Kurucz

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This is a combined Web/outgoing-FTP site, KURUCZ.HARVARD.EDU or CFAKU5.CFA.HARVARD.EDU. It provides up-to-date public access to my data and programs. These are the same programs and files that I use in my research. Many bugs and problems have been corrected but there are still many more errors remaining to be found. Programs and data that I would not use myself because they are still under development are not on this computer. Many of the files are large and are also available on CDs or DVDs, and I am willing to write DVDs on demand. Some files taken from Kurucz CD-ROMs 1-26 are given for historical checks although many have been replaced by new versions. Binary versions will eventually be replaced by (much larger) ASCII versions. I am willing to rewrite them in ASCII on demand. Neither the programs nor data are "black boxes". You should not be using them if you do not have some understanding of the physics and of the programming in the source code.

#### The Kurucz web site

#### Kurucz/Linelists \*\*\* See /ATOMS or /MOLECULES for new calculations (now underway). At the time these qf files were made all the laboratory data in the Table of Contents literature were considered and laboratory data were substituted for computed data when they appeared to be better than the computed. All of the files, atomic and molecular, need to be updated. GF10: wavelength-sorted atomic lines in 10 nm intervals wavelength-sorted atomic lines in 100 nm intervals GF100: 1. News GFALL: wavelength-sorted atomic lines in one file per spectrum and also Vita and Bibliography all merged into one file 3. Papers GFHYPER10: wavelength-sorted atomic lines in 10 nm intervals with hyperfine Atoms splitting for levels that have been measured 5. Molecules Linelists GFHYPER100: wavelength-sorted atomic lines in 100 nm intervals with hyperfine splitting for levels that have been measured Opacities 8. Grids of model atmospheres GFHYPERALL: wavelength-sorted atomic lines in one file per spectrum with hyperfine splitting for levels that have been measured 9. Sun and also all merged into one file 10. Stars LINES: Sample programs for reading the files. References. 11. Programs 12. CD-ROMs LINESCD: binary files from CD-ROMs 1 and 15 that have 58 million atomic Temporary files and diatomic linss packed 16 bytes per line wavelength sorted diatomic molecular lines in various large files LINESMOL: with extension .ASC . The same data also are given divided into smaller wavelength intervals in files with extension .100 .

There are more data than anonymous FTP can digest. Instead there is a user account with username GUEST and password CFAGUEST that can be accessed by FTP and TELNET. Simple OpenVMS commands like "TYPE file", "SEARCH file string", and "HELP" will work. The directories [NEWS], [VITABIB], [PAPERS], [ATOMS], [MOLECULES], [LINELISTS], [PROGRAMS], and [CDROMS] are on disk KU5E. [OPACITIES],[GRIDS],[SUN], and [STARS], are on KU5D, [TEMP] is on KU5C. and other directories and disks may be added. FTP does not execute the login so the logical names are not defined, but TELNET does. To go to a new directory "SET DEFAULT [name]". Case does not matter.

### A very good alternate "compilation" site; more tools for applications to stellar spectra *but be careful of multiple gf sources*

#### Welcome to VALD

Please enter your registered email address :



#### Rationale

The Vienna Atomic Line Database (VALD) is a collection of atomic line parameters of astronomical interest and provides tools for selecting subsets of lines for typical astrophysical applications: line identification, chemical composition and radial velocity measurements, model atmosphere calculations etc.

Reset

Login

The VALD Electronic Mail Service (VALD-EMS) is the main interface for accessing VALD by external users. VALD-EMS is aimed to endorse the following main principles of VALD access.

- subsets of spectral line lists are extracted with tools consistent with the specific astronomical problem. VALD strongly discourages bulk data transfer for the case of an external
  access to the data base and concentrates more on intelligent search and extraction procedures.
- VALD provides data sets and extraction tools suitable for several spectroscopic applications.
- VALD is regularly updated with critically evaluated data sets. The VALD project team experts investigate the statistical properties of the data, extensively compare the results
  obtained with different data sources, and establish the quality rating for each new source.
- VALD computers are not dedicated to the VALD project alone, so the correct scheduling is important.

Mail access lets VALD automatically process requests and queue them for execution on VALD computers at the most convenient time. It also allows us to have control over the size of the data traffic and to register VALD users.

Apart from the mail service, this WWW interface has been developed to facilitate extraction of data from VALD and to contact the VALD staff for troubleshooting and registration.

http://vald.astro.univie.ac.at/~vald/php/vald.php

## linemake: a curated "special-purpose" database

- a single database with U. Wisconsin and Old Dominion U. relevant LABORATORY transiton data for:
  - atomic neutrals and ions
  - diatomic molecules (CH, CN, OH, MgH
- friendly format for stellar spectroscopy
- simple code to generate synthetic spectrum linelists

0	vmplacco Update README.md		c430a57 on May 12	172 commits
	mooglists	updates April 2021 from lan		5 months ago
Ľ	README.md	Update README.md		4 months ago
Ľ	linemake.f	updated mooglists path		5 months ago

#### E README.md

#### **linemake** Atomic and Molecular Line List Generator

#### About

linemake is an open-source atomic and molecular line list generator. Rather than a replacement for a number of well-established atomic and molecular spectral databases, linemake aims to be a lightweight, easy-to-use tool to generate formatted and curated lists suitable for spectral synthesis work. We stress that the users of should be *in charge* of all of their transition data, and should cite the appropriate sources in their published work, given below.

I	H 1.00794 Hydrogen																	He 4.002602 Helium
П	3 Li 6.941 Lithium	4 Be 9.012182 Beryllum											5 B 10.811 Boron	6 C 12.0107 Carbon	7 N 14.0067 Nitrogen	8 0 15.9994 Oxygen	9 F 18.9984032 Fluorine	10 Ne 20.1797 Neon
ш	11 Na 22.98976928 Sodium	12 Mg 24.3050 Magnesium											13 AI 26.9815386 Aluminum	14 Si 28.0855 Silicon	15 P 30.973762 Phosphorus	16 S 32.085 Sulfur	17 CI 35.453 Chlorine	18 Ar <sup>39.948</sup> Argon
IV	19 K <sup>39.0983</sup> Potassium	20 Ca 40.078 Calcium	21 Sc 44.955912 Scandium	22 <b>Ti</b> <sup>47.867</sup> Titanium	23 V 50.9415 Vanadium	24 <b>Cr</b> 51.9961 Chromium	25 Mn 54.938045 Manganese	26 Fe 55.845 Iron	27 <b>CO</b> 58.933195 Cobalt	28 Ni 58.6934 Nickel	29 Cu <sup>63.546</sup> Copper	30 Zn 65.38 Zinc	31 Ga 69.723 Gallium	32 Ge 72.64 Germanium	33 As 74.92160 Arsenic	34 Se 78.96 Selenium	35 Br <sup>79.904</sup> Bromine	36 Kr 83.798 Krypton
v	37 <b>Rb</b> 85.4678 Rubidium	38 Sr 87.62 Strontium	39 Y 88.90585 Yttrium	40 <b>Zr</b> <sup>91.224</sup> Zirconium	41 Nb 92.90638 Niobium	42 Mo 95.96 Molybdenum	43 TC <sup>[98]</sup> Technetium	44 Ru 101.07 Ruthenium	45 Rh 102.90550 Rhodium	46 Pd 106.42 Palladium	47 Ag 107.8682 Silver	48 Cd 112.411 Cadmium	49 In 114.818 Indium	50 <b>Sn</b> <sup>118.710</sup> Tin	51 Sb 121.760 Antimony	52 <b>Te</b> 127.60 Tellurium	53   126.90447 lodine	54 Xe <sup>131,293</sup> Xenon
VI	55 <b>CS</b> 132.9054519 Cesium	56 <b>Ba</b> <sup>137,327</sup> Barium	La	72 Hf 178.49 Hafnium	73 <b>Ta</b> 180.94788 Tantalum	74 W 183.84 Tungsten	75 Re 186.207 Rhenium	76 <b>OS</b> 190.23 Osmium	77 Ir 192.217 Iridium	78 Pt 195.084 Platinum	79 Au 196.966569 Gold	80 Hg 200.59 Mercury	81 <b>TI</b> 204.3833 Thallium	82 Pb 207.2 Lead	83 Bi 208.98040 Bismuth	84 Po <sup>[209]</sup> Polonium	85 At [210] Astatine	86 Rn [222] Radon
VII	87 Fr [223] Francium	88 <b>Ra</b> [226] Badium	Ac	104 <b>Rf</b> [267] Rutherfordium	105 <b>Db</b> [268] Dubnium	106 Sg [271] Seaborgium	107 Bh [272] Bohrium	108 HS [270] Hassium	109 Mt [276] Meitnerium	110 Ds [281] Darmstadtium	111 Rg [280] Roentgenium	112 Cn [285] Copernicium	113 <b>Nh</b> [284] Nihomium	114 FI [289] Flerovium	115 MC [288] Moscovium	116 LV [293] Livermorium	117 <b>TS</b> [294] Tennessine	118 Og [294] Oganesso
La				57 La 138.90547 Lanthanum	58 <b>Ce</b> 140.116 Cerium	59 Pr 140.90765 Praseodymium	60 Nd 144.242 Neodymium	61 Pm [145] Promethium	62 Sm 150.36 Samarium	63 Eu 151.964 Europium	64 Gd <sup>157.25</sup> Gadolinium	65 <b>Tb</b> 158.92535 Terbium	66 Dy 162.500 Dysprosium	67 Ho 164.93032 Holmium	68 Er 167.259 Erbium	69 <b>Tm</b> 168.93421 Thulium	70 <b>Yb</b> 173.054 Ytterbium	71 Lu 174.9668 Lutetium
Ac				89 Ac (227) Actinium	90 <b>Th</b> 232.03806 Thorium	91 Pa 231.03588 Protactinium	92 U 238.02891 Uranium	93 Np [237] Neptunium	94 <b>Pu</b> [244] Plutonium	95 <b>Am</b> [243] Americium	96 <b>Cm</b> [247] Curium	97 <b>Bk</b> <sup>[247]</sup> Berkelium	98 Cf [251] Californium	99 Es [252] Einsteinium	100 <b>Fm</b> [257] Fermium	101 Md <sup>[258]</sup> Mendelevium	102 No [259] Nobelium	103 Lr [262] Lawrenciu
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
								not a	vailable	neutra	l and ion	ionize	ed species	s neu	tral speci	es 🗾 m	olecular s	pecies

- combines with Kurucz database transitions
- adds low-temperature molecules (like TiO, H<sub>2</sub>O) for M star spectroscopy
- published: Placco+ 2021, RNAAS, 5, 92
- public; easy to expand

## other useful line list compilations



https://ui.adsabs.harvard.edu/abs/2019Atoms...7..105L/abstract



#### Article The Belgian Repository of Fundamental Atomic Data and Stellar Spectra (BRASS)

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#### the "Kentucky" site (Gary Ferland+): especially good for high-energy emission lines



#### Welcome to the atomic line list.

This is a compilation of approximately 923,000 allowed, intercombination and forbidden atomic transitions with wavelengths in the range from 0.5 Å to 1000  $\mu$ m. It's primary intention is to allow the identification of observed atomic absorption or emission features. The wavelengths in this list are all calculated from the difference between the energy of the upper and lower level of the transition. No attempt has been made to include observed wavelengths. Most of the atomic energy level data have been taken from the <u>Atomic Spectra Database</u> provided by the National Institute of Standards and Technology (NIST).

https://www.pa.uky.edu/~peter/atomic/

#### Remember our starting spectrum synthesis



#### Remember our starting spectrum synthesis

Lab  $\lambda$ 's and gf's: adopted without change

Identified (or guessed-at) lines without lab data: changed  $\lambda$ 's and gf's to fit Sun Unknown lines: added fake lines (Fe I,  $\chi$ = 3.5 eV, log (gf) set to match observed line)



This finishes the line list preparation, to be applied to the stellar spectra



Makes sense out of strange spectra: isotopes

> Vertical line sizes give relative strengths of hyperfine components

FIG. 1.—Observed and synthetic spectra of the Eu II 4205.04 Å line in the three program stars. The observed spectra (*filled circles*) are compared to synthetic spectra with  $fr(^{151}\text{Eu}) = 0.000$  (*dotted line*); 0.350 (*short-dashed line*); 0.478 (*solid line*); 0.650 (*long-dashed line*); and 1.000 (*dot-dashed line*). As Eu has only two stable isotopes,  $fr(^{153}\text{Eu}) = 1.0 - fr(^{151}\text{Eu})$ . In the top panel vertical lines are added to indicate the wavelengths and relative strengths of the hyperfine components of the isotopes  $^{151}\text{Eu}$  (*dotted lines*) and  $^{153}\text{Eu}$  (*solid lines*). The absolute vertical line lengths are normalized by an arbitrary constant for display purposes.



Sneden et al. 2002

# The one isotopic analysis that can be done well with atomic lines: Eu



# Note the hyperfine vs isotopic structures for rare earths



#### MUCH more difficult: barium isotopes

<sup>121</sup> Ba <sup>122</sup> B	a <sup>123</sup> Ba <sup>124</sup> Ba <sup>125</sup> Ba <mark>126</mark> Ba	127Ba <mark>128Ba</mark>	129Ba <mark>130</mark> Ba <mark>13</mark>	<sup>31</sup> Ba <sup>132</sup> Ba <sup>1</sup>	33 <mark>Ba</mark> 134Ba <mark>135</mark>	3a 136 Ba 137 <mark>Ba</mark>	a <mark>138Ba</mark> 139Bal	40Ba <sup>141</sup> Ba <sup>14</sup>	2Ba <sup>143</sup> Ba
		_							
	Isotopic mix	130	132	134	135	136	137	138	
	Solar (mostly "s)	0.1%	0.1%	2.4%	6.6%	7.9%	11.2%	71.7%	
	Pure "r"	0.0%	0.0%	0.0%	40.0%	0.0%	12.2%	47.8%	
						e bi	lemental reakdown		
					N=82	~	r s		
				Nd	8	-> 4	<b>2%</b> 58%		
			141 <i>s</i> , <i>r</i> 100%	5	1% 49%				
			Ce		140 <i>s</i> , <i>r</i> 88.5%	142 r 1 11.2%	<mark>9% 81%</mark>		
		La			139 <i>s</i> ,r 99.9%	2	5 <mark>% 7</mark> 5%		
		Ba	134 s 2.4%	135 136 s,r s 6.6% 7.9%	137 138 s,r s,r 11.2% 71.7%	1	5% 85%		
	Cs		133 <i>s,r</i>	2		8	<mark>5% 15</mark> %		
	Xe 126	129 130 s,r s 26.4% 4.1%	131 132 s,r s,r 21.2% 26.9%	134 r 10.4%	136 r 8.9%	8	0% 20%		
		Dalp Ce		$\langle \rangle$	Path oce	$\langle \rangle$			
					· · · · · · · · · · · · · · · · · · ·	$\cdot$ $\land$ $\land$	5	Sneden et al.	2008



Solid line:  $f_{odd} = 0.31$ Dashed lines: changing  $f_{odd}$  by ±0.21

Lambert & Allende Prieto 2004

# Ni isotopes are detectable in the Sun and can be accounted for



Sneden et al. 2014

#### Isotopic ratios are much easier for molecular features



Let's talk about molecular equilibrium ...

Gay & Lambert 2000

## simplified molecular equilibrium: H-C-N-O

P(H) = p(H) + 2p(H2) + p(CH) + p(NH) + p(OH) + 2p(H2O) + ... P(C) = p(C) + p(CH) + 2p(C2) + p(CN) + p(CO) + p(CO2) + ...P(N) = p(N) + p(NH) + p(CN) + 2p(N2) + p(NO) + ...

P(O) = p(O) + p(OH) + p(CO) + p(NO) + 2p(O2) + 2p(CO2) + ...

But (happily!) the importance of each depends on abundance of the element(s) and the molecular dissociation energy

$$\frac{p(AB)}{p(A)p(B)} = const \left(\frac{M(AB)}{M(A)M(B)}\right)^{3/2} \left(\frac{U(AB)}{U(A)U(B)}\right) T^{-5/2} \exp\left(\frac{D_0}{kT}\right)$$

- P(H) = p(H) + 2p(H2) + ...
- P(C) = p(C) + p(CO) + ...
- P(N) = p(N) + 2p(N2) + ...
- P(O) = p(O) + p(CO) + ...

(H cares only about itself)(C cares only about O)(N cares only about itself)(O cares only about C)

#### A sample isotopic analysis



Relative Intensity

Spectrum of HD 23439A from 5134.0 to 5136 Å and from 5138 to 5140.5 Å. The observed spectrum (circles) is shown. Synthetic spectra are shown for the isotopic ratios 24Mg : 25Mg : 26Mg = 100 : 0 : 0 (dashed lines), 78 : 13 : 9 (solid lines, best fit to the recommended features), and 72 : 16 : 12 and 83 : 10 : 6 (dotted lines).

## Fundamental problem: is LTE a good assumption?

Non-local thermodynamical equilibrium (NLTE or non-LTE) is a loose term which implies that the assumption of LTE fails. Often one then assumes statistical equilibrium implicitly, usually with the Maxwell distribution and complete redistribution in frequency and angle. However, the populations are now permitted to differ from the local Saha-Boltzmann equilibrium values.

#### 2.6.1 Statistical equilibrium

**Rate equations.** Statistical equilibrium (SE) implies that the radiation fields (in all directions and on all frequencies) and level populations do not vary with time, as expressed in the statistical equilibrium equations (population equations, rate equations):

$$\frac{\mathrm{d}n_i(\vec{r})}{\mathrm{d}t} = \sum_{j\neq i}^N n_j(\vec{r}) P_{ji}(\vec{r}) - n_i(\vec{r}) \sum_{j\neq i}^N P_{ij}(\vec{r}) = 0, \qquad (2.100)$$

with  $n_i$  the population of a particular level, N the total number of levels that are important for the population of level  $n_i$  one way or another, and j stepping over all those levels. The transition rates  $P_{ij}$  for radiative and collisinal processes, respectively, are given per particle in state i or j by:

$$P_{ij} = R_{ij} + C_{ij}.$$
 (2.101)

For a bound-bound transition the radiative rate per particle is:

$$R_{ij} = A_{ij} + B_{ij}\overline{J}_{\nu_0}.$$
 (2.102)

#### Fundamental problem: is LTE a good assumption?

$$b_l = n_l / n_l^{\text{LTE}}$$
  $b_u = n_u / n_u^{\text{LTE}}$   $S_{
u_0}^l = rac{2h
u_0^3}{c^2} rac{1}{rac{b_l}{b_u}} \, \mathrm{e}^{h
u_0/kT} - 1$ 

**Bound-bound extinction.** The monochromatic line extinction coefficient (2.63) on page 23 becomes:

$$\alpha_{\nu}^{l} = \frac{h\nu}{4\pi} b_{l} n_{l}^{\text{LTE}} B_{lu} \varphi(\nu - \nu_{0}) \left[ 1 - \frac{b_{u} n_{u}^{\text{LTE}} B_{ul} \chi}{b_{l} n_{l}^{\text{LTE}} B_{lu} \varphi} \right]$$
(2.108)

$$= \frac{h\nu}{4\pi} b_l n_l^{\text{LTE}} B_{lu} \varphi(\nu - \nu_0) \left[ 1 - \frac{b_u}{b_l} \frac{\chi}{\varphi} e^{-h\nu/kT} \right]$$
(2.109)

$$= b_l n_l^{\text{LTE}} \sigma_{\nu}^l \left[ 1 - \frac{b_u}{b_l} \frac{\chi}{\varphi} \, \mathrm{e}^{-h\nu/kT} \right]$$
(2.110)

$$= \frac{\pi e^2}{m_{\rm e}c} b_l n_l^{\rm LTE} f_{lu} \varphi(\nu - \nu_0) \left[ 1 - \frac{b_u}{b_l} \frac{\chi}{\varphi} \,\mathrm{e}^{-h\nu/kT} \right]$$
(2.111)

# First issue when facing departures from LTE: continuum scattering

CS 22892-052 ( $T_{eff}$ =4800, log g=1.5, [Fe/H]=-2.9)



When scattering is important, you can't use the simple integral radiative transfer solution

#### Situation is better for warmer stars



Can go into deep UV before scattering is important

Here is an example of a spectrum warning



Preston et al. 2006
The abundances appear to be superficially normal, but why the scatter in silicon abundances?

Like compared to Ca I or Ti II????



#### Change of axes reveals the problem



# Turns out this problem had not been "unnoticed" in earlier data sets



# Surely this is a non-LTE symptom; energylevel diagrams give clues



$$\left[rac{n_{r,s}}{n_{r,t}}
ight]_{ ext{LTE}} = rac{g_{r,s}}{g_{r,t}} \, \mathrm{e}^{-(\chi_{r,s}-\chi_{r,t})/kT}$$

The 3905Å line is almost the only line used for Si abundances in very metal-poor stars

Sneden et al. 2008

#### Grotrian diagram for Si I



# We even have trouble deriving the solar oxygen abundance

#### Choices for analysis:

- [O I] 6300.3 Å (χ=0.0eV) and more rarely 6363.7Å (χ=0.0eV)
- O I triplet 7771.9, 7774.2, 7775.4 Å (χ=9.2eV)
  - more rarely a triplet near 6156Å (χ=10.7eV)
- OH vibration/rotation bands in the infrared
- OH electronic/vibration/rotation bands in near-UV
- NO: CO because this molecule is more sensitive to carbon abundance

## Headaches

- [O I] lines 0.0eV should be best (why?) but are very weak in Sun & dwarfs
- O I triplets are very high excitation (so what?) and have LTE departures
- OH is minor part of oxygen; IR bands not strong
- OH electronic/vibration/rotation bands are in the very crowded near-UV

Sun: partial pressures (arbitrary units) of major oxygen components at  $\tau \sim 0.5$ log p(O I) = 1.9 log p(CO) = -0.3 log p(OH) = -1.2 log p(O<sub>2</sub>) = -4.7 log p(ON) = -3.5 log p(H<sub>2</sub>O) = -4.7 log p(CO<sub>2</sub>) = -7.5

#### Grotrian diagram for O I



Moore & Merrill 1956

### a challenge from two decades ago ... just as relevant today

"So, even if the study of these surface layers appears rather boring to many of the astrophysicists, it cannot be neglected. As we have shown, even the most fundamental parameters of the most basic representation of stellar atmospheres suffer from significant uncertainties. The theoretical and observational tools needed to solve these problems are, to a large extent, available

It is therefore mostly a matter of will: there is still a lot to be done in the study of stellar atmospheres, what is needed is researchers who wish to tackle these problems."

**Pierre Magain, 1995**, in "Stellar Evolution: What Should be Done", Proc. 32nd Liège Int. Astrophysical Colloq, ed. A. Noels, D. Fraipont-Caro, M. Gabriel, N. Grevesse, and P. Demarque. Liege: Universite de Liege, Institut d'Astrophysique, 1995., p.139

# remember: our work is supposed to be about astrophysics, not big data manipulation

Not covered in detail here, but will be discussed a little/lot by other speakers

grid syntheses pragmatic approaches to non-LTE studies automated EW analyses tangled molecular equilibria normalizing different samples to a common system machine learning for very large samples magnetic field derivations de-convolution of velocity broadening components

Thanks for inviting me to speak here!

# Slide heading