Theory of optically thin emission line spectroscopy

1 Important definitions

In general the spectrum of a source consists of a continuum and several line components. Processes which give raise to the continuous part of the spectrum involve situations where the radiation emitters (or absorbers) are left free to vary their energy without constraints. These include free – free, bound – free and free – bound processes. Electrons which jump between bound levels of an ion, instead, can only vary their energy by well defined amounts and, therefore, they produce spectral lines, either in absorption (if the arrival level is higher than the starting level) or in emission (if the arrival level is lower than the starting level).

We call ground level of an ion the lowest energy configuration of its electrons. It is a state with very long lifetime, in which the electrons experience the highest binding energy to the nucleus.

We call permitted line a spectral line that corresponds to a transition following the selection rules. Such transitions are very fast and the levels being connected to the ground level by permitted lines only live for extremely short times.

We call forbidden line a spectral line that corresponds to a transition violating one or more selection rules.

We call meta-stable level an excited level of a heavy ion that is located a few eV above the ground level and is connected to it only by forbidden transitions. Such a level lives for a relatively long time, before radiating back to the ground level, because its spontaneous decay is unlikely. If the spontaneous transition actually occurs, the emitted photon is never re-absorbed, because the forbidden transition would require the photon and the ion to stay close for a long time, which is obviously impossible.

2 The transport of radiation

Electromagnetic radiation is a form of propagating energy, which, while traveling along a path from a source to the observer, can be affected by interactions with the intervening medium. The intensity of radiation, measured over a frequency range, produces the spectrum of a source and it carries information on the physics of the source and of the intervening medium.

If we consider a radiation beam of specific intensity I_ν, traveling along an elementary path dr, we can describe the change of intensity occurring at frequency ν by taking into account the amount of energy that is added to the beam (emission) and the one that is subtracted from it:

$$\mathrm{d}I_\nu = \epsilon_\nu \mathrm{d}r - k_\nu I_\nu \mathrm{d}r, \tag{2.1}$$

where ϵ_ν represents the emission coefficient and k_ν represents the absorption coefficient. If we define the optical depth of the medium as:

$$\tau_\nu = -k_\nu r \Rightarrow \mathrm{d}\tau_\nu = -k_\nu \mathrm{d}r, \tag{2.2}$$

where the negative sign arises from the fact that we observe the radiation beam looking towards the source, while radiation propagates in the opposite direction, we can divide Equation (2.1) by dτ_ν and obtain the differential form of the transfer equation:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = I_\nu - \frac{\epsilon_\nu}{k_\nu}. \tag{2.3}$$

Defining the source function as $S_\nu = \epsilon_\nu / k_\nu$, the general solution of the transfer equation becomes:

$$I_\nu(\tau_\nu = 0) = I_{\nu 0} e^{-\tau_\nu^*} + \int_0^{\tau_\nu^*} S_\nu(\tau_\nu) e^{-\tau_\nu} \mathrm{d}\tau_\nu, \tag{2.4}$$

where $I_\nu(\tau_\nu = 0)$ is the observed emergent radiation intensity, $I_{\nu 0}$ is the background radiation intensity and τ_ν^* is the total optical depth of the encountered medium. The solution of the transfer equation can be read as follows: *the intensity of the observed radiation, emerging from a cloud, is given by the sum of the background radiation intensity, absorbed by the full length of the cloud, and of all the contributions emitted by the cloud layers, each one absorbed by the path corresponding to its depth in the cloud.*

If we make the simplifying assumption that S_ν is spatially constant and, therefore, not depending on τ_ν, we can solve the integral getting to the solution:

$$I_\nu(\tau_\nu = 0) = I_{\nu 0} e^{-\tau_\nu^*} + S_\nu(1 - e^{-\tau_\nu^*}), \tag{2.5}$$

which has two limits, depending on τ_ν^*:

Optically thick case $(\tau_\nu^* >> 1) \Rightarrow I_\nu(\tau_\nu = 0) = S_\nu$

in this case all the exponential terms are lost, no background is visible and the observed intensity is simply the source function of the outermost layer of the cloud.

Optically thin case $(\tau_\nu^* << 1) \Rightarrow I_\nu(\tau_\nu = 0) = I_{\nu 0} + \tau_\nu^* S_\nu$

this is obtained by plugging the approximation $e^{-\tau_\nu^*} \approx 1 - \tau_\nu^*$, holding when $\tau_\nu^* << 1$, into equation (2.5). The meaning of this solution is that in the optically thin case we see the radiation coming from behind the cloud, with the addition of a faint emission contribution. It is the case of the optically thin emission lines.

In general, the intensity of an emission line is defined as:

$$I_\nu^L = I_\nu(\tau_\nu = 0) - I_{\nu 0}, \tag{2.8}$$

that is the observed intensity without the intensity of the background source. It should be noted however that we can neglect the background source intensity if we look at a medium in a direction where there is no source in the background (for example, the border of an ionized nebula, far away from the central star) or in conditions of dilution of radiation.

3 Dilution of radiation

Dilution of radiation is a concept that applies whenever we are far away from a radiation source (with respect to the source size). It is commonly the situation that we deal with in the optical / UV domain, where sources are point-like, but it cannot be used in radio, where the whole sky is a source of background radiation. It is expressed by applying a dilution factor W to the radiation field intensity I_ν. The definition of the dilution factor is *the ratio between the solid angle subtended by the source from the observing point with respect to the whole solid angle of the sky.* Numerically:

$$W = \frac{\Omega}{4\pi}, \tag{3.1}$$

where Ω is the solid angle subtended by the radiation source (which scales with the inverse square of distance), while 4π corresponds to the whole-sky solid angle. In most cases of interest, it is a very tiny quantity (it is $W \sim 10^{-5}$ for the Sun as seen from Earth and $W \sim 10^{-16}$ for a point located in an ionized nebula at approximately 1pc from the ionizing star). In the case of thermal sources, dilution of radiation means that:

$$I_\nu = W B_\nu(T), \tag{3.2}$$

implying that all terms containing an interaction with the radiation field can be neglected in the balance equations, effectively decoupling the system from the transport equation and simplifying the solution of analytical problems.

4 Equilibrium conditions in ionized nebulae

The theory that we develop on the Physics of ionized nebulae is based on the assumption that the medium can achieve:

1. thermal equilibrium (defined by a temperature that is constant in time): it requires that the heating and the cooling of the medium have the same efficiency;

2. ionization equilibrium, meaning that the number of electrons that are released in ionization processes is equal to the number of recombinations, so that the ionization degree does not change in time;

3. steady state statistical equilibrium, meaning that the population of the ion excitation levels does not change with time (so that the number of electrons which leave a specific level in the unit of time is equal to the number of electrons which come to that same level in the same time).

In this situation (which IS NOT a strict condition of Thermodynamic Equilibrium), we can still apply some of the Thermodynamic Equilibrium relations and in particular we assume that the particles have a Maxwell-Boltzmann velocity distribution. This is possible because the elastic collision cross-section is by far the most relevant at the typical energies of thermal astrophysical plasmas. The above assumptions are based on the observational evidence that the spectra of photo-ionized nebulae, like H II regions and planetary nebulae, do not change appreciably over short time scales. Should any of the conditions above be violated, we would expect changes in the spectrum, as well. Indeed there are peculiar environments where such assumptions DO NOT hold. We can mention for example:

- nova and supernova explosions
- compact regions in Active Galactic Nuclei
- shock waves

The spectra of most of these objects are actually variable and they must be studied with a somewhat different formalism.

5 The two-level system

The two-level system is a simplified representation of the transitions that can occur between the energy levels of an ion, under specific circumstances. In order to apply this formalism, we need the equilibrium conditions described in the previous sections. In addition we neglect

- ionizations
- recombinations

and we only consider the transitions between two bound states, a lower level 1 (ground level) and an upper level 2 (excited level). In these conditions the steady state rule implies that the number of electrons that undergo the transition $1 \to 2$ (excitation) equals the number of electrons that follow the opposite transition $2 \to 1$ (de-excitation). The general expression of steady state for a two-level system, therefore, is:

$$N_1(B_{12}U_\nu + N'Q_{12}) = N_2(A_{21} + B_{21}U_\nu + N'Q_{21}), \tag{5.1}$$

where N_1 and N_2 are the occupation numbers of levels 1 and 2, Q_{12} and Q_{21} are the collisional efficiency rates for excitation and de-excitation, N' is the collisional partners number density, B_{12} is the radiation absorption probability, B_{21} the stimulated emission probability, A_{21} the spontaneous emission probability and U_ν is the radiation density. The general definition of U_ν is:

$$U_\nu = \frac{1}{c}\int_{4\pi} I_\nu \mathrm{d}\omega. \tag{5.2}$$

This simply reduces to:

$$U_\nu = \frac{4\pi}{c} I_\nu \tag{5.3}$$

if I_ν is isotropic or it can be expressed through the *equivalent isotropic radiation field*. Solving the steady state equation (5.1) gives the population ratio of the two considered levels under specific physical conditions. If we are able to connect any spectral properties (mainly intensity of continuum or emission lines) with the level occupation numbers, we are finally able to constrain the physics of gas.

Although oversimplified, the two-level system well describes the physics of isolated transitions. It has two very important applications, namely to forbidden optical emission lines and to radio emission lines.

5.1 The optical case

We consider the case when the transition connecting levels 1 and 2 corresponds to a forbidden optical line. Since we are far from radiation sources, we put ourselves in dilution of radiation (which implies that we can neglect all terms depending on U_ν from equation 5.1). In this case, the steady state equation (5.1) becomes:

$$N_1 N' Q_{12} = N_2(A_{21} + N'Q_{21}). \tag{5.4}$$

We can infer the population ratio as:

$$\frac{N_2}{N_1} = \frac{N'Q_{12}}{A_{21} + N'Q_{21}}. \tag{5.5}$$

Now, recalling that in thermodynamic equilibrium (TDE) every process is exactly balanced by its opposite process, the collisional efficiency rates must obey the relation:

$$N_1^* Q_{12} = N_2^* Q_{21}, \tag{5.6}$$

where N_1^* and N_2^* are the occupation numbers of levels 1 and 2 in thermodynamic equilibrium, meaning that in TDE every collisional excitation must be followed by a corresponding collisional de-excitation. Since, however, the collisional efficiency rates are intrinsic to the ions, their relation is independent on whether the system is in TDE or not, so that:

$$\frac{Q_{12}}{Q_{21}} = \frac{N_2^*}{N_1^*} = \frac{g_2}{g_1} \exp\left(-\frac{h\nu_{21}}{k_B T}\right) \tag{5.7}$$

is a general expression and we used the Boltzmann formula for the ratio of the two levels occupation numbers in TDE. Using Equation (5.7) to express Q_{12} as function of Q_{21} in Equation (5.5) and dividing numerator and denominator by $N'Q_{21}$, we get:

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} \exp\left(-\frac{h\nu_{21}}{k_B T}\right) \cdot \frac{1}{1 + A_{21}/N'Q_{21}}. \tag{5.8}$$

We immediately recognize that Equation (5.8) is a generalized form of the Boltzmann formula, where the factor:

$$\frac{1}{1 + A_{21}/N'Q_{21}} = \frac{b_2}{b_1} \tag{5.9}$$

represents the ratio between the departure coefficients from TDE of the two levels, which are defined as:

$$b_i = \frac{N_i}{N_i^*}. \tag{5.10}$$

If we compare the rate of spontaneous radiative decays A_{21} with that of collisional de-excitations $N'Q_{21}$, we immediately see that

when $A_{21} >> N'Q_{21}$ **(radiation dominated case)** the departure coefficient ratio of Equation (5.9) is much smaller than 1, all the ions sit in the ground level, because every excitation is followed by radiation emission, and the system is far from TDE;

when $A_{21} << N'Q_{21}$ **(collision dominated case)** the departure coefficient ratio of Equation (5.9) is approximately 1 (Equation (5.8) reduces to the Boltzmann formula), all collisional excitations are followed by collisional de-excitation and the system retains its energy, staying close to TDE.

Following these considerations, we define the critical density of an emission line as:

$$N_c = \frac{A_{21}}{Q_{21}}. \tag{5.11}$$

At this density, half of the ions which get excited to level 2 are also collisionally de-excited back to level 1. This is an extremely useful reference, because at higher density values than N_c the emission of a specific line is effectively suppressed by collisional de-excitations. We conclude that there are 3 fundamental conditions to emit a forbidden line:

1. the density of collisional partners must be $N' < N_c$;

2. the temperature of the gas must be high enough for collisions to excite the high energy level 2;

3. the radiation field must be diluted (otherwise the excited level can be destroyed by an incoming photon, before it radiates back the emission line photon).

6 Temperature and density determination in ionized nebulae

There are two main ways to measure the temperature and the density of a photo-ionized cloud and they are based on the observation of:

1. OPTICAL FORBIDDEN LINES

2. RADIO CONTINUUM

Here, we only deal with the first method. The determination from optical lines is based on the two-level system formalism. Indeed, solving the transport equation in the optically thin case we have:

$$I_\nu^L = I_\nu(\tau_\nu = 0) - I_{\nu 0} = \int_0^{\tau_\nu^*} S_\nu \mathrm{d}\tau_\nu. \tag{6.1}$$

Since we can express the source function as:

$$S_\nu = \frac{\epsilon_\nu^{cont} + \epsilon_\nu^{line}}{k_\nu^{cont} + k_\nu^{line}}, \tag{6.2}$$

keeping in mind that it is $\epsilon_\nu^{cont} << \epsilon_\nu^{line}$ (because continuum radiation is diluted), $k_\nu^{cont} >> k_\nu^{line}$ (because the line is forbidden and therefore never re-absorbed) and that $\mathrm{d}\tau_\nu = k_\nu \cdot \mathrm{d}r$, we have that:

$$S_\nu \mathrm{d}\tau_\nu = \frac{\epsilon_\nu^{line}}{k_\nu^{cont}} k_\nu^{cont} \mathrm{d}r. \tag{6.3}$$

Plugging Eq. (6.3) into (6.1), we find:

$$I_\nu^L = \int_0^{r^*} \epsilon_\nu^L \mathrm{d}r, \tag{6.4}$$

where we can use the general expression of a line emission coefficient:

$$\epsilon_\nu^L = \frac{1}{4\pi} h\nu_{21} N_2 A_{21} \psi(\nu), \tag{6.5}$$

where $\psi(\nu)$ is a function of order unity, expressing the normalized line profile over frequency. It is clear that:

$$I_\nu^L = \frac{1}{4\pi} h\nu_{21} A_{21} \psi(\nu) \int_0^{r^*} N_2 \mathrm{d}r, \tag{6.6}$$

so that, if we consider the average gas density, which does not depend on r, and we take into account the ratio of two emission lines coming from one specific ion species that have the same profile, it is:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{\nu_{nm}}{\nu_{n'm}} \frac{A_{nm}}{A_{n'm}} \frac{N_n}{N_{n'}}. \tag{6.7}$$

Using the population ratio derived in Equation (5.8) for the optical case of the two level system, applied to the ratio $N_n/N_{n'}$ that appears in Equation (6.7), we obtain:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{g_n}{g_{n'}} \frac{\nu_{nm}}{\nu_{n'm}} \frac{A_{nm}}{A_{n'm}} \frac{1 + A_{nm}/N'Q_{nm}}{1 + A_{n'm}/N'Q_{n'm}} \exp\left[-\frac{h(\nu_{nm} - \nu_{n'm})}{k_B T}\right]. \tag{6.8}$$

The choice of lines with very similar frequencies reduces Equation (6.8) to:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{g_n}{g_{n'}} \frac{A_{nm}}{A_{n'm}} \frac{1 + A_{nm}/N'Q_{nm}}{1 + A_{n'm}/N'Q_{n'm}}, \tag{6.9}$$

which changes between two constant values depending mainly on density and it is therefore a strong indicator of gas density (case of [S II] and [O II] emission lines). On the contrary, taking lines that are far away in frequency, like in the case of the [O III], the ratio expressed in Equation (6.8) is strongly controlled by the exponential term, which depends mainly on temperature.

The complete solution of the nebula is to assume a guess to the temperature (10000K is a good starting point for most ionized nebulae), to calculate the density and to use it in the calculation of a more precise temperature. The process can be iterated until convergence is achieved.

7 Recombination lines

Due to the equilibrium conditions that apply in photo-ionized nebulae, in order to keep the ionization degree to a constant value, the number of electrons that are released in photo-ionization processes must be equal to the number of electrons that recombine with ions. In principle, recombinations can occur to an arbitrary energy level of the ions, but those electrons, which directly recombine to the ground level, give back to the radiation field a single photon, whose energy is high enough to ionize another particle. We shall see later that this re-ionization occurs very close to the recombination point (on the spot), so that recombinations to the ground level do not participate to the overall balance of the level occupation numbers. The electrons that recombine to higher energy levels, on the other hand, follow a very quick transition cascade to the ground level, going through a series of permitted transitions, which results in the emission of recombination lines.

To study the recombination lines, we put ourselves in the typical conditions of a hydrogen dominated astrophysical cloud, where:

- all H atoms sit in the ground level and they are photo-ionized from there
- the radiation field is diluted and the gas is optically thin (no stimulated emission or radiation absorptions are present)
- there is no collisional excitation of levels (this is reasonable because the energy gap between the ground level and the first excited level of H is 10.4eV, which is far too high to be covered by the collision with a thermal partner)
- the excited levels can only be populated by direct recombination or by recombination to higher levels, followed by transition cascade coming to the level.

In these conditions, the statistical balance is expressed by:

$$N_n \sum_{m=1}^{n-1} A_{nm} = \sum_{m=n+1}^{\infty} N_m A_{mn} + N_p N_e \alpha_{0n}(T_e), \tag{7.1}$$

where $\alpha_{0n}(T_e)$ is the effective recombination coefficient at level n, which is a function of temperature. Since in TDE every level would be described by a Saha-Boltzmann distribution, we can generalize Equation (7.1) simply by introducing the departure coefficients in every term containing an occupation number. The result is an equation system with unknown departure coefficients that can be numerically solved in order to determine the actual level occupation numbers and to predict the intensities of the recombination lines.

8 Ionization equilibrium

Let's consider, as a starting point, the case of a pure hydrogen nebula. In this case, the electron density is equal to the ion number density and the only relevant source of continuous opacity is the bound – free absorption (photoionization) cross-section:

$$a_\nu = 3 \cdot 10^{29} n^{-5} \nu^{-3}, \tag{8.1}$$

where n is the principal quantum number of the level that is being photo-ionized (meaning that photo-ionizations from excited levels are highly disfavoured with respect to those from the ground level). The absorption coefficient is obtained by multiplying Equation (8.1) by the density of absorbers:

$$k_\nu^k(n-f) = 3 \cdot 10^{29} n^{-5} \nu^{-3} N_{0n}. \tag{8.2}$$

Since the lifetimes of excited levels are very short, we can conclude that all photo-ionizations occur from the ground level and write that the ratio between ionized and neutral particles is:

$$\frac{N_1}{N_0} = \frac{R_{01}}{N_e \alpha_0}, \tag{8.3}$$

where $R_{01} \approx 10^{-8}\,\mathrm{s}^{-1}$ is the ionization rate and $\alpha_0 \approx 4 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$ is the effective recombination coefficient. Taking advantage from the pure hydrogen assumption ($N_e \approx N_1$), we have:

$$N_0 = \frac{N_e^2}{2.5 \cdot 10^4\,\mathrm{cm}^{-3}}. \tag{8.4}$$

Once we know the number density of neutral H atoms, we can put it into equation (8.2) to evaluate the absorption coefficient. Forcing an optical depth of 1, we can estimate the size at which a gaseous cloud becomes optically thick to the Lyman series and to the Lyman continuum photons. It turns out that typical sizes to achieve the optically thick regime are between 10^{-1} pc and 10^{-3} pc, much smaller than the size of a real cloud. As a consequence, real clouds are optically thick to Lyman photons.