

Non-LTE line formation for trace elements in stellar atmospheres,
July 30 – August 4, 2007, Nice, France

Few notes to the subject of our workshop

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Non-LTE

line formation

for trace elements in stellar atmospheres

- Which elements at given stellar parameters can be treated as trace elements?
- Thermal absorption and emission processes and scattering.
- Spectral line formation. Basic definitions. Scattering in line formation.

Trace element?

- Line formation for **trace element** can be considered for the fixed atmospheric structure.
- *At given stellar parameters*, variations in the excitation and ionization state of the **trace element** have no significant effect on the atmospheric structure.
- *In the model atmosphere calculations*, **trace element** can be treated under the LTE assumption.

Trace element is not necessary very rare element.

The classical stellar atmosphere problem

In this workshop,

stellar atmosphere is considered as the surface layers of a star where *most frequency-integrated radiation forms*.

1. The atmosphere is composed of **homogeneous layers**.
1-D geometry: plane-parallel (PP) or spherically-symmetric (SS).
2. The atmosphere is **static**.
3. **Energy conservation**. The transfer of energy through the atmosphere is done by radiation and convection.
4. Thermodynamic state: LTE or non-LTE.

Basic equations

- The hydrostatic equilibrium (HE) equation $\rightarrow N(r)$.

$$\frac{dp_g}{dr} + \frac{dp_R}{dr} = -g\rho$$

the PP atmosphere: $g = \text{const}$,

the SS atmosphere: $g = G M/r^2$

The surface ratio of radiative acceleration g_R to gravity:

$$\frac{g_R}{g} = 10^{-4.51} \frac{L / L_{Sun}}{M / M_{Sun}}$$

The atmosphere is stable if

$$\log g > 4 \log T_{eff} - 15.12$$

Type	$\log g$
Main sequence star	4.0 4.7
Sun	4.44
Supergiants	0 1
White dwarfs	~8
Neutron stars	~15
Earth	3.0

A5 and earlier type stars.

- The radiative equilibrium (RE) equation $\rightarrow T(r)$.

$$\int_0^{\infty} (\eta_{\nu} - \chi_{\nu} J_{\nu}) d\nu = 0$$

$$\chi_{\nu} = f(n_i^A, n_j^B, \dots, n_k^Z)$$

Later type stars.

- Radiative and convective equilibrium $\rightarrow T(r)$.

$$F = F_{rad} + F_{conv} = \sigma_R T_{eff}^4$$

The effects of convection are treated in an approximate way, while keeping the assumptions of 1-D geometry and HE.

The mixing-length theory (MLT) is the simplest and most widely used convection theory in astrophysics.

LTE:

- The Saha-Boltzmann equations $\rightarrow n_{A,r,i} = f(T, p)$

Non-LTE:

The SE equations for all those atoms which are important sources of opacity and/or important donors of free electrons. $\rightarrow n_i$

$$\sum_{j \neq i} n_j (R_{ji} + C_{ji}) = n_i \sum_{j \neq i} (R_{ij} + C_{ij}) \quad i = 1, \dots, NL$$

- The charge conservation equation. $\rightarrow n_e$
- The particle conservation equation.

The codes for model atmosphere calculations.

Non-LTE models.

TLUSTY (*Hubeny & Lanz 1995, 2003*)

$T_{eff} = 27500 - 55000$ K; $\log g = 3.0 - 4.75$ ($L < L_{Edd}$)

PP, HE, RE, SE for 40 chemical species

(complete linearization / ALI, super levels, super lines)

PHOENIX (*Hauschildt, et al. 1996, 1997*)

is the multipurpose code.

PP and SS, MLT, line blanketing (5-20 mln. atomic lines + 15-300 mln. molecular lines) is taken into account by explicitly including it in the calculations, SE for 15 elements (ALI).

The code of Kubát (2003)

for hot stars of arbitrary chemical composition.

PP and SS, HE, RE.

LTE models

ATLAS9 (*Kurucz 1993; Castelli & Kurucz 2004*)

for extended range of stellar parameters,

$T_{\text{eff}} = 3500 - 50000 \text{ K}$; $\log g = 0 - 5$ ($g > g_R$; $L < L_{\text{Edd}}$);

$[M/H] = (+0.5) - (-3)$

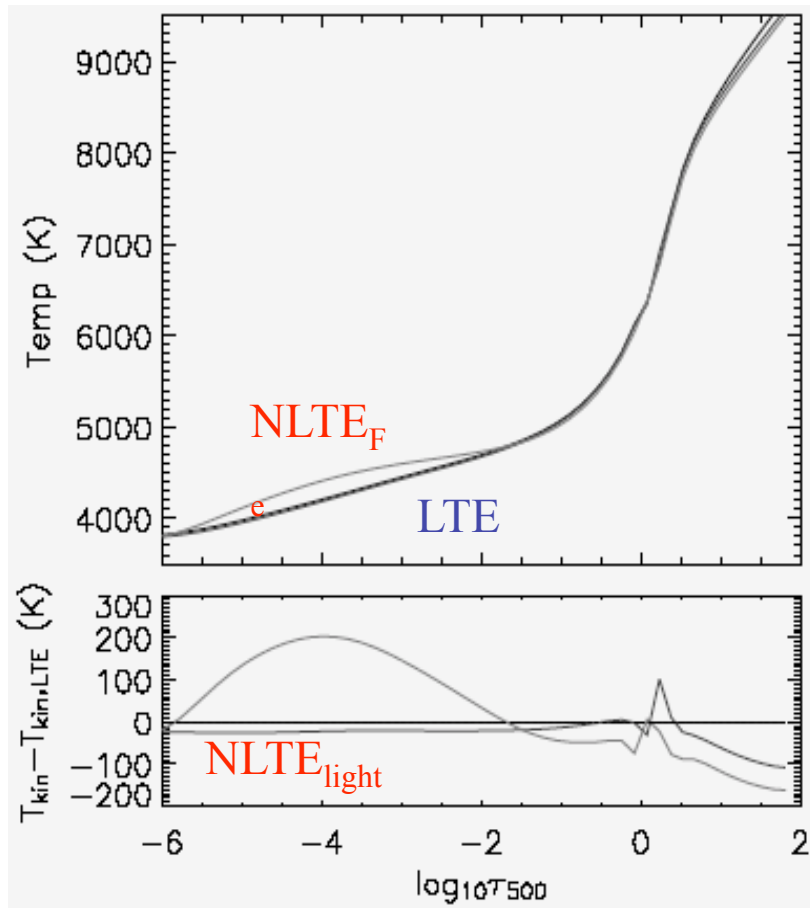
PP, HE, MLT, ODF for line opacity (~ 50 mln. lines).

New generation of codes and models

is based on either OS or line-by-line (LL) technique for calculations of line blanketing.

- **ATLAS12** (*Kurucz 1996*),
- **MARCS-OS** (*Gustafsson et al. 2003*),
- **MAFAGS-OS** (*Grupp 2004*),
- **the LL code** (*Shulyak et al. 2004*).

The effect of a given chemical element on the atmospheric structure depends on stellar parameters.



A difference in T between the NLTE and LTE models is up to 200K.

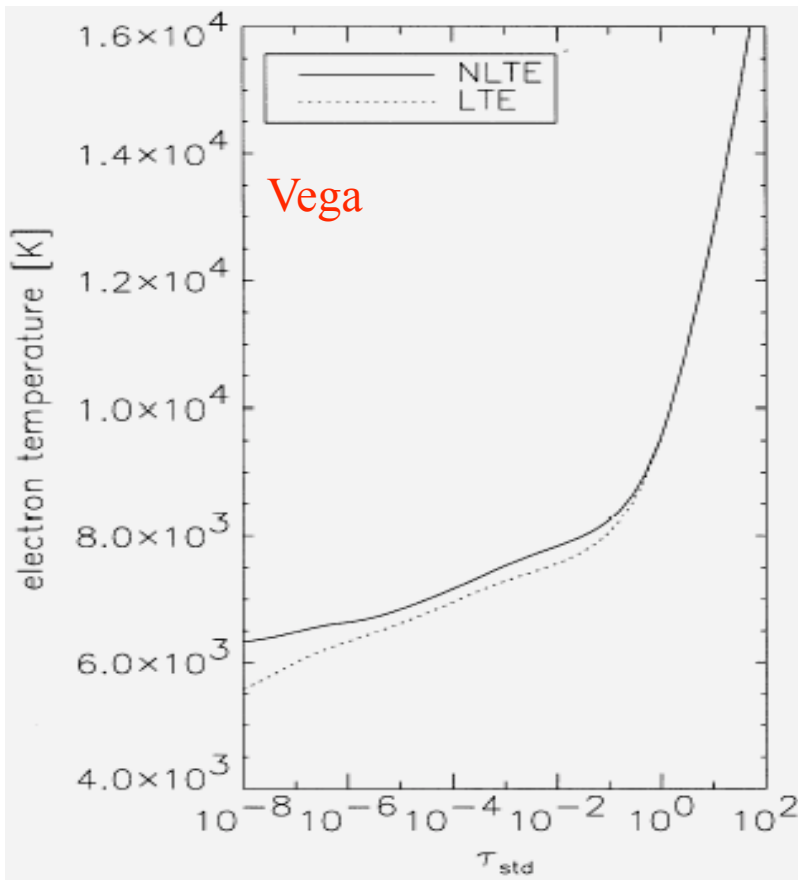
Sun (*Short & Hauschildt, 2005*):

- light metals in NLTE, small effect,
 - light metals and Fe group in NLTE, the model is warmer in $\log \tau < -2$.
- H^- determines the opacity and the transport of radiative energy.
 - $n(\text{H}^-) \sim n(\text{H I}) \cdot n_e$ is close to LTE.
 - H I is the majority species,
 - n_e is mainly contributed by metals (Mg, Si, Ca, Fe) which are already strongly ionized.

Vega

A difference in T between the non-LTE and LTE models is up to 500 K in the outermost zones.

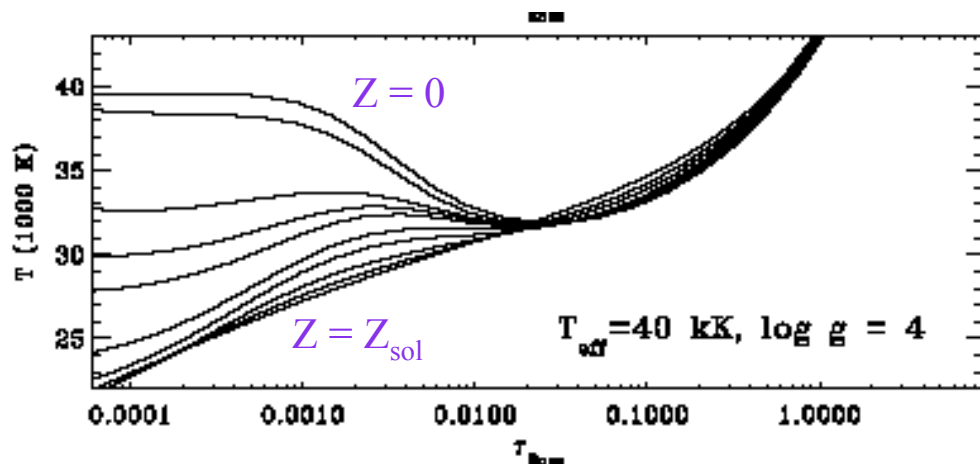
- H I determines the opacity and the transport of radiative energy.
- $n = 1, 2, 3$ depart from LTE and result in heating the outermost layers.



Hauschildt et al. (1999)

For A and later type stars, most chemical elements can be treated as trace elements. In solar type stars, even H.

Hot models



Temperature distribution
in the non-LTE models of
various metallicity.

$T_{\text{eff}} = 40000 \text{ K}, \log g = 4.$

Lanz & Hubeny (2003), TLUSTY

ΔT (H-He model – solar metallicity model) is up to 18000 K !

ΔT (non-LTE – LTE) is up to 400 K.

Even for the hottest stars, line blanketing
effect on the atmospheric structure is more
important than non-LTE effects.

Radiation transfer:
thermal absorption-emission processes and scattering

$$\mu \frac{dI_{\nu}(\tau_{\nu}, \mu)}{d\tau_{\nu}} = I_{\nu}(\tau_{\nu}, \mu) - S_{\nu}(\tau_{\nu})$$

When the atmospheric structure is fixed a problem of the radiation transfer is reduced to a determination of

$$S_{\nu}(z) = \frac{\eta_{\nu}(z)}{\chi_{\nu}(z)}$$

The source function depends on the physical nature of the interaction between matter and radiation.

Thermal (true) absorption and emission processes

- Photon is destroyed (thermalized) / generated.
- Radiation energy \longleftrightarrow thermal energy of gas.
$$S_{\nu}(\tau_{\nu}) = B_{\nu}(T_e)$$
- Local rate of energy emission depends on local value T .
 - photoionization / photorecombination,
 - free-free absorption / bremsstrahlung,
 - photoexcitation followed by collision de-excitation / collision excitation followed by radiative decay.

True absorption and emission tend to produce local equilibrium between the radiation and matter.

Scattering processes

- Photon interacts with a scattering center.
- Emerges in a new direction with the same or slightly altered energy.
- No energy exchange with gas,
only weak coupling to local conditions !

$$S_{\nu} \sim f(J_{\nu'})$$

- Thomson scattering,
- Rayleigh scattering,
- photoexcitation followed by the radiative decay directly to the initial state.

*Scattering processes tend to destroy
local equilibrium between the radiation and matter.*

Example

Scattering in the continuum is coherent and isotropic:

$$\eta_{\nu}^S = \sigma_{\nu} J_{\nu}$$

σ_{ν} is the scattering coefficient.
 χ_{ν}^t is the thermal absorption coefficient.

$$S_{\nu} = \frac{\chi_{\nu}^t B_{\nu}(T) + \sigma_{\nu} J_{\nu}}{\chi_{\nu}^t + \sigma_{\nu}}$$

In this case, scattering can be taken into account even in LTE calculations.

Spectral line formation

Line absorption coefficient in the transition $i - j$:

$$\chi_{\nu}^l = n_i \alpha_{ij}^{tot} \phi_{\nu} \left(1 - \frac{g_i n_j \psi_{\nu}}{g_j n_i \phi_{\nu}} \right)$$

ϕ_{ν} is the absorption profile,
 ψ_{ν} is the emission profile.

The correction for stimulated emission.

Line emission

coefficient:

$$\eta_{\nu}^l = n_j A_{ji} \psi_{\nu} h\nu_{ij} / 4\pi$$

$$a_{ij}^{tot} = \frac{\pi e^2}{mc} f_{ij}$$

Line source function:

$$S_{\nu}^l = \frac{2h\nu_{ij}^3}{c^2} \frac{1}{\frac{n_i g_j \phi_{\nu}}{n_j g_i \psi_{\nu}} - 1}$$

Absorption profile for various broadening mechanisms

$$\phi_\nu = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-[(\nu - \nu_0)/\Delta\nu_D]^2} \quad \text{Doppler broadening, } \Delta\nu_D^2 = \Delta\nu_t^2 + \Delta\nu_{turb}^2$$

$$\phi_\nu = \frac{\Gamma / 4\pi^2}{(\nu_0 - \nu)^2 + (\Gamma / 4\pi)^2} \quad \begin{array}{l} \text{natural damping with } \Gamma = \Gamma_R \text{ and} \\ \text{pressure broadening with } \Gamma = \Gamma_n, \\ n = 3, 4, 6. \end{array}$$

A combined effect is described by a Voigt profile.

$$\phi_\nu = V(u, a) = \frac{1}{\sqrt{\pi} \Delta\nu_D} \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-y^2}}{(u - y)^2 + a^2} dy \quad u = \frac{\nu - \nu_0}{\Delta\nu_D}, \quad a = \frac{\Gamma_R + \Gamma_4 + \Gamma_6}{4\pi\Delta\nu_D}$$

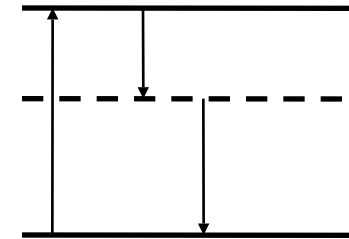
ϕ_ν in tabular form for the linear Stark effect broadening.

The line absorption coefficient is expressed explicitly!

How to compute the line emission coefficient?

- Which part of the absorbed photons is destroyed and which one is scattered?

There are also combinations of processes which can be referred to neither as scattering nor as true absorption.



Non-LTE: all these processes are automatically taken into account.

LTE: either pure thermal absorption and emission processes or pure scattering.

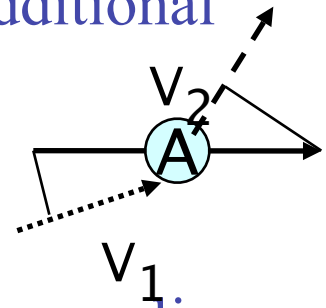
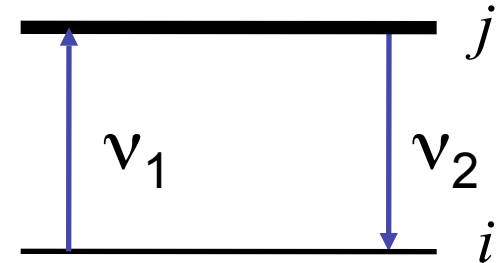
- How to specify an emission profile for scattered photons?

Scattering in line formation

Scattering in a line is **non-coherent**.

ν_1 is not exactly equal ν_2 , because

- the lower level i has a finite energy width,
- perturbations by nearby particles result in additional broadening of the levels i and j ,
- atom moves and leads to Doppler effect.



- Scattering is particularly important for the resonance lines. Non-coherence in their cores is only due to the Doppler redistribution.
- For the subordinate lines, non-coherence is mainly due to pressure effects.

Frequency redistribution over line profile

The angle-averaged redistribution function $R(\nu', \nu)$ is the probability that a photon absorbed in frequency range $(\nu', \nu' + d\nu')$ is reemitted in the range $(\nu, \nu + d\nu)$. $R(\nu', \nu)$ is symmetric and normalized.

By definition,

$$\phi(\nu') = \int_0^{\infty} R(\nu, \nu') d\nu; \quad \Psi(\nu) = \int_0^{\infty} R(\nu, \nu') d\nu';$$

The line emission coefficient contributed by scattering:

$$\eta_{\nu}^S = \sigma_{tot}^l \int_0^{\infty} R(\nu', \nu) J_{\nu'} d\nu'$$

$R(\nu', \nu)$ for the specific cases see e.g. in Mihalas (1978).

Complete redistribution

No correlation between the frequencies of incoming (ν') and scattered (ν) photons.

$$R(\nu, \nu') = f_1(\nu) f_2(\nu') \longrightarrow R(\nu, \nu') = \phi(\nu) \phi(\nu'), \quad \Psi(\nu) = \phi(\nu)$$

$$\eta_{\nu}^S = \sigma_{\nu}^l \int_0^{\infty} \phi(\nu') J(\nu') d\nu' = \sigma_{\nu}^l \bar{J}_l$$

$$\bar{J}_l = \int \phi_{\nu} J_{\nu} d\nu$$

the mean intensity
averaged over line profile.

A good approximation to scattering in subordinate lines.

In deep layers, atoms are so strongly perturbed by elastic collisions with nearby particles that the excited electrons are randomly redistributed over substates of the upper

$$S_{\nu}^l = \frac{2h\nu_{ij}^3}{c^2} \frac{1}{\frac{n_i}{n_j} \frac{g_j}{g_i} - 1}$$

The line source function
is frequency-independent
inside a spectral line.