## **Non-LTE**



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



### **LTE versus non-LTE?**

- 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*<sub>e</sub>. However, LTE strictly holds only 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 = pop(non-LTE)/pop(LTE)

## What does non-LTE mean?

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 ( <i>R</i> <sub>ij</sub> )	Photoionization ( $R_{ik}$ )
Spontaneous + stimulated emission ( <i>R</i> <sub>ji</sub> )	Spontaneous + stimulated recombination $(R_{ki})$
COLLISIONAL	
Excitation (C <sub>ij</sub> )	Ionization (C <sub>ik</sub> )
De-excitation (C <sub>ji</sub> )	Recombination (C <sub>ki</sub> )

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<sub>i</sub> = n<sub>i</sub> (T, n<sub>e</sub>)
- NLTE: population numbers depend on radiation field
   n<sub>i</sub> = n<sub>i</sub> ( T, n<sub>e</sub>, 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:

 $-n_i \left| \frac{\sum_{j>i} (R_{ij} + C_{ij}) +}{\sum_{i \neq i} (R_{ij} + C_{ij})} \right|$ + $\sum_{j>i} n_j (R_{ji} + C_{ji}) + \sum_{j<i} n_j (R_{ji} + C_{ji})$  $= \frac{dn_i}{dt}$ 

excitation and ionization
rates out of *i*de-excitation and recombination

de-excitation and recombination

rates into *i*

excitation and ionization

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



• 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**

Let's consider schematic lineformation cases with easy solution.

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



It is highly simplified:

not accurate, but provide insight into the mechanisms at work in real stellar atmospheres. It well approximates the situation for some lines, *e.g.* resonance lines from the ground state.



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:

Einstein coefficients:  $n_{\rm l}B_{\rm lu}J_{\nu} = n_{\rm u}A_{\rm ul} + n_{\rm u}B_{\rm ul}J_{\nu}$ 

$$n_l(B_{lu}\int_{\mathbf{0}}^{\infty}\varphi_{\nu}J_{\nu}d\nu + C_{lu}) = n_u(A_{ul} + B_{ul}\int_{\mathbf{0}}^{\infty}\varphi_{\nu}J_{\nu}d\nu + C_{ul})$$

Transition Probabilities: Radiative Processes

$$R_{ij} = B_{ij} \int_{0}^{\infty} \varphi_{ij}(\nu) J_{\nu} d\nu$$
$$R_{ji} = A_{ji} + B_{ji} \int_{0}^{\infty} \varphi_{ij}(\nu) J_{\nu} d\nu$$

Absorption

Spontaneous and stimulated Emission

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# **Calculation of the line source function**

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

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

$$S_{\nu}^{line} = \frac{\varepsilon_{\nu}^{line}}{\alpha_{\nu}^{line}} = \frac{n_{u}A_{ul}}{n_{l}B_{lu} - n_{u}B_{ul}} = \frac{A_{ul}}{\frac{n_{l}}{n_{u}}B_{lu} - B_{ul}}$$

Einstein Coefficients:

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

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

Note: this is the general expression for the line source function in **NLTE**. We have not made use of any equilibrium condition. It is always valid (not only in 2-level approximation). What is different in the general case, is how  $n_l$  and  $n_u$  are computed.

## **Calculation of the line source function**

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If we substitute

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

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**

313)

Substituting  $n_l/n_u$  in  $S_v$ :

1 – ε

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

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

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

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



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

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  $\zeta \equiv \frac{\alpha_{abs}}{\alpha_{abs} + \alpha_{sc}}$ 

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



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

 $\begin{array}{ccc} C_{ul} \ll A_{ul} & \epsilon \approx 0 & \overrightarrow{\phantom{a}} & S_{\nu} = \int \phi_{\nu \prime} \, J_{\nu \prime} \, d\nu' & \text{Extreme non-LTE} \end{array}$ 

From the previous lecture:  $S_v = J_v$  for pure *coherent* scattering now  $S_v = \int \varphi_{v'} J_{v'} dv'$  *non-coherent* scattering 316

*T* is the kinetic

temperature

For an electron with kinetic energy *E* exciting an atom

Excitation:

$$C_{ij} = n_e \int_{E_{ij}}^{\infty} \sigma_{ij}(u) u f(u) du = n_e \int_{E_{ij}}^{\infty} \sigma_{ij}(E) \sqrt{\frac{2E}{m}} f(E) dE \propto \frac{n_e}{T^{3/2}} \int_{E_{ij}}^{\infty} \sigma_{ij}(E) e^{-E/kT} E dE \propto \frac{n_e}{T^{1/2}} e^{-E_{ij}/kT} dE \sim \frac{n_e}{T^{1/2$$

• 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

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

In TE, the principle of detailed balance gives

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

• Even if there is no TE, but we have a Maxwellian velocity distribution  $\frac{C_{ij}}{C_{ji}} = \frac{g_j}{g_i} e^{-E_{ij}/kT}$  $\frac{C_{ul}}{C_{iu}} = \frac{g_u}{g_i} e^{-(E_u - E_l)/kT}$ 



- Thus, if the excitations and de-excitations are due to collisions, the occupation numbers follow the Boltzmann formula for the kinetic temperature.
- We can conclude that in gases with high enough densities to make collisional excitations and de-excitations more important than the radiative processes, the occupation numbers follow the Boltzmann formula for the kinetic temperature.
- This means that the excitation temperature equals the kinetic temperature, which in turn means that the source function equals the Planck function for the kinetic temperature, which means **we have LTE**.

## **Two-level approximation**

- 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)

→  $J_{\nu}$  decreases with height →  $S_{\nu}$  decreases with height → absorption line

- line absorption coefficient larger at line center ightarrow 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  $J_v$ ,  $n_i$  and  $S_v$  is far more complicated

### NLTE: Occupation numbers (1)

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We obtain a system of linear equations for  $n_i$ :

$$A \cdot \begin{pmatrix} n_1 \\ n_2 \\ \dots \\ n_p \end{pmatrix} = \mathbf{X} \quad \begin{array}{l} \text{Where matrix A} \\ \text{contains terms:} \\ n_p \end{pmatrix} \overset{\infty}{\underset{0}{\longrightarrow}} \varphi_{ij}(\nu) \int_{4\pi} I_{\nu}(\omega) \frac{d\omega}{4\pi} d\nu$$

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 (2)

#### 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

$$\kappa_{
u}^{
m b-f}=n_l\;\sigma_{lk}(
u)$$

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

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

1) Collisional rates **dominate** for all transitions

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

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

Solution of rate equations -> LTE

2)  $J_v = B_v$  is a good approximation at all frequencies

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

Solution of rate equations -> LTE

#### **Non-LTE**



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<sub>eff</sub> of very cool stars (in which electron densities are low)
   (d) nebulae
   (e) ISM

## **Non-LTE effects in scattering**

- 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.



## **Non-LTE in the Sun**



- 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<sup>6</sup> K.
- 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 disc 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

- 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(0/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?**

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**

Radiation field is so intense in hot stars (O-type, OBA supergiants, WDs) that their populations are only weakly dependent on local ( $T_{eff}$ ,  $N_e$ ), 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

Difference between NLTE and LTE in H $\gamma$  line profile for an O-star model with T<sub>eff</sub> = 45000K and log g = 4.5





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





## **Non-LTE in OBA stars**



- 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



#### LTE underpopulated

#### LTE overpopulated



LTE overpopulated



## **NLTE effects & stellar parameters**



#### Summary



- 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).

# Spectral type sequence

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## **Spectral Types: temperature sequence**



T ~ 4000K Molecules!

Mainly neutral

T~6000K

Ionised Metal

Dominated by

T ~ 30 000K Highly ionised

#### **Line Broadenings**



For example: Stark Effect



## **He and Metals**

Metal are strongests when temperature is low enough that lower ionization stages are populated. The metal lines become progressively stronger as the

temperature cools and dominate in the F, G, K stars.

Helium is the second most abundant element, but only in the hottest stars (O and B) do He atoms show up in their excited levels where they can absorb visible light. For the very hottest O stars we also see HeII lines.



#### **Molecular Bands**

For very cool stars (M, L, T type) the atmospheres are sufficiently cool that simple molecules can form. These can absorb not only in electronic transitions, but also in vibrational and rotational modes. These create "bands" of absorption which can reduce the flux in vast portions of the spectrum. In M stars, TiO is a common important molecule. In L and T stars, other molecules such as CO,  $H_2O$  and  $CH_4$  become important.





