7. Non-LTE – basic concepts

- LTE vs NLTE
- occupation numbers
- rate equation
- transition probabilities: collisional and radiative
- examples: hot stars, A supergiants
LTE vs NLTE

LTE

each volume element separately in thermodynamic equilibrium at temperature $T(r)$

1. $f(v) \, dv = \text{Maxwellian with } T = T(r)$
2. Saha: $(n_p \, n_e)/n_1 = T^{3/2} \exp(-h\nu_1/kT)$
3. Boltzmann: $n_i / n_1 = g_i / g_1 \exp(-h\nu_{1i}/kT)$

However:

volume elements not closed systems, interactions by photons

$\Rightarrow$ LTE non-valid if absorption of photons disrupts equilibrium
Equilibrium: LTE vs NLTE

Processes:

**radiative** – photoionization, photoexcitation
- Establish equilibrium if radiation field is Planckian and isotropic
- Valid in innermost atmosphere
- However, if radiation field is non-Planckian these processes drive occupation numbers away from equilibrium, if they dominate

**collisional** – collisions between electrons and ions (atoms) establish equilibrium if
- Velocity field is Maxwellian
- Valid in stellar atmosphere

*Detailed balance*: the rate of each process is balanced by inverse process
LTE vs NLTE

NLTE if

rate of photon absorptions $\gg$ rate of electron collisions

$I_v(T) \gg T^\alpha, \alpha > 1 \quad \Rightarrow \quad n_e T^{1/2}$

LTE

valid: low temperatures & high densities
non-valid: high temperatures & low densities
LTE vs NLTE in hot stars

Kudritzki 1978
NLTE
1. \( f(v) \, dv \) remains Maxwellian
2. Boltzmann – Saha replaced by \( \frac{dn_i}{dt} = 0 \) (statistical equilibrium)
   for a given level \( i \) the rate of transitions out = rate of transitions in

rate out = rate in

\[
n_i \sum_{j \neq i} P_{ij} = \sum_{j \neq i} n_j P_{ji}
\]

rate equations
\( P_{i,j} \) transition probabilities
Calculation of occupation numbers

**NLTE**

1. $f(v) \ dv$ remains Maxwellian

2. Boltzmann – Saha replaced by $\frac{dn_i}{dt} = 0$ (statistical equilibrium)

   for a given level $i$ the rate of transitions **out** = rate of transitions **in**

\[
n_i \sum_{j \neq i} P_{ij} = \sum_{j \neq i} n_j P_{ji}
\]

**Rate Equations**

\[
n_i \sum_{j \neq i} (R_{ij} + C_{ij}) = \sum_{j \neq i} n_j (R_{ji} + C_{ji}) + n_e (R_{ki} + C_{ki})
\]

Transition probabilities

radiative

\begin{align*}
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
\end{align*}

collisional

absorption

\[
C_{ij} = n_e \int_0^\infty \sigma_{\text{coll}}(\nu) v f(\nu) d\nu
\]

emission

\[
C_{ji} = g_i / g_j e^{E_{ji}/kT} C_{ij}
\]
Occupation numbers

can prove that if \( C_{ij} \gg R_{ij} \) or \( J_\nu \to B_\nu (T) \): \( n_i \to n_i (\text{LTE}) \)

We obtain a system of linear equations for \( n_i \):

\[
A \cdot \begin{pmatrix}
  n_1 \\
  n_2 \\
  \vdots \\
  n_p 
\end{pmatrix} = X
\]

Where matrix \( A \) contains terms:

\[
\int_0^\infty \varphi_{ij}(\nu) \int I_\nu(\omega) \frac{d\omega}{4\pi} d\nu
\]

combine with equation of transfer:

\[
\frac{dI_\nu(\omega)}{dr} = -\kappa_\nu I_\nu(\omega) + \epsilon_\nu
\]

\[
\kappa_\nu = \sum_{i=1}^{N} \sum_{j=i+1}^{N} \sigma_{ij}^{\text{line}}(\nu) \left( n_i - \frac{g_i}{g_j} n_j \right) + \sum_{i=1}^{N} \sigma_{ik}(\nu) \left( n_i - n_i^* e^{-h\nu/kT} \right) + n_e n_p \sigma_{kk}(\nu, T) \left( 1 - e^{-h\nu/kT} \right) + n_e \sigma_e
\]

\[
\epsilon_\nu = \ldots
\]

*non-linear system of integro-differential equations*
complex atomic models for O-stars (Pauldrach et al., 2001)
Occupation numbers

Iteration required:
radiative processes depend on radiation field
radiation field depends on opacities
opacities depend on occupation numbers

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
Transition probabilities: collisions

Probability of collision between atom/ion (cross section $\sigma$) and colliding particles in time $dt$: $\sim \sigma v dt$

Rate of collisions = flux of colliding particles relative to atom/ion ($n_{coll} v$) $\times$ cross section $\sigma$.

For excitations: $C_{ij} = n_{coll} \int_0^\infty \sigma_{ij}^{coll}(v)vf(v)dv$

$\sigma^{coll}$ from complex quantum mechanical calculations

and similarly for de-excitation
Transition probabilities: collisions

in a hot plasma free electrons dominate: \( n_{\text{coll}} = n_e \)

\( v_{\text{th}} = \langle v \rangle = (2kT/m)^{1/2} \) is largest for electrons \( (v_{\text{th}, e} \sim 43 \ v_{\text{th}, p}) \)

\[
C_{ij} = n_e \int_0^\infty \sigma_{ij}^{\text{coll}}(v) v f(v) dv = n_e \ q_{ij}
\]

\( f(v) \ dv \) is Maxwellian in stellar atmospheres established by fast belastic e-e collisions.

One can show that under these circumstances the collisional transition probabilities for excitation and de-excitation are related by

\[
C_{ij} = \frac{g_j}{g_i} e^{-E_{ij}/kT} C_{ji}
\]
Transition probabilities: collisions

for bound-free transitions:

\[ C_{ki} = C_{ik} n_e \frac{g_i}{g_1^+} \frac{1}{2} \left( \frac{h^2}{2\pi mkT} \right)^{3/2} e^{E_i/kT} \]

collisional recombination (very inefficient 3-particle process) =

collisional ionization (important at high T)

In LTE:

\[ \left( \frac{n_j}{n_i} \right)^* = \frac{g_j}{g_i} e^{-E_{ij}/kT} \quad \text{Boltzmann} \]

\[ \left( \frac{n_1}{n_1^+} \right)^* = n_e \phi_1(T) \quad \text{Saha} \]

\[ C_{ij} = \left( \frac{n_j}{n_i} \right)^* C_{ji} \quad C_{ki} = \left( \frac{n_i}{n_1^+} \right)^* C_{ik} \]
Transition probabilities: collisions

Approximations for $C_{ji}$

\[ C_{ji} = n_e \frac{8.631 \times 10^{-6} \Omega_{ji}}{T_e^{1/2}} \frac{s}{g_j} \]

$\Omega_{ji} = \text{collision strength}$

for \textit{forbidden transitions}: $\Omega_{ji} \approx 1$

for \textit{allowed transitions}: $\Omega_{ji} = 1.6 \times 10^6 \left(\frac{g_i}{g_j}\right) f_{ij} \lambda_{ij} \Gamma(E_{ij}/kT)$

\[ \max (g', 0.276 \exp(E_{ij}/kT) E_{1}(E_{ij}/kT) \]

$g' = 0.7$ for $nl \to nl'$

$=0.3$ for $nl \to n'l'$
Transition probabilities: collisions

for ionizations

\[ C_{ik} = n_e \frac{1.55 \times 10^{13}}{T_e^{1/2}} g'_i \sigma_{ik}^{\text{phot}}(\nu_{ik}) \frac{e^{-E_i/kT}}{E_i/kT} \]

= 0.1 for Z=1
= 0.2 for Z=2
= 0.3 for Z=3

photoionization cross section at ionization edge
Transition probabilities: radiative processes

Line transitions

**absorption**  \( i \rightarrow j \ (i < j) \)

probability for absorption

\[
dW_{ij} = B_{ij} I_x \frac{d\omega}{4\pi} \varphi(x) dx \quad x = \frac{\nu - \nu_0}{\Delta \nu_D}
\]

integrating over \( x \) and \( d\omega \) (\( d\omega = 2\pi d\mu \))

\[
R_{ij} = B_{ij} \tilde{J}_{ij} \quad \tilde{J}_{ij}(r) = \frac{1}{2} \int_{-\infty}^{1} \int_{-1}^{1} I(x, \mu, r) \varphi(x) d\mu dx
\]

**emission**  \( i \rightarrow j \)

\[
R_{ji} = A_{ji} + B_{ji} \tilde{J}_{ji}
\]
Transition probabilities: radiative processes

**Bound-free**

*photo-ionization* $i \rightarrow k$

$$R_{ik} = \int_{\nu_{ik}}^{\infty} \sigma_{ik}(\nu) c n_{\text{phot}}(\nu) d\nu$$

$\sigma \times v$ for photons

$$u_\nu = h \nu n_{\text{phot}}(\nu) = \frac{4\pi}{c} J_\nu$$ energy density

$$R_{ik} = 4\pi \int_{\nu_{ik}}^{\infty} \frac{\sigma_{ik}(\nu)}{h \nu} J_\nu d\nu$$

*photo-recombination* $k \rightarrow i$

$$R_{ki} = \left( \frac{n_i}{n_1^+} \right)^* \tilde{R}_{ki}$$

$$\tilde{R}_{ki} = 4\pi \int_{\nu_{ik}}^{\infty} \frac{\sigma_{ik}}{h \nu} \left( \frac{2h \nu^3}{c^2} + J_\nu \right) e^{-h \nu/kT} d\nu$$
LTE vs NLTE in hot stars

Kudritzki 1979
LTE vs NLTE in hot stars

Kudritzki 1979

difference between NLTE and LTE in Hγ line profile for an O-star model with Teff = 45000K and log g = 4.5
LTE vs NLTE in hot stars

Kudritzki 1979

difference between NLTE and LTE $H_\gamma$ equivalent width as a function of log $g$ for $T_{\text{eff}} = 45,000$ K

NLTE and LTE temperature stratifications for two different Helium abundances at $T_{\text{eff}} = 45,000$ K, log $g = 5$
LTE vs NLTE: departure coefficients - hydrogen

\[ b_i = \frac{n_{i}^{\text{NLTE}}}{n_{i}^{\text{LTE}}} \]

\( \beta \) Orionis (B8 Ia)

\( T_{\text{eff}} = 12,000 \text{ K} \)

\( \log g = 1.75 \) (Przybilla 2003)
Nitrogen atomic models
Przybilla, Butler, Kudritzki
2003
LTE vs NLTE: departure coefficients - nitrogen
LTE vs NLTE: line fits – nitrogen lines
\[
\log \left\{ \frac{n_i}{n_i^{\text{LTE}}} \right\}
\]
LTE vs NLTE: line fits – hydrogen lines in IR

Brackett lines
J-band spectroscopy of red supergiants

Cosmic abundance probes out to 70 Mpc distance

α Her

Red supergiants, NLTE model atom for TiI

Bergemann, Kudritzki et al., 2012
Bergemann, Kudritzki et al., 2012
Red supergiants, IR lines and connected transitions for TiI

Bergemann, Kudritzki et al., 2012
Red supergiants, IR lines fine structure levels for TiI

Bergemann, Kudritzki et al., 2012
Red supergiants, IR lines departure coefficient for TiI

Bergemann, Kudritzki et al., 2012
Red supergiants, IR lines for TiI: NLTE vs. LTE

Bergemann, Kudritzki et al., 2012
Red supergiants, IR lines NLTE abundance corrections for TiI

\[ D(\text{NLTE-LTE}) = \log \left( \frac{N(\text{Ti})}{N(\text{H})} \right)_{\text{NLTE}} - \log \left( \frac{N(\text{Ti})}{N(\text{H})} \right)_{\text{LTE}} \]

Bergemann, Kudritzki et al., 2012
complex atomic models for O-stars (Pauldrach et al., 2001)
consistent treatment of expanding atmospheres along with spectrum synthesis techniques allow the determination of stellar parameters, wind parameters, and abundances

Pauldrach, 2003, Reviews in Modern Astronomy, Vol. 16