The non-LTE Rate Equations

Statistical equations

Population numbers

LTE: population numbers follow from Saha-Boltzmann equations, i.e. purely local problem

$$n_i^* = n_i^*(T, n_e)$$

Non-LTE: population numbers also depend on radiation field. This, in turn, is depending on the population numbers in all depths, i.e. non-local problem.

$$n_i = n_i(T, n_e, J)$$

The Saha-Boltzmann equations are replaced by a detailed consideration of atomic processes which are responsible for the population and de-population of atomic energy levels:

$$\left.\begin{array}{l}\text{Excitation and de-excitation}\\ \\ \text{Ionization and recombination}\end{array}\right\}\text{ by radiation or collisions}$$

Statistical Equilibrium

Change of population number of a level with time:
= Sum of all population processes into this level
- Sum of all de-population processes out from this level

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

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

One such equation for each level

The transition rate P_{ij} comprises radiative rates R_{ij}
and collision rates C_{ij}

In stellar atmospheres we often have the stationary case:

$$\frac{d}{dt}n_i = 0 \quad \text{hence} \quad \boxed{\sum_{j\neq i} n_j P_{ji} = n_i \sum_{j\neq i} P_{ij}} \quad \text{for all levels } i$$

These equations determine the population numbers.

Radiative rates: bound-bound transitions

Two alternative formulations:

a) Einstein coefficients $B_{ij}\ B_{ji}\ A_{ji}$

b) Line absorption coefficients $\sigma_{ij}(\nu)$

advantage a): useful for analytical expressions with simplified model atoms

advantage b): similar expressions in case of bound-free transitions: good for efficient programming

Number of transitions $i \rightarrow j$ induced by intensity I_ν in frequency interval $d\nu$ und solid angle $d\omega$

$$n_i B_{ij} \varphi_\nu I_\nu d\nu d\omega / 4\pi \quad \text{(absorbed Energy / } h\nu\text{)}$$

Integration over frequencies and angles yields

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

Or alternatively

$$\text{with } \sigma_{ij}(\nu) = B_{ij}\varphi(\nu) h\nu / 4\pi \quad \boxed{n_i R_{ij} = n_i 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} J_\nu d\nu}$$

Radiative rates: bound-bound transitions

In analogy, number of stimulated emissions:

$$n_j R'_{ji} = n_j B_{ji} \int_0^\infty \varphi_\nu J_\nu d\nu = n_j B_{ij} \frac{g_i}{g_j} \int_0^\infty \varphi_\nu J_\nu d\nu$$

$$\boxed{n_j R'_{ji} = n_j 4\pi \frac{g_i}{g_j} \int_0^\infty \frac{\sigma_{ij}}{h\nu} J_\nu d\nu}$$

Number of spontaneous emissions:

$$n_j R''_{ji} = n_j \int_0^\infty A_{ji} \varphi_\nu d\nu = n_j B_{ji} \int_0^\infty \frac{2h\nu^3}{c^2} \varphi_\nu d\nu$$

$$\boxed{n_j R''_{ji} = n_j 4\pi \frac{g_i}{g_j} \int_0^\infty \frac{\sigma_{ij}}{h\nu} \frac{2h\nu^3}{c^2} d\nu}$$

Total downwards rate:

$$n_j \bar{R}_{ji} = n_j \left(R'_{ji} + R''_{ji} \right) = n_j 4\pi \frac{g_i}{g_j} \int_0^\infty \frac{\sigma_{ij}}{h\nu} \left(\frac{2h\nu^3}{c^2} + J_\nu \right) d\nu$$

$$\boxed{n_j \bar{R}_{ji} = n_j \left(\frac{n_i}{n_j} \right)^* R_{ji} = n_j \left(\frac{n_i}{n_j} \right)^* [4\pi] \int_0^\infty \frac{\sigma_{ij}}{h\nu} \left(\frac{2h\nu^3}{c^2} + J_\nu \right) e^{-h\nu/kT} d\nu}$$

Radiative rates: bound-free transitions

Also possible: ionization into excited states of parent ion

Example C III:

Ground state $2s^2\ {}^1S$

Photoionisation produces C IV in ground state $2s\ {}^2S$

C III in first excited state $2s2p\ {}^3P^o$

Two possibilities:

Ionization of 2p electron → C IV in ground state $2s\ {}^2S$

Ionization of 2s electron → C IV in first excited state $2p\ {}^2P$

C III two excited electrons, e.g. $2p^2\ {}^3P$

Photoionization only into excited C IV ion $2p\ {}^2P$

Radiative rates: bound-free transitions

Number of photoionizations = absorbed energy in dν, divided by photon energy, integrated over frequencies and solid angle

$$\int_0^\infty \oint n_i p_\nu I_\nu d\omega d\nu \rightarrow \boxed{n_i R_{ij} = n_i 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} J_\nu d\nu}$$

Number of spontaneous recombinations:

$$\int_0^\infty \oint n_j n_e(\mathrm{v}) F(\mathrm{v}) d\omega \mathrm{v} d\mathrm{v} \rightarrow n_j R_{ji} = n_j 4\pi \int_0^\infty n_e(\mathrm{v}) \frac{2h\nu^3}{c^2} G(\mathrm{v}) \frac{h}{m} d\nu$$

$$n_j R_{ji} = n_j 4\pi \int_0^\infty n_e(\mathrm{v}) \frac{2h\nu^3}{c^2} p_\nu \frac{m}{h} e^{-h\nu/kT} \left(\frac{n_i}{n_j}\right)^* \frac{1}{n_e(\mathrm{v})} \frac{h}{m} d\nu$$

$$\boxed{n_j R_{ji} = n_j \left(\frac{n_i}{n_j}\right)^* 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} \frac{2h\nu^3}{c^2} e^{-h\nu/kT} d\nu}$$

Radiative rates: bound-free transitions

Number of induced recombinations

$$\int_0^\infty \oint n_j n_e(\mathrm{v}) G(\mathrm{v}) I_\nu d\omega \mathrm{v} d\mathrm{v} \rightarrow n_j R_{ji} = n_j 4\pi \int_0^\infty n_e(\mathrm{v}) G(\mathrm{v}) J_\nu \frac{h}{m} d\nu$$

$$n_j R_{ji} = n_j 4\pi \int_0^\infty n_e(\mathrm{v}) p_\nu \frac{m}{h} e^{-h\nu/kT} \left(\frac{n_i}{n_j}\right)^* \frac{1}{n_e(\mathrm{v})} J_\nu \frac{h}{m} d\nu$$

$$\boxed{n_j R_{ji} = n_j \left(\frac{n_i}{n_j}\right)^* 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} J_\nu e^{-h\nu/kT} d\nu}$$

Total recombination rate

$$\boxed{n_j \left(\frac{n_i}{n_j}\right)^* R_{ji} = n_j \left(\frac{n_i}{n_j}\right)^* 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} \left(\frac{2h\nu^3}{c^2} + J_\nu\right) e^{-h\nu/kT} d\nu}$$

Radiative rates

Upward rates:

$$n_i R_{ij} \quad \text{with}$$

$$R_{ij} = 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} J_\nu d\nu$$

Downward rates:

$$n_j \left(\frac{n_i}{n_j}\right)^* R_{ji} \quad \text{with}$$

$$R_{ji} = 4\pi \int_0^\infty \frac{\sigma_{ij}(\nu)}{h\nu} \left(\frac{2h\nu^3}{c^2} + J_\nu\right) e^{-h\nu/kT} d\nu$$

Remark: in TE we have $J_\nu = B_\nu \Rightarrow R_{ij}^* = R_{ji}^* \Rightarrow \frac{n_i}{n_j} = \left(\frac{n_i}{n_j}\right)^*$

Stellar Atmospheres: Non-LTE Rate Equations

Collisional rates

Stellar atmosphere: Plasma, with atoms, ions, electrons

Particle collisions induce excitation and ionization

Cool stars: matter mostly neutral ⇒ frequent collisions with neutral hydrogen atoms

Hot stars: matter mostly ionized ⇒ collisions with ions become important; but much more important become electron collisions

$$\frac{\mathrm{v}_{electron}}{\mathrm{v}_{ion}} = \left(\frac{\text{ion mass}}{\text{electron mass}}\right)^{1/2} = \left(\frac{m_H A}{m_e}\right)^{1/2} \approx 43\sqrt{A}$$

Therefore, in the following, we only consider collisions of atoms and ions with electrons.

Electron collisional rates

Transition $i \rightarrow j$ (j: bound or free), $\sigma_{ij}(\mathrm{v})$ = electron collision cross-section, v = electron speed

Total number of transitions $i \rightarrow j$:

$$n_i C_{ij} = n_i n_e \int_{\mathrm{v}_0}^{\infty} \sigma_{ij}(\mathrm{v}) f(\mathrm{v}) \mathrm{v} d\mathrm{v} = n_i n_e \Omega_{ij}(T)$$

v_0 minimum velocity necessary for excitation (threshold)

$f(\mathrm{v})d\mathrm{v}$ velocity distribution (Maxwell)

In TE we have therefore

$$\mathrm{n}_i^* C_{ij} = \mathrm{n}_j^* C_{ji}$$

Total number of transitions $j \rightarrow i$:

$$\mathrm{n}_j C_{ji} = \mathrm{n}_j \left(\frac{n_i}{n_j}\right)^* C_{ij}$$

Electron collisional rates

We look for: collisional cross-sections $\sigma_{ij}(\mathrm{v})$

- experiments
- quantum mechanical calculations

Usually: Bohr radius πa_0^2 as unit for cross-section $\sigma_{ij}(\mathrm{v})$

$\sigma_{ij}(\mathrm{v}) = \pi a_0^2 \, Q_{ij}$

Q_{ij} usually tabulated as function of energy of colliding electron

$$\Omega_{ij}(T) = \int_{\mathrm{v}_0}^{\infty} \sigma_{ij}(\mathrm{v}) f(\mathrm{v}) \mathrm{v} d\mathrm{v} \quad \text{with} \quad 1/2\, m\mathrm{v}^2 = E \quad \text{and} \quad f(\mathrm{v})d\mathrm{v} = \left(\frac{\mathrm{m_e}}{2\pi \mathrm{kT}}\right)^{1/2} e^{-m\mathrm{v}^2/2kT} 4\pi \mathrm{v}^2 d\mathrm{v}$$

$$= C_0 \sqrt{T} \int_{\mathrm{u}_0}^{\infty} Q_{ij}(\mathrm{ukT}) u e^{-u} d\mathrm{u} \quad \text{with} \quad \mathrm{u} := \mathrm{E}/kT \quad \text{and} \quad C_0 = \pi a_0^2 \left(\frac{8k}{m_e \pi}\right)^{1/2} = 5.456 \cdot 10^{-11}$$

$$\boxed{\Omega_{ij}(T) = C_0 \sqrt{T} e^{-u_0} \Gamma_{ij}(T)} \quad \text{with} \quad \Gamma_{ij}(T) = \int_0^{\infty} Q_{ij}(E_0 + \mathrm{xkT})(x + u_0) e^{-x} dx, \quad \mathrm{x} := (\mathrm{E}/kT - \mathrm{E}_0/kT)$$

Electron collisional rates

$$\boxed{\Omega_{ij}(T) = C_0 \sqrt{T} e^{-u_0} \Gamma_{ij}(T)}$$

$$n_i C_{ij} = n_i n_e \Omega_{ij}(T)$$

Advantage of this choice of notation:

Main temperature dependence is described by $\sqrt{T} e^{-E_0/kT}$

$\Gamma_{ij}(T)$ only weakly varying function of T

Hence, simple polynomial fit possible

$\Rightarrow$ Important for numerical application

Now: examples how to compute the C_{ij}

Computation of collisional rates: Excitation

Van Regemorter (1962): Very useful approximate formula for allowed dipole transitions

$$\boxed{C_{ij} = C_0 n_e \sqrt{T} 14.5 f_{ij} \left(\frac{E_H}{E_0}\right)^2 u_0 e^{-u_0} \Gamma(u_0)}$$

E_H hydrogen ionization energy

f_{ij} oscillator strength of radiative transition

$E_0 = h\nu_{ij} \quad u_0 = E_0 / kT \quad \Gamma(u_0) = \max\left[\bar{g}, 0.276 e^{u_0} E_1(u_0)\right]$

$$\bar{g} = \begin{cases} 0.7 & \text{for transitions between levels with equal principal quantum number} \\ 0.2 & \text{else} \end{cases}$$

There exist many formulae, made for particular ions and transitions, e.g., (optically) forbidden transitions between n=2 levels in He I (Mihalas & Stone 1968)

$$\boxed{C_{ij} = C_0 n_e \sqrt{T} e^{-u_0} \Gamma(T)}$$

with $\log \Gamma = c_0 + c_1 \log T + c_{-2} (\log T)^{-2}$ coefficients **c** tabulated for each transition

Computation of collisional rates: Ionization

The Seaton formula is in analogy to the van-Regemorter formula in case of excitation. Here, the photon absorption cross-section for ionization is utilized:

$$\boxed{C_{ij} = 1.55 \cdot 10^{13} \sigma_0 \bar{g} \frac{n_e}{\sqrt{T}} \frac{e^{-u_0}}{u_0}}$$

$\sigma_0 =$ threshold photon cross-section for ionization

$$\bar{g} = \begin{cases} 0.1 & \text{for ions with charge } Z = 1 \\ 0.2 & \text{for ions with charge } Z = 2 \\ 0.3 & \text{for ions with charge } Z > 2 \end{cases}$$

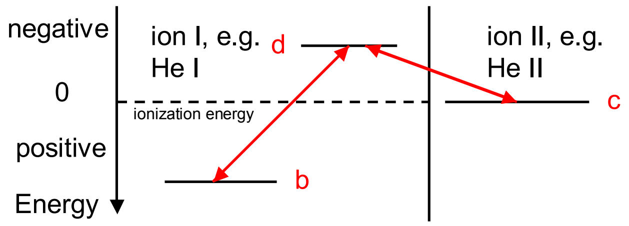
Alternative: semi-empirical formula by Lotz (1968):

$$\boxed{C_{ij} = C_0 n_e \sqrt{T}\, 2.5a \left(\frac{E_H}{E_0}\right)^2 u_0 \left[E_1(u_0) - b e^c u_0 E_1(u_1)/u_1\right]}$$

$u_1 = u_0 + c \quad a,b,c$ empirical quantities, adjusted to individual atoms

For H und He specific fit formulae are used, mostly from Mihalas (1967) and Mihalas & Stone (1968)

Autoionization and dielectronic recombination



b bound state, d doubly excited state, autoionization level

c ground state of next Ion

d $\rightarrow$ c: Autoionization. d decays into ground state of next ionization stage plus free electron

c $\rightarrow$ d $\rightarrow$ b: Dielectronic recombination. Recombination via a doubly excited state of next lower ionization stage. d auto-ionizes again with high probability: $A_{auto}=10^{13}...10^{14}$/sec! But sometimes a stabilizing transition d $\rightarrow$ b occurs, by which the excited level decays radiatively.

Computation of rates

Number of dielectronic recombinations from c to b:

$$n_c R_{cb} = n_d A_s \quad A_s = \text{probability for spontaneous stabilizing transition}$$

In the limit of weak radiation fields the reverse process can be neglected. Then we obtain (Bates 1962):

$$n_d = n_d^* A_a / (A_a + A_s) \quad \text{with } n_d^* = n_c n_e C_1 T^{-3/2} e^{E_{\text{Ion}}^{\text{d}} / kT} = n_c n_e \Phi_{cd}(T)$$
$$A_a = \text{transition probability for autoionization}$$

So, the number of dielectronic recombinations from c to b is:

$$\boxed{n_c R_{cb} = n_c n_e \Phi_{cd}(T) A_s A_a / (A_a + A_s)}$$

Computation of rates

There are two different regimes:

a) high temperature dielectronic recombination **HTDR**

b) low temperature dielectronic recombination **LTDR**

for the cases that the autoionizing levels are close to the ionization limit (b) or far above it (a)

a) Most important recombination process He II → He I in the solar corona ($T \sim 2 \cdot 10^6$K)

b) Very important for specific ions in photospheres ($T < 10^5$K) e.g. N III λ4634-40Å emission complex in Of stars

Reason: upper level is overpopulated, because a stabilizing transition is going into it.

Because in case b) $A_a >> A_s \rightarrow n_d = n_d^*$

LTDR

The radiation field in photospheres is **not** weak, i.e., the reverse process b → d is induced

Recombination rate:

$$\boxed{n_c R_{cb} = n_c n_e \Phi_{cd}(T) A_s \left(1 + \frac{c^2}{2h\nu^3}\bar{J}\right)}$$

$\bar{J}$ mean intensity in stabilizing transition, i.e.,
given by continuum value (line very broad, because short lifetime)

Reverse process:

$$\boxed{n_b R_{bc} = n_b B_{bd} \bar{J} = n_b A_s \frac{c^2}{2h\nu^3} \frac{g_d}{g_b} \bar{J}}$$

These rates are formally added to the usual ionization and recombination rates and do not show up explicitly in the rate equations.

Complete rate equations

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

$$n_i \sum_{j \neq i} P_{ij} - \sum_{j \neq i} n_j P_{ji} = 0$$

In detail:

$$n_i \left[\sum_{j>i} \left(R_{ij} + C_{ij}\right) \right.$$ ↑ excitation and ionization

rates out of ***i***

$$\left. + \sum_{j<i} \left(\frac{n_j}{n_i}\right)^* \left(R_{ij} + C_{ji}\right) \right]$$ ↓ de-excitation and recombination

$$- \sum_{j>i} n_j \left(\frac{n_i}{n_j}\right)^* \left(R_{ji} + C_{ij}\right)$$ ↓ de-excitation and recombination

rates into ***i***

$$- \sum_{j<i} n_j \left(R_{ji} + C_{ji}\right)$$ ↑ excitation and ionization

$$= 0$$

Closure equation

One equation for each chemical element is redundant, e.g., the equation for the highest level of the highest ionization stage; to see this, add up all equations except for the final one: these rate equations only yield population **ratios**.

We therefore need a closure equation for each chemical species:

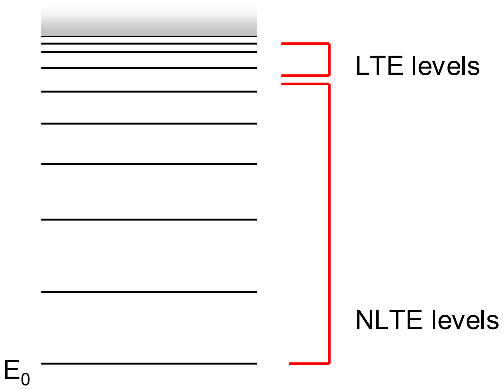
Abundance definition equation of species k, written for example as number abundance y_k relative to hydrogen:

$$y_k = \frac{\sum \text{population numbers of species k}}{\sum \text{population numbers of hydrogen}}$$

Abundance definition equation

Notation:

Population number of level i in ionization stage l : $n_{l,i}$



do not appear explicitly in the rate equations; populations depend on ground level of next ionization stage:

$$n_{l,i}^{*} = n_e n_{l+1,1} \Phi_{l,i}(T)$$

Abundance definition equation

Notation:

$NION$ number of ionization stages of chemical element k

$NL(l)$ number of NLTE levels of ion l

$LTE(l)$ number of LTE levels of ion l

$$\sum_{l=1}^{NION}\left[\sum_{i=1}^{NL(l)} n_{l,i} + \sum_{i=1}^{LTE(l)} n_{l,i}^{*}\right] = y_k\left[\sum_{i=1}^{NL(H)} n_i + \sum_{i=1}^{LTE(H)} n_i^{*} + n_{protons}\right] \Rightarrow$$

$$\boxed{\sum_{l=1}^{NION}\left[\sum_{i=1}^{NL(l)} n_{l,i} + n_{l+1,1} n_e \sum_{i=1}^{LTE(l)} \Phi_{li}(T)\right] = y_k\left[\sum_{i=1}^{NL(H)} n_{l,i} + n_{protons}\left(1 + n_e \sum_{i=1}^{LTE(H)} \Phi_i(T)\right)\right]}$$

Also, one of the abundance definition equations is redundant, since abundances are given relative to hydrogen (other definitions don't help) $\Rightarrow$ charge conservation

Charge conservation equation

Notation:

Population number of level ***i***, ion ***l***, element ***k***: n_{kli}

$NELEM$ number of chemical elements

$q(l)$ charge of ion ***l***

$$\sum_{k=1}^{NELEM}\sum_{l=1}^{NION} q(l)\left[\sum_{i=1}^{NL(l,k)} n_{kli} + \sum_{i=1}^{LTE(l,k)} n_{kli}^{*}\right] = n_e \Rightarrow$$

$$\boxed{\sum_{k=1}^{NELEM}\sum_{l=1}^{NION} q(l)\left[\sum_{i=1}^{NL(l,k)} n_{kli} + n_{k,l+1,1} n_e \sum_{i=1}^{LTE(l)} \Phi_{kli}(T)\right] = n_e}$$

Complete rate equations: Matrix notation

Vector of population numbers

$\underline{n} = (n_1, n_2, \cdots, n_{\mathrm{NLALL}})$ NLALL= total number of NLTE levels

$\boxed{\underline{\underline{A}}\,\underline{n} = \underline{b} \quad \text{rate equation in matrix notation}}$

One such system of equations per depth point

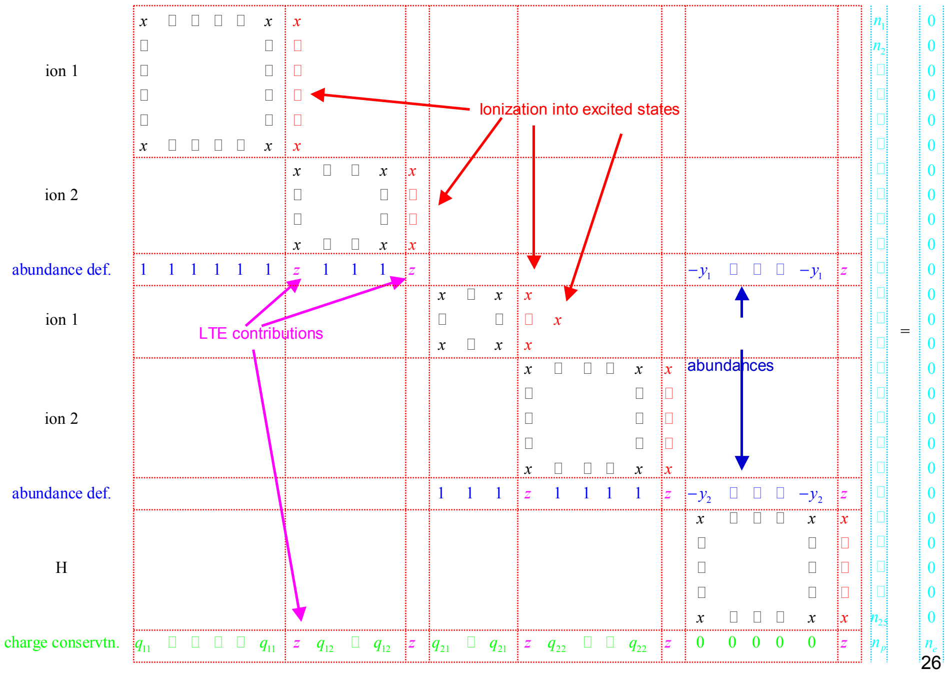
Example: 3 chemical elements

Element 1: NLTE-levels: ion1: 6, ion2: 4, ion3: 1

Element 2: NLTE-levels: ion1: 3, ion2: 5, ion3: 1

Element 3: NLTE-levels: ion1: 5, ion2: 1, hydrogen

Number of levels: NLALL=26, i.e. 26 x 26 matrix



Elements of rate matrix

For each ion l with $NL(l)$ NLTE levels one obtains a sub-matrix with the following elements:

$$A_{ij} = \begin{cases} -\left(R_{ji}+C_{ji}\right) & j<i \text{ lower left} \\ -\left(\dfrac{n_i}{n_j}\right)^{*}\left(R_{ji}+C_{ij}\right) & j>i \text{ upper right} \\ \sum\limits_{m<i}\left(\dfrac{n_m}{n_i}\right)^{*}\left(R_{im}+C_{mi}\right)+\sum\limits_{m>1}^{k}\left(R_{im}+C_{im}\right) & j=i \text{ diagonal} \end{cases}$$

$i=1\ldots NL(l) \quad j=1\ldots NL(l)\ldots k \quad k$ highest level in parent ion, into which ion l can ionize; does not have to be $= NL(l)+1$!

Elements corresponding to abundance definition eq.

Are located in final row of the respective element:

$$i=\sum_{l=1}^{NION} NL(l)$$

$$A_{ij} = \begin{cases} 1 & j=1\ldots\sum\limits_{l=1}^{NION} NL(l) \text{ except of ground state of excited ions} \\ 1+n_e \sum\limits_{m=LTE(l-1)} \Phi_{l-1,m} & j= \text{ ground state of excited ions} \\ -y_k & j=[NLALL\text{ - }NL(H)]\ldots[NLALL-1] \\ -y_k\left(1+n_e \sum\limits_{m=LTE(H)} \Phi_m\right) & j=NLALL \end{cases}$$

Elements corresponding to charge conservation eq.

Are located in the very final row of rate matrix, i.e., in

$$i = NLALL$$

$$A_{ij} = \begin{cases} q(l) & j = 1 \ldots NLALL, \text{ except of ground state of excited ions} \\ q(l) + q(l-1) \sum\limits_{m=LTE(-1)} \Phi_{l-1,m} & \text{else} \end{cases}$$

Note: the inhomogeneity vector **b** (right-hand side of statistical equations) contains zeros except for the very last element (i=NLALL): electron density $\mathbf{n_e}$ (from charge conservation equation)

Solution by linearization

The equation system $\underline{\underline{A}}\underline{n} = \underline{b}$ is a linear system for $\underline{n}$ and can be solved if, n_e, T, J_ν are known. But: these quantities are in general unknown. Usually, only approximate solutions within an iterative process are known.

Let all these variables change by $\delta n_e, \delta T, \delta J_\nu$ e.g. in order to fulfill energy conservation or hydrostatic equilibrium.

Response of populations $\delta \underline{n}$ on such changes:

Let $\underline{\underline{A}}\underline{n} = \underline{b}$ with actual quantities

And $\left(\underline{\underline{A}} + \delta \underline{\underline{A}}\right)\left(\underline{n} + \delta \underline{n}\right) = \left(\underline{b} + \delta \underline{b}\right)$ with new quantities n_e, T, J_ν

Neglecting 2nd order terms, we have:

$$\underline{\underline{A}}\underline{n} - \underline{b} = -\delta \underline{n} - \underline{n}\delta \underline{\underline{A}} + \delta \underline{b}$$

Linearization of rate equations

Needed: expressions for: $\delta \underline{\underline{A}}, \delta \underline{b}$

$J\nu$ discretized in **NF** frequency points

One possibility:

$$\boxed{\delta \underline{\underline{A}} = \frac{\partial \underline{\underline{A}}}{\partial T}\delta T + \frac{\partial \underline{\underline{A}}}{\partial n_e}\delta n_e + \sum_{k=1}^{NF}\frac{\partial \underline{\underline{A}}}{\partial J_k}\delta J_k}$$

If in addition to $\underline{n}$ the variables n_e, T, J_k are introduced as unknowns, then we have the

$\rightarrow$ Method of Complete Linearization

Other possibility: eliminates J_k from the equation system by expressing J_k through the other variables n_e, T :

$J_k = f\left(\underline{n}, T, n_e\right)$

As an approximation one uses $J_k^d \sim S_k^d(\underline{n}, T, n_e)$

(and iterates for exact solution)

Stellar Atmospheres: Non-LTE Rate Equations

Linearization of rate equations

$$\boxed{\begin{aligned} \delta \underline{\underline{A}} &= \frac{\partial \underline{\underline{A}}}{\partial T}\delta T + \frac{\partial \underline{\underline{A}}}{\partial n_e}\delta n_e + \sum_{k=1}^{NF}\frac{\partial \underline{\underline{A}}}{\partial S_k}\delta S_k \\ \delta S_k &= \frac{\partial S_k}{\partial T}\delta T + \frac{\partial S_k}{\partial n_e}\delta n_e + \sum_{j=1}^{NLALL}\frac{\partial S_k}{\partial n_j}\delta n_j \end{aligned}}$$

Method of approximate Λ-operators (Accelerated Lambda Iteration)

analogous, $\delta \underline{b}$:

$$\delta \underline{b} = \frac{\partial \underline{b}}{\partial T}\delta T + \frac{\partial \underline{b}}{\partial n_e}\delta n_e + \sum_{k=1}^{NF}\frac{\partial \underline{b}}{\partial S_k}\delta S_k = \left(0, \cdots, 0, \delta n_e\right)$$

Linearization of rate equations

$$\underline{\underline{A}}\,\underline{n}-\underline{b}=-\delta\underline{n}\,\underline{\underline{A}}\quad+\delta T\left[-\frac{\partial\underline{\underline{A}}}{\partial T}\underline{n}-\sum_{k=1}^{NF}\underline{n}\frac{\partial\underline{\underline{A}}}{\partial S_k}\frac{\partial S_k}{\partial T}\right]$$
$$+\delta n_e\left[-\frac{\partial\underline{\underline{A}}}{\partial n_e}\underline{n}-\sum_{k=1}^{NF}\underline{n}\frac{\partial\underline{\underline{A}}}{\partial S_k}\frac{\partial S_k}{\partial n_e}\right]$$
$$+\sum_{j=1}^{NLALL}\delta n_j\left[-\sum_{k=1}^{NF}\underline{n}\frac{\partial\underline{\underline{A}}}{\partial S_k}\frac{\partial S_k}{\partial n_j}\right]$$

Linearized equation for response $\delta\underline{n}$ as answer on changes $\delta n_e, \delta T, \delta J_\nu$

Expressions $\sum_{k=1}^{NF}\underline{n}\frac{\partial\underline{\underline{A}}}{\partial S_k}\frac{\partial S_k}{\partial n_j}$ show the complex coupling of all variables. A change in the radiation field and, hence, the source function at any frequency causes a change of populations of all levels, even if a particular level cannot absorb or emit a photon at that very frequency!

Linearization of rate equations

In order to solve the linearized rate equations we need to compute these derivatives:

$$\frac{\partial}{\partial n_e},\frac{\partial}{\partial T},\frac{\partial}{\partial n_j},\frac{\partial}{\partial S_k}\quad\text{with respect to}\quad\underline{\underline{A}},\underline{b},S_k$$

All derivatives can be computed analytically!

Increases accuracy and stability of numerical solution. More details later.

LTE or NLTE?

When do departures from LTE become important?

LTE is a good approximation, if:

1) Collisional rates dominate for all transitions

$$R_{ij} << C_{ij} \rightarrow P_{ij} = R_{ij} + C_{ij} \approx C_{ij}$$

$$\text{because } \frac{C_{ij}}{C_{ji}} = \left(\frac{n_i}{n_j}\right)^*$$

solution of rate equations $\rightarrow$ LTE

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

$$R_{ij} = R_{ji}$$

$$\rightarrow \frac{n_i}{n_j} = \left(\frac{n_i}{n_j}\right)^*$$

solution of rate equations $\rightarrow$ LTE

LTE or NLTE?

When do departures from LTE become important?

LTE is a bad approximation, if:

1) Collisional rates are small $C_{ij} \sim n_e / \sqrt{T}$ $\quad n_e \downarrow, T\uparrow \;\Rightarrow\; C_{ij}\downarrow$

2) Radiative rates are large $R_{ij} \sim T^\alpha,\ \alpha > 1$ $\quad T\uparrow \;\Rightarrow\; R_{ij}\uparrow$

3) Mean free path of photons is larger than that of electrons

Example: pure hydrogen plasma

$\Delta z \sim 1/n_H$ (density of neutral H)

$$\text{Saha: } n_H \sim n_e n_p T^{-3/2} e^{\Delta E/kT} \rightarrow \Delta z \sim \frac{T^{3/2}}{n_e n_p} e^{-\Delta E/kT}$$

$$n_e \downarrow, T\uparrow \;\Rightarrow\; \Delta z \uparrow$$

Departures from LTE occur, if temperatures are high and densities are low

LTE or NLTE?

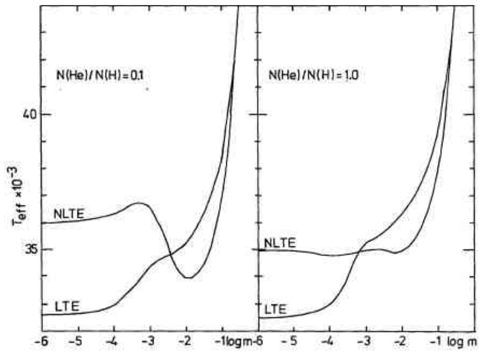


Fig. 4. Temperature stratification in NLTE and LTE for T_{eff} = 45000 K, $\log g = 5$ and two different helium abundances (N(He)/N(H) = 0.1 and 1.0)

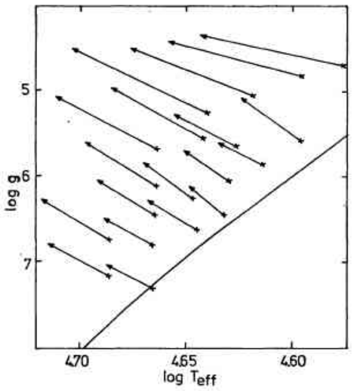


Fig. 8. "Non-LTE vectors" [Displacement due to non-LTE effects in the ($\log g$, $\log T_{eff}$)-diagram] for N(He)/N(H) = 0.1

LTE or NLTE?

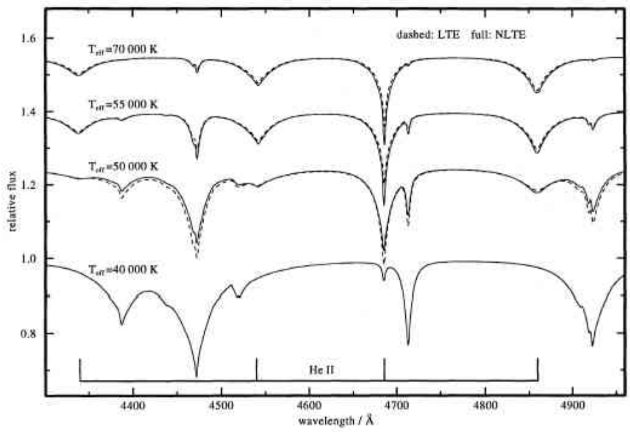
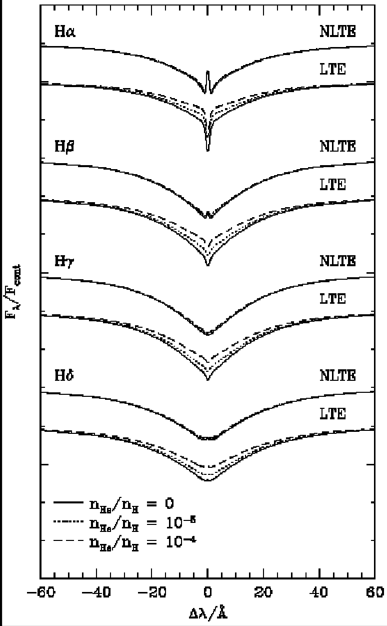
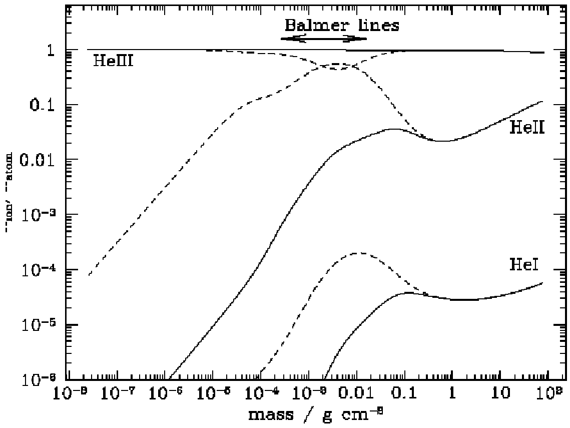


Fig. 3. NLTE effects on synthetic DO line profiles (convoluted by a 2 Å Gauss profile) at various effective temperatures. The two hotter models are calculated at log g=7.5, the cooler ones at log g=8.0. Significant deviations between LTE (dashed) and NLTE spectra occur down to T_{eff}=50 000 K. At T_{eff}=40 000 K the NLTE effects disappear completely, justifying LTE analyses for DB white dwarfs

LTE or NLTE?

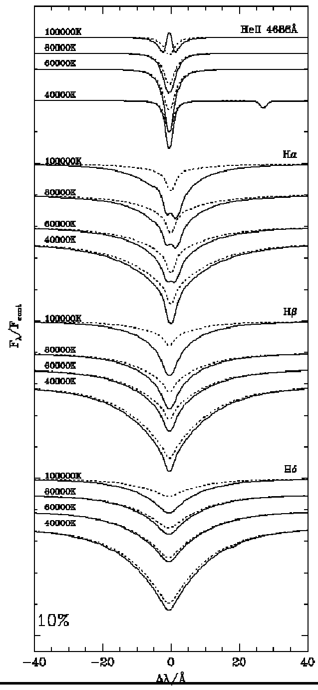


DA white dwarf, T_{eff}= 60000K, log g= 7.5

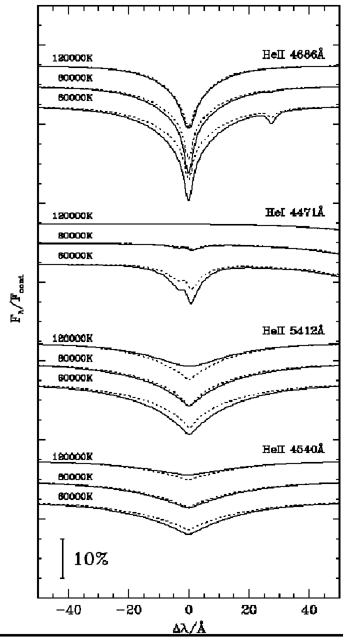


LTE or NLTE?

DAO with log g= 6.5



DO with log g= 7.5



Summary: non-LTE Rate Equations

Complete rate equations

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

$$n_i \sum_{j \neq i} P_{ij} - \sum_{j \neq i} n_j P_{ji} = 0$$

In detail:

$$
\begin{aligned}
& n_i \left[\sum_{j>i} \left(R_{ij} + C_{ij} \right) \right. \\
& \left. + \sum_{j<i} \left(\frac{n_j}{n_i} \right)^* \left(R_{ij} + C_{ji} \right) \right] \\
& - \sum_{j>i} n_j \left(\frac{n_i}{n_j} \right)^* \left(R_{ji} + C_{ij} \right) \\
& - \sum_{j<i} n_j \left(R_{ji} + C_{ji} \right) \\
& = 0
\end{aligned}
$$

excitation and ionization

rates out of i

de-excitation and recombination

de-excitation and recombination

rates into i

excitation and ionization