Basics of the NLTE physics

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Outline

Analysis of observed spectra

assume you have observed and reduced spectrum (using some spectrograph, telescope and some reduction software, e.g. IRAF)

steps of analysis

1. calculation of model atmosphere (ATLAS9, TLUSTY)
   - solution of structural equations
2. calculation of synthetic spectrum (SYNTHE, SYNSPEC)
   - solution of the radiative transfer equation for *given* model
3. comparison with observations (printing, screen, SME)
   - using the synthetic spectra for comparison

Analysis of observed spectra

assume you have observed and reduced spectrum (using some spectrograph, telescope and some reduction software, e.g. IRAF)

steps of analysis

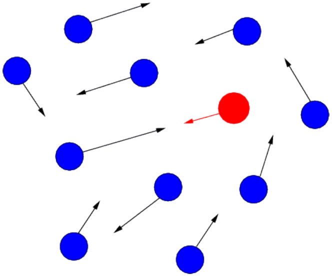
1. calculation of model atmosphere (ATLAS9, TLUSTY)
    - solution of structural equations
    - fully LTE / NLTE dependent
2. calculation of synthetic spectrum (SYNTHE, SYNSPEC)
    - solution of the radiative transfer equation for *given* model
    - partially LTE / NLTE dependent
3. comparison with observations (printing, screen, SME)
    - using the synthetic spectra for comparison
    - LTE / NLTE independent

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

- $t_{\text{relaxation}} \ll t_{\text{macroscopic changes}}$
- $l_{\text{macroscopic changes}} \ll \bar{l}_{\text{free path}}$
- $t_{\text{relaxation}} \ll t_{\text{inelastic collisions}}$
- if $t_{\text{relaxation}} \gtrsim t_{\text{inelastic collisions}} \Rightarrow$
  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*

$$B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{kT}}-1}$$

Thermodynamic equilibrium

distributions in equilibrium

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

Thermodynamic equilibrium

distributions in equilibrium

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radiation field	–	Planck distribution
		contradicts observations

Thermodynamic equilibrium

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Thermodynamic equilibrium

distributions in equilibrium

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

not suitable approximation for stellar atmospheres

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

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electron velocities	–	Maxwellian distribution
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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

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

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 ???

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Statistical equilibrium (NLTE or non-LTE)

locally equilibrium distribution

electron velocities – Maxwellian distribution

non-equilibrium distributions

level populations – statistical equilibrium
radiation field – calculated by RTE solution

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

η_ν and χ_ν determined using level populations

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 $\Rightarrow$ usually 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

scattering

- 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): $\nu + \mathrm{X} \rightarrow \nu + \mathrm{X}$
  - bound with frequency change (Raman): $\nu + \mathrm{X} \rightarrow \nu' + \mathrm{X}$

LTE and NLTE

maxwellian velocity distribution – silent background

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

LTE and NLTE

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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

- elastic collisions (E)

Saha-Boltzmann equilibrium

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

LTE versus NLTE

LTE 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 $J_\nu \neq B_\nu$ (as in stellar atmospheres) $\Rightarrow$ LTE not acceptable approximation, we can not reach detailed balance in radiative transitions

Equations of statistical equilibrium

change of the state *i* of each element

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

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

Equations of statistical equilibrium

change of the state i of each element

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

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

Summing over all levels $\rightarrow$ continuity equation for element k,

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

gas continuity equation ($\rho = N_k m_k$)

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

Equations of statistical equilibrium

change of the state *i* of each element

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

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

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

Equations of statistical equilibrium

change of the state *i* of each element

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

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

- stationary state or negligible changes with time – without $\partial/\partial t$
- static state ($\vec{v} = 0$) or negligible advection – also without ∇

Equations of statistical equilibrium

change of the state *i* of each element

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

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

- stationary state or negligible changes with time – without $\partial/\partial t$
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Equations of statistical equilibrium

change of the state i of each element

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

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

- $P_{ij} = R_{ij} + C_{ij}$
- R_{ij} – radiative rates (depend on J_ν)
- C_{ij} – collisional rates (depend on T, n_e)

Equations of statistical equilibrium

change of the state i of each element

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

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 $b_i = 1$

two definitions 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
   $b_{i,j}$ describes actual departure from LTE for given level i

first choice – seems more natural; second choice – more descriptive

System of statistical equilibrium equations

$\forall$ level i

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

linearly dependent equations

supplementary equations

- charge conservation $\sum_k \sum_j q_j N_{jk} = n_e$
  example: pure hydrogen $n_{\mathrm{H\,II}} = n_{\mathrm{e}}$
- particle number conservation $\sum_k \sum_j N_{jk} = N_N$
  example: pure hydrogen $n_{\mathrm{H\,I}} + n_{\mathrm{H\,II}} = N_N$
  N_N – total number density of all neutral atoms and ions
- abundance equation $\sum_j N_{jk} = \frac{\alpha_k}{\alpha_H} \sum_j N_{jH}$

System of statistical equilibrium equations

System of equations

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

$$\sum_k \sum_j q_j N_{jk} = n_e \qquad \sum_k \sum_j N_{jk} = N_N \qquad \sum_j N_{jk} = \frac{\alpha_k}{\alpha_H} \sum_j N_{jH}$$

can be formally written

$$\mathcal{A} \cdot \vec{n} = \mathcal{B}$$

- matrix $\mathcal{A}$ contains all rates – rate matrix
- vector $\mathcal{B}$ is 0 except rows with conservation laws
- $\vec{n} = (n_1, \ldots, n_{\mathrm{NL}})$ – vector of all populations

Solution of the system of ESE

$$\mathcal{A} \cdot \vec{n} = \mathcal{B}$$

for *given* $\mathcal{A}$ and $\mathcal{B}$ set of linear equations

$\mathcal{A}(I_{\mu\nu}) \quad \Rightarrow \quad$ add solution of the radiative transfer equation

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

$\eta_\nu(\vec{n}), \chi_\nu(\vec{n}) \quad \Rightarrow \quad$ systems mutually coupled

- nonlinear system of equations
- "natural" iteration scheme: $\vec{n} \to J_\nu \to \vec{n} \to J_\nu \to \ldots$ does not converge (Λ-iteration, $J_\nu = \Lambda S_\nu$)
- necessary to solve both systems of equations at once

Solution of the system of ESE

- nonlinear system of equations
- "natural" iteration scheme: $\vec{n} \rightarrow J_\nu \rightarrow \vec{n} \rightarrow J_\nu \rightarrow \ldots$ does not converge (Λ-iteration, $J_\nu = \Lambda S_\nu$)

methods of solution

- Newton-Raphson method – linearization of
  - all equations of statistical equilibrium
  - radiation transfer equation for all frequency points
- accelerated Λ-iteration (ALI)
  - similar scheme to Λ-iteration
  - uses approximate Λ-operator (ALO)
  - approximate solution of radiative transfer used in equations of statistical equilibrium

Summary

- NLTE (non-LTE) means
  - radiation is not in TE – determined from radiative transfer equation
  - exictation and ionization is not in TE – determined from equations of statistical equilibrium
  - particles are in LTE – Maxwellian distribution
- equations of
  - radiation transfer
  - statistical equilibrium

  solved simultanously