

# Astrophysics with the Computer: Temperature Fluctuations in Ionized Nebulae

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## 1 Astrophysics

Planetary nebulae, H II regions, and supernova remnants consist of warm ionized gas which emits many bright emission lines. Many of the lines are produced by excitation of the ions following collisions with the free electrons in the plasma. The intensities of these lines depends on the ionic abundance and the temperature and density of the electrons. The intensity ratios of certain lines depend strongly on the electron temperature  $T_e$  (such as [O III] 5007/4363 Å, [N II] 6584/5755 Å), others are sensitive to the electron density  $n_e$  ([O II] 3727/3729, [S II] 6717/6731). Therefore it is possible to deduce from observed line intensity ratios the average values of  $T_e$  and  $n_e$  in a nebula. If one assumes that these values are representative for the entire object, one can compute the emissivities for all lines and thus determine from the observed spectrum the chemical composition of the nebula. For instance, the H II regions allow to study the present state of the interstellar gas, whereas planetary nebulae can tell us the chemical composition of the gas from which the central star had been born, which can be several  $10^9$  years ago.

The collisionally excited lines are very sensitive to the electron temperature. In order to get accurate abundances, one would want to measure  $T_e$  as accurately as possible. However, it is known from theoretical models that in such a nebula the electron temperature is unfortunately **not** constant. Furthermore, in some well-observed objects one finds that the temperatures derived from different line ratios do not agree with each other. Finally, high resolution images shows that many nebulae are not a body of uniform density, but instead they contain many small blobs and condensations. Thus, the idea that there are fluctuations of the electron temperature has been around for many years. How does this affect the interpretation of the spectra?

It has also been known for quite a while that in the presence of temperature fluctuations the apparent temperature is somewhat higher than the true average value. In this project we shall consider the line ratio [O III]5007/4363 and measure this effect.

## 2 The equations

### 2.1 Excitation of the Ion

We can model the  $O^{++}$  ion as a three-level ion; the 5007 line is emitted when the ion goes from its first excited state (level 2) into the ground state (level 1). The 4363 Å line is the transition from level 3 to level 2. The transition from level 3 to 1 is a line in the ultraviolet, and observable only from space. The data is given in this table. Note that the energies are in the spectroscopist's favoured unit, inverse centimetres, which comes

from  $E = h\nu = hc/\lambda$ .

level	energy [cm <sup>-1</sup> ]	statistical weight $g$
1	0.0	9
2	19967.1	5
3	42879.6	1

This model is somewhat simplified, but it is accurate enough to be used even in serious interpretation of spectra.

The three transitions are radiative ones, due to spontaneous emission. They are characterized by the Einstein A-value, which is the inverse lifetime of the upper state. Between all levels there are collisional transitions caused by the electrons, which are described by the collision strength  $\Omega$ . Both atomic constants can be computed by quantum mechanical models of the ion, and are listed in the following table:

transition	A [s <sup>-1</sup> ]	$\Omega$
2 $\rightarrow$ 1	0.0196	2.17
3 $\rightarrow$ 1	0.223	0.276
3 $\rightarrow$ 2	1.78	0.617

In a gaseous nebula there is no thermal equilibrium, because the densities are so low, between 10 and 10000 atoms per cubic centimetre. But we can assume that there is a statistical equilibrium for the states of atoms and ions, i.e. there is a stationary balance between the sum of the processes that populate and those which depopulate a level. This condition allows us formulate a system of linear equations ("rate equations" or "statistical equations") from which we can compute the population numbers, i.e. what fraction of ions can be found in each state.

In general the rate equations should include all processes between the levels, whether it be radiative or collisional. Because of the low densities in nebulae, we can simplify the problem:

- we need to consider only the lowest levels (here: 3), which includes the ground state and a few essential excited states. For many ions such as oxygen, nitrogen, neon etc. the excited states are meta-stable states. The only radiative deexcitation to the ground state are "forbidden" transitions, which cannot proceed via the usual electric dipole radiation. Therefore they have much longer lifetimes (order of seconds) than normal states (10<sup>-8</sup>s).
- radiative processes are only due to spontaneous emission. Because the gas is far away from the central star, all other radiative processes: absorption and induced emission can be neglected.
- the transitional probabilities for the electron collision induced transitions can be computed from simple formulae which depend on electron density and temperature.

For a two-level system one gets these rate equations:

$$0 = \frac{dn_1}{dt} = -n_1 C_{12} + n_2 (A_{21} + C_{21}) \quad (1)$$

$$0 = \frac{dn_2}{dt} = n_1 C_{12} - n_2 (A_{21} + C_{21}) \quad (2)$$

where  $n_1$  and  $n_2$  are the number densities of ions in the levels 1 (ground state) and 2.  $A_{21}$  is the Einstein coefficient for spontaneous emission of the line produced by the transition  $2 \rightarrow 1$ . The rate coefficients for collisions with electrons  $C_{12}$  (for excitation) and  $C_{21}$  (de-excitation) are proportional to the density of the electrons:

$$C_{ik} = n_e q_{ik} \quad (3)$$

with

$$q_{21} = \frac{8.629 \cdot 10^{-6} \Omega_{12}}{\sqrt{T_e} g_2} \quad (4)$$

and

$$q_{12} = q_{21} \frac{g_2}{g_1} \exp\left(-\frac{E_2 - E_1}{kT_e}\right) \quad (5)$$

Here the  $g_i$  are the statistical weights and  $E_i$  the energies of level  $i$ . The ground state has  $E_1 = 0$ . The collision strength  $\Omega_{12}$  is a measure for the effective cross-section for the ion-electron interaction.

The resulting homogeneous system of linear equations is linearly dependent, but it already permits to compute the ratio of the level populations:

$$\frac{n_2}{n_1} = \frac{C_{12}}{A_{21} + C_{21}} \quad (6)$$

To get a unique solution, we need to add the condition that the total number of ions in all states shall be conserved

$$n_1 + n_2 = n_{ion} \quad (7)$$

The solution of this simple two-level ion is possible by hand, and it constitutes an important tool to check your program!

In an analogous way, we obtain the equations for a multi-level system: in stationary equilibrium for level  $i$  the total loss rate (left hand side) is balanced by the sum of all gains (right hand side)

$$n_i \sum_{k \neq i}^m P_{ik} = \sum_{k \neq i}^m n_k P_{ki} \quad (8)$$

with the rate coefficients  $P_{ik}$  for the transition  $i \rightarrow k$ . Written as a matrix, we have (for  $m = 5$ )

$$(n_1 \dots n_5) \begin{pmatrix} -\sum_{k \neq 1} P_{1k} & P_{12} & P_{13} & P_{14} & P_{15} \\ P_{21} & -\sum_{k \neq 2} P_{2k} & P_{23} & P_{24} & P_{25} \\ P_{31} & P_{32} & -\sum_{k \neq 3} P_{3k} & P_{34} & P_{35} \\ P_{41} & P_{42} & P_{43} & -\sum_{k \neq 4} P_{4k} & P_{45} \\ P_{51} & P_{52} & P_{53} & P_{54} & -\sum_{k \neq 5} P_{5k} \end{pmatrix} = 0 \quad (9)$$

The diagonal terms of the matrix are the loss terms. The upper-right triangle are the gains by excitations from lower levels, the lower-left triangle are the gains by de-excitations from higher levels. The rate coefficients are

$$P_{ik} = \begin{cases} A_{ik} + C_{ik} & \text{for } i > k \\ C_{ik} & \text{for } i < k \end{cases} \quad (10)$$

To get a unique solution, we can substitute for example the first line by the particle conservation:

$$\sum_{k=1}^m n_k = 1 \quad (11)$$

Since we shall only be interested in the intensity ratios of lines, we do not need the absolute population numbers. It is sufficient to normalize the sum of all levels to unity.

## 2.2 Line emissivity

The solution of the rate equations gives us the population numbers. These are used to compute the rate of emission  $n_i A_{ik}$  of photons in a line  $i \rightarrow k$  and the emissivity of the gas (unit:  $\text{erg cm}^{-3} \text{ s}^{-1} \text{ sterad}^{-1}$ )

$$j_{ik} = \frac{h\nu_{ik}}{4\pi} n_i A_{ik} \quad (12)$$

This is the power which a unit volume of the gas radiates per unit solid angle (in all directions: solid angle =  $4\pi$ ) in this line.

Fortunately, gaseous nebulae are optically thin in almost all lines; this means that the total emitted power and hence the observed intensity are just the sum of all the emissivities, integrated over the entire volume of the object. And thus the intensity ratio of two lines is equal to the ratio of their emissivities:

$$I_{ik}/I_{lm} = j_{ik}/j_{lm} \quad (13)$$

And there is a small correction about the wavelengths: for optical lines one prefers the wavelength in air, which is 1.0003 times smaller than the vacuum wavelength from the energies ...

## 3 How to do it

The main idea is to consider a line of sight over which the electron temperature fluctuates with a given amplitude. We sum up from all these emitting gas elements the emissivities of the 5007 and the 4363 line and compute their ratio. From this ratio we can derive the temperature, if we interpret it with a model of a constant temperature.

We do not need to consider really the extend in space of this line of sight; we can simply compute the emissivities from gas with different temperatures and sum up their results. The temperatures are randomly picked, with a gaussian distribution about a given value and with a certain dispersion. Thus we do a kind of Monte Carlo simulation.

- The best thing is to start with the heart of the problem: the assembly and the solution of the rate equations. For the solution of a system of linear equations you can either write your own subprogram for a Gauss elimination method or take a routine from the ‘Numerical Recipes’. It is best to start with a two-level system and to check it against your hand calculations. Then you add the ”real” O<sup>++</sup> ion. Make sure that you get all the indices right ... is is very easy to make mistakes here and spend hours finding the errors!
- With the real oxygen data, you should be able to reproduce the relation of the intensity ratio with electron temperature (e.g. Osterbrock ”Astrophysics of Gasous Nebulae” or other books). Often, the ratio is given as (5007+4959)/4363 ... the intensity ratio of 5007/4959 is 3.0 independent of temperature or density.
- This relation can be fitted with a simple formula

$$\frac{I(5007)}{I(4363)} = 6.0 \exp\left(\frac{32500\text{K}}{T_e}\right) \quad (14)$$

Determine the two fit constants as accurately as possible using your results. You shall later use this formula to ’measure’ the temperature from the ratio of the average line intensities.

- For the Monte Carlo approach we need a random number generator: in Java, it is `Math.random()`, you can use routines from ’Numerical Recipes’ or from the Internet. But check whether they work properly on your machine and generate random numbers uniformly distributed between 0 and 1.
- Since we want to distribute the temperatures with a gaussian fluctuation about a central value, we need to modify the generated random numbers. This is done by the transformation method, described in ‘Numerical Recipes’: Consider

$$y(t) = \int_{x_{\min}}^t f(x) dx \quad (15)$$

$y$  is an invertible function between 0 and 1. For a uniform random numbers  $r$  the values  $t = y^{-1}(r)$  will be distributed as  $f(x)$ . So before any computations, we compute at the start of the program for a sufficiently fine grid of values of  $t$  the values  $y$ , and store them in arrays. Whenever we need a new random number, we get a uniform random number  $r$ , look up the nearest position in the  $y$  array, and take the corresponding value of the  $t$  array, perhaps with a linear interpolation. For the gaussian distribution, ‘Numerical Recipes’ also gives other methods.

- After putting these things together, you can compute the emissivities of the 5007 and 4363 lines from an assembly of many gas elements at temperatures which are randomly distributed about the central value. Sum up the emissivities for each line separately – this is what we do when we look with the spectrograph at a position in a nebula – and compute the ratio.

- determine with your fit formula the apparent electron temperature. How does it differ from the central value that you had assumed? How does this change with different values for the dispersion in the temperature?

## 4 Further possibilities

### 4.1 Density fluctuations

Fluctuations in the density are not so important, because the OIII line ratio does not depend strongly on that parameter. However, at higher densities this becomes more important. One could also think of using a gaussian distribution in the logarithm of the density. How does this show up?

### 4.2 N<sup>+</sup>

Here are the data for ionized nitrogen. The lines of this ion are a bit more sensitive to electron density. It would be interesting to see whether the difference between true average temperature and apparent mean temperature compares with OIII.

level	energy [cm <sup>-1</sup> ]	statistical weight $g$		
1	0.0	9		
2	15185.4	5		
3	32558.0	1		

  

transition	$\lambda$ [Å]	A [s <sup>-1</sup> ]	$\Omega$
2 → 1	6584	0.0030	2.68
3 → 1	...	0.038	0.353
3 → 2	5755	1.12	0.411

## 5 Literature

D.E.Osterbrock: "Astrophysics of Gaseous Nebulae ...".

The book "Numerical Recipes" is available in the MS2 library.

There may be a test version of a Java applet - but still without any explanations - is available at

<http://astro.u-strasbg.fr/~koppen/tempfluct/>