Non-LTE line formation for trace elements in stellar atmospheres,
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Stellar atmospheres

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- Basic definitions. Basic equations. The assumptions and restrictions in modelling the atmospheres.
- Which elements at given stellar parameters can be treated as trace elements?
- Radiation transfer: thermal absorption-emission processes and scattering.
- Spectral line formation. Basic definitions. Scattering in line formation.

- Effective temperature T_{eff}, surface gravity log g, chemical composition: from fitting theoretical spectra to the observed spectral data.

- Theoretical spectra: from modelling of the temperature- and pressure-stratification of the surface layers of a star and solving the radiation transfer equation.

- Layers from which radiation can escape into space are called stellar atmosphere.

The *complete* atmosphere of a star
can be constituted of the regions different in the sources of heating and cooling, different in dynamics:

- – photosphere,
- – chromosphere,
- – corona,
- – stellar wind.

In order to model the complete atmosphere we have to understand all the physics involved.

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

Modelling of stellar atmospheres.

Basic assumptions.

I. Geometry.

Assume the atmosphere is composed of

homogeneous layers. $\rightarrow$ 1-D geometry

- Plane-parallel (PP) layers for MS stars and giants

  where the atmosphere is geometrically thin.

  E.g. a height of the solar photosphere, h $\cong$ 500 km,

  $\sim 10^{-3}$ of stellar radius.

- Spherical shells (SS) for supergiants.

II. Dynamics.

Assume the atmosphere is static.

The hydrostatic equilibrium (HE) equation:

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

the PP atmosphere: $g = const$,

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

III. Energy balance.

The transfer of energy through the atmosphere is done by radiation and convection.

The radiation transfer (RT) equation:

$$\mu \frac{dI_\nu(z)}{dz} = -\chi_\nu(z) I_\nu(z,\mu) + \eta_\nu(z) \qquad \text{(PP)}$$

$\mu = cos\,\theta$

$$\frac{\partial I_\nu}{\partial r}\mu + \frac{\partial I_\nu}{\partial \mu}\frac{1-\mu^2}{r} = -\chi_\nu(r) I_\nu(r,\mu) + \eta_\nu(r) \qquad \text{(SS)}$$

χ_ν is absorption coefficient, or opacity, or extinction coefficient per unit volume.

η_ν is emission coefficient, or emissivity.

χ_ν and η_ν are strongly state- and frequency-dependent, isotropic for static media.

Radiative equilibrium (RE)

A5 and earlier type stars:

the transfer of energy is done entirely by photons.

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

- In the PP atmosphere, the total radiation flux F is conserved over atmospheric depths.

$$F = \int_0^\infty F_\nu \, d\nu = const = \sigma T_{eff}^{\,4}$$

- In the SS atmosphere, $F\, r^2 = const = L/4\pi$

Other definitions of flux: $\left\{ \begin{array}{l} \mathrm{F}_\nu \text{ is astrophysical flux} \\ H_\nu \text{ is Eddington flux} \end{array} \right.$

$$F_\nu = \pi\, \mathrm{F}_\nu = 4\pi\, H_\nu$$

Radiative and convective equilibrium

- Convective transport of energy becomes important in the middle F type stars and dominates in later types.
- The classical stellar atmosphere problem treats the effects of convection 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.

- The total flux is transported by radiation and convection together:

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

IV. Thermodynamic state

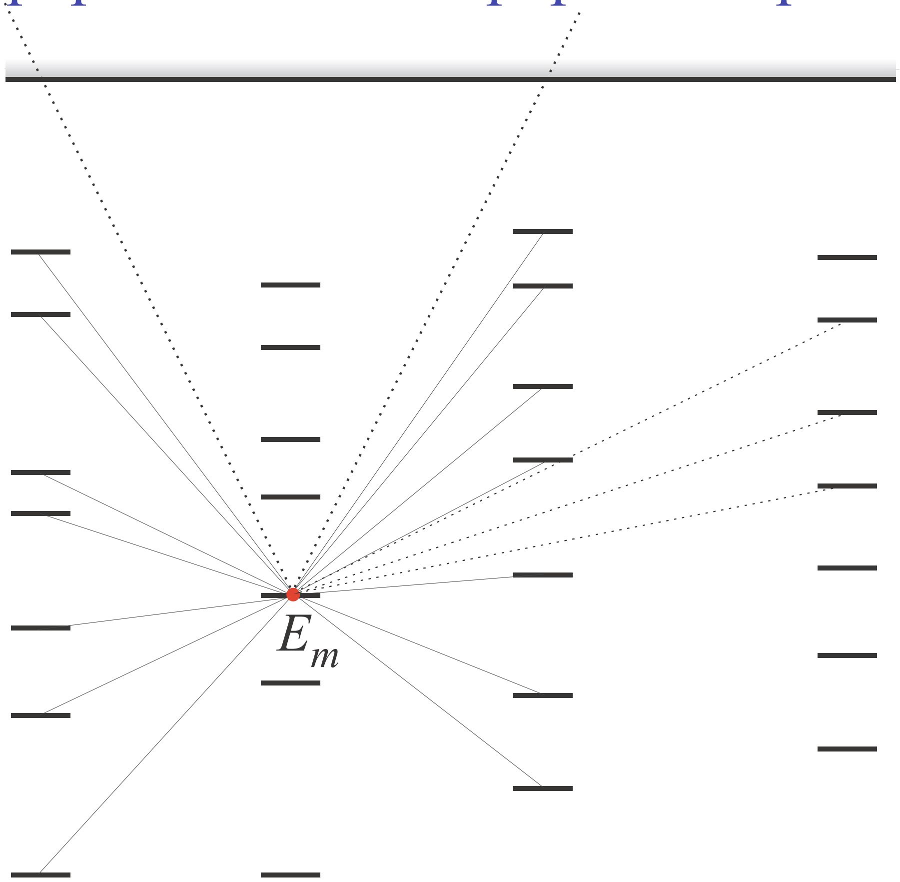
- TE is not fulfilled,
  - stellar atmosphere is open system,
  - temperature gradient.

- Local Thermodynamic Equilibrium (LTE) is based on the assumption that TE can be applied in small volume elements.

  For atom A in the ionization stage $\boldsymbol{r}$ in the level $\boldsymbol{i}$,

  $n_{A,r,i} = f(T, p)$ from the Saha-Boltzmann equations.

• In general, occupation numbers of atomic levels must be determined from a balance among radiative and collisional population and de-population processes:



Typical energy level diagram with interactions indicated

Given level is populated from the lower levels

- in photo- and collision excitation

and the upper levels

- in photo- and collision de-excitation,
- photorecombination and 3-body collisions;

depopulated to the lower levels and the upper levels

- in inverse processes.

Assuming $dn_i / dt = 0$

we investigate the statistical equilibrium (SE) of an atom.

The statistical equilibrium equations

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

in given atom,
and for all atoms
$A_1, A_2, \ldots, A_N$

$$n_{i,d} = f\left(n_1, \ldots, n_{NL}, J_1, \ldots, J_{NF}\right)_d$$

The excitation and ionization state of the matter
at any depth point *d* depends on the physical conditions throughout the atmosphere.

Basic equations
for the classical non-LTE stellar atmosphere problem

- HE $\rightarrow$ $N(z)$,
- RT equations for the grid $\{\nu_1, \nu_2, \ldots, \nu_{NF}\}$
  covering the radiative transitions in the SE equations and necessary for a calculation of the total flux. $\rightarrow$ J_ν
- RE equation or $F = F_{rad} + F_{conv}$ $\rightarrow$ $T(z)$,
- The charge conservation equation. $\rightarrow$ n_e
- SE equations for all those atoms which are important sources of opacity and/or important donors of free electrons. $\rightarrow$ n_i
- The particle conservation equation.

Fundamental parameters.

PP: T_{eff}, log g, chemical composition,

SS: L, M, chemical composition.

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_{eff} = 3500 – 50000 K; log g = 0 – 5 ($g > g_R$; $L < L_{Edd}$);
[M/H] = (+0.5) – (-3)
PP, HE, MLT, ODF for line opacity (~50 mln. lines).

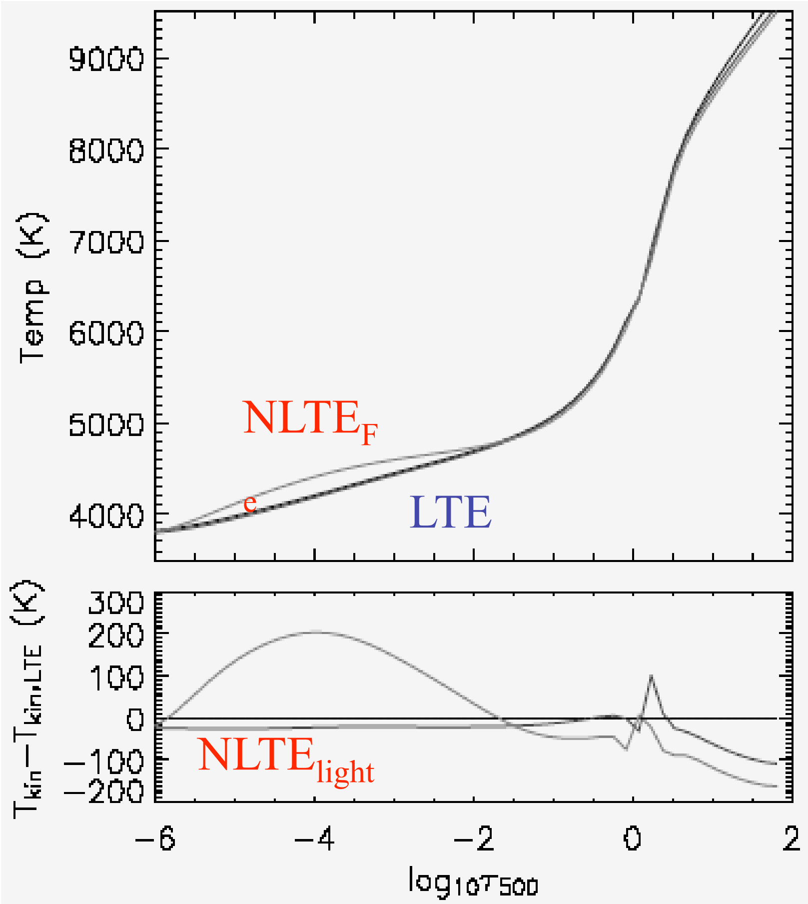
New generation of codes and models
is based on either OS or line-by-line (LL) technique for calculations of line blanketing.

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

Which elements at given stellar parameters can be treated as trace elements?

- **The atoms that, *at given stellar parameters*, contribute only a little to the opacity of the matter and/or to free electron reservoir are treated under the LTE assumption *in the model atmosphere calculations*.**
- **Non-LTE line formation for such an atom can be considered for the fixed atmospheric structure.**
- **Such element is referred to as trace element.**

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 $\tau < -2$.

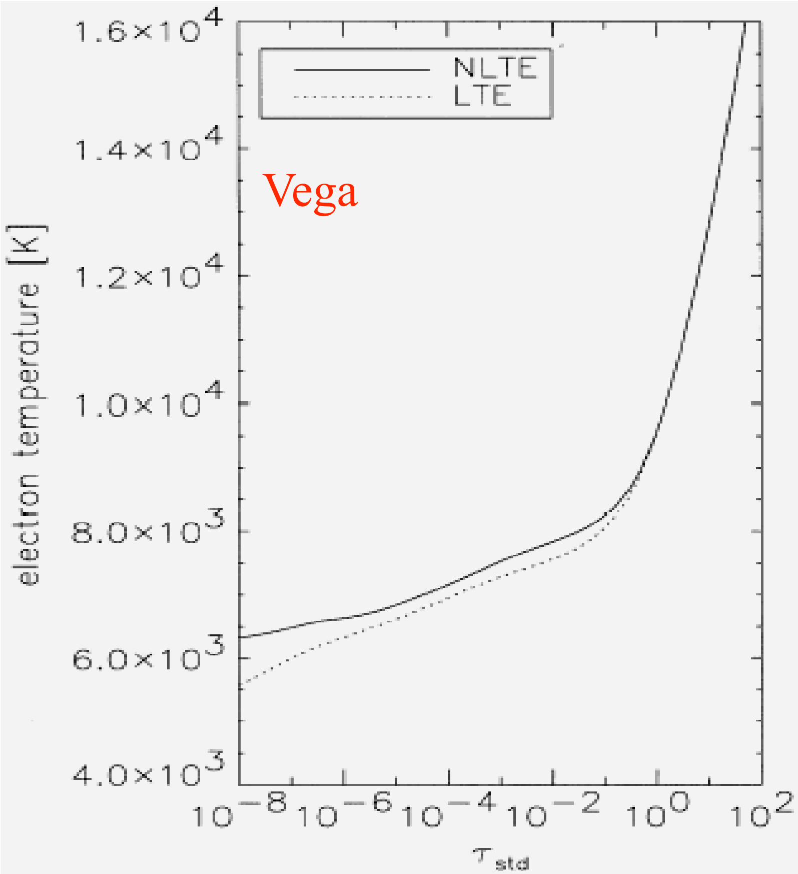
• H^- determines the opacity and the transport of radiative energy.

• $n(H^-) \sim n(H\ I) \cdot n_e$ 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.

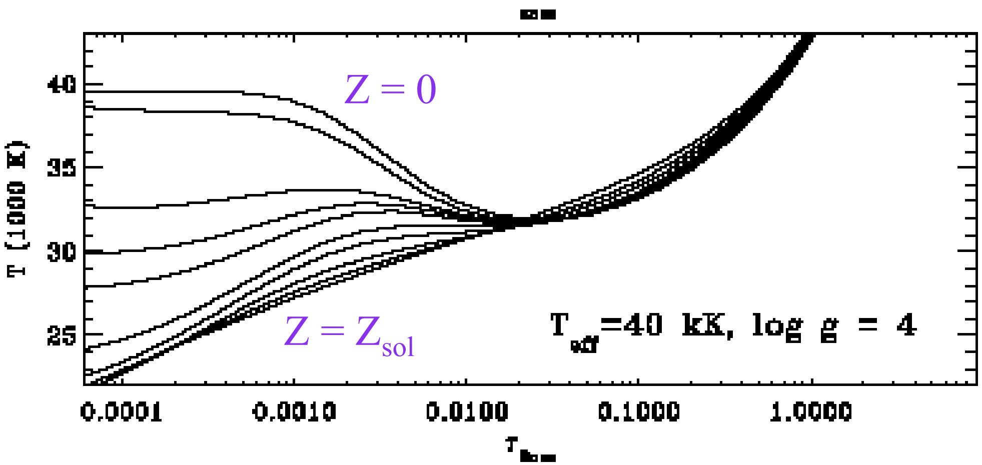


Hauschildt et al. (1999)

- 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.

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_{eff} = 40000 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

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

The source function

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

Optical depth is the integrated absorptivity

$$\tau_\nu(z) = \int_z^{z\,\max} \chi_\nu(z)dz \qquad d\tau_\nu = -\chi_\nu(z)dz$$

$S_\nu(\tau_\nu)$ - ?

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 ⟷ 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 $i - j$:

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

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:

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

Absorption profile for various broadening mechanisms

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

Doppler broadening, $\Delta\nu_D^2 = \Delta\nu_t^2 + \Delta\nu_{turb}^2$

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

natural damping with $\Gamma = \Gamma_R$ and pressure broadening with $\Gamma = \Gamma_n$, $n = 3, 4, 6.$

A combined effect is described by a Voigt profile.

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

ϕ_ν in tabular form for the linear Stark effect broadening.

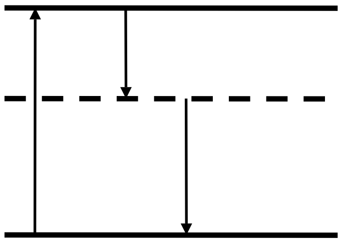
The line absorption coefficient is expressed explicitly!

The situation with atomic data has improved significantly in recent years.

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.



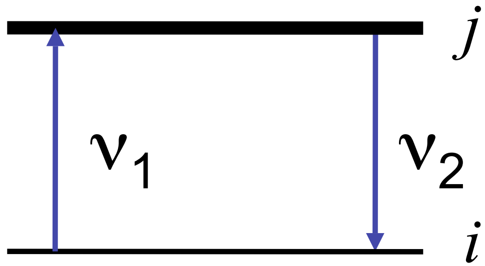
  Non-LTE: all these processes are automatically taken into account.

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

- How to specify an emission profile for scattered photons?

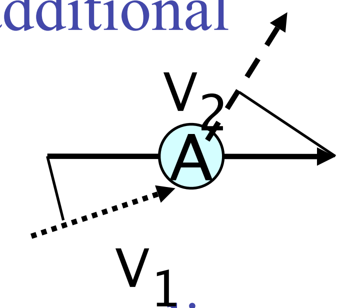
Scattering in line formation

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(ν‘,ν)* is the probability that a photon absorbed in frequency range $(\nu', \nu' + d\nu')$ is reemitted in the range $(\nu, \nu + d\nu)$.
R(ν‘,ν) is symmetric and normalized.

By definition,

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

The line emission coefficient contributed by scattering:

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

R(ν‘,ν) for the specific cases see e.g. in Mihalas (1978).

Complete redistribution

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

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

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

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

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 level.

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

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