STATISTICAL EQUILIBRIUM EQUATIONS FOR TRACE ELEMENTS IN STELLAR ATMOSPHERES

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Abstract. The conditions of thermodynamic equilibrium, local thermodynamic equilibrium, and statistical equilibrium are discussed in detail. The equations of statistical equilibrium and the supplementary equations are shown together with the expressions for radiative and collisional rates with the emphasize on the solution for trace elements.

1 Introduction: Stellar atmosphere problem

Solution of the stellar atmosphere problem is usually considered as the determination of spatial dependence of basic macroscopic quantities (see also Kubát, 2010, these proceedings) also be understood (following Hubeny, 1976) as aiming at finding three basic microscopic distributions, namely, the momentum distribution (distribution of velocities of all particles), distribution of particle internal degrees of freedom (populations of atomic excitation stages), and distribution of internal degrees of freedom of the electromagnetic field (radiation field for all frequencies and directions).

2 From thermodynamic equilibrium to NLTE

2.1 Thermodynamic equilibrium

To maintain thermodynamic equilibrium, several necessary conditions have to be met (see Hubeny, 1976, also Hubeny, 1997). First, the characteristic time for macroscopic changes of the medium has to be much larger than the relaxation time ($t_{\text{relaxation}} \ll t_{\text{macroscopic changes}}$). Second, macroscopic changes of the medium must be small on the scale of a particle mean free path ($l_{\text{macroscopic changes}} \ll \bar{l}_{\text{free path}}$). Then, the relaxation time has to be much less than the time interval between inelastic collisions ($t_{\text{relaxation}} \ll t_{\text{inelastic collisions}}$). And, finally, if the

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latter condition is violated, then colliding particles need to have equilibrium distributions.

If the medium is in thermodynamic equilibrium, then all three distributions mentioned in Introduction (momentum, internal, and radiation) have their equilibrium form. Velocities $v_a$ of particles $a$ follow the Maxwellian distribution,

$$f(v_a) dv_a = \frac{1}{v_a \sqrt{\pi}} e^{-\left(\frac{v_a^2}{\bar{v}_a^2}\right)} dv_a,$$

(2.1)

where $\bar{v}_a = \sqrt{2kT_a/m_a}$ is their most probable speed, $T_a$ is the corresponding particle temperature, $m_a$ is its mass, and $k$ is the Boltzmann constant. In thermodynamic equilibrium all temperatures $T_a$ are the same and in the following we denote them as $T$.

Individual atomic energy levels $i$ are populated according to the Boltzmann distribution (see Mihalas, 1978, Eq. 5-4),

$$\frac{n_i}{n_0} = \frac{g_i}{g_0} e^{-\chi_i/kT},$$

(2.2)

where $n_i$ is the population of the $i$-th level, $n_0$ is the population of the ground level, asterisks (*) denote equilibrium values, $g_i$ is the statistical weight of the level $i$, and $\chi_i$ is its excitation energy. The ionization equilibrium is described by the Saha equation (see Mihalas, 1978, Eq. 5-15)

$$\frac{N_j^*}{N_{j+1}^*} = n_e \frac{U_j(T)}{2U_{j+1}(T)} \left(\frac{h^2}{2\pi m_e kT}\right)^{\frac{3}{2}} e^{\frac{\chi_{ij}}{kT}},$$

(2.3)

where $N_j^*$ is the total population (number density) of the ion $j$, $U_j(T)$ is its partition function, $n_e$ is the electron number density, $\chi_{ij}$ is the ground state ionization energy, and $h$ is the Planck constant.

Finally, the radiation field energy is distributed in frequency $\nu$ according to the Planck law

$$B_\nu(T) = \frac{2h\nu}{c^2} \frac{1}{e^{h\nu/kT} - 1}.$$

(2.4)

2.2 Local thermodynamic equilibrium (LTE)

The fact that we can observe stellar light and the shape of the stellar spectrum clearly show that the stellar radiation is far from that of a blackbody. Therefore, the assumption of radiation field energy equilibrium is not valid and we have to include detailed radiative transfer. However, simple relaxing of the equilibrium condition for radiation does not help, since if the first two distributions are in equilibrium in a homogeneous medium, then also the radiation field is forced to have the equilibrium value.

To allow the light to escape from the star, we have to allow spatial dependence of temperature and density. We assume local equilibrium distributions of particle
Statistical equilibrium equations for trace elements

velocities (2.1) and level populations (2.2 and 2.3), which means that the equilibrium condition ignores possible gradients of $T(\vec{r})$ and $N(\vec{r})$. Then, the equilibrium conditions change from point to point. This approximation is usually called local thermodynamic equilibrium (LTE).

To determine the specific radiation field intensity ($I_{\mu\nu}$) distribution, we solve the radiative transfer equation. For the simple case of a plane-parallel horizontally homogeneous atmosphere (1D case with the only spatial coordinate $z$), the transfer equation along the ray determined by $\mu = \cos \theta$, where $\theta$ (see Fig. 1 in Kubát, 2010, these proceedings) is the ray angle with the coordinate axis $z$, reads

$$\mu \frac{dI_{\mu\nu}}{dz} = \eta_{\nu} - \chi_{\nu} I_{\mu\nu},$$

where $\eta_{\nu}$ and $\chi_{\nu}$ are the emissivity and opacity, respectively. The condition of local thermodynamic equilibrium implies that $\eta_{\nu} = \chi_{\nu} B_{\nu}(T(z))$ at each depth $z$.

2.3 Statistical equilibrium (NLTE)

The non-equilibrium distribution of the radiation field obtained by solution of (2.5) affects in turn the atomic level population distribution. If this influence becomes strong, the Saha-Boltzmann ionization and excitation distribution is no longer in equilibrium. But even if this influence is weak, it is better to assume that the excitation distribution can generally be a non-equilibrium one.

Doing this, we assume that the excitation and ionization states distribution does not follow from the Saha (2.3) and Boltzmann (2.2) equations. For its determination we have to explicitly consider all individual level populating and depopulating processes. Such treatment is usually referred to as NLTE or non-LTE.

Assuming NLTE we still assume an equilibrium (i.e. Maxwellian - Eq. 2.1) distribution of particle velocities, especially of electrons. The radiation field and level populations are allowed to have non-equilibrium distributions, which for the radiation field is determined by solution of the radiative transfer equation (2.5) and for the level populations by solution of statistical equilibrium equations (2.3) described later in the Section.

2.3.1 Microscopic processes

Due to the non-equilibrium nature of level population distribution it is necessary to take into account all processes influencing level populations on a microscopic level. The most important processes for hot star atmospheres are listed in Table.

2.4 Between LTE and NLTE

2.4.1 Elastic collisions

In both LTE and NLTE, a Maxwellian velocity distribution of particles (2.1) is assumed however it is never explicitly stated. Elastic collisions between particles tend to maintain their equilibrium velocity distribution. These collisions are
Table 1. List of most important microscopic processes affecting the equilibria in stellar atmospheres. In this table, $\nu$ means photon, $e$ stands for electron, $X$ means a particular atom. Superscript $^+$ denotes the ion and $^*$ the excited state. $E$ (in the rightmost column) means that the process tends to establish equilibrium of population numbers, $M$ denotes processes that tend to establish equilibrium velocity distributions.

| collisions          | elastic (e–e, e–H, e–H$^+$, e–He, H–H, H–He, ...) | M     |
|---------------------|--------------------------------------------------|-------|
| inelastic with electrons |                                                   |       |
| excitation          | $e(\nu) + X \rightarrow e(\nu' < \nu) + X^*$  | $E$   |
| de-excitation       | $e(\nu) + X^* \rightarrow e(\nu' > \nu) + X$  | $E$   |
| ionization          | $e(\nu) + X \rightarrow e(\nu' < \nu) + e(\nu'') + X^+$ | $E$   |
| recombination       | $e + e(\nu) + X^+ \rightarrow e(\nu' \neq \nu) + X$ | $E$   |
| inelastic with other particles | less frequent $\Rightarrow$ neglected |       |
| interaction with radiation |                                                   |       |
| excitation          | $\nu + X \rightarrow X^*$                        |       |
| de-excitation       | spontaneous                                     |       |
|                     | $X^* \rightarrow \nu + X$                        |       |
|                     | stimulated                                       |       |
|                     | $\nu + X^* \rightarrow 2\nu + X$                 |       |
| ionization          | $\nu + X \rightarrow X^+ + e$                    |       |
| autoionization      | $\nu + X \rightarrow X^{**} \rightarrow X^+ + e$|       |
| Auger ionization    | $\nu + X \rightarrow X^{**} + e$                 |       |
| recombination       | spontaneous                                      |       |
|                      | $e + X^+ \rightarrow \nu + X$                    | $E$   |
|                      | stimulated                                       |       |
|                      | $\nu + e + X^+ \rightarrow 2\nu + X$             | $E$   |
| dielectronic recombination | $X^+ + e \rightarrow X^{**} \rightarrow \nu + X$ | $E$   |
| free-free transitions |                                                   |       |
| electron scattering | free (Compton, Thomson)                          |       |
|                     | $\nu + e \leftrightarrow \nu + e$                |       |
| bound (Rayleigh)    | $\nu + X \rightarrow \nu + X$                   |       |

rarely explicitly considered both in LTE and in NLTE calculations. Usually, it is sufficient to assume that they are frequent enough to balance all non-equilibrium processes that tend to destroy the Maxwellian velocity distribution. For stellar atmospheres, the equilibrium velocity distribution is a reasonable assumption (see Mihalas [1978]).

2.4.2 Inelastic collisions

Inelastic collisions play a key equilibrium role in the atomic level populations. If the velocity distribution is in equilibrium, then the inelastic collisions push the atomic level populations also to their equilibrium. On the other hand, inelastic collisions change the electron kinetic energy and so cause departures from the Maxwellian velocity distributions. Equilibrium velocity distribution is recovered only if there is enough elastic collisions. Luckily, in most astrophysical cases the time between two inelastic collisions is much larger than the time necessary for rebuilding the equilibrium velocity distribution – the relaxation time (the inequality $t_{\text{relaxation}} \ll$
t_{inelastic
collisions} holds), so we can safely adopt Maxwellian velocity
distribution. However, there are exceptions, for example there is
evidence that the electron velocity distribution differs from the
Maxwellian in the solar transition region (Shoup, 1983) and in the
corona (Cranmer, 1998). In such cases we would have to solve
an additional kinetic equation, namely the equation for electrons.

2.4.3 Level populations

In the following, we assume a Maxwellian velocity distribution for all
particles. The distribution of the radiation field is, on the other hand,
ot in equilibrium and must be determined by solution of the
radiative transfer equation. Whether level populations will have their
equilibrium value or not (in other words, if the atmosphere will be “LTE” or
“NLTE”) depends on the balance between processes connected
with the equilibrium part – inelastic collisions with electrons having
Maxwellian distribution – and processes connected with the non-equilibrium
part – radiative processes, which connect the level populations with a
generally non-equilibrium radiation field. In Table 1 the letter (E) denotes
processes that aim at maintaining equilibrium of level populations.

If the equilibrium processes dominate (e.g. in a collisionally dominated
atmosphere), then level populations will have or will be close to the equilibrium
Saha-Boltzmann values. In such case, all processes are in detailed balance, which
means that the rate of each process is balanced by the rate of the reverse process.
For a Maxwellian velocity distribution, the collisional processes are always
in detailed balance. Note that all radiative processes involving a free electron
(recombination, free-free transition) are in principle collisional. On the other hand,
radiative processes can hardly be in detailed balance, they may be in detailed balance
only for the case when radiation has its equilibrium, i.e. Planck, distribution,
which happens only in the deepest parts of stellar atmospheres. When the radiation
intensity is different from Planckian, $J_\nu \neq B_\nu$, then LTE is not an acceptable
approximation.

If the non-equilibrium processes dominate, then a quite complicated game begins.
The medium may reach states very far from equilibrium.

3 Trace elements

Solution of the NLTE problem for trace elements may be considered as a simplification
of the standard model atmosphere problem, where we aim to determine the
temperature and density structures of the atmosphere (see Kubát, 2010,
these proceedings). Here we assume that we have a given model atmosphere (either LTE or NLTE), i.e. given temperature ($T(r)$) and density ($n_e(r)$) structures,
given chemical composition, and if the given model atmosphere is a NLTE one,
also occupation numbers of atomic levels for the most important atmosphere constituents.
This implies that also the background opacities (which are calculated
from the given model atmosphere) are known. Then we solve simultaneously the
radiative transfer and statistical equilibrium equations for a trace element (or trace elements).

There are several conditions, which have to be met to enable the element to be a trace element. The basic requirement is that the influence of the trace element on the atmospheric structure is really negligible. The trace element may, of course, have influence on emergent radiation in some parts of the spectrum. More exactly, there is a requirement that inclusion of the NLTE trace element does not change the atmospheric structure, which may also allow to include the case of a change from an LTE treatment of the element to the NLTE one. This may sometimes enable to consider even hydrogen as a trace element (see also Przybilla, 2010, these proceedings), but this is not generally recommended. Stellar atmospheric structure is usually sensitive to changes in the dominant ions, even if such changes are relatively small. Sometimes it is very difficult to predict the final effect caused by a change of the basic assumption from LTE to NLTE, so after any NLTE trace element calculation it is necessary to check if the assumptions we made at the beginning are still met.

This also means that we have always to check if a trace element is really a trace element. For example, changes in ionization equilibrium alter also the free electron density, which may have an impact on the ionization structure of the initial model atmosphere. Background opacities have to be the same in the solution of the trace element as in the model atmosphere.

There is one principal warning for using background LTE models, which is based on physical grounds. As a commonly used case we have an LTE model atmosphere, it means that we assume that in the whole atmosphere there are sufficient collisions with electrons to maintain equilibrium values of population numbers. If we then choose one of elements as a trace element and solve the NLTE problem, we implicitly say that the equilibrium may be violated for this particular element. But since the number of free electrons is the same as for all other elements (which populations have their LTE values thanks to the assumption of the LTE background model atmosphere), we simultaneously assume that for the same physical conditions there exists detailed balance for all transitions that belong to non-trace elements, but at the same time it is lacking for the trace element. Thus we are using two contradictory physical assumptions for the same region. Since LTE is a special case of a more general NLTE case, there may be regions in the atmosphere, where this very specific condition is fulfilled, but it hardly happens for the whole atmosphere. Using an LTE model atmosphere and assuming NLTE for a trace element is highly inconsistent and one has always to prefer NLTE model atmospheres as background models.
4 Equations of statistical equilibrium

For the change of the occupation number \( n_i \) of the state \( i \) of each element in the stellar atmosphere we may write (Mihalas, 1978, Eq. 5-48)

\[
\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \vec{v}) = \sum_{l=1 \atop l \neq i}^{N_{l \text{tot}}} (n_i P_{li} - n_l P_{il}),
\]

(4.1)

where \( N_{l \text{tot}} \) is the total number of energy levels considered, \( P_{il} \) is the probability (per time unit) of a transition from the state (level) \( i \) to the state (level) \( l \). This probability consist of two parts, namely of the probability that the transition is caused by absorption or emission of radiation (the radiative probability \( R_{il} \)), or that the transition is caused by a collision with a neighbouring particle, mostly with an electron (the collisional probability \( C_{il} \)). Then, the probability \( P_{il} \) can be expressed as a sum of radiative and collisional probabilities, \( P_{il} = R_{il} + C_{il} \). If these probabilities are multiplied with the starting level population, then we call them radiative and collisional rates, respectively.

For the case of a stationary atmosphere, i.e. if the time variations of the medium are negligible, we may neglect the time derivative in the equation (4.1) and we obtain the time independent set of the statistical equilibrium equations,

\[
\nabla \cdot (n_i \vec{v}) = \sum_{l \neq i} (n_i P_{li} - n_l P_{il}).
\]

(4.2)

This set of equations has to be used in stationary moving atmospheres, which includes the common case of a stellar wind. However, due to simplicity, the advective term is very often neglected. As a result we obtain an equation, which is valid in static atmospheres exactly,

\[
\sum_{l \neq i} (n_i P_{li} - n_l P_{il}) = 0.
\]

(4.3)

We say that the particular transition \( i \leftrightarrow l \) is in detailed balance, if \( n_i P_{li} = n_l P_{il} \). If this condition is fulfilled for all \( i, l \), then all transitions are in detailed balance, which is the case of LTE. Then, also the level populations have their equilibrium values \( n_i^* \) given by Eq. (2.2).

4.1 Equilibrium level populations

Equilibrium level populations are calculated using the assumption of thermodynamic equilibrium or local thermodynamic equilibrium. They are usually denoted as \( n_i^* \) and referred to as LTE populations. However, Mihalas (1978) uses the quantity \( n_i^* \) in a different meaning. The LTE populations are calculated with respect to the ground level of the next higher ion using the equation (Eq.5-14 in Mihalas, 1978)

\[
n_{i,j}^* = n_{0,j+1} n_e \frac{g_{ij}}{g_{0,j+1}} \frac{1}{2} \left( \frac{\hbar^2}{2 \pi m_e k T} \right) ^{\frac{3}{2}} e^{-\frac{x_{lj}-x_{ij}}{k T}}.
\]

(4.4)
Here $j$ is the index of the corresponding ion and $n_{0,j+1}$ is the actual population of the ground level of the next higher ion, which is not necessarily an LTE value. Equation (4.4) is used as a definition of LTE populations in NLTE calculations. Then, if we are using the departure coefficients $b_i = n_i/n_i^*$ [Menzel, 1937], it is necessary to know which definition of LTE population is used. Note that for both definitions of LTE populations the equation (2.2) holds and that for the case of LTE, $b_i = 1$.

4.2 Radiative rates

The expressions for radiative rates shown here closely follow the book of Mihalas (1978).

4.2.1 Photoionization and photorecombination transitions

**Photoionization:** The radiative rate for a photoionization transition is obtained by expressing the amount of absorbed energy $E$ during photoionization from the bound state $i$ to the free state $k$, $E = 4 \pi J_\nu \alpha_{ik}(\nu) d\nu$. The number of photoionizations is obtained by dividing the energy $E$ by $h\nu$ and integrating from the ionization frequency $\nu_0$ to $\infty$,

$$n_i R_{ik} = n_i 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ik}(\nu)}{h\nu} J_\nu d\nu$$  \hspace{1cm} (4.5)$$

**Photorecombination:** Photorecombination is a collisional process, since the ion catches the free electron during this process. If the medium is in a thermodynamic equilibrium, then from the detailed balance it follows that $J_\nu = B_\nu$. The number of recombinations has its equilibrium value

$$(n_i R_{ik})^* = (n_k R_{ki})^* = n_i^* 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ik}(\nu)}{h\nu} B_\nu d\nu.$$  \hspace{1cm} (4.6)$$

By adding and subtracting the expression $B_\nu e^{-\frac{h\nu}{kT}}$ under the integral and using the expression for the Planck function (2.4), we obtain

$$(n_k R_{ki})^* = n_k^* 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ik}(\nu)}{h\nu} \left[ \frac{2h\nu^3}{c^2} + B_\nu \right] e^{-\frac{h\nu}{kT}} d\nu.$$  \hspace{1cm} (4.7)$$

Dividing (4.7) by $n_k^*$ yields an expression for a rate per ion (the probability). This expression has to be valid also outside LTE, so we replace the Planck function $B_\nu$ by actual mean radiation intensity $J_\nu$. Finally, multiplying the result by actual population of the free state $n_k$ we obtain

$$n_k R_{ki} = n_k \left( \frac{n_i^*}{n_k^*} \right) 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ik}(\nu)}{h\nu} \left[ \frac{2h\nu^3}{c^2} + J_\nu \right] e^{-\frac{h\nu}{kT}} d\nu$$  \hspace{1cm} (4.8)$$

where $n_i^*/n_k^* = n_e \Phi_{ik}(T)$ is the so called Saha-Boltzmann factor.
4.2.2 Bound-bound transitions

We consider transitions from the level \( i \) to the level \( l \). The number of transitions caused by intensity \( J(\nu) \) in the interval \( d\nu d\omega \) is \( n_i B_{il} \phi_{il}(\nu) \, d\nu \), where \( \phi_{il}(\nu) \) is the line profile function for the given transition, and \( B_{il} \) is the Einstein coefficient for absorption. Since \( \alpha_{il}(\nu) = \alpha_{0l}^2 \phi(\nu) = \frac{h \nu}{4\pi} B_{il} \phi_{il}(\nu) \), we may express the total number of absorptions obtained by integration over the line profile as

\[
n_i R_{il} = n_i B_{il} \int \phi_{il}(\nu) \, J_{\nu} \, d\nu = n_i 4\pi \int \frac{\alpha_{il}(\nu)}{h \nu} \, J_{\nu} \, d\nu.
\]  

(4.9)

The total number of emissions is given by a sum of spontaneous and stimulated emissions

\[
n_l R_{li} = n_l \left( A_{li} + B_{li} \int \phi_{il}(\nu) \, J_{\nu} \, d\nu \right) = n_l 4\pi \frac{g_i}{g_l} \alpha_{0l}^2 \left[ \frac{2h \nu_i^3}{c^2} + \int \frac{\phi_{il}(\nu)}{h \nu} \, J_{\nu} \, d\nu \right].
\]  

(4.10)

Using the Boltzmann equation (2.2), we may write the total number of de-excitations as

\[
n_l R_{li} = n_l \frac{n_i^*}{n_i} 4\pi \int \frac{\alpha_{il}(\nu)}{h \nu} \left( \frac{2h \nu^3}{c^2} + J_{\nu} \right) e^{-\frac{h \nu}{kT}} \, d\nu.
\]  

(4.11)

4.2.3 Net radiative bracket

The net rate for the transition \( i \leftrightarrow l \) may be obtained by subtracting upward and downward radiative rates

\[
n_l \left( A_{li} + B_{li} \int \phi_{il}(\nu) \, J_{\nu} \, d\nu \right) - n_i B_{il} \int \phi_{il}(\nu) \, J_{\nu} \, d\nu \equiv n_j A_{li} Z_{li}.
\]  

(4.12)

We have introduced the net radiative bracket \( Z_{li} \) as

\[
Z_{li} = 1 - \frac{n_i B_{il} - n_j B_{li}}{n_i A_{li}} \int \phi_{il}(\nu) \, J_{\nu} \, d\nu = 1 - \frac{\int \phi_{il}(\nu) \, J_{\nu} \, d\nu}{S_{il}},
\]  

(4.13)

where \( S_{il} \) is the source function (independent of \( \nu \)) of the transition \( i \leftrightarrow l \). For the case of detailed radiative balance \( Z_{li} = 0 \).

4.3 Collisional rates

Inelastic collisions transfer energy between the thermal particle motion energy and the internal energy of atoms. Although collisions between all particles occur in stellar atmospheres, it is mostly sufficient to consider only collisions with electrons, because the ratio between electron and ion thermal velocities is \( v_{th,e}/v_{th,i} \approx 43 \sqrt{A} \), consequently, the ion contribution to collisions can be neglected.

The upward collisional rate from the level \( i \) to the level \( l \) is obtained by integration of the total cross section of the transition \( \sigma_{il}(v) \) over the electron velocity distribution \( f(v) \), which is Maxwellian in our case,

\[
n_i C_{il} = n_i n_e \int_{v_0}^{\infty} \sigma_{il}(v) f(v) \, dv = n_i n_e q_{il}(T),
\]  

(4.14)
where the quantity $q_{il}(T)$ is called the effective collision strength (see, e.g., Mihalas, 1978, Eq. 5-68). The downward rate follows from the detailed balance in thermodynamic equilibrium, $n_i^e C_{il} = n_i^r C_{il}$, and is

$$n_i C_{li} = n_i \left( \frac{n_i^e}{n_i^r} \right) C_{il} = n_i \left( \frac{n_i^e}{n_i^r} \right) n_e q_{il}(T).$$ \hfill (4.15)

Thus, for calculation of both upward and downward collisional rates we need to know only the effective collision strength $q_{il}(T)$.

Details of calculations of collisional rates can be found elsewhere in these proceedings (Butler, 2010; Mashonkina, 2010).

### 4.4 Set of statistical equilibrium equations

Let us consider an element having NL levels. For each level $i$ we may write an equation

$$n_i \sum_{l \neq i}^{NL} (R_{il} + C_{il}) + \sum_{l \neq i}^{NL} n_l (R_{li} + C_{li}) = 0,$$ \hfill (4.16)

where $R_{il}$ and $C_{il}$ are given by equations (4.5), (4.8), (4.9), (4.11), (4.14), and (4.15). Since the system of these equations for all levels is linearly dependent (for NL levels only NL – 1 levels are linearly independent), we must supplement the equations by some additional equation.

For model atmosphere calculations, we have two equivalent options (both physically and numerically). We can use either the charge conservation equation,

$$\sum_k \sum_j jN_{jk} = n_e,$$ \hfill (4.17)

where $N_{jk}$ means the number density of ions $j$ of the element $k$, or the particle conservation,

$$\sum_k \sum_j N_{jk} = (N - n_e),$$ \hfill (4.18)

where $N$ is the total number density in the atmosphere, are being used.

For the case of the solution of the NLTE problem for the trace element, the abundance equation

$$\sum_j N_{jk} = \frac{\alpha_k}{\alpha_{ref}} \sum_j N_{j,ref}$$ \hfill (4.19)

can be used. Here $\alpha_k$ is the abundance of the element $k$ and $\alpha_{ref}$ is the abundance of the reference atom, which is usually (but not necessarily) hydrogen. Equation (4.19) relates the abundances of the studied and reference elements.
4.5 Non-explicit levels

Usually the atoms that exist in reality have much more complicated structure than we are able to include in our models. As a consequence, some energy levels are not explicitly considered in the statistical equilibrium equations. This mainly concerns highly excited levels. However, it does not mean that they do not exist and we have to include them in the system of the statistical equilibrium equations somehow. There are several possibilities of how to handle this task. We may, of course, neglect them. However, it is better to include them in the total number density and to assume that they are in LTE with respect to the next higher ion. Also the corresponding collisional excitation rates to these levels can then be included in the generalised (or modified) collisional ionization rate [for a detailed description of this approximation see Hubeny (1988) Hubeny et al. (1994)]. The radiative rates to these levels are assumed to be in detailed radiative balance and they do not enter into the equations of statistical equilibrium.

Alternatively, they may be merged into one or more superlevels (see Hubeny & Lanz, 1995), which can then be included in the set of energy levels and in the equations of statistical equilibrium to allow their departures from the local thermodynamic equilibrium.

5 Conclusions

In this review we summarized the basic equations for the solution of the NLTE line formation problem with a focus on the solution of the problem for trace elements in stellar atmospheres. It has to be emphasized that in NLTE calculations for trace elements preference should be given to background NLTE model atmospheres, since using LTE model atmospheres is inconsistent with the condition of NLTE. It must be carefully decided which elements can be treated as a trace element and for which such treatment is questionable. After obtaining the numerical results all assumptions have to be verified, especially that of the traceness.

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