

Stellar Atmospheres

Lecture 18



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Non-LTE

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NON-LTE
STATISTICAL EQUILIBRIUM
TWO-LEVEL APPROXIMATION
THE LINE SOURCE FUNCTION
LTE VERSUS NON-LTE

LTE versus non-LTE?

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- Most studies of stellar atmospheres are performed under LTE, where the thermodynamic state of the plasma is described via the Saha-Boltzmann equation as a function of **local T and N_e** . However, LTE strictly holds deep in the interior when collisions dominate and the photon mean-free-path is small.
- For a more accurate physical description, the **non-local** nature of the radiation field and its interaction with the plasma has to be accounted for. This requires consideration of the detailed atomic processes for excitation and ionization, as expressed in the **rate equations of statistical equilibrium** (non-LTE case).
- Departure coefficients **$b = \text{pop}(\text{non-LTE})/\text{pop}(\text{LTE})$**

What does non-LTE mean?

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The level populations of atoms are governed by the rates of all (**collisional** and **radiative**) processes, by which an atom leaves a certain state i to some other state j (if bound) or k (if unbound) and vice versa

Bound-bound	Bound-free
RADIATIVE	
Photoabsorption(R_{ij})	Photoionization(R_{ik})
Spontaneous + stimulated emission (R_{ji})	Spontaneous + stimulated recombination (R_{ki})
COLLISIONAL	
Excitation (C_{ij})	Ionization (C_{ik})
De-excitation(C_{ji})	Recombination(C_{ki})

The total upward rate $P_{ij} = C_{ij} + R_{ij}$, whilst the total downward rate is $P_{ji} = C_{ji} + R_{ji}$

LTE vs NLTE

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- LTE: population numbers follow Saha-Boltzmann Equation
 $n_i = n_i(T, n_e)$
- NLTE: population numbers depend on radiation field
 $n_i = n_i(T, n_e, J)$
- Need to take into account the sum of all processes that decrease and increase population for a given level i :

$$\frac{d}{dt}n_i = \sum_{j \neq i} n_j P_{ji} - n_i \sum_{j \neq i} P_{ij}$$

In stellar atmospheres typically:
 $dn_i / dt = 0$ (stationary)

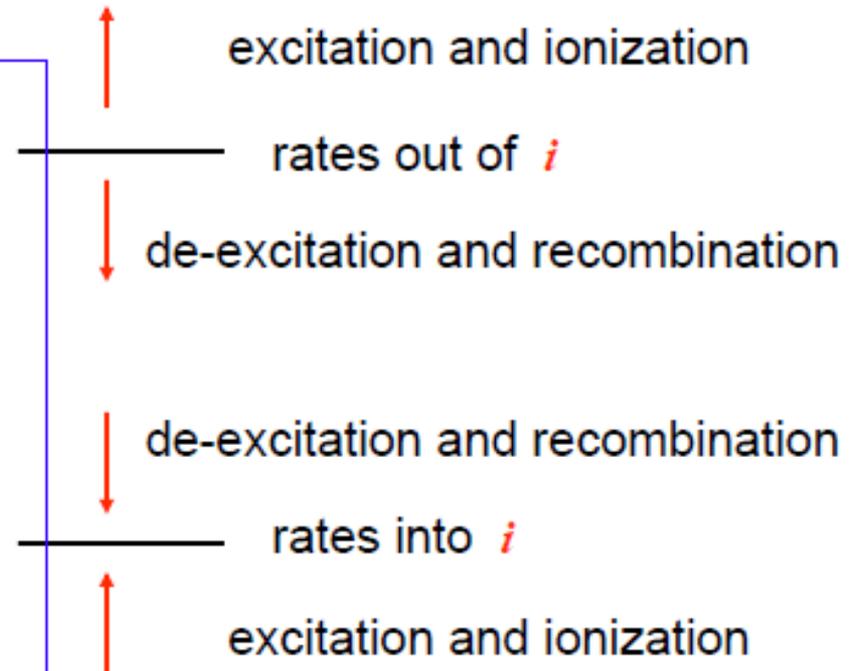
Complete rate equations

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For each atomic level i of each ion, of each chemical element we have:

$$\begin{aligned}
 & -n_i[\sum_{j>i}(R_{ij} + C_{ij}) + \\
 & \sum_{j<i}(R_{ji} + C_{ji})] \\
 & + \sum_{j>i}n_j(R_{ij} + C_{ij}) \\
 & + \sum_{j<i}n_j(R_{ji} + C_{ij}) = dn_i/dt
 \end{aligned}$$

In steady-state: $dn_i/dt=0$



Statistical equilibrium

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- Statistical equilibrium, also known as rate equations:

$$\frac{dn_i}{dt} = \sum_{j \neq i}^N n_j P_{ji} - n_i \sum_{j \neq i}^N P_{ij} = \sum_{j \neq i}^N n_j (R_{ji} + C_{ji}) - n_i \sum_{j \neq i}^N (R_{ij} + C_{ij}) = 0$$

- Particle conservation:

$$\sum_{i=1}^N n_i = n_T$$

- By “non-LTE”, we refer to the solution of these equations of statistical equilibrium or rate equations. This is **much** more challenging computationally than LTE...
- Rate equations represent a non-linear system of equations, we look for the solution vector via linearization, based **on Newton-Raphson iteration**.

Two-level approximation

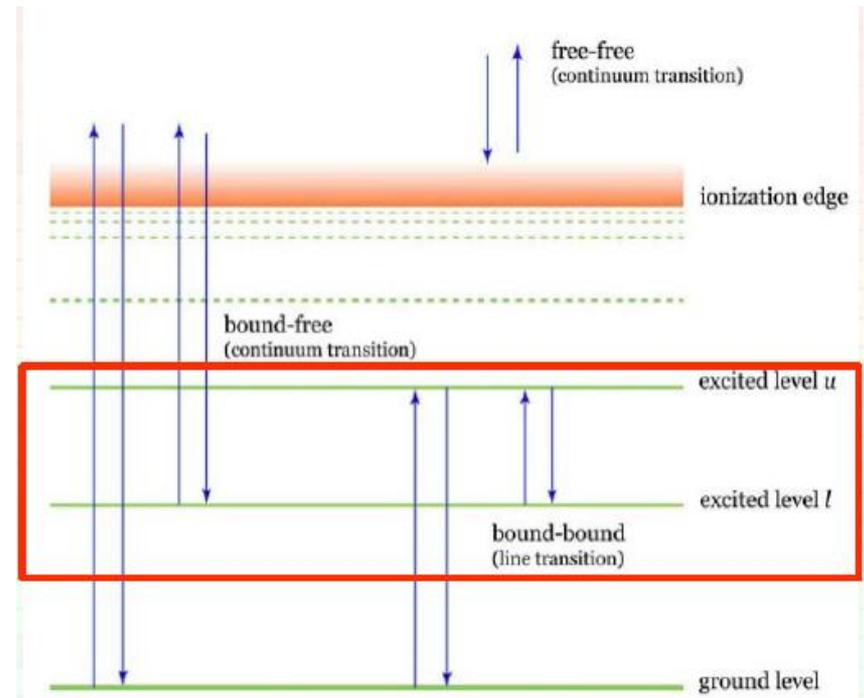
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Let's consider schematic line-formation cases with easy solution

It is highly simplified:
not accurate, but provide insight into the mechanisms at work in real stellar atmospheres.

Consider an atomic model with only two important levels:
lower l and upper u .

Although highly simplified, it well approximates the situation for some lines, *e.g.* resonance lines from the ground state.



Two-level approximation

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Rate equations (statistical equilibrium)

$$n_i \underbrace{\sum_{j \neq i} (R_{ij} + C_{ij})}_{\text{lines}} + n_i \underbrace{(R_{ik} + C_{ik})}_{\text{ionization}} = \sum_{j \neq i} \underbrace{n_j (R_{ji} + C_{ji})}_{\text{lines}} + \underbrace{n_p (R_{ki} + C_{ki})}_{\text{recombination}}$$

Consider two levels u and l : isolating the transitions between them:

$$n_l (R_{lu} + C_{lu}) + n_l \sum_{j \neq l, u} (R_{lj} + C_{lj}) + n_l (R_{lk} + C_{lk}) = n_u (R_{ul} + C_{ul}) + \sum_{j \neq l, u} n_j (R_{jl} + C_{jl}) + n_p (R_{kl} + C_{kl})$$

and **neglecting** all transitions involving $j \neq l, u$, plus recombinations/ionizations:



$$n_l (R_{lu} + C_{lu}) = n_u (R_{ul} + C_{ul})$$

Two-level approximation

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$$n_l(R_{lu} + C_{lu}) = n_u(R_{ul} + C_{ul})$$

substituting for the R coefficients:

$$n_l(B_{lu} \int_0^{\infty} \varphi_{\nu} J_{\nu} d\nu + C_{lu}) = n_u(A_{ul} + B_{ul} \int_0^{\infty} \varphi_{\nu} J_{\nu} d\nu + C_{ul})$$

Einstein coefficients:

$$n_l B_{lu} J_{\nu} = n_u A_{ul} + n_u B_{ul} J_{\nu}$$

Transition Probabilities: Radiative Processes

$$R_{ij} = B_{ij} \int_0^{\infty} \varphi_{ij}(\nu) J_{\nu} d\nu$$

Absorption

$$R_{ji} = A_{ji} + B_{ji} \int_0^{\infty} \varphi_{ij}(\nu) J_{\nu} d\nu$$

Spontaneous and stimulated Emission

Two-level approximation

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$$n_l(R_{lu} + C_{lu}) = n_u(R_{ul} + C_{ul})$$

Einstein coefficients:
 $n_l B_{lu} J_\nu = n_u A_{ul} + n_u B_{ul} J_\nu$

substituting for the R coefficients:

$$n_l \left(B_{lu} \int_0^\infty \varphi_\nu J_\nu d\nu + C_{lu} \right) = n_u \left(A_{ul} + B_{ul} \int_0^\infty \varphi_\nu J_\nu d\nu + C_{ul} \right)$$

assuming collision rates dominate over radiative rates $n_l C_{lu} = n_u C_{ul}$

Sanity check:
LTE case

remembering that $C_{lu} = \left(\frac{n_u}{n_l} \right)^* C_{ul} = \frac{g_u}{g_l} e^{-E_{ul}/kT} C_{ul}$

$$\Rightarrow n_l \frac{g_u}{g_l} e^{-E_{ul}/kT} C_{ul} = n_u C_{ul}$$

$$\Rightarrow \frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-E_{ul}/kT} = \left(\frac{n_u}{n_l} \right)^{\text{LTE}}$$

Calculation of the line source function

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$$\alpha_{\nu}^{line} = (n_l B_{lu} - n_u B_{ul}) J_{\nu}$$

$$\epsilon_{\nu}^{line} = n_u A_{ul} J_{\nu}$$

$$S_{\nu}^{line} = \frac{\epsilon_{\nu}^{line}}{\alpha_{\nu}^{line}} = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} = \frac{A_{ul}}{\frac{n_l}{n_u} B_{lu} - B_{ul}}$$

Einstein Coefficients:

$$B_{lu} = \frac{g_u}{g_l} B_{ul} \quad A_{ul} = \frac{2h\nu^3}{c^2} B_{ul}$$

$$S_{\nu}^{line} = \frac{2h\nu^3}{c^2} \frac{1}{\frac{n_l g_u}{n_u g_l} - 1}$$

Note: this is the general expression for the line source function in **NLTE**. It is **always** valid (not only in 2-level approximation). What is different in the general case, is how n_l , n_u are computed

Two-level approximation

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If we substitute $\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-E_{ul}/kT} = \left(\frac{n_u}{n_l}\right)^*$ $E = h\nu$

we recover the Planck function $S_\nu^{\text{line}} = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} = B_\nu(T)$

For the 2-level atom we found $n_l(B_{lu} \int_0^\infty \varphi_\nu J_\nu d\nu + C_{lu}) = n_u(A_{ul} + B_{ul} \int_0^\infty \varphi_\nu J_\nu d\nu + C_{ul})$

$$\frac{n_l}{n_u} = \frac{1 + \frac{c^2}{2h\nu^3} \int \varphi_{\nu'} J_{\nu'} d\nu' + C_{ul}/A_{ul}}{\frac{g_u}{g_l} \left[\frac{c^2}{2h\nu^3} \int \varphi_{\nu'} J_{\nu'} d\nu' + e^{-h\nu/kT} C_{ul}/A_{ul} \right]}$$

Calculation of the line source function

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Substituting n_l/n_u in S_ν :

$$S_\nu^{\text{line}} = \frac{2h\nu^3}{c^2} \frac{1}{\frac{n_l g_u}{n_u g_l} - 1}$$

$$S_\nu^{\text{line}} = \frac{2h\nu^3}{c^2} \frac{\frac{c^2}{2h\nu^3} \int \varphi_{\nu'} J_{\nu'} d\nu' + e^{-h\nu/kT} C_{ul}/A_{ul}}{1 + \frac{C_{ul}}{A_{ul}}(1 - e^{-h\nu/kT})} =$$

$$= \underbrace{\frac{1}{1 + \frac{C_{ul}}{A_{ul}}(1 - e^{-h\nu/kT})}}_{1 - \varepsilon} \int \varphi_{\nu'} J_{\nu'} d\nu' + \underbrace{\frac{2h\nu^3}{c^2} \frac{e^{-h\nu/kT} C_{ul}/A_{ul}}{1 + \frac{C_{ul}}{A_{ul}}(1 - e^{-h\nu/kT})}}_{\varepsilon}$$

$1 - \varepsilon$

$$\frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT} - 1} \underbrace{\frac{(1 - e^{-h\nu/kT}) C_{ul}/A_{ul}}{1 + \frac{C_{ul}}{A_{ul}}(1 - e^{-h\nu/kT})}}_{\varepsilon}$$

$B_\nu(T)$

$:= \varepsilon$

Calculation of the line source function

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$$S_{\nu}^{\text{line}} = \underbrace{(1 - \epsilon) \int_0^{\infty} \varphi_{\nu'} J_{\nu'} d\nu'}_{\text{scattering term}} + \underbrace{\epsilon B_{\nu}(T)}_{\text{thermal term}} = \frac{\int_0^{\infty} \varphi_{\nu'} J_{\nu'} d\nu' + \epsilon' B_{\nu}(T)}{1 + \epsilon'}$$

$$\epsilon := \frac{(1 - e^{-h\nu/kT}) C_{ul}/A_{ul}}{1 + \frac{C_{ul}}{A_{ul}} (1 - e^{-h\nu/kT})} = \frac{\epsilon'}{1 + \epsilon'}$$

destruction probability

Photons are either destroyed into thermal pool or scattered photons are created in thermal processes

From the previous lecture:

$$S(\tau) = \zeta B + (1 - \zeta)J(\tau)$$

absorption fraction $\zeta \equiv \frac{\alpha_{\text{abs}}}{\alpha_{\text{abs}} + \alpha_{\text{sc}}}$

Now we obtained that Line source function has similar terms except that we also allow for non-coherent scattering

Two-level approximation

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$$\epsilon := \frac{(1 - e^{-h\nu/kT}) C_{ul}/A_{ul}}{1 + \frac{C_{ul}}{A_{ul}} (1 - e^{-h\nu/kT})} = \frac{\epsilon'}{1 + \epsilon'}$$

$$S_{\nu}^{\text{line}} = (1 - \epsilon) \int_0^{\infty} \varphi_{\nu'} J_{\nu'} d\nu' + \epsilon B_{\nu}(T) = \frac{\int_0^{\infty} \varphi_{\nu'} J_{\nu'} d\nu' + \epsilon' B_{\nu}(T)}{1 + \epsilon'}$$

Deep layers: collisions dominate $\rightarrow \epsilon' \gg 1$ or $\epsilon = 1$ **thermal** term dominant

$$C_{ul} \gg A_{ul} \quad \epsilon = 1 \quad \rightarrow \quad S_{\nu} = B_{\nu}(T) \quad \text{LTE}$$

Higher layers: collisions non-important $\rightarrow \epsilon' \approx 0$ or $\epsilon = 0$ **scattering** term dominant

$$C_{ul} \ll A_{ul} \quad \epsilon \approx 0 \quad \rightarrow \quad S_{\nu} = \int \varphi_{\nu'} J_{\nu'} d\nu' \quad \text{Extreme non-LTE}$$

From the previous lecture: $S_{\nu} = J_{\nu}$ for pure *coherent* scattering

now $S_{\nu} = \int \varphi_{\nu'} J_{\nu'} d\nu'$ *non-coherent* scattering

Collisional rates

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For an electron with kinetic energy E exciting an atom

- Excitation:

$$C_{ij} = n_e \int_{E_{ij}}^{\infty} \sigma_{ij}(u) u f(u) du = n_e \int_{E_{ij}}^{\infty} \sigma_{ij}(E) \sqrt{\frac{2E}{m}} f(E) dE \propto \frac{n_e}{T^{3/2}} \int_{E_{ij}}^{\infty} \sigma_{ij}(E) e^{-E/kT} E dE \propto \frac{n_e}{T^{3/2}} e^{-E_{ij}/kT}$$

$$\sigma_{ij}(E) \propto 1/E$$

- De-excitation:

$$C_{ji} = n_e \int_0^{\infty} \sigma_{ji}(u) u f(u) du = n_e \int_0^{\infty} \sigma_{ji}(E) \sqrt{\frac{2E}{m}} f(E) dE$$

where $f(E)$ is the (Maxwellian) energy distribution of the colliding particles.

- In TE, the principle of detailed balance gives

$$n_i C_{ij} = n_j C_{ji} \Rightarrow \frac{C_{ij}}{C_{ji}} = \frac{n_j}{n_i} = \frac{g_j}{g_i} e^{-E_{ij}/kT}$$

- Even if there is no TE, but we have a Maxwellian velocity distribution

$$\frac{C_{ij}}{C_{ji}} = \frac{g_j}{g_i} e^{-E_{ij}/kT}$$

Two-level approximation

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- Moving outward in the photosphere scattering term dominates.
- At some point we reach the region where photons are being lost from the star (small optical depth)
 - J_ν decreases with height
 - S_ν decreases with height
 - absorption line
- line absorption coefficient larger at line center → see higher layers
- wings form in deeper layers than line core

Wing can form in LTE conditions whilst a line core in non-LTE

- 2-level atom is a special NLTE case
- in general the coupling between J_ν , n_i and S_ν is far more complicated

NLTE: Occupation numbers

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We obtain a system of linear equations for n_i :

$$A \cdot \begin{pmatrix} n_1 \\ n_2 \\ \dots \\ n_p \end{pmatrix} = \mathbf{X}$$

Where matrix A contains terms:

$$\int_0^{\infty} \varphi_{ij}(\nu) \int_{4\pi} I_{\nu}(\omega) \frac{d\omega}{4\pi} d\nu$$

combine with equation of transfer:

$$\mu \frac{dI_{\nu}(\omega)}{dr} = -\kappa_{\nu} I_{\nu}(\omega) + \epsilon_{\nu}$$

$$\kappa_{\nu} = \sum_{i=1}^N \sum_{j=i+1}^N \sigma_{ij}^{\text{line}}(\nu) \left(n_i - \frac{g_i}{g_j} n_j \right) + \sum_{i=1}^N \sigma_{ik}(\nu) \left(n_i - n_i^* e^{-h\nu/kT} \right) + n_e n_p \sigma_{kk}(\nu, T) \left(1 - e^{-h\nu/kT} \right) + n_e \sigma_e$$

$$\epsilon_{\nu} = \dots$$

non-linear system of integro-differential equations

NLTE: Occupation numbers

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Iteration required:

radiative processes depend on radiation field

$$R_{ij} = B_{ij} \int_0^{\infty} \varphi_{ij}(\nu) J_{\nu} d\nu$$



radiation field depends on opacities

$$\mu \frac{dI_{\nu}(\omega)}{dr} = -\kappa_{\nu} I_{\nu}(\omega) + \epsilon_{\nu}$$



opacities depend on occupation numbers

$$\kappa_{\nu}^{\text{b-f}} = n_l \sigma_{lk}(\nu)$$

requires database of atomic quantities: energy levels, transitions, cross sections

20...1000 levels per ion – 3-5 ionization stages per species – » 30 species

→ fast algorithm to calculate radiative transfer required

LTE

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LTE is a **good** approximation, if:

1) Collisional rates dominate for all transitions

$$R_{ij} \ll C_{ij} \text{ so } P_{ij} (= R_{ij} + C_{ij}) \sim C_{ij}$$

$$\text{Since } C_{ij}/C_{ji} = (n_i/n_j)^*$$

Solution of rate equations \rightarrow LTE

2) $J_\nu = B_\nu$ is a good approximation at all frequencies

$$n_i R_{ij} = n_j R_{ji} \text{ so } n_i/n_j = (n_j/n_i)^*$$

Solution of rate equations \rightarrow LTE

Non-LTE

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LTE is a **bad** approximation, if:

- 1) Collisional rates are small
 - 2) Radiative rates are large
 - 3) Mean free path of photons is larger than that of electrons
- Large deviations from LTE may be expected for low density gas in which the radiation field deviates strongly from the Planck function for the kinetic temperature.
 - Non-LTE needs to be considered for (a) **hot stars**, whose atmospheres are rapidly expanding; (b) low density **chromospheres** and **coronae** of Solar-type stars; (c) low T_{eff} of very **cool stars** (in which electron densities are low); (d) nebulae; (e) ISM.

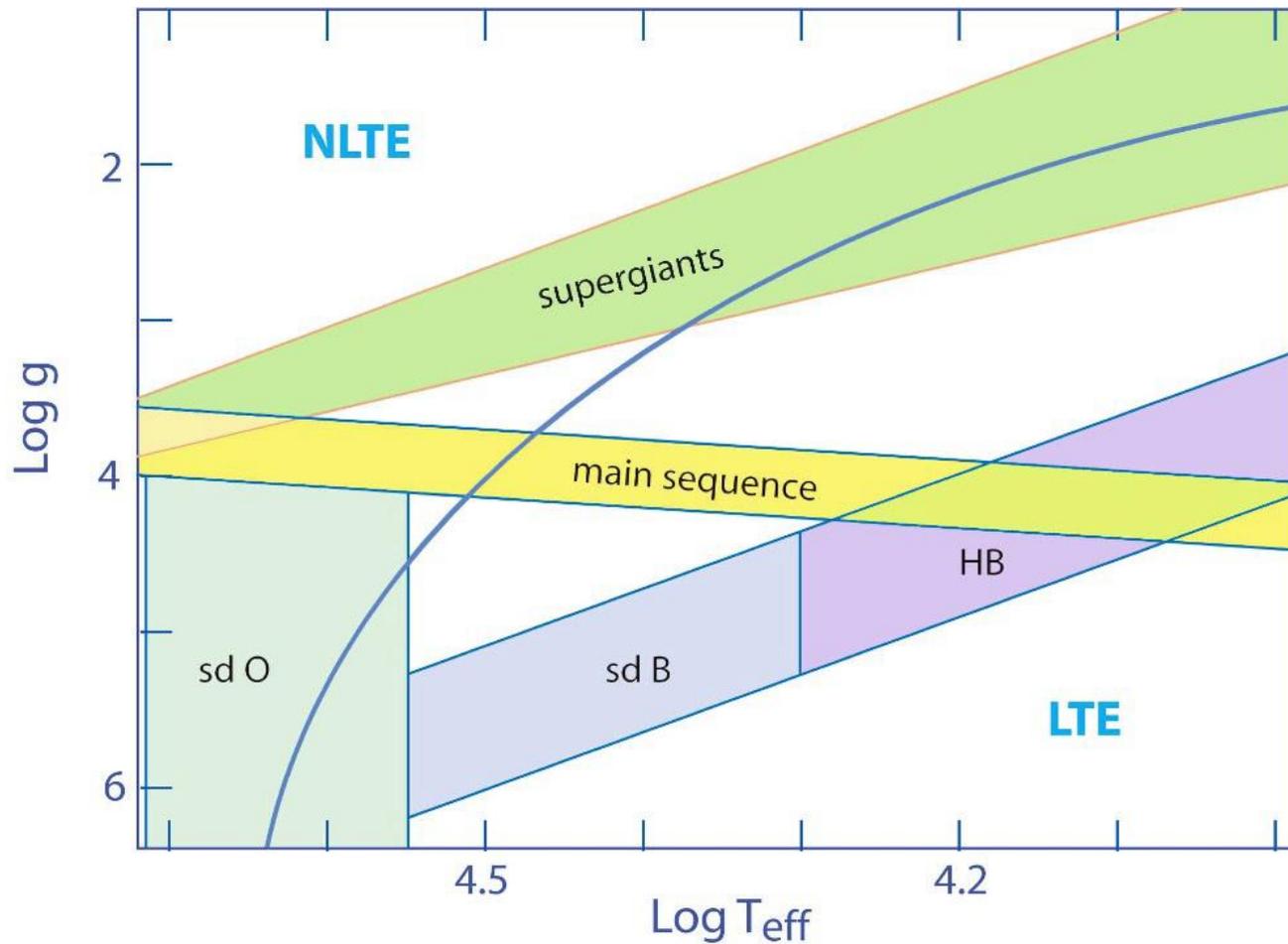
Non-LTE effects in scattering

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- Deep in the atmosphere, collisions are frequent, radiation field is close to Planck and populations follow Boltzmann law. → LTE.
- Close to the boundary, radiation can escape freely, density drops, collisional rates decrease, radiative rates are not enough to populate upper levels. As a result, the **upper** level can be underpopulated. Therefore the source function deviates from Planck function.
- Even if the only scattering (no true absorption) occurs in the atmosphere, an absorption line forms.

LTE vs NLTE

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Non-LTE in the Sun

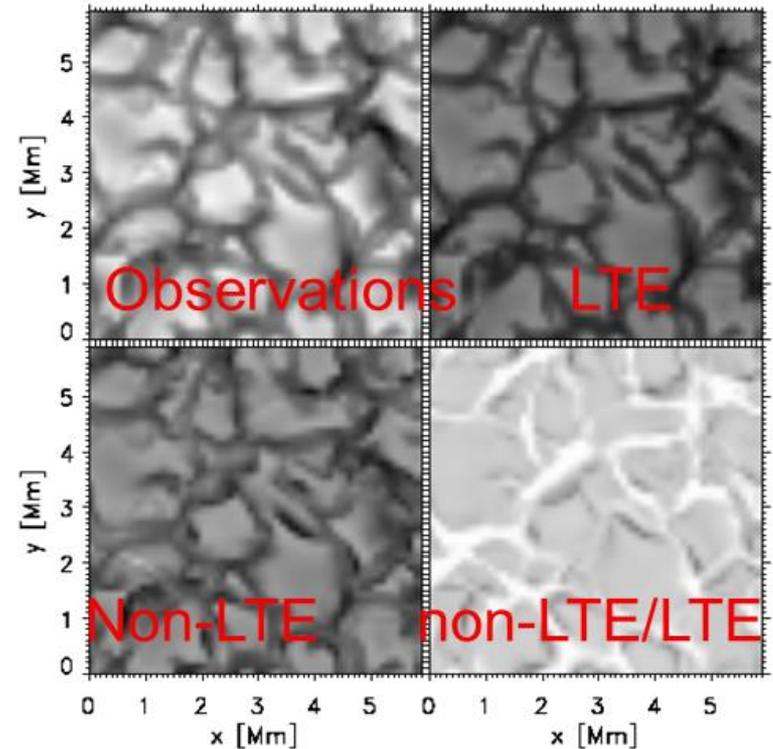
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- **Chromosphere & corona** in non-LTE, since the radiation field corresponds to a diluted Planck function for the effective temperature of the Sun, whilst the kinetic temperature in the coronae may be several 10^6K .
- **Photospheric departures from LTE occur.** Weak lines of low-abundance species often show departures from LTE (e.g. they reverse to emission lines on the solar disk just inside the limb). Cores of strong lines may depart from LTE, while the wings may remain in LTE.
- Non-LTE is most relevant in the Solar context via **inaccuracies** in elemental **abundances** obtained with the LTE assumption (typically 0.05 dex), although effect is greatest from comparison between latest 3D vs earlier 1D models.

Solar Oxygen abundance

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- Until recently, commonly adopted Solar oxygen abundance was $\log(O/H)+12=8.93$ suggested by analyses of [OI] 6300Å (Lambert 1978) and OH lines in IR using 1D LTE models.
- Asplund et al. (2004) has used 3D analyses of the [OI] and OH lines, revealing significant departures from LTE, indicating a much lower abundance of $\log(O/H)+12=8.66$.
- Ar and Ne aren't seen in the Solar photosphere, so deduced from coronal material, relative to oxygen. The decrease in oxygen also causes Ar and Ne to be scaled down.



Consequences?

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The Solar metal mass fraction falls from $Z=0.019$ to $Z=0.013$, **reconciling** some long standing problems (e.g. agreement with local ISM abundances, e.g. Orion nebula), BUT there is now a helioseismology (sound speed, density below convective zone) **discrepancy** for the Sun, which can be reconciled in following ways:

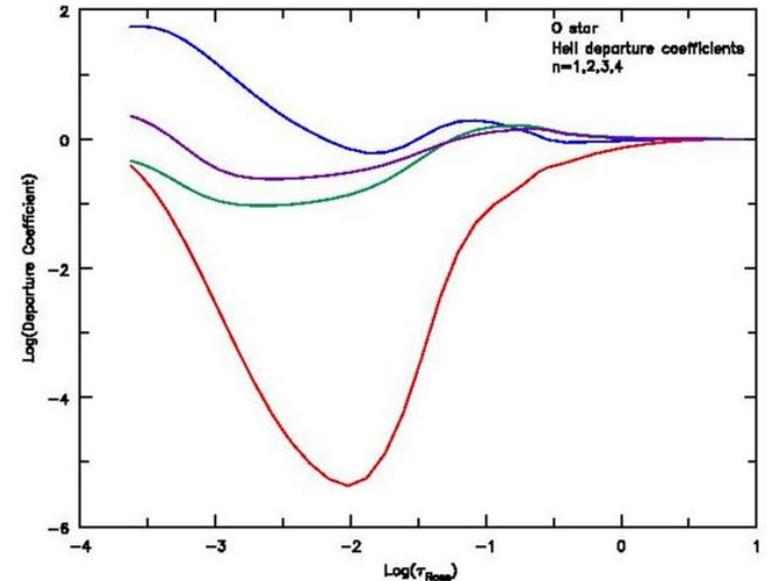
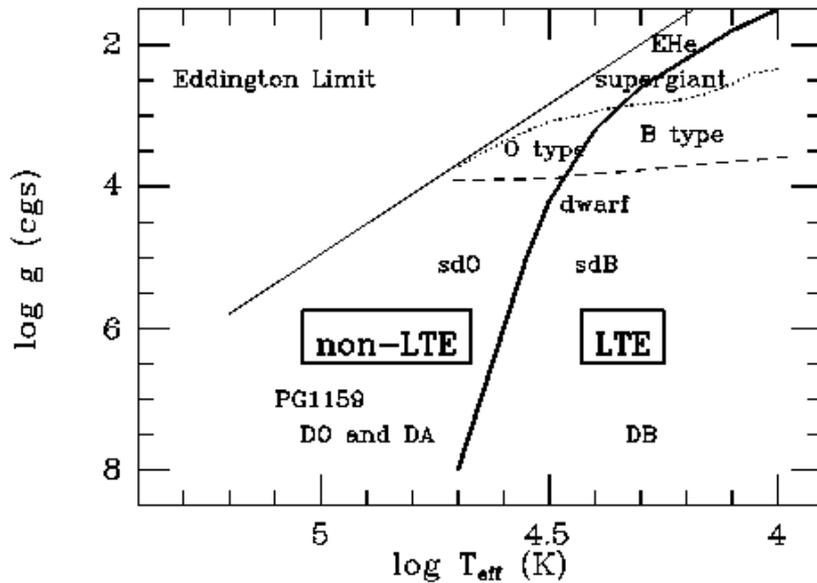
- Missing opacity from OPAL calculations? Need 7% at $\log T=6.4$, though new OP calculations suggest $<2.5\%$ missing in OPAL.
- Problems with diffusion in interior models?
- Problems with abundance of Ne (indirectly inferred from Ne/O in solar corona). Needs factor 3 increase!

Overall, experience from Solar analysis suggests that determination of stellar abundances may be less certain than is normally considered!

Non-LTE for hot stars

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Radiation field is so **intense** in hot stars (O-type, OBA supergiants, WDs) that their **populations** are only **weakly** dependent on **local** (T_e , N_e), consequently LTE represents a poor assumption.

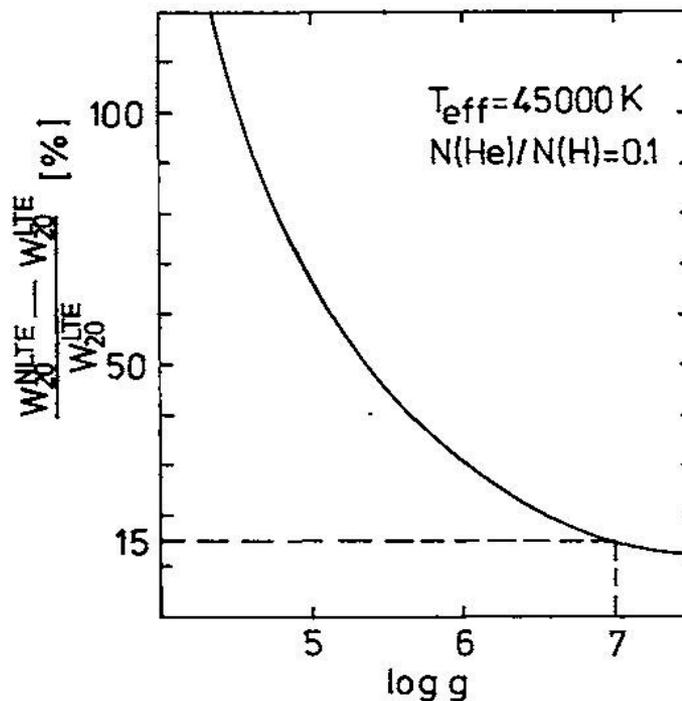
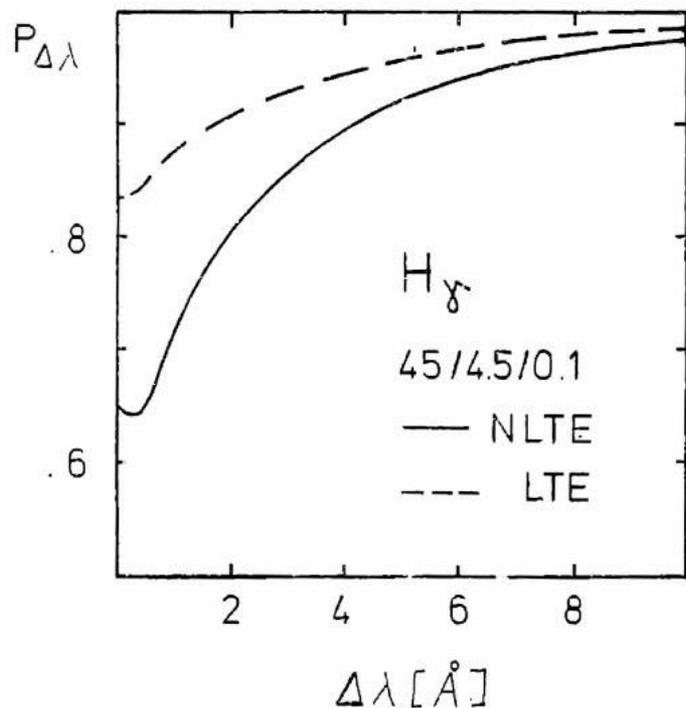


In O stars, LTE profiles are much too weak. Departure coefficients (non-LTE/LTE-pop) shown here for $n=1, 2, 3, 4$ for HeII can differ greatly in wind and photosphere, making HeI & HeII lines *much* stronger.

LTE vs NLTE in hot stars

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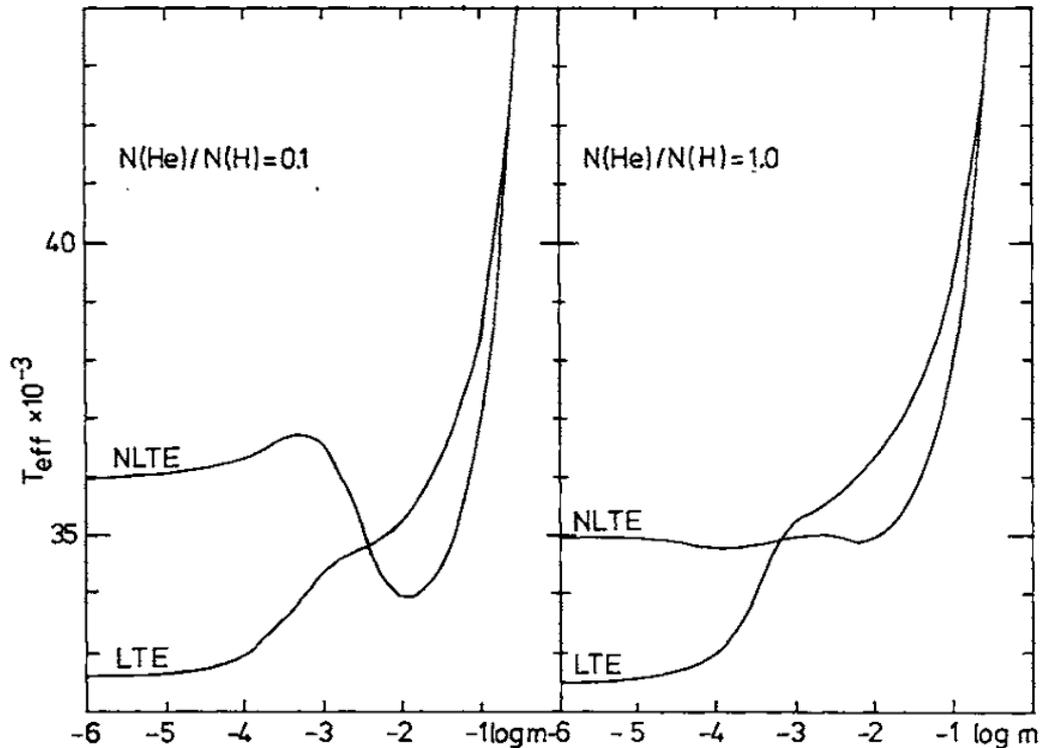
Difference between NLTE and LTE in H_γ line profile for an O-star model with $T_{\text{eff}} = 45000\text{K}$ and $\log g = 4.5$



Difference between NLTE and LTE H_γ equivalent width as a function of $\log g$ for $T_{\text{eff}} = 45,000\text{K}$ for subluminal O stars

LTE vs NLTE in hot stars

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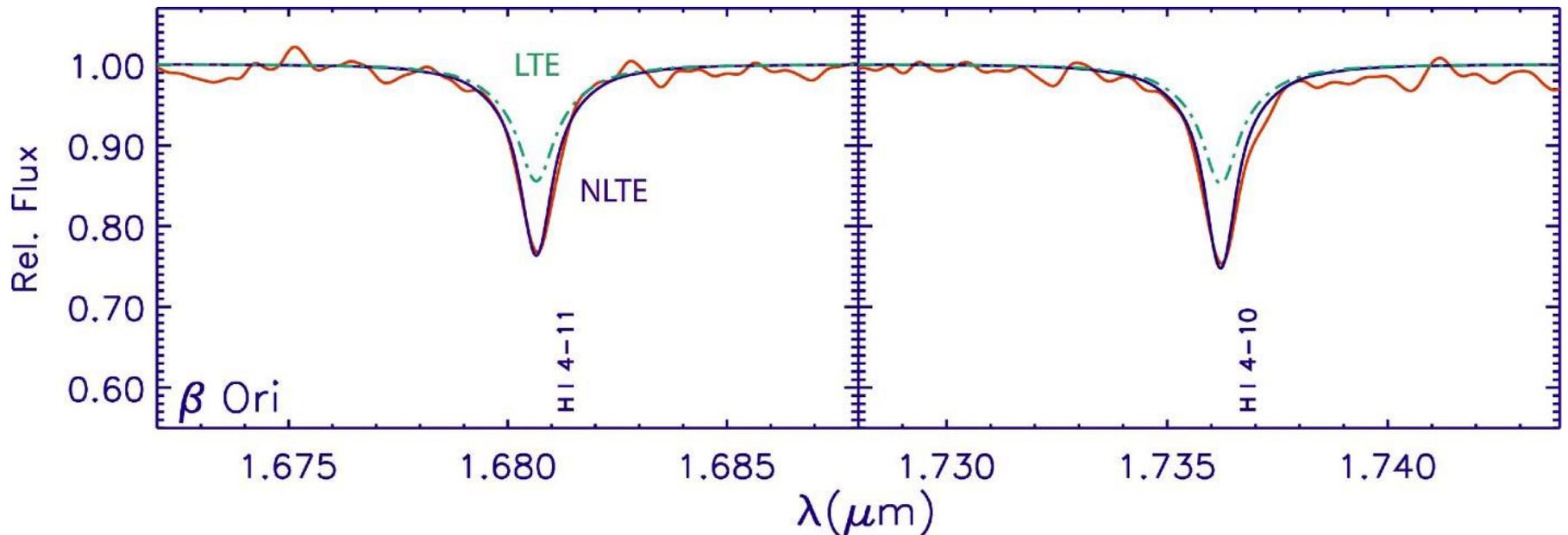


NLTE and LTE temperature stratifications for two different Helium abundances at $T_{\text{eff}} = 45,000 \text{ K}$, $\log g = 5$

LTE vs NLTE: hydrogen lines in IR

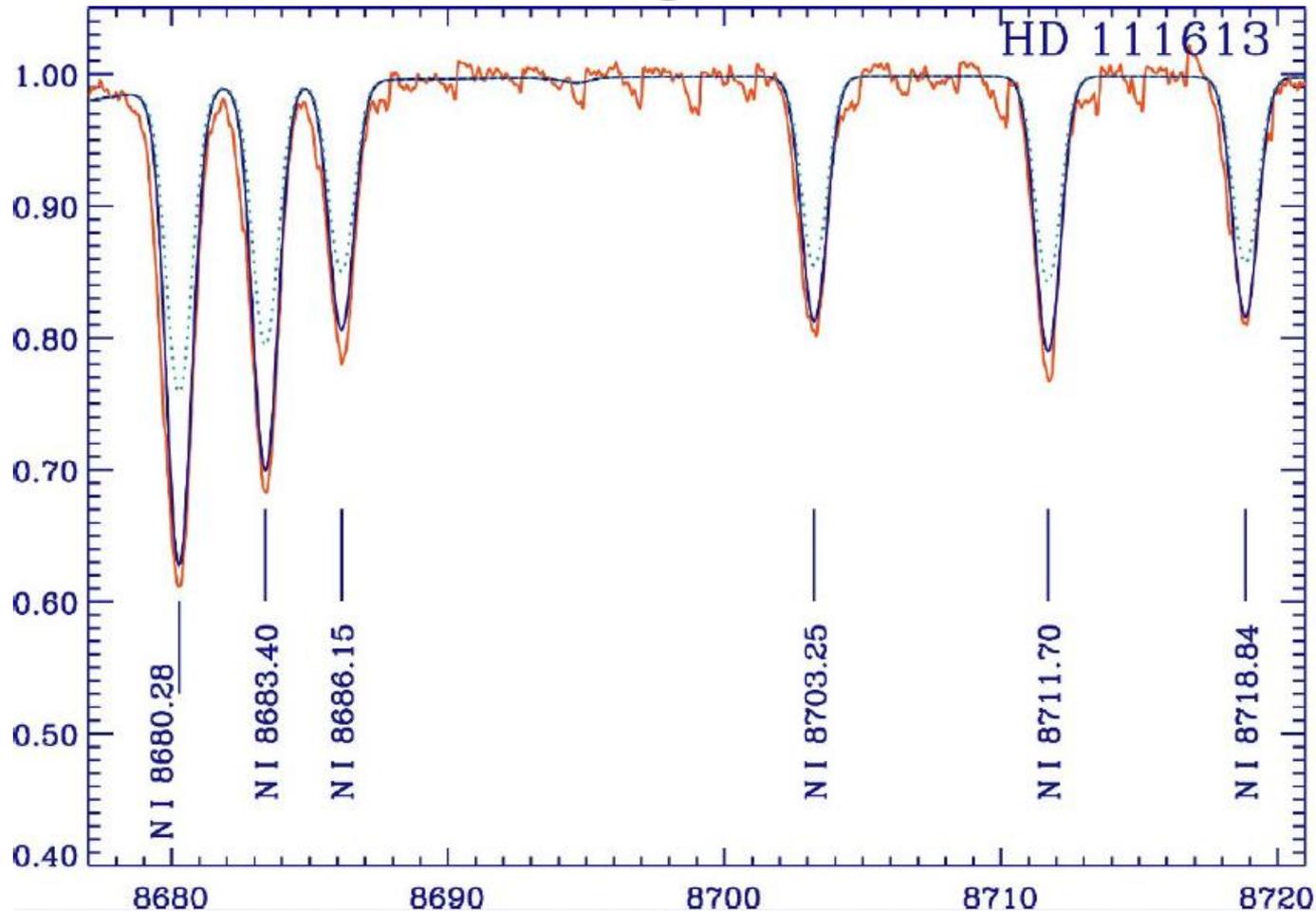
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Brackett lines



LTE vs NLTE: nitrogen lines

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Non-LTE in OBA stars

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- Hydrostatic equilibrium is invalid in OBA supergiants – their tenuous atmospheres lead to a drop in the line source function below LTE (Planckian) value.
- In the blue-violet spectra of B stars, some He I lines are formed in LTE, however red and IR lines are not collision dominated, instead photoionization-recombination processes dominate, so non-LTE is necessary.
- In A supergiants, reliable metal abundance determinations require non-LTE treatment – lines become stronger in non-LTE with corrections of up to factor of 10 for strong lines.

LTE vs NLTE in cool stars

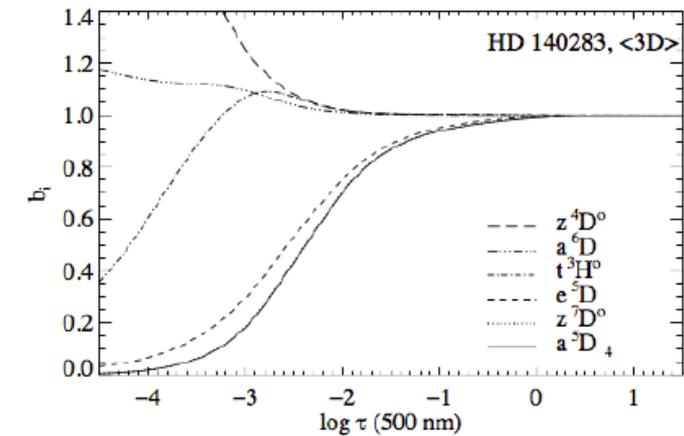
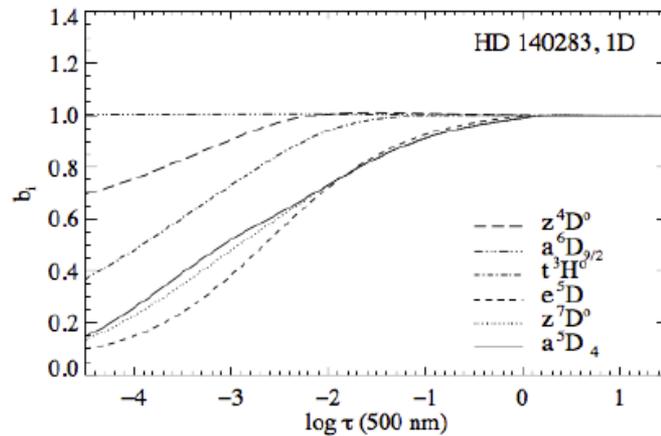
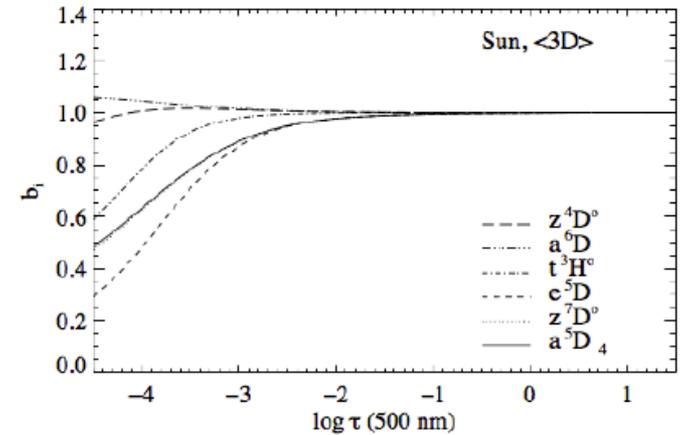
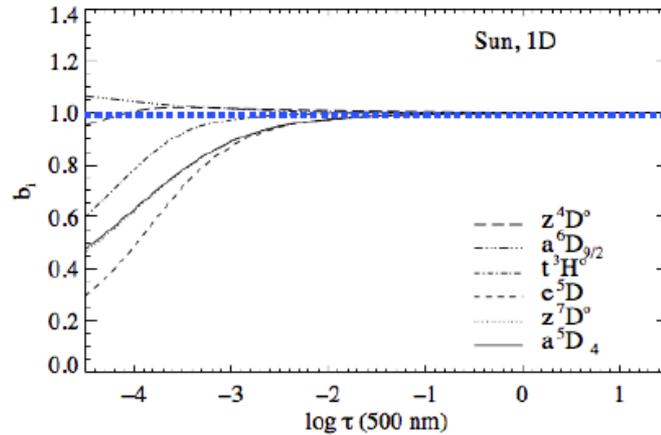
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LTE
underpopulated

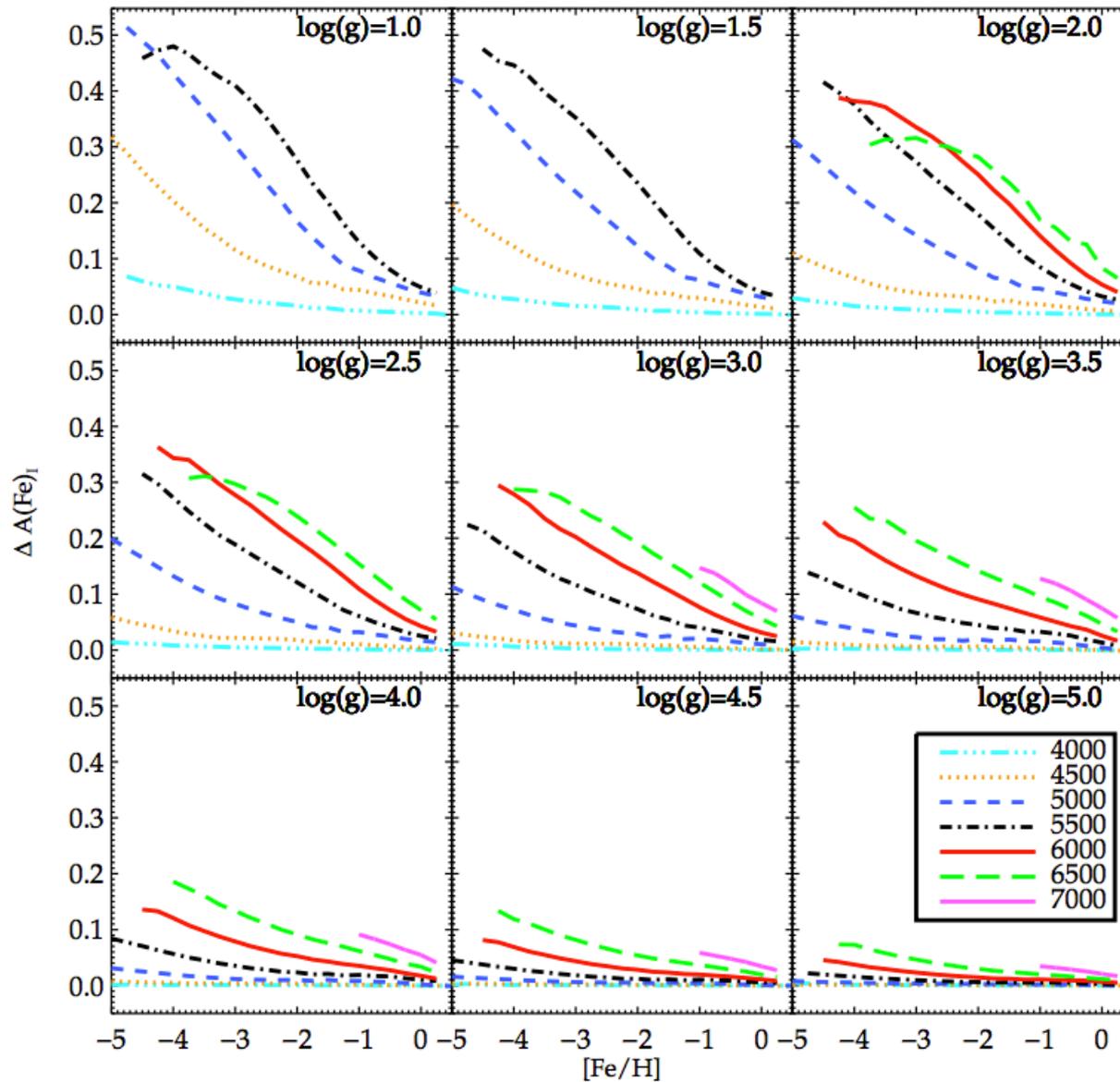
LTE
overpopulated

LTE
underpopulated

LTE
overpopulated



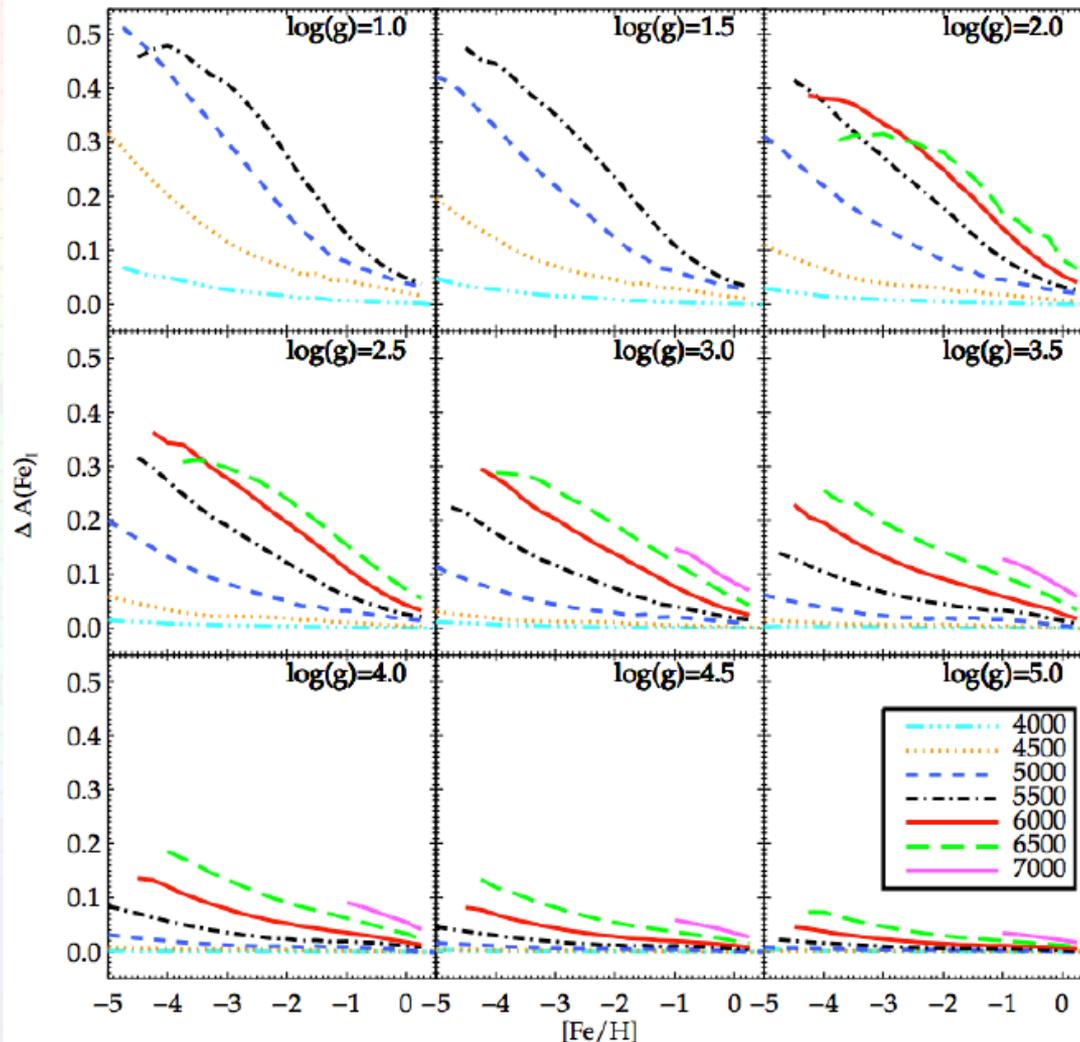
NLTE effects & stellar parameters



NLTE effects & stellar parameters

decreasing $[\text{Fe}/\text{H}]$ (less metal line blocking)

decreasing $\log(g)$
(collisional processes
become
less
important)



increasing
temperature
(radiative
processes
become
more
important)

Summary

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- If LTE does not hold, Saha-Boltzmann no longer describes excitation and ionization conditions – **need to solve rate equations for statistical equilibrium** – much more complicated!
- Non-LTE is necessary for **hot stars**, **coronae** of cool stars, **M-type** stars (as well as in nebulae and ISM).