Statistical equilibrium for trace elements in stellar atmospheres

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Outline

1. Stellar atmosphere problem
2. Comparison of LTE and NLTE
   (a) Thermodynamic equilibrium
   (b) Local thermodynamic equilibrium (LTE)
   (c) Statistical equilibrium (NLTE)
   (d) Microscopic processes
3. Trace elements
4. Equations of statistical equilibrium
   (a) Radiative rates
   (b) Collisional rates
5. Conclusions

Stellar atmosphere problem

solution of the stellar atmosphere problem – searching for distributions:

- momentum distribution (velocities of all particles)
- distribution of particle internal degrees of freedom (populations of atomic excitation stages)
- distribution of internal degrees of freedom of the electromagnetic field (radiation field for all frequencies, directions, polarization)

Thermodynamic equilibrium

conditions for equilibrium

- $t_{\text{relaxation}} \ll t_{\text{macroscopic changes}}$
- $l_{\text{macroscopic changes}} \ll \bar{l}_{\text{free path}}$
- $t_{\text{relaxation}} \ll t_{\text{inelastic collisions}}$
- for $t_{\text{relaxation}} \gtrsim t_{\text{inelastic collisions}}$ colliding particles have to be in equilibrium

Hubený 1976, PhD thesis

Thermodynamic equilibrium

distributions in equilibrium

- electron (and other particle) velocities
  – *Maxwellian distribution*

$$f(v)\,\mathrm{d}v = \frac{1}{v_0\sqrt{\pi}} e^{-\frac{v^2}{v_0^2}}\,\mathrm{d}v$$

most probable speed: $v_0 = \sqrt{\frac{2kT}{m_e}}$

Thermodynamic equilibrium

distributions in equilibrium

- atomic level populations
  - *Boltzmann distribution*

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

- ionization degrees distribution
  - *Saha equation*

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

Thermodynamic equilibrium

distributions in equilibrium

- radiation field – *Planck distribution*

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

Thermodynamic equilibrium

distributions in equilibrium

electron velocities	–	Maxwellian distribution
level populations	–	Saha-Boltzmann distribution
radiation field	–	Planck distribution

Thermodynamic equilibrium

distributions in equilibrium

electron velocities	–	Maxwellian distribution
level populations	–	Saha-Boltzmann distribution
radiation field	–	Planck distribution
		contradicts observations

Thermodynamic equilibrium

distributions in equilibrium

electron velocities	–	Maxwellian distribution
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		contradicts observations

Local thermodynamic equilibrium

- locally equilibrium distributions
  (we ignore the dependence $T(\vec{r})$, $N(\vec{r})$)

  electron velocities – Maxwellian distribution

  level populations – Saha-Boltzmann distribution

- non-equilibrium distribution

  radiation field – calculated by RTE solution

$$\mu \frac{\mathrm{d}I_{\mu\nu}}{\mathrm{d}z} = \eta_\nu - \chi_\nu I_{\mu\nu}$$

with the source function equal to the Planck function

$$S_\nu = \frac{\eta_\nu}{\chi_\nu} = B_\nu$$

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Statistical equilibrium

usually called NLTE or non-LTE

- equilibrium distribution
  electron velocities – Maxwellian distribution
- non-equilibrium distributions
  level populations – statistical equilibrium
  radiation field – calculated by RTE solution

Microscopic processes

particle collisions

- elastic collisions (e–e, e–H, e–H$^+$, e–He, H–H, H–He, ...) maintain equuilibrium velocity distribution
- inelastic collisions with electrons
  - excitation: $\mathrm{e}(v) + \mathrm{X} \rightarrow \mathrm{e}(v' < v) + \mathrm{X}^*$
  - deexcitation: $\mathrm{e}(v) + \mathrm{X}^* \rightarrow \mathrm{e}(v' > v) + \mathrm{X}$
  - ionization: $\mathrm{e} + \mathrm{X} \rightarrow 2\mathrm{e} + \mathrm{X}^+$
  - recombination: $2\mathrm{e} + \mathrm{X}^+ \rightarrow \mathrm{e} + \mathrm{X}$
- inelastic collisions with other particles less frequent
  $\Rightarrow$ neglected

Microscopic processes

interaction with radiation

- excitation: $\nu + \mathrm{X} \rightarrow \mathrm{X}^*$
- deexcitation:
  - spontaneous: $\mathrm{X}^* \rightarrow \nu + \mathrm{X}$
  - stimulated: $\nu + \mathrm{X}^* \rightarrow 2\nu + \mathrm{X}$
- ionization: $\nu + \mathrm{X} \rightarrow \mathrm{X}^+ + \mathrm{e}$
- recombination:
  - spontaneous: $\mathrm{e} + \mathrm{X}^+ \rightarrow \nu + \mathrm{X}$
  - stimulated: $\nu + \mathrm{e} + \mathrm{X}^+ \rightarrow 2\nu + \mathrm{X}$

Microscopic processes

interaction with radiation

- excitation: $\nu + \mathrm{X} \rightarrow \mathrm{X}^*$
- deexcitation:
  - spontaneous: $\mathrm{X}^* \rightarrow \nu + \mathrm{X}$
  - stimulated: $\nu + \mathrm{X}^* \rightarrow 2\nu + \mathrm{X}$
- ionization: $\nu + \mathrm{X} \rightarrow \mathrm{X}^+ + \mathrm{e}$
  - autoionization: $\nu + \mathrm{X} \rightarrow \mathrm{X}^{**} \rightarrow \mathrm{X}^+ + \mathrm{e}$
  - Auger ionization: $\nu + \mathrm{X} \rightarrow \mathrm{X}^{+*}$
- recombination:
  - spontaneous: $\mathrm{e} + \mathrm{X}^+ \rightarrow \nu + \mathrm{X}$
  - stimulated: $\nu + \mathrm{e} + \mathrm{X}^+ \rightarrow 2\nu + \mathrm{X}$
  - dielectronic recombination: $\mathrm{X}^+ + \mathrm{e} \rightarrow \mathrm{X}^{**} \rightarrow \nu + \mathrm{X}$

Microscopic processes

- free-free transitions $\nu + \mathrm{e} + \mathrm{X} \leftrightarrow \mathrm{e} + \mathrm{X}$
- electron scattering
  - free (Compton, Thomson): $\nu + \mathrm{e} \rightarrow \nu + \mathrm{e}$
  - bound (Rayleigh): $\nu + \mathrm{X} \rightarrow \nu + \mathrm{X}$

LTE and NLTE

- silent background – maxwellian velocity distribution
  - inelastic collisions (collisional ionizations and excitations) destroy equilibrium velocity distribution
  - equilibrium is maintained by elastic collisions
  - $t_{\text{relaxation}} \ll t_{\text{inelastic collisions}}$ for most situations
  - exceptions: medium with few electrons

in the following we assume maxwellian (i.e. equilibrium) velocity distribution for all particles
radiation field is not in equilibrium – determined via the solution of the radiative transfer equation

LTE versus NLTE

maxwellian velocity distribution

- processes entering the game
  - collisional excitation and ionization (E)
  - radiative recombination (E)
  - free-free transitions (E)
  - photoionization
  - radiative excitation and deexcitation
  - elastic collisions (E)
  - Auger ionization
  - autoionization
  - dielectronic recombination (E)

LTE versus NLTE

detailed balance

- rate of each process is balanced by rate of the reverse process
- maxwellian distribution of electrons $\Rightarrow$ collisional processes in detailed balance
- radiative transitions in detailed balance only for Planck radiation field
- if $J_\nu \neq B_\nu \Rightarrow$ LTE not acceptable approximation

Trace elements

we have a model atmosphere (LTE or NLTE)

- assume that our model atmosphere is correct
- trace elements
  1. negligible effect on the atmospheric structure
  2. effect only on emergent radiation, but [1] must be valid
- given $T(r)$, $n_e(r)$,$n_i^{\mathrm{back}}(r) \Rightarrow$ background opacities
- solve RTE+ESE for trace elements

Trace elements – some warnings

- always check, if the trace element is really a trace element
- electrons from more abundant “trace” elements (C,N,O,. . .) may change the total number of free electrons
- background opacities should be the same as in the model atmosphere calculation
- LTE model atmosphere inconsistent with NLTE for trace elements
  - LTE $\Rightarrow$ enough collisions with e^- for H, He; why not for a trace element?
  - equilibrium can be maintained only via detailed balance
  - once detailed balance is violated, equilibrium is away
  - there may be regions, where equilibrium is met
- NLTE model atmosphere highly preferable

Equations of statistical equilibrium

change of the state i of each element

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i \vec{v}) = \sum_{j \neq i} (n_j P_{ji} - n_i P_{ij})$$

P_{ij} – transition probability from the level i to the level j

Equations of statistical equilibrium

change of the state i of each element

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P_{ij} – transition probability from the level i to the level j
continuity equation for element k,

$$\frac{\partial N_k}{\partial t} + \nabla \cdot (N_k \vec{v}) = 0.$$

gas continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0.$$

Equations of statistical equilibrium

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- stationary state or negligible changes with time – without $\partial/\partial t$

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- static state ($\vec{v} = 0$) or negligible advection (used in stellar winds) – also without ∇

Equations of statistical equilibrium

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

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Equations of statistical equilibrium

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

P_{ij} – transition probability from the level i to the level j

- $P_{ij} = R_{ij} + C_{ij}$
- R_{ij} – radiative rates
- C_{ij} – collisional rates

Equations of statistical equilibrium

change of the state i of each element

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

P_{ij} – transition probability from the level i to the level j

- detailed balance is for $n_j P_{ji} = n_i P_{ij}$, for $\forall i, j$
- equilibrium populations n_i^*,

Equilibrium level populations

- n_i^* – LTE level population
- departure coefficients $b_i = \frac{n_i}{n_i^*}$, for LTE $b_i = 1$

definition of $n_{i,j}^*$ (level i of ion j)

1. population with the assumption of LTE
2. $n_{i,j}^* = n_{0,j+1} n_e \frac{g_{ij}}{g_{0,j+1}} \frac{1}{2} \left(\frac{h^2}{2\pi mkT} \right)^{\frac{3}{2}} e^{-\frac{\chi_{Ij} - \chi_{ij}}{kT}}$

   $n_{0,j+1}$ – ***actual*** population of the ground level of the next higher ion

Radiative rates – bound-free

photoionization from the state i:
amount of absorbed energy: $4\pi J_\nu \alpha_{ik}(\nu)\,\mathrm{d}\nu$
number of photoionization is obtained dividing by $h\nu$ and integrating from 0 to ∞:

$$n_i R_{ik} = n_i 4\pi \int_{\nu_0}^{\infty} \frac{\alpha_{ik}}{h\nu} J_\nu \,\mathrm{d}\nu$$

Radiative rates – free-bound

photorecombination – collisional process

for TE $\Rightarrow$ detailed balance and $J_\nu = B_\nu$

$$n_k^* R_{ki}^* = n_i^* R_{ik}^* = n_i^* 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} B_\nu \, \mathrm{d}\nu$$

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$$n_k^* R_{ki}^* = n_i^* 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[B_\nu \left(1 - e^{-\frac{h\nu}{kT}} \right) + B_\nu e^{-\frac{h\nu}{kT}} \right] \mathrm{d}\nu$$

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$$n_k^* R_{ki}^* = n_i^* 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + B_\nu \right] e^{-\frac{h\nu}{kT}} \, \mathrm{d}\nu$$

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for TE ⇒ detailed balance and $J_\nu = B_\nu$

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per ion

$$R_{ki}^* = \frac{n_i^*}{n_k^*} 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + B_\nu \right] e^{-\frac{h\nu}{kT}} \, \mathrm{d}\nu$$

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for TE $\Rightarrow$ detailed balance and $J_\nu = B_\nu$

per ion

$$R^*_{ki} = \frac{n^*_i}{n^*_k} 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + B_\nu\right] e^{-\frac{h\nu}{kT}} \, \mathrm{d}\nu$$

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for TE $\Rightarrow$ detailed balance and $J_\nu = B_\nu$

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$$R_{ki} = R^*_{ki} = \frac{n^*_i}{n^*_k} 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + B_\nu \right] e^{-\frac{h\nu}{kT}} \, \mathrm{d}\nu$$

valid also outside TE

Radiative rates – free-bound

photorecombination – collisional process

for TE $\Rightarrow$ detailed balance and $J_\nu = B_\nu$

per ion

$$R_{ki} = R^*_{ki} = \frac{n^*_i}{n^*_k} 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + B_\nu \right] e^{-\frac{h\nu}{kT}} \, \mathrm{d}\nu$$

valid also outside TE

replace $B_\nu \rightarrow J_\nu$ and multiply by actual number of ions n_k

$$n_k R_{ki} = n_k \frac{n^*_i}{n^*_k} 4\pi \int_0^\infty \frac{\alpha_{ik}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + J_\nu \right] e^{-\frac{h\nu}{kT}} \, \mathrm{d}\nu$$

Radiative rates – bound-bound (up)

number of transitions $i \to j$ caused by intensity I in $\mathrm{d}\nu\,\mathrm{d}\omega$

$$n_i B_{ij} \phi_\nu I_\nu \,\mathrm{d}\nu \frac{\mathrm{d}\omega}{4\pi} = n_i B_{ij} \phi_\nu J_\nu \,\mathrm{d}\nu$$

total number of absorptions by integration over the profile

$$n_i R_{ij} = n_i B_{ij} \int \phi_\nu J_\nu \,\mathrm{d}\nu = n_i 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} J_\nu \,\mathrm{d}\nu$$

since $\alpha_\nu = \frac{h\nu}{4\pi} B_{ij} \phi_\nu$

Radiative rates – bound-bound (down)

number of stimulated emissions

$$n_j R_{ji}^{\text{stim}} = n_j B_{ji} \int \phi_\nu J_\nu \, \mathrm{d}\nu = n_i 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} J_\nu \, \mathrm{d}\nu$$

Radiative rates – bound-bound (down)

number of stimulated emissions

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number of spontaneous emissions

$$n_j R_{ji}^{\mathrm{spont}} = n_j A_{ji} = n_j \frac{2h\nu_{ij}^3}{c^2} B_{ji} = n_j \frac{g_i}{g_j} \frac{2h\nu_{ij}^3}{c^2} B_{ij} = n_j \frac{g_i}{g_j} \frac{4\pi}{h\nu_{ij}} \frac{2h\nu_{ij}^3}{c^2} \alpha_{ij}$$

Radiative rates – bound-bound (down)

number of stimulated emissions

$$n_j R_{ji}^{\mathrm{stim}} = n_j B_{ji} \int \phi_\nu J_\nu \,\mathrm{d}\nu = n_i 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} J_\nu \,\mathrm{d}\nu$$

number of spontaneous emissions

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total number of emissions

$$n_j R_{ji} = n_j \left(A_{ji} + B_{ji} \int \phi_\nu J_\nu \,\mathrm{d}\nu \right)$$

Radiative rates – bound-bound (down)

total number of emissions

$$n_j R_{ji} = n_j \left(A_{ji} + B_{ji} \int \phi_\nu J_\nu \, \mathrm{d}\nu \right)$$

Radiative rates – bound-bound (down)

total number of emissions

$$n_j R_{ji} = n_j \left(A_{ji} + B_{ji} \int \phi_\nu J_\nu \, \mathrm{d}\nu \right)$$

$$= n_j \frac{4\pi}{h\nu_{ij}} \frac{g_i}{g_j} \alpha_{ij} \left[\frac{2h\nu_{ij}^3}{c^2} + \int \phi_\nu J_\nu \, \mathrm{d}\nu \right]$$

Radiative rates – bound-bound (down)

total number of emissions

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the Boltzmann equation

$$\frac{n_i^*}{n_j^*} = \frac{g_i}{g_j} \exp\left(\frac{h\nu_{ij}}{kT} \right)$$

Radiative rates – bound-bound (down)

total number of emissions

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$$= n_j \frac{n_i^*}{n_j^*} 4\pi \int \frac{\alpha_{ij}(\nu)}{h\nu} \left[\frac{2h\nu^3}{c^2} + J_\nu \right] e^{-\frac{h\nu}{kT}} \,\mathrm{d}\nu$$

the Boltzmann equation

$$\frac{n_i^*}{n_j^*} = \frac{g_i}{g_j} \exp\left(\frac{h\nu_{ij}}{kT} \right)$$

Radiative rates – total

upward $i \to l$:

$$n_i R_{il} = n_i 4\pi \int \frac{\alpha_{il}(\nu)}{h\nu} J_\nu \, \mathrm{d}\nu$$

downward $l \to i$:

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

Collisional rates

sufficient to consider only electrons, because $v_{\rm th,e}/v_{\rm th,i} \approx 43\sqrt{A}$

rate up

$$n_i C_{ij} = n_i n_e \int_{v_0}^{\infty} \sigma_{ij}(v) f(v) v \, \mathrm{d}v = n_i n_e q_{ij}(T)$$

$\sigma_{ij}(v)$ – total cross section of the transition $i \rightarrow j$

rate down from the detailed balance $n_j^* C_{ji} = n_i^* C_{ij}$

$$n_j C_{ji} = n_j \left(\frac{n_i^*}{n_j^*} \right) C_{ij} = n_j \left(\frac{n_i^*}{n_j^*} \right) n_e q_{ij}(T)$$

System of statistical equilibrium equations

$\forall$ level

$$n_i \sum_l (R_{il} + C_{il}) + \sum_l n_l (R_{li} + C_{li}) = 0 \qquad (1)$$

linearly dependent equations
supplementary equations

- charge conservation $\sum_k \sum_j j N_{jk} + n_p = n_e$
- particle number conservation $\sum_k \sum_j N_{jk} = N_N$
- abundance equation $\sum_j N_{jk} = \frac{\alpha_k}{\alpha_H} \sum_j N_{jH}$

this system of equations is solved using methods described yesterday

Conclusions

- prefer NLTE model atmospheres
- decide, which element is a trace one and which one not
- verify your assumptions after calculations

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never use any code as a black box