

# Introduction to NLTE radiative transfer in gases

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# What kind of a gas?

- The most general case of a gas is a bunch of particles of various types flying around in all directions and with various velocities (in the observer's frame).
- Since we want to deal with radiation there are also a bunch of photons cruising around in different directions and with some wavelength (in the observer's frame).

# A near-Maxwellian gas

- If that is all we know we have to just simulate all particles and photons and try to figure out what all that means to us. Normally the number of particles is huge and simulating them is not an alternative.
- But many gases are nicer in that particles interact with each other efficiently, and do not travel too far before they reach an almost Maxwellian velocity distribution.

# The “macroscopic” description

- At this point we have a statistical description of the particles microscopic velocities and we can use hydrodynamic equations to find the density, mean velocity, and the “kinetic” temperature.
- So we do know quite a bit about the gas and although details on the particles positions and velocities are not there, we don’t need to know them.

# Still, the photons

- However, the photons do not “interact” with each other (their interactions in interference processes do not change them).
- Thus, for the photons we are still on the same situation, a bunch of them flying around, and by themselves will never “thermalize”.
- Again there are too many of photons and we only care about how many we can find at each location traveling in each direction, and with which wavelength.
- The radiation intensity describes that.

# The gas “composition”

- Conservation equations describe the gas composition of various types of particles. They just state the particles may come in and out of a volume element by their mean velocity. The density may increase or decrease in time at this element. Besides, particles can transform between different types by chemical reactions or excitation-de-excitation.

$$\frac{\partial n_i}{\partial t} + \nabla \cdot [n_i (\mathbf{V}_i + \mathbf{U})] = \sum_j (P_{j,i} n_j - P_{i,j} n_i)$$

# Photons may be involved in composition changes

- These processes are of many kinds and some may involve the absorption or emission of a photon but others do not.
- Those that do not involve photons eventually tend towards a chemical “equilibrium” at the kinetic temperature.
- Those involving photons couple them with the gas and are responsible by the “absorption” and “emission” of photons used in radiative transfer.

# Thermodynamic Equilibrium

- In a very dense or large uniform gas the photons distribution (i.e. intensity) would eventually settle to the equilibrium if not too many are coming in or out of the uniform region. This requires the optical thickness of the uniform region to be very large for all photons.
- That is why in TE there is a single temperature value that describes the particle velocities distribution, the reacting particles equilibrium, and also the photons distribution (or intensity).
- In TE the photons follow the Planck function and radiative transfer is not needed.

# Local Thermodynamic Equilibrium

- The most common situation in gases is where the optical thickness of the uniform region is not large enough, at least at some relevant wavelengths.
- But often reactions that are not photon dependent can establish a local (in a volume element) composition equilibrium regardless of the photons not reaching their equilibrium distribution.
- In this case one can use the LTE radiative transfer by assuming the source function (ratio between absorption coefficient and emissivity) given by the Planck function. Here a transport equation is only needed for photons.

# When we can use LTE radiative transfer

- There are two cases:
  - The particle interactions drive the composition much faster than the photon interactions and the composition reached equilibrium at a particles temperature.
  - When the optical thickness of the uniform region at the wavelengths that affect the particle reactions is large. But at other wavelengths maybe the optical thickness is not large and radiative transfer has to be carried out.

## But in other common cases...

- Two things can prevent the gas from reaching equilibrium chemical composition.
  - Too many particles come in or go out of the volume element and the reactions inside have no time to settle the equilibrium.
  - Interactions with photons are disturbing the equilibrium.
- In these cases the composition needs to be calculated with the statistical equilibrium (conservation) equation.

# The “coupled” calculations

- In the first case one can first calculate the composition and from that the absorption coefficient and source function independently of the photons. Then one can calculate the photons distribution.
  - This is often called optically thin approach
- In the second case there no other way than to determine the composition and photons distribution at once since they are intimately coupled.

# The NLTE

- The “coupled” situation is the main issue the so-called NLTE addresses. (The optically thin would also be NLTE but is trivial.)
- For NLTE the statistical equation has to be solved in concert with the radiative transfer equation at the relevant wavelengths.

# Lambda iteration

- The so-called Lambda iteration was the first thing tried.
- This scheme consists of:
  - An initial guess of the gas composition (e.g. LTE)
  - Radiative transfer computation of the photons
  - Computing the composition with these photons
  - Iterate again the radiative transfer
- Although it may work in some special cases, in general should not be used because it converges so slowly that one may think a solution is achieved when it is very far from a correct solution.

# A very simple problem

- A very simple problem is that of a two level atom, and this can be solved analytically.
- An offspring of this is the “equivalent two level atom” that some people still uses for more complicated cases although has slow convergence.
- This method is not considered very good these days but it works and does not have the problem of the Lambda iteration.

# Simple two-level atom

- It is assumed the gas formed by 2 types of an atom. The two types are the two excitation levels it can be found:
  - the “ground level” (i.e. the lowest energy level  $E=0$ )
  - The “excited level” (with an energy  $E$ )
- Atoms of one type may transition to the other by absorption or emission of a photon of frequency  $\nu$  in a certain narrow range.

# Formalism of two-level atom

The statistical equilibrium is assumed as:

$$0 = P_{12}n_1 - P_{21}n_2$$

Which in the present case, considering collisional and radiative excitation and de-excitation gives:

$$0 = (C_{12}n_e + B_{12}\bar{J})n_1 - (C_{21}n_e + A_{21})n_2$$

$$\varepsilon_\nu = \varphi_\nu \frac{A_{21}}{4\pi} n_2$$

$$\kappa_\nu = \varphi_\nu \frac{B_{12}}{4\pi} n_1$$

# Developing the two-level atom

Working the equations the statistical equilibrium gives:

$$S_{\nu} = S = \frac{A_{21} n_2}{B_{12} n_1}$$

$$(C_{12}n_e + B_{12}\bar{J}) = (C_{21}n_e + A_{21})S \frac{B_{12}}{A_{21}}$$

The second equation gives a direct relationship between the mean intensity,  $J$ , and the source function,  $S$

# The usual result for two-level atom

Replacing S in the second equation it gives:

$$S = \frac{A_{21} (C_{12}n_e + B_{12}\bar{J})}{B_{12} (C_{21}n_e + A_{21})} = \frac{(\varepsilon \text{ Planck}'(T) + \bar{J})}{(\varepsilon + 1)}$$

$$\varepsilon = \frac{C_{21}n_e}{A_{21}}$$

$$\text{Planck}'(T) = \frac{A_{21} C_{12}n_e}{B_{12} C_{21}n_e} = \frac{A_{21} g_2}{B_{12} g_1} e^{-\frac{E}{kT}}$$

Thus, S is given in terms of the averaged (over angle and frequencies) intensity, the scattering term, and the Planck function (thermalization term). This can be incorporated in the radiative transfer equation and solved.

# Current methods for complex NLTE

- Numerical methods are currently in use for NLTE:
  - Complete Linearization technique (Mihalas & Auer ~1970). Solves simultaneously in a very big system of equations the statistical equilibrium and radiative transfer equations for all relevant wavelengths
  - Accelerated Lambda Iteration is somewhat similar to the Lambda iteration but uses a “pre-conditioning scheme to avoid the convergence problems.
  - Formal Replacement of the radiative transfer equations into the statistical equilibrium equations. This is the method I use and runs in small computers solving complicated problems very effectively

# Which are “correct” methods

- Whatever works for you and provides correct results, all the three above do
- Others methods exist but are not often used.
- CL is used by people with big computers and a lot of money.
- ALI is used a lot because of freely available code (MULTI) from Carlsson.
- FR replacement is used by me and few other people in small computers. Can deal with particle diffusion and transport while ALI currently cannot.

# Difference from LTE & NLTE in the solar spectrum, e.g. the Ca II H line

