Lecture Notes for Astronomical Spectroscopy

1 Fundamentals of atomic spectroscopy

1.1 Quantum number definitions

Let's consider an atom or ion with 1 valence electron. Valence electrons are defined as those electrons which lie outside the atomic core, that consists of the stable group of electrons filling a complete shell. The elements that have only 1 valence electron are H and alcaline metals (Li, Na, K, Ru, Ce). Ions with only 1 electron are, instead, He^+, Li^{++} etc. The state of an atom or ion with only 1 valence electron is defined by the following quantum numbers:

- n principal quantum number ($n = 1, 2, 3, \ldots\ \infty$)
- l azimuthal quantum number ($l = 0, 1, \ldots\ n - 1$)
- s spin quantum number ($s = \pm 1/2$)
- j inner quantum number ($j = l + s$)
- m_j magnetic quantum number ($-j \leq m_j \leq j$)

Each quantum number is connected with some characteristics of the electron in its level. n defines the energy level in which the electron can be found. l is related to the angular momentum associated to the orbital motion and the states with $l = 0, 1, 2, 3, 4$ ... are also named s (sharp), p (principal), d (diffuse), f, g ... The angular momentum quantum numbers l, s and j are associated with the actual angular momentum vectors $\vec{L}$, $\vec{S}$ and $\vec{J}$ by the relations:

$$|\vec{L}| = \sqrt{l(l+1)}\hbar \tag{1}$$

$$|\vec{S}| = \sqrt{s(s+1)}\hbar \tag{2}$$

$$|\vec{J}| = \sqrt{j(j+1)}\hbar \tag{3}$$

Electron states are defined by means of their quantum numbers n, l, s, j (and m_j if a magnetic field is present) and each state corresponds to a different binding energy.

1.2 Bohr atomic model

According to Bohr's model, electrons can be interpreted as classical particles orbiting about the atomic nucleus only on trajectories which give raise to an angular momentum that is a multiple of $\hbar$. If we consider, for example, an atom of Na I ($Z = 11$), the electron configuration is

$$\underbrace{1s^2 2s^2 2p^6}_{\text{atomic core}}\ 3s^1$$

where $1s^2 2s^2 2p^6$ is the electron configuration of the atomic core, while $3s^1$ represents the valence electron in its ground state.

1.3 Russell-Saunders coupling

If an atom or ion features more than 1 valence electron, the interaction between the vectors of the system leads to coupling of the electron properties. In particular, if for any pair of electrons i, j the conditions

$$l_i - l_j >> l_i - s_i \tag{4}$$

$$s_i - s_j > l_i - s_i \tag{5}$$

we can perform a vectorial sum of the orbital and spin angular momenta and, thus, define the total azimuthal quantum number:

$$\vec{L} = \sum_i \vec{l_i} \qquad |\vec{L}| = \sqrt{L(L+1)}$$

and the total spin quantum number:

$$\vec{S} = \sum_i \vec{s_i} \qquad |\vec{S}| = \sqrt{S(S+1)},$$

where the sums are calculated on the valence electrons only.

We can therefore define the term state of an ion as it is described by the quantum number set n, L, S. In general, lower orbits have higher binding energy and, for the hydrogen atom, it turns out that $E_n = E_0 \cdot n^{-2}$ (with $E_0 = -13.6\,\text{eV}$). Each nLS term naturally splits into $r = 2J + 1$ sub-levels, characterized by different values of J:

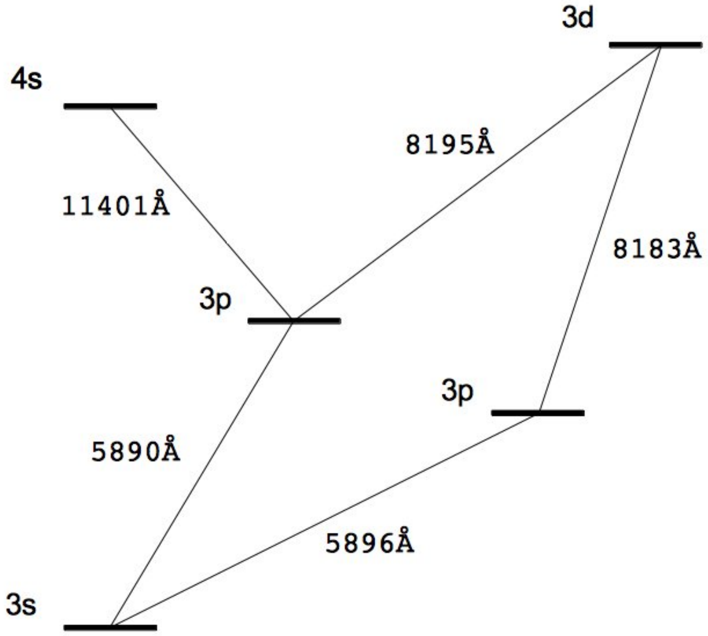

Figure 1: Energy diagram for the electron configurations of the Na I atom.

- if $L \geq S$ $\quad J = L + S, L + (S-1) \ ... \ L - (S-1), L - S \quad r = 2S + 1$
- if $L < S$ $\quad J = S + L, S + (L-1) \ ... \ S - (L-1), S - L \quad r = 2L + 1$

so that, in absence of any external field, the term nLS is split in a multiplet $nLSJ$. Each multiplet term is represented by the notation:

$$^{2S+1}L_J$$

Knowing the state of an ion, we can derive the statistical weights of its levels (which are equal to the number of different ways an electron can fill the level) and, in conditions of thermodynamical equilibrium, we can calculate the ratio between the occupation numbers.

We also define the parity of a state to be odd or even, depending on the parity of the sum $\sum_i l_i$, so that the term is represented by:

$$^{2S+1}L_J^{(o,e)}$$

Example on Na I terms:

there is 1 valence electron of configuration $3s^1$, therefore

$$L = 0 \qquad S = \frac{1}{2} \Rightarrow J = \frac{1}{2}$$

${}^2S^e_{1/2}$ $\quad s$ term

$L < S \qquad r = 2L + 1 = 1 \rightarrow$ singlet term

If the electron is in a higher angular momentum state, however, the situation may be different, as, for example in the cases with:

$$L = 1 \qquad S = \frac{1}{2} \qquad J = \begin{cases} L + S = 3/2 \\ L - S = 1/2 \end{cases}$$

a doublet of P terms, or

$$L = 2 \qquad S = \frac{1}{2} \qquad J = \begin{cases} L + S = 5/2 \\ L - S = 3/2 \end{cases}$$

representing a doublet of D terms. The detailed notation of the Na I ground level is $1s^2 2s^2 2p^6\ 3^2S_{1/2}$ and the Na I doublet at $\lambda\lambda 5890, 5896$ comes from the transitions

$$3^2S^e_{1/2} \rightarrow 3^2P^o_{1/2} \qquad \lambda = 5895.92\,\text{Å}$$

$$3^2S^e_{1/2} \rightarrow 3^2P^o_{3/2} \qquad \lambda = 5889.95\,\text{Å}$$

which are illustrated in the electron configuration diagram given in Fig. 1.

1.4 Grötrian diagrams

Grötrian diagrams represent a means of illustration of the energy levels of ions, through the introduction of two distinct scales. The first one gives the energy difference of the considered level with respect to the ground state, in eV. A second scale, called the *term scale*, provides the ratio between the absolute value of the binding energy and the product $h\,c$, given in *kaiser* or $\mathrm{cm}^{-}1$. An example is illustrated in Fig. 2. By the definition of the term scale, it turns out that it is:

$$T_m = \frac{|\text{Binding energy}|}{hc} \tag{6}$$

and, recalling that:

$$h = 4.13 \cdot 10^{-15}\,\mathrm{eV\,s^{-1}} = 6.626 \cdot 10^{-27}\,\mathrm{erg\,s^{-1}}$$

Figure 2: Example of a Grötrian diagram

$$c = 2.99792 \cdot 10^{10}\,\mathrm{cm\,s^{-1}}$$

$$1\,\mathrm{eV} = 1.6022 \cdot 10^{-12}\,\mathrm{erg}$$

it turns out that:

$$T_m = \frac{1}{\lambda} = \frac{E\,(\mathrm{eV})}{12398 \cdot 10^{-8}\,(\mathrm{eV\,cm})} \tag{7}$$

T_m measures the wave number corresponding to the transition between the m level and the free state. For a transition between two levels m and n, on the contrary, it is:

$$|T_m - T_n| = \frac{|E_m - E_n|}{hc} = \frac{1}{\lambda_{mn}} = \frac{\Delta E\,(\mathrm{eV})}{12398 \cdot 10^{-8}\mathrm{eV\,cm}} \tag{8}$$

so that an energy difference of 1 eV corresponds to a radiation wavelength of 12398 Å.

1.5 Fine structure

In the presence of an external magnetic field, each multiplet term splits in $g = 2J + 1$ simple terms, due to the various possible orientations of the angular momentum $\vec{J}$ with respect to the field lines. If there is no external magnetic field, we still have to weigh each energy levels g times, in the statistics of occupation numbers. In this case, it is said that the LSJ term is g-times degenerate. Fig. 3 summarizes the hierarchy of terms.

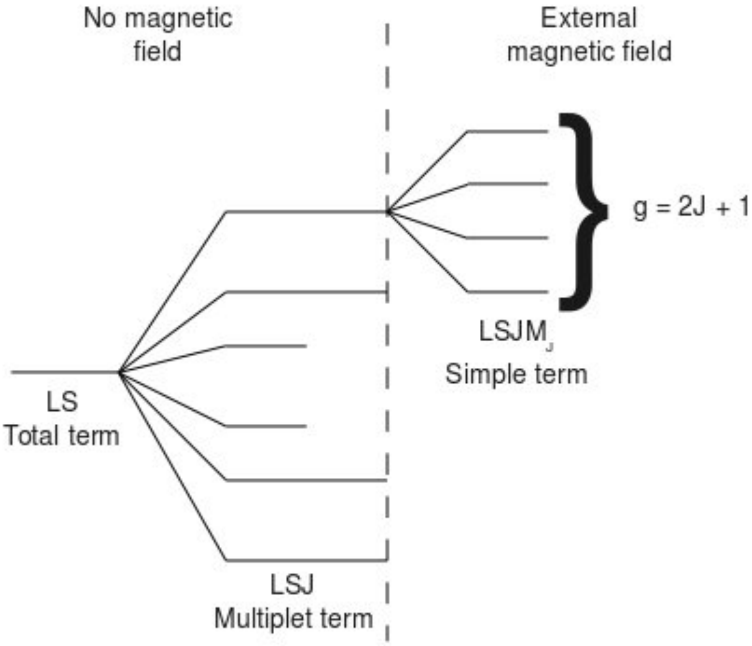

Figure 3: Electron configuration term hierarchy.

The statistical weight of a total term LS is calculated as the sum of the weights of its multiplet terms LSJ:

$$g = \sum_{J=L-S}^{L+S} (2J+1) = \sum_{k=0}^{2S} [2(L-S+k)+1] \tag{9}$$

This sum is an arithmetic progression of terms with step 1 and it equals the product between the number of members and the arithmetic mean of the first and the last member:

$$g = (2S+1)\frac{(2L-2S+1)+(2L-2S+4S+1)}{2} = (2S+1)(2L+1) \tag{10}$$

In the case of the hydrogen atom, with $S = 1/2$ and $g = 2(2L+1)$, each total term LS corresponds to a statistical weight of:

$$g_n = \sum_{L=0}^{n-1} 2(2L+1) = 2n^2 \tag{11}$$

Therefore, in the hydrogen atom, all the LS terms with the same principal quantum number n have the same energy. This occurs because the hydrogen atom has only one electron and there is no mantle affecting the binding energy according to the orbit's eccentricity. Of course, this situation changes for more complex ions.

1.6 Selection rules

An ion with a particular electron configuration may change to a different one, provided that it can exchange the amount of energy corresponding to the energy difference of the initial and final configurations. For transitions involving energy exchanges with radiation, through the emission or absorption of photons, the following selection rules apply:

1. only transitions connecting states with the same parity are permitted
2. $\Delta J = \pm 1$, 0 but $J = 0 \rightarrow J = 0$ is forbidden
3. $\Delta L = \pm 1$, 0 but it must always be $\Delta l = \pm 1$ for the jumping electron
4. $\Delta S = 0$ (if $L \geq S$ this means that transitions between states with different multiplicity are forbidden)
5. $\Delta M_J = \pm 1$, 0 but $M_J = 0 \rightarrow M_J = 0$ is forbidden, if it is also $\Delta J = 0$

The conditions 1 and 2 hold in dipole approximation, while 3 and 4 are valid in Russell-Saunders coupling.

1.7 Level population - the Boltzmann equation

If we consider a sample of atoms and ions, we can introduce the following definitions:

- N_{in} number of i-times ionized atoms in the energy level n per cubic centimeter (cm^{-3})
- $N_i = \sum_n N_{in}$ number of i-times ionized atoms (cm^{-3})
- $N = \sum_i N_i$ number of atoms and ions of an element (cm^{-3})
- χ_{in} excitation energy of the level n from the ground state of the i-times ionized atom

- $\chi_i = \chi_{i\infty}$ ionization energy from the ground state of the i-times ionized atom

- g_{in} statistical weight of the n level in the i-times ionized atom

In conditions of Thermodynamical Equilibrium, where every energy exchange process is perfectly balanced by its own inverse, the distribution of the ions of a given element in the available energy levels is given by the Boltzmann formula:

$$\frac{N_{in}}{N_{i1}} = \frac{g_{in}}{g_{i1}} \exp\left(-\frac{\chi_{in}}{k_B T}\right) \tag{12}$$

where $k_B = 1.38 \cdot 10^{-16}\,\mathrm{erg\,K^{-1}}$. It can be easily seen from Eq. (12) that the population of excited levels decreases exponentially with their excitation energy, though an increase of temperature brings to an higher population of the excited levels, because of the higher average energy of particles, that can therefore fill more easily the excitation energy gap through collisional processes.

Summing Eq. 12 over all the excitation states n, we have that:

$$\frac{N_i}{N_{i1}} = \frac{1}{g_{i1}} \sum_n g_n \exp\left(-\frac{\chi_{in}}{k_b T}\right) \tag{13}$$

and, dividing Eq. (12) by Eq. (13), we get:

$$\frac{N_{in}}{N_i} = \frac{g_{in}}{U_i(T)} \exp\left(-\frac{\chi_{in}}{k_b T}\right), \tag{14}$$

where we have introduced the *partition function*

$$U_i(T) = \sum_n g_n \exp\left(-\frac{\chi_{in}}{k_b T}\right). \tag{15}$$

$U_i(T)$ is a converging function because of the exponential factor (which quickly drops toward the high energy levels) and of the level broadening effects (such as natural broadening, collisional broadening and Doppler effects) which limit the number of discrete energy levels to a finite n, above which any further level melts in a continuous band.

Eq. (14) is the Boltzmann formula for the population of the generic level n, relative to the total ion abundance N_i, in thermodynamical equilibrium. For computational purposes, it is useful to express Eq. (12) in logarithmic form:

$$\log \frac{N_{in}}{N_i} = \log \frac{g_{in}}{g_i} - \chi_{in}\theta \tag{16}$$

with $\theta = 5040 \cdot T^{-1}$.

1.8 Ionization - the Saha equation

The Saha equation is the relationship which describes the equilibrium established for the reactions of ionization and recombination and it can be regarded as the extension of the Boltzmann's formula to the region of space where the levels are continuously distributed with positive energy. Assuming that χ_0 is the ionization potential of a particular species, indeed, we can represent the state of a free electron with kinetic energy K as:

$$E = \chi_0 + K = \chi_0 + \frac{p^2}{2m_e v} \tag{17}$$

Recalling from Quantum Mechanics that we cannot define the properties of an electron with an accuracy better than:

$$\mathrm{d}p_x \mathrm{d}x \geq h \tag{18}$$

we have to subdivide the six-dimensional phase space[1] in cells with a volume of h^3, each one being able to contain up to 2 electrons. The number of atoms in the ground level which lost an electron, whose position in the phase space is in the range $\vec{x} - \vec{x} + \mathrm{d}\vec{x}$ and $\vec{p} - \vec{p} + \mathrm{d}\vec{p}$ is given by:

$$\frac{\mathrm{d}N_{11}}{N_{01}} = 2\frac{g_{01}}{g_{11}} \exp\left\{-\frac{1}{k_b T}\left[\frac{1}{2m_e}(p_x^2 + p_y^2 + p_z^2) + \chi_0\right]\right\} \frac{\mathrm{d}^3x\mathrm{d}^3p}{h^3}, \tag{19}$$

where the factor 2 expresses the number of electrons that can share the same phase space cell. If we integrate Eq. (19) over the whole phase space, we have:

$$\frac{N_{11}}{N_{01}} = 2\frac{g_{11}}{g_{01}} \int_{-\infty}^{+\infty} \int_V \exp\left[-\frac{1}{K_B T}\left(\frac{1}{2m_e}|p|^2\right)\right] \frac{\mathrm{d}^3x\mathrm{d}^3p}{h^3}, \tag{20}$$

where V is the volume averagely available for one electron. If we consider the approximation in which 1 ion corresponds to 1 electron, we can use the expression:

$$V = N_e^{-1} = \frac{p_e}{k_b T}, \tag{21}$$

with p_e representing the electron pressure. Integration of Eq. (20) over the momentum yields a factor $(2\pi m_e k_B T)^{3/2}$ and, since there is no function of the spatial coordinates, with the introduction of Eq. (21) in Eq. (20), the result is:

$$\frac{N_{11} p_e}{N_{01}} = 2\frac{g_{11}}{g_{01}} \frac{(2\pi m_e)^{3/2}(k_B T)^{5-2}}{h^3} \exp\left(-\frac{\chi_0}{k_B T}\right). \tag{22}$$

[1]Remember that we must use vectorial quantities to describe the phase space. Therefore $\vec{x}$ will be the three-dimensional position vector and $\vec{p}$ provides the additional three dimensions of the velocity space.

This relation gives the ratio between the occupation number of the ground level of the singly ionized atom, with respect to the occupation number of the ground level of the neutral atom. Summing over all the possible excitation levels and considering the more general case of subsequent ionization states, we get the Saha equation:

$$\frac{N_{i+1}p_e}{N_i} = 2\frac{U_{i+1}(T)}{U_i(T)}\frac{(2\pi m_e)^{3/2}(k_BT)^{5-2}}{h^3}\exp\left(-\frac{\chi_i}{k_BT}\right), \tag{23}$$

which has a logarithmic expression:

$$\log\left(\frac{N_{i+1}p_e}{N_i}\right) = \log\left[2\frac{U_{i+1}(T)}{U_i(T)}\right] - \chi_i\theta + \frac{5}{2}\log T - 0.48, \tag{24}$$

provided that χ_i is measured in eV and p_e in $\mathrm{dyn\,cm^{-2}}$.

Notice from equations (23) and (24) that the effect of increasing the electron pressure is to reduce the degree of ionization (recombinations are favored and there are fewer cells for free electrons), while increasing temperature raises the ionization.

2 Radiation transport

2.1 The Radiative Transport Equation

We now want to consider the case in which a gaseous nebula is ionized, either by a shock wave, or by radiation coming from a thermal or a non-thermal source. The main difference between the cases of thermal (e. g. stellar) and non-thermal (e. g. AGN) radiation is the *Spectral Energy Distribution* (SED) of the ionizing photons. In the case of a star, the SED is well represented by a Black Body function of appropriate temperature, while in the AGN case the spectrum is essentially given by a combination of power-law continuum and of emission lines (mainly H lines, with a prominent Balmer series and several forbidden lines of [O III], [O I], [S II], [N II], [Ne III]). The most important consequence of the different spectral shapes is the excess of high frequency photons, produced by power law SEDs, illustrated in Fig. 4.

Let's now consider the case, illustrated in Fig. 5, of a radiation beam which crosses a gas cloud and describe what happens during the interaction between the gas cloud and the low density radiation field. In particular, we need to

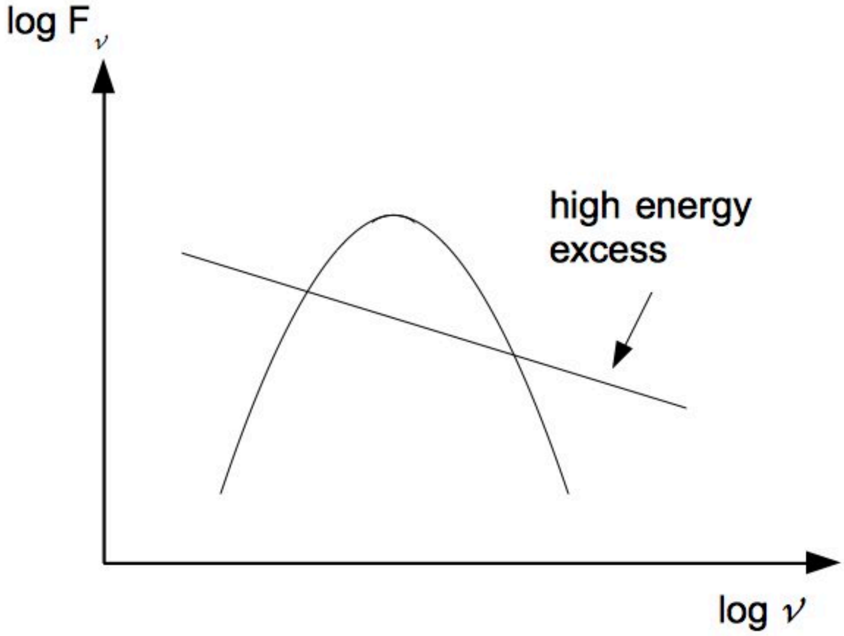

Figure 4: Ionizing photons SEDs for a thermal (curve) and a non-thermal (straight line) radiation source.

introduce some parameters to describe the radiation field. To do this, let's take into account a surface Σ and an area element $\mathrm{d}A$ on it (see Fig. 6). The energy flowing through the area $\mathrm{d}A\cos\theta$ per unit time, unit frequency in a beam propagating in the solid angle $\mathrm{d}\Omega$ is given by the *specific intensity*:

$$I_\nu = \frac{\mathrm{d}E_\nu}{\mathrm{d}A\cos\theta\mathrm{d}\nu\mathrm{d}\Omega\mathrm{d}t}\ [\mathrm{erg\,cm^{-2}s^{-1}Hz^{-1}}] \tag{25}$$

As the beam passes through the cloud, energy may either be absorbed or emitted due to the interactions of radiation with the atoms. We define the *emission coefficient*:

$$\epsilon_\nu = \frac{\mathrm{d}E_\nu}{\mathrm{d}s\mathrm{d}A\cos\theta\mathrm{d}\Omega\mathrm{d}t\mathrm{d}\nu}\ [\mathrm{erg\,cm^{-3}s^{-1}Hz^{-1}}] \tag{26}$$

as the amount of energy added to the beam while crossing the element volume $\mathrm{d}s\mathrm{d}A\cos\theta$ (per unit frequency and time), while we introduce an *absorption coefficient* through the expression:

$$k_\nu I_\nu = -\frac{\mathrm{d}E_\nu}{\mathrm{d}s\mathrm{d}A\cos\theta\mathrm{d}\nu\mathrm{d}\Omega\mathrm{d}t} \tag{27}$$

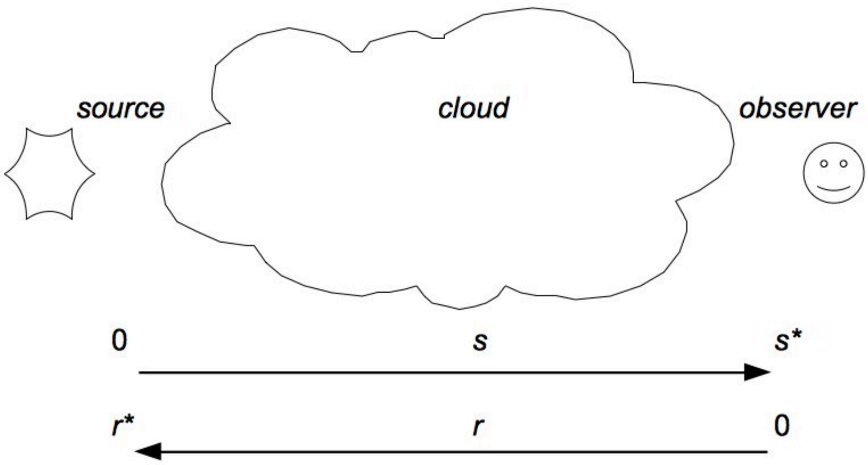

Figure 5: Scheme of a radiation source observed behind an intervening gas cloud. The line of sight to the source defines the r coordinate of the problem.

Notice that, while the emission coefficient ϵ_ν is an amount of energy, the absorption coefficient represents the fraction of energy that will be absorbed from a beam of specific intensity I_ν and it is measured in units of cm^{-1}.

If we take into account a radiation beam which propagates into a medium for a path of length $\mathrm{d}s$, in the most general situation its specific intensity will be affected by the emissions and absorptions of energy according to:

$$\mathrm{d}I_\nu = -k_\nu I_\nu \mathrm{d}s + \epsilon_\nu \mathrm{d}s. \tag{28}$$

Dividing Eq. (28) by the length element $\mathrm{d}s$, we obtain the *Radiative Transport Equation* in its differential form:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -k_\nu I_\nu + \epsilon_\nu. \tag{29}$$

In the case of pure absorption (i. e. $\epsilon_\nu = 0$) Eq. (29) becomes

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -k_\nu I_\nu \tag{30}$$

and, if s^* is the geometrical thickness of the cloud, its solution is:

$$I_\nu(s^*) = I_\nu(0) \exp\left(- \int_0^{s^*} k_\nu(s)\mathrm{d}s \right). \tag{31}$$

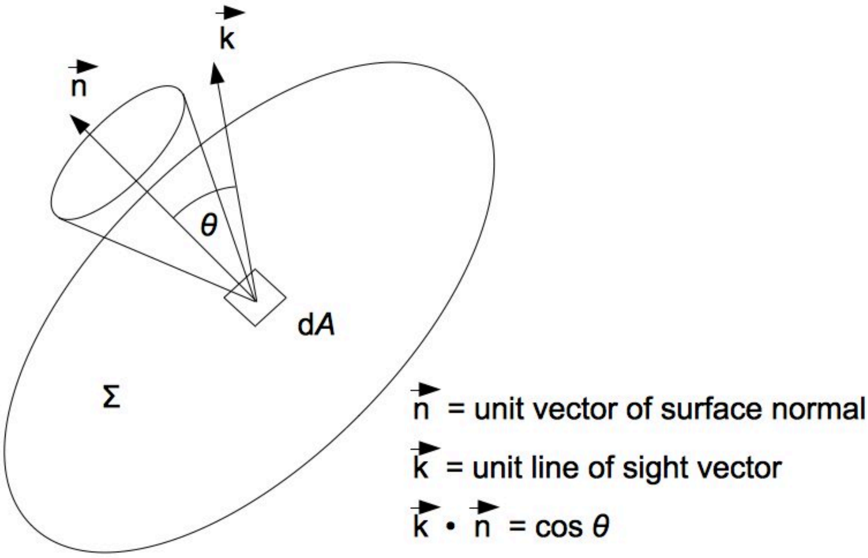

Figure 6: Geometry of a radiation beam crossing a surface Σ.

The exact solution of Eq. (31), therefore, requires a detailed knowledge of $k_\nu(s)$ in each point within the cloud.

In order to solve the radiative transport problem in a more general case, we introduce the *optical depth* of the medium through the definition:

$$\mathrm{d}\tau_\nu = k_\nu \mathrm{d}r = -k_\nu \mathrm{d}s \tag{32}$$

(notice that the optical depth is a dimensionless quantity that, for our geometry, is null at the observer's side of the cloud, while it is maximum deep in the cloud, on the source's side). The total optical depth of the medium is, thus:

$$\tau_\nu^* = \int_0^{r^*} k_\nu(r)\mathrm{d}r = -\int_{s^*}^0 k_\nu(s)\mathrm{d}s. \tag{33}$$

Dividing Eq. (29) by $-k_\nu$, we have:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = I_\nu - \frac{\epsilon_\nu}{k_\nu}. \tag{34}$$

The quantity $S_\nu = \epsilon_\nu / k_\nu$ is a characteristic of the cloud, fairly independent from the properties of the radiation source, that is called *source function.* Eq. (34) can be re-arranged in

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

and, multiplying both members by a factor $e^{-\tau_\nu}$, we get

$$\frac{\mathrm{d}}{\mathrm{d}\tau_\nu}[I_\nu e^{-I_\nu}] = -S_\nu e^{-\tau_\nu} \tag{35}$$

that can be integrated to:

$$I_\nu(\tau_\nu = 0) = \int_0^{\tau_\nu^*} S_\nu(\tau_\nu) e^{-\tau_\nu} \mathrm{d}\tau_\nu + I_{\nu 0} e^{-\tau_\nu^*}, \tag{36}$$

where we have called $I_{\nu 0} = I_\nu(\tau_\nu^*)$ the specific intensity of the initial radiation beam, as it strikes the cloud on the source's side. It can be seen from Eq. (36) that the emergent intensity is the sum of the original specific intensity, emitted by the source and attenuated by the whole path across the cloud, and of any contribution arising within the cloud itself and attenuated by a path corresponding to its own depth. Recalling the expression of source function, indeed, the integral on the right hand side of Eq. (36) turns out to be:

$$\int_0^{\tau_\nu^*} S_\nu e^{-\tau_\nu} \mathrm{d}\tau_\nu = \int_0^{r^*} \epsilon_\nu e^{-\tau_\nu} \mathrm{d}r,$$

meaning that the overall emitted radiation is a sum of contributions attenuated by the proper $e^{-\tau_\nu}$ factor.

If we now assume $S_\nu = \mathit{const}$ inside the cloud, the integration of Eq. (34) yields:

$$I_\nu(0) = S_\nu(1 - e^{-\tau_\nu^*}) + I_{\nu 0} e^{-\tau_\nu^*}. \tag{37}$$

This solution has two fundamental limits:

- $\tau_\nu >> 1$ (optically thick case), which implies $I_\nu(0) = S_\nu$ (i. e. we only see the cloud, through its source function)
- $\tau_\nu << 1$ (optically thin case), that, in the approximation $e^{-\tau_\nu} \approx 1 - \tau_\nu$, gives $I_\nu(0) = \tau_\nu^*(S_\nu - I_{\nu 0}) + I_{\nu 0}$.

Taking into account the optically thin case, if we do not look along the direction to the radiation source, it is $I_{\nu 0} = 0$ and, therefore

$$I_\nu(0) = \tau_\nu^* S_\nu = \epsilon_\nu r*$$

meaning that all the radiation produced in any element ds emerges from the cloud without being absorbed.

In conditions of Thermodynamical Equilibrium the energy absorbed in a volume element dV must be equal to the energy emitted in the same region:

$$k_\nu I_\nu = \epsilon_\nu \tag{38}$$

and the source function is given by the Planck distribution:

$$\frac{\epsilon_\nu}{k_\nu} = I_\nu = B_\nu(T) \tag{39}$$

where we recall that:

$$B_\nu(T) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/k_B T} - 1}. \tag{40}$$

When this condition is carried out in the continuum, outside the lines, we can describe the level population with the Boltzmann equation (14), the ionization degree with the Saha equation (23) and the source function with the Black Body distribution. The temperature to be used in these relations must be the same and coincident with the kinetic temperature of the gas.

2.2 The Equivalent Thermodynamic Equilibrium

A fundamental question is the problem of under which conditions the assumption of Thermodynamic Equilibrium is valid. A particular region is in thermodynamic equilibrium when each process has exactly the same probability to occur as its opposite one. Energy is constantly exchanged in all its forms and a steady state is reached if the translational kinetic energy is exchanged between all the particles, without being transformed into other forms of energy (for instance, when elastic scatterings dominate). The particle velocity distribution is then very similar to the Maxwell law:

$$\phi(v,T)\mathrm{d}v = \frac{4}{\pi}\left(\frac{m}{2k_B T}\right)^{3/2} v^2 \exp\left(-\frac{mv^2}{2k_B T}\right)\mathrm{d}v. \tag{41}$$

In a real astrophysical plasma the translational energy of particles is transformed in radiating energy as a consequence of the collisional excitation of the levels of ions or molecules and of the subsequent spontaneous de-excitation with the emission of a photon. However, this process is quite rare, with respect to elastic collisions, as it can be seen from a simple comparison of the characteristic process cross-sections (being $\sigma_{el} \sim 10^{-13}\,\mathrm{cm}^{-2}$ for elastic scattering, $\sigma_{rec} \sim 10^{-20}\,\mathrm{cm}^{-2}$ for electron–ion recombinations and $\sigma_{forb} \sim 10^{-15}\,\mathrm{cm}^{-2}$ to

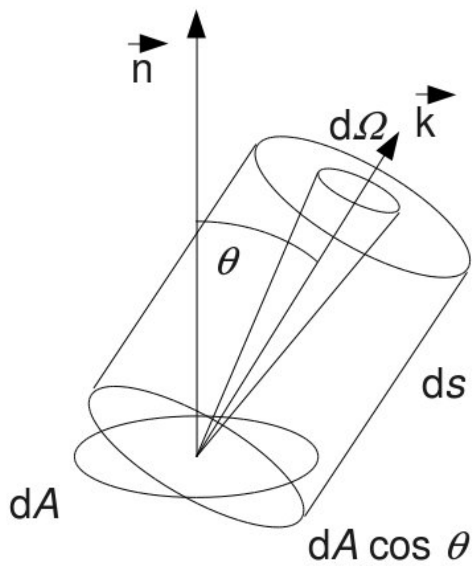

Figure 7: Geometry of a radiation beam flowing through a surface element dA.

excite a nebular line). In general, then, atoms and electrons in the interstellar gas have a velocity distribution that looks very similar to the Maxwellian expression of Eq. (41) and the same value of the temperature can be used to describe the different kinds of particles that compose the gas. As a consequence, the relative population of levels will be very similar to the one the gas would have in thermodynamic equilibrium, if collisional excitations and de-excitations dominate over the radiative processes.

We, therefore, define a condition of *Equivalent Thermodynamic Equilibrium* as a situation in which

- there is thermal equilibrium (all the particles are described by the same temperature)
- translational kinetic energy is NOT converted into other forms of energy

2.3 Radiation density

If a radiation beam flows with the speed of light c through a surface element dA in a direction oriented with an angle θ with respect to the surface normal, like it is shown in Fig. 7, we have that $\mathrm{d}t = \mathrm{d}s/c$ and we can write the expression of the specific intensity of Eq. (25) in the form:

$$I_\nu = \frac{c\mathrm{d}E_\nu}{\mathrm{d}A\cos\theta\mathrm{d}\nu\mathrm{d}\Omega\mathrm{d}s}, \tag{42}$$

but, since $\mathrm{d}A\cos\theta\mathrm{d}s = \mathrm{d}V$, the presence of a radiation beam implies the existence of an energy density per unit frequency:

$$\frac{\mathrm{d}E_\nu}{\mathrm{d}V\mathrm{d}\nu} = \frac{I_\nu\mathrm{d}\Omega}{c}. \tag{43}$$

Integrating over all the possible propagation directions, we define the radiation density as:

$$U_\nu = \frac{1}{c}\int_{4\pi} I_\nu\mathrm{d}\Omega, \tag{44}$$

so that, for an isotropic radiation field, it is:

$$U_\nu = \frac{4\pi}{c}I_\nu. \tag{45}$$

2.4 Radiation transport in the lines

Let's consider again the general solution of the transport equation (36):

$$I_\nu(0) = \int_0^{\tau^*_{nu}} S_\nu(\tau_\nu)e^{-\tau_\nu}\mathrm{d}\tau_\nu + I_{\nu 0}e^{-\tau^*_\nu}.$$

In order to determine I_ν, we have to know the source function $S_\nu = \epsilon_\nu/k_\nu$ in each point. In general, the absorption and emission of radiation are due to continuous processes, which arise from free-free, free-bound and bound-free transitions, and to discrete ones, generated only by bound-bound transitions. We can therefore separate the two contributions and write:

$$S_\nu(\tau_\nu) = \frac{\epsilon^K_\nu + \epsilon^L_\nu}{k^K_\nu + k^L_\nu}. \tag{46}$$

If we now focus on the line contribution, the total energy emitted in a certain direction per unit volume per unit time, due to a transition $n \to m$, is:

$$\int_{line} \epsilon_\nu\mathrm{d}\nu = \frac{1}{4\pi}h\nu_{nm}A_{nm}N_n, \tag{47}$$

where A_{nm} is the spontaneous transition probability coefficient (numerically equal to the number of transitions $n \to m$ which can occur per unit time, or, equivalently, to the inverse mean life time of the level n) and N_n is the particle densities of ions in the level n. It is convenient to define the normalized line profile as a function of frequency $\psi(\nu)$, such that:

$$\int_{line} \psi(\nu)\mathrm{d}\nu = 1 \tag{48}$$

so that the line emission coefficient can be expressed as:

$$\epsilon_\nu^L = \psi(\nu)\int_{line} \epsilon_\nu \mathrm{d}\nu = \frac{1}{4\pi} h\nu_{nm} A_{nm} N_n \psi(\nu). \tag{49}$$

On the other hand, the energy absorbed in a transition $m \to n$ per unit time, per unit volume, per unit solid angle is:

$$\int_{line} k_\nu I_\nu \mathrm{d}\nu = \frac{1}{4\pi} h\nu_{nm} N_m B_{mn} U_{\nu_{nm}} - \frac{1}{4\pi} h\nu_{nm} N_n B_{nm} U_{\nu_{nm}}, \tag{50}$$

where B_{mn} and B_{nm} are, respectively, the absorption probability coefficient and the stimulated emission coefficient, so that the right hand side of Eq. (50) accounts for the energy that is subtracted from the beam by absorptions and the energy that is added back to it, because of stimulated emissions. If we assume that I_ν is constant and isotropic in the line, we can assume $U_\nu = 4\pi I_\nu / c$ (Eq. 45) and, taking the intensity out of integration in Eq. (50), we get:

$$\int_{line} k_\nu \mathrm{d}\nu = \frac{h\nu_{nm}}{c}(B_{mn}N_m - B_{nm}N_n). \tag{51}$$

To find the line absorption coefficient, we simply have to multiply this integral by the normalized line profile $\psi(\nu)$, so that it is:

$$k_\nu^L = \frac{h\nu_{nm}}{c}(B_{mn}N_m - B_{nm}N_n)\psi(\nu). \tag{52}$$

The spontaneous and stimulated transition probabilities A_{nm}, B_{nm} and B_{mn} are named *Einstein coefficients* and are related together by general expressions, that can be derived in conditions of thermodynamic equilibrium. In such conditions, indeed, all the reactions relating levels $n \rightleftharpoons m$ ($n > m$) are perfectly balanced, and we can set up a statistical balance equation between the radiative transitions connecting the levels:

$$U_\nu B_{mn} N_m = N_n[A_{nm} + U_\nu B_{mn}]. \tag{53}$$

Solving Eq. (53) for U_ν, we get:

$$U_\nu = \frac{N_n A_{nm}}{N_m B_{mn} - N_n B_{nm}}$$

that can be re-arranged in:

$$U_\nu = \frac{A_{nm}}{\frac{N_m}{N_n}B_{mn} - B_{nm}}. \tag{54}$$

For an isotropic radiation field of low frequency, the thermodynamical equilibrium condition implies that:

$$\frac{N_m}{N_n} = \frac{g_m}{g_n}e^{-\frac{h\nu_{nm}}{k_B T}} \approx \frac{g_m}{g_n}\left(1 - \frac{h\nu_{nm}}{k_B T}\right) \tag{55a}$$

$$U_\nu = \frac{4\pi}{c}I_\nu \approx \frac{4\pi}{c}2\left(\frac{\nu}{c}\right)^2 k_B T = \frac{8\pi\nu^2}{c^3}k_B T, \tag{55b}$$

where we made use of the Rayleigh-Jeans approximation of the black body distribution:

$$B_\nu(T) = I_\nu \approx 2\left(\frac{\nu}{c}\right)^2 k_B T$$

that holds at low frequencies. Since Eq. (54) must be equal to Eq. (55b), it turns out that:

$$\frac{A_{nm}}{\frac{N_m}{N_n}B_{mn} - B_{nm}} = \frac{8\pi\nu^2}{c^3}k_B T,$$

which is satisfied by the solution:

$$A_{nm} = \frac{8\pi h\nu^3}{c^3}B_{nm}, \tag{56a}$$

$$g_n B_{nm} = g_m B_{mn} \tag{56b}.$$

Using Eq. (56a,b), we can write the expression of k_ν^L in Eq. (52) in the form:

$$k_\nu^L = \frac{h\nu_{nm}}{c}\psi(\nu)N_m B_{mn}\left[1 - \frac{g_m N_n}{g_n N_m}\right] \tag{57}$$

and, introducing Eq. (56a) in the expression of ϵ_ν^L (Eq. 49):

$$\epsilon_\nu^L = \frac{2h^2\nu^4}{c^3}N_n\psi(\nu)\frac{g_m}{g_n}B_{mn}. \tag{58}$$

The source function in the line is then given by the ratio between Eq. (58) and Eq. (57):

$$S_\nu^L = \frac{2h\nu^3}{c^2}\left(\frac{g_n N_m}{g_m N_n} - 1\right)^{-1}. \tag{59}$$

Since in thermodynamic equilibrium the level population follows the Boltzmann distribution:

$$\frac{N_n}{N_m} = \frac{g_n}{g_m}\exp\left(-\frac{h\nu_{nm}}{k_B T}\right), \tag{60}$$

the expression of S_ν^L reduces to:

$$S_\nu^L = \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu_{nm}}{k_B T}} - 1}$$

that is the Planck distribution, in agreement with the solution of the transport equation in thermodynamical equilibrium of Eq. (39).

2.5 Deviations from thermodynamic equilibrium

Equations (57), (58) and (59) give us the general expressions of the absorption coefficient, of the emission coefficient and of the source function within a spectral line. We now want to determine the ratio between the level populations, without assuming our system to be in thermodynamic equilibrium. Instead, we assume a *steady state*, i.e. a condition where there are **no temporal variation of the level population**.

We define:

- R_{nm} the velocity of radiative transitions $n \to m$
- C_{nm} the velocity of collisional transitions $n \to m$

The steady state assumption implies that the condition:

$$\frac{\mathrm{d}N_n}{\mathrm{d}t} = N_n \sum_m (R_{nm} + C_{nm}) - \sum_m N_m (R_{mn} + C_{mn}) = 0 \tag{61}$$

is satisfied for each level n. To obtain the level population, we must solve a system of equations like Eq. (61), called *statistical equations*, for each level. In addition, the complete solution would require the sums over m to be extended and to include the continuously distributed states, in order to account also for ionizations from the level n. A similar system of equations canbe introduced to describe the *ionization equilibrium*, for which we have that the number of ionizations equals the number of recombinations.

For the moment, let's just consider the statistical equations for bound state only, under the effect of radiative and collisional transitions. The transition rates can be expressed as:

$n > m$ departures	$n < m$ departures
$R_{nm} = A_{nm} + B_{nm}U_\nu$	$R_{nm} = B_{nm}U_\nu$
$C_{nm} = N'Q_{nm}$	$C_{nm} = N'Q_{nm}$
$n > m$ arrivals	$n < m$ arrivals
$R_{mn} = B_{mn}U_\nu$	$R_{mn} = A_{mn} + B_{mn}U_\nu$
$C_{mn} = N'Q_{mn}$	$C_{mn} = N'Q_{mn}$

where we have introduced the collision partner density N' and the rate of the collisional efficiency Q_{nm}, expressing the frequency of effective collisions for a gas of unit density (therefore measured in $\mathrm{cm^3s^{-1}}$).

With this distinction and an isotropic radiation field, we can set up the steady state equation for each level n:

$$N_n \left\{ \sum_m B_{nm} \frac{4\pi}{c} I_\nu + \sum_{m<n} A_{nm} + N' \sum_m Q_{nm} \right\} =$$

$$= \sum_m N_m B_{mn} \frac{4\pi}{c} I_\nu + \sum_{m>n} N_m A_{mn} + N' \sum_m N_m Q_{mn}. \tag{62}$$

The complete solution of the level populations is achieved by solving Eq. (62) for all the levels, together with the transport equation, accounting for the presence of the radiation field, which, in this case, becomes:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -\frac{h\nu_{nm}}{c} B_{mn} N_m \left(1 - \frac{g_m N_n}{g_n N_m} \right) \psi(\nu) I_\nu + \frac{h\nu_{nm}}{4\pi} A_{nm} N_n \psi(\nu). \tag{63}$$

We shall see later on how these equations can be used to solve some specific problems, under suitable assumptions for the cases of astrophysical environments.

3 Scattering processes and kinetic temperature

3.1 The cross-section of collisional interactions

In §2.2, while comparing the processes that can occur in astrophysical plasmas, we met the concept of cross-section. In general, a cross-section is the area that must be hit in order for a certain process to take place. For particle interactions, we can practically define the particle cross-section as a surface having the same radius as the particle radius. The particle radius, in its turn, is defined as

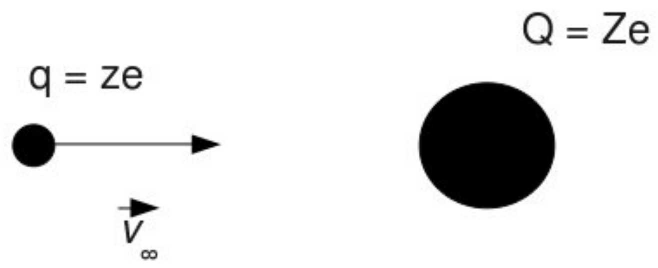

Figure 8: A test particle q approaching a target particle Q with initial velocity v_∞.

the minimum distance that can be reached by a particle of the same sign, approaching from infinity with a velocity v_∞. Considering the situation illustrated in Fig. 8, the minimum distance is reached when the initial kinetic energy of the approaching particle has been fully converted into positional energy in the target particle's field:

$$\frac{m_q v_\infty^2}{2} = \frac{zZe^2}{r_0^2}. \tag{64}$$

Solving for r_0, it is:

$$r_0 = 2\frac{zZe^2}{mv_\infty^2} \tag{65}$$

and the cross-section is simply $\sigma = \pi r_0^2$.

It can be immediately seen that the cross-section depends on the particle potentials and relative velocities. Let's assume that, in a gaseous nebula, the ions (or molecules) and their collisional partners have, respectively, the average velocities v_A and v_S. Clearly, their relative velocity will be $v = v_A - v_S$. If $\sigma(v)$ is the cross-section of the ions with respect to their collisional partners, the volume swept by one particle in a second is:

$$V = \sigma(v)v \tag{66}$$

and, being N' the density of collisional partners, the rate of collisions becomes:

$$C(v) = N'v\sigma(v). \tag{67}$$

The quantity $C(v)/N'$ has the same dimensions of the rate of collisional efficiency $Q(v)$, thus we can define:

$$Q(v) = v\sigma(v) \tag{68}$$

and write:

$$C(v) = N'Q(v).$$

When we are dealing with inelastic scattering, we express the cross-section of the transition $n \to m$ as $\sigma_{nm}(v)$ and the related coefficients Q_{nm} are obtained averaging over all the relative velocities between atoms and their collisional partners. If we only had elastic scatterings, the distribution of relative velocities would become a Maxwellian function. Deviations from this distribution are due to the inelastic scatterings that can occur when collisional excitations are followed by radiative de-excitations. This process subtracts energy from the gas and, for this reason, the high energy tail of the velocity field is missing.

Concerning the rates of collisional efficiency, we said that $Q_{mn} =< v\sigma_{mn}(v) >$. For particles such as H I, H II, He I and He II that interact with e^-, the collisions are elastic up to energies of $\sim 10\,\mathrm{eV}$ and anelastic scatterings, due to collisions with heavier ions or molecules, are less frequent, because of their lower abundances. As a consequence, in H I and H II regions we should expect relative variations from a Maxwellian distribution of velocities to be in the order of $\sim 10^{-5}$. In addition, within a volume of a few mean free paths, all the particles have the same kinetic temperature, so that we can assume that all the kinds of particles present follow a Maxwellian velocity distribution. This is of fundamental importance, because it implies that also the relative velocities v follow the same distribution, given by:

$$\phi(v,T)\mathrm{d}v = \frac{1}{\sigma^3(2\pi)^{3/2}} e^{-\frac{v^2}{2\sigma^2}} \mathrm{d}v_x \mathrm{d}v_y \mathrm{d}v_z, \tag{69}$$

or, in polar coordinates:

$$\phi(v,T)\mathrm{d}v = \frac{4\pi}{\sigma^3(2\pi)^{3/2}} v^2 e^{-\frac{v^2}{2\sigma^2}} \mathrm{d}v, \tag{70}$$

where we have:

$$v^2 = v_x^2 + v_y^2 + v_z^2$$
$$\frac{1}{2}\frac{m_A m_e}{m_A + m_e}\overline{v_x^2} = \frac{1}{2}k_B T$$
$$\sigma^2 = \overline{v_x^2} = \left(\frac{1}{m_A} + \frac{1}{m_e}\right) k_B T \approx \frac{k_B T}{m_e}.$$

3.2 The rate of collisional efficiency

Taking into account the transition $n \to m$ $(n > m)$, the rate of collisional efficiency is given by:

$$Q_{nm} = \overline{v\sigma_{nm}(v)} = \int_0^\infty v\sigma_{nm}(v)\phi(v,T)\mathrm{d}v. \tag{71}$$

If excitations and de-excitations are dominated by collisional processes, we can assume the system to be in thermodynamic equilibrium and we can derive a general relation between Q_{nm} and Q_{mn}. Indeed, from the balance of the processes, we have:

$$Q_{nm}N_nN_e = Q_{mn}N_mN_e \tag{72}$$

and, since the population ratio is again following the Boltzmann distribution:

$$\frac{Q_{mn}}{Q_{nm}} = \frac{N_n}{N_m} = \frac{g_n}{g_m}e^{-\frac{h\nu_{nm}}{k_BT}}. \tag{73}$$

In the case of collisions of atoms or ions with electrons, due to the low electron mass, with respect to that of any atom, and since

$$E_e = E_A \to v_{e^-} = \frac{m_A}{m_e}v_A$$

we can consider the atoms as non moving targets and take the relative velocities to be coincident with the electron velocities. If we consider a collision in which the kinetic energy of the electron is higher than the excitation energy of the ion's first excited level, part of the kinetic energy is converted into ion excitation energy and the electron flies away with a lower velocity (energy). In conditions of thermodynamic equilibrium, the number of excitation per unit volume and time, which occur by collisions with electrons in a particular energy range, must be equal to the number of de-excitations per unit volume and time, which send back the electrons to the same energy range (super-elastic scattering). If this happens in the range

$$v_1 - v_1 + \mathrm{d}v_1 \text{ for incoming } e^-$$
$$v_2 - v_2 + \mathrm{d}v_2 \text{ for outcoming } e^-$$

then:

$$N_eN_1v_1\sigma_{12}(v_1)\phi(v_1)\mathrm{d}v_1 = N_eN_2v_2\sigma_{21}(v_2)\phi(v_2)\mathrm{d}v_2. \tag{74}$$

Given that, in thermodynamic equilibrium it is:

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} e^{-\frac{\chi_{21}}{k_B T}} \tag{75}$$

and, from the energy balance:

$$\frac{1}{2} m_e v_1^2 = \chi_{21} + \frac{1}{2} m_e v_2^2 \tag{76}$$

we can derive:

$$v_1 \mathrm{d}v_1 = v_2 \mathrm{d}v_2, \tag{77}$$

introducing Eq. (75) and (77) into Eq. (74), we get:

$$\sigma_{12}(v_1)\phi(v_1) = \frac{g_2}{g_1} e^{-\frac{\chi_{21}}{k_B T}} \sigma_{21}(v_2)\phi(v_2). \tag{78}$$

Recalling Eq. (70), we can calculate the ratio:

$$\frac{\phi(v_2)}{\phi(v_1)} = \left(\frac{v_2}{v_1}\right)^2 \exp\left(\frac{m_e(v_2^2 - v_1^2)}{k_B T}\right) = \left(\frac{v_2}{v_1}\right)^2 \exp\left(\frac{\chi_{21}}{k_B T}\right). \tag{79}$$

Finally, we can write:

$$\sigma_{12}(v_1) = \frac{g_2}{g_1} \left(\frac{v_2}{v_1}\right)^2 \sigma_{21}(v_2). \tag{80}$$

The interaction cross-section of a collisional excitation is known from quantum mechanics to be:

$$\sigma_{12}(v_1) = \frac{\pi \hbar^2}{m_e^2 v_1^2} \frac{\Omega(1,2)}{g_1}, \tag{81}$$

where the quantity $\Omega(1,2)$ is called the collisional strength and gives the probability that the wavelength associated with the electron motion ($\lambda = h/p = h/mv$) can interact with the ion at different distances during the encounter. Comparing Eq. (80) and (81), we can also write:

$$\sigma_{21}(v_2) = \frac{\pi \hbar^2}{m_e^2 v_2^2} \frac{\Omega(1,2)}{g_2}. \tag{82}$$

The collisional de-excitation efficiency coefficient is, then:

$$Q_{21} = \int_0^\infty v \sigma_{21}(v)\phi(v) \mathrm{d}v =$$

$$= \int_0^\infty v \left[\frac{\pi \hbar^2}{m_e^2 v_2^2} \frac{\Omega(1,2)}{g_2}\right] \cdot \left[\frac{4}{\sqrt{\pi}} \left(\frac{m_e}{2 k_B T}\right)^{3/2} v^2 \exp\left(-\frac{m_e v^2}{2 k_B T}\right)\right] \mathrm{d}v =$$

$$= \frac{4 \pi^{1/2} \hbar^2}{g_2 m_e^{1/2} (2 k_B T)^{3/2}} \int_0^\infty \Omega(1,2) \exp\left(-\frac{m_e v^2}{2 k_B T}\right) \mathrm{d}v. \tag{83}$$

Plugging in the numbers, we get:

$$Q_{21} = \frac{8.629 \cdot 10^{-6}}{T^{1/2}} \frac{< \Omega(1,2) >}{g_2}. \tag{84}$$

Assuming that the factor $< \Omega(1,2) > /g_2$ lies between 1 and 10, and for temperatures in the range $10^4\,\mathrm{K} - 2{\cdot}10^4\,\mathrm{K}$ (achieved when photo-ionization is the main heating mechanism), it is found that $Q_{21} \sim 10^{-7}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$. For the typical densities of gaseous nebulae ($N_e \sim 10^4\,\mathrm{cm}^{-3}$), we have that $Q_{21}N_e \sim 10^{-3}\,\mathrm{s}^{-1}$. Even in the high density environment of the cores of Active Galactic Nuclei, where $N_e \sim 10^9\,\mathrm{cm}^{-3}$, it is $Q_{21}N_e \sim 10^2\,\mathrm{s}^{-1}$ and the emission of radiation through spontaneous radiative decays, which has a probability coefficient $A_{21} \sim 10^8\mathrm{s}^{-1}$, turns out to be 10^6 time more efficient in de-populating the first excited level of H.

4 Study of the population ratio in a two-level system

4.1 Dilution of radiation

The dilution factor is defined to account for the weakening of the radiation field at large distances from the source. If a star has radius R^* and the field is evaluated at a distance r from its center ($r >> R^*$), then the solid angle subtended by the star, as seen from the point of observation, is:

$$\Omega^* = \frac{\pi R^{*2}}{r^2}. \tag{85}$$

If the flux received in the observation point is $\Phi_\nu(r)$, then the mean specific intensity of the stellar disk at distance r is:

$$\overline{I_\nu^*}(r) = \frac{\Phi_\nu(r)}{\Omega^*}. \tag{86}$$

Therefore, at the surface of the star, we have:

$$\overline{I_\nu^*}(R^*) = \frac{\Phi_\nu(R^*)}{\pi} \tag{87}$$

but, because of energy conservation, we also have:

$$\frac{\overline{I_\nu^*}(r)}{\overline{I_\nu^*}(R^*)} = \frac{\Phi_\nu(r)\pi r^2}{\Phi_\nu(R^*)\pi R^{*2}} = 1 \tag{88}$$

i. e. **the specific intensity does not depend on distance.** The energy density is defined as:

$$U_\nu = \frac{1}{c}\int_{\Omega^*} \overline{I^*_\nu}\mathrm{d}\Omega = \frac{\overline{I^*_\nu}}{c}\Omega^* \tag{89}$$

and it is not isotropic. For use in the statistical equations, however, we have to deal with the radiation field as it were actually isotropic, so we define an equivalent isotropic radiation field I_ν, having the same energy density of the real one:

$$\frac{4\pi}{c} I_\nu = \frac{\Omega^*}{c}\overline{I^*_\nu}, \tag{90}$$

having:

$$I_\nu = \frac{\Omega^*}{4\pi}\overline{I^*_\nu}, \tag{91}$$

where we define the dilution factor:

$$W = \frac{\Omega^*}{4\pi}. \tag{92}$$

The dilution factor can be easily interpreted as the percentage of the celestial sphere that is covered by the source, as seen from the observing point.

We can compute, as an example, the dilution factor of the Sun, at the distance of the Earth. Since $\Omega^\odot = \pi R_\odot^2/r^2$, from Eq. (92) we have

$$W = \frac{\pi R_\odot^2}{4\pi r^2} \approx \frac{(7\cdot 10^5 \mathrm{km})^2}{4\cdot(150\cdot 10^6 \mathrm{km})^2} \approx 5.5\cdot 10^{-6}$$

It turns out that the dilution factors of radiation fields in the optical are generally very small numbers, as soon as the distance from the source exceeds a some tens of source radii. In other frequency ranges, on the other hand, the situation can be very different. In the radio domain, for instance, the dilution factor is $W \sim 1$ because nearly the entire sky can be source of radiation.

4.2 The two-level system in the optical range

Ions and molecules are characterized by complex energy structures, with many levels connected by different transitions. However, the mechanisms which are at the basis of spectral line formation and propagation can be better understood if we consider the transitions as independent from each other, sending back the treatment of further details to later sections. A single transition can be generally represented by only 2 levels (departure and arrival, with, in our notation, $E_2 > E_1$). We also make the following simplifying assumptions:

1. there are **no ionizations or recombinations**
2. the transitions $1 \rightleftharpoons 2$ occur in the optical range
3. the radiation field which surrounds the atom is a *diluted* black body of the form:

$$I_\nu = W B_\nu(T^*), \tag{93}$$

where $W << 1$ (because of assumption 2) is the dilution factor.

Under such assumptions, in the statistical equilibrium between the two levels:

$$N_1 \left(N_e Q_{12} + \frac{4\pi}{c} I_\nu B_{12} \right) = N_2 \left(A_{21} + N_e Q_{21} + \frac{4\pi}{c} I_\nu B_{21} \right) \tag{94}$$

we can neglect all the terms in which there is a contribution from I_ν and write:

$$N_1 N_e Q_{12} = N_2 (A_{21} + N_e Q_{21}), \tag{95}$$

that gives:

$$\frac{N_2}{N_1} = \frac{N_e Q_{12}}{N_e Q_{21} + A_{21}}. \tag{96}$$

Since in thermodynamical equilibrium it is:

$$N_1 Q_{12} = N_2 Q_{21} \tag{97}$$

we have that:

$$Q_{12} = Q_{21} \frac{g_2}{g_1} e^{-\frac{h\nu_{12}}{k_B T}}, \tag{98}$$

substituting Q_{12} in Eq. (95) and dividing by $N_e Q_{21}$ yields:

$$\frac{N_2}{N_1} = \frac{1}{1 + A_{21}/N_e Q_{21}} \frac{g_2}{g_1} e^{-\frac{h\nu_{12}}{k_B T}}. \tag{99}$$

We can therefore define a departure coefficient from thermodynamic equilibrium in the level n as:

$$b_n = \frac{N_n}{N_n^*}, \tag{100}$$

where N_n^* is the equilibrium population of level n. From Eq. (99), it turns out that the ratio:

$$\frac{b_2}{b_1} = \frac{1}{1 + A_{21}/N_e Q_{21}} \tag{101}$$

represents the deviation from thermodynamic equilibrium. Indeed, if collisional processes dominate over radiative ones, it is $N_e Q_{21} >> A_{21}$ and $b_2/b_1 \sim 1$, meaning that the relative populations of the two levels set as they would be in equilibrium. When, on the contrary, $A_{21} = N_e Q_{21}$ half of the de-excitations of collisionally excited levels occur via spontaneous radiative decay. For each transition, thus, we can define a *critical density*:

$$N_c = \frac{A_{21}}{Q_{21}}$$

such that if $N_e > N_c$ collisional de-excitations dominate and we do not see photons emitted in the line, while, if $N_e < N_c$ the spontaneous radiative decays can take place and the line is emitted by the medium. Therefore, the simple presence or absence of a spectral line is already an indicator of the density range where the ion species we are studying lies in.

4.3 The departure coefficients of permitted and forbidden lines

The most abundant element in the Universe is H. The transition $2^2p \rightarrow 1^2s$ leads to the emission of a photon of frequency $\nu = 2.46 \cdot 10^{15}\,\mathrm{Hz}$ ($\lambda = 1216\,\text{Å}$, Lyman α), with an average lifetime of the excited level of $t \sim 10^{-8}\,\mathrm{s}$. The transition probability is given by the inverse lifetime and it is $A_{21} \sim 10^{8}\,\mathrm{s}$. These orders of magnitude apply fairly well to permitted transitions. If the gas temperature approaches the typical value of a photo-ionized nebula ($T \sim 10^4\,\mathrm{K}$) the collisional de-excitation was estimated in $Q_{21} \sim 10^{-7}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$ (cfr. §3.2) and, with an electron density $N_e \sim 10^4\,\mathrm{cm}^{-3}$, we have:

$$\frac{b_2}{b_1} = \frac{1}{1 + A_{21}/N_e Q_{21}} \sim 10^{-11}$$

and all the atoms are in their ground level.

If we now consider a different ion, that is commonly found in photo-ionized nebulae, namely O III, there is a complex transition system, that is illustrated in the Grötrian diagram of Fig. 9. The transitions plotted on the diagram are forbidden by violation of the illustrated selection rules. The involved levels, that are called *metastable*, are not populated via cascade recombination from higher levels, since we do not observe the corresponding emission lines, neither they can be excited by absorption of radiation, because the transition is forbidden. Therefore, they can only be populated by collisional excitation from the ground

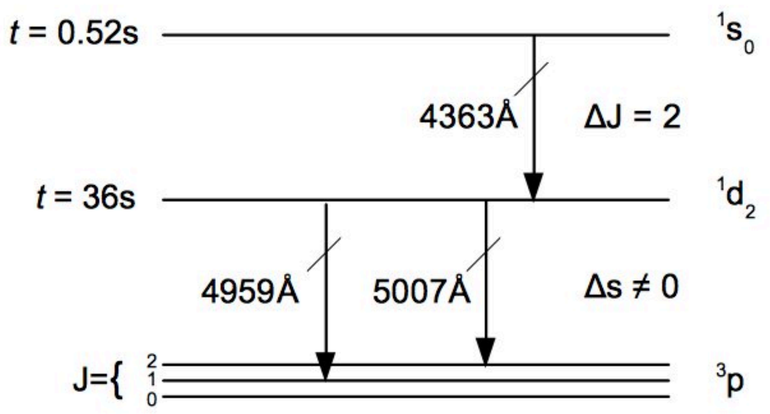

Figure 9: Grötrian diagram for the forbidden transitions of [O III] in the optical spectrum.

level (a bound-bound process). Under the assumption of a diluted radiation field, we can still neglect ionizations and recombinations, and just take collisions into account.

Assuming again $T \sim 10^4\,\mathrm{K}$ and $N_e \sim 10^4\,\mathrm{cm}^{-3}$ and considering the transition system $2 \to 1$, for which we have:

$$A_{21}(5007) \approx 2.1 \cdot 10^{-2}\mathrm{s}^{-1}$$

$$A_{21}(4959) \approx 0.7 \cdot 10^{-2}\mathrm{s}^{-1}$$

it is:

$$\frac{b_2}{b_1} = \frac{1}{1 + A_{21}/N_e Q_{21}} \sim 10^{-1}$$

which is 10 good orders of magnitude than the value that we found for the permitted transitions of H. This means that the population of the excited level of an ion with forbidden transitions is favored by a factor 10^{10} with respect to the case of permitted transitions. If we compare the emission coefficients of the forbidden and permitted lines, we find that:

$$\frac{\epsilon^L_{\nu\ (permitted)}}{\epsilon^L_{\nu\ (forbidden)}} = \frac{(N_2 A_{21})_{(permitted)}}{(N_2 A_{21})_{(forbidden)}} \sim 1$$

(remember the fundamental assumption of low density radiation field), meaning that, in the case of a line emitting nebula of proper density, we can expect the forbidden lines to be as strong as the permitted ones.

4.4 Conditions for the emission of forbidden lines

In the case of photons arising from forbidden lines, the nebula is transparent and the radiation we observe is the whole radiation produced by all the ions in the nebula. As a consequence there is no need to solve the transport equation and we simply get:

$$I_\nu = \int_0^{\tau_\nu^*} S_\nu \mathrm{d}\tau_\nu + I_{\nu 0}, \tag{102}$$

where we called $I_{\nu 0}$ the intensity of the continuum under the emission line. Recalling the definition of the source function and the expression of the optical depth (Eq. 32), since radiation is not re-absorbed, from Eq. (102) we can estimate the intensity of the emission line as:

$$I_\nu^L = I_\nu - I_{\nu 0} = \epsilon_\nu r^* \tag{103}$$

and what we observe is the real intensity of the line over the continuum produced throughout the nebula. Introducing the expression of the line emission coefficient (Eq. 49):

$$I_\nu^L = \frac{1}{4\pi} N_2 A_{21} h\nu_{21} \psi(\nu) r^*. \tag{104}$$

Therefore, the intensity of a forbidden line depends on the population of the excited level and on the coefficient of spontaneous emission.

We can try to estimate the number of emitted photons per ion J. This number will be equal to the number of collisional excitations that are not subsequently de-excited by another collision and can, therefore, decay through a spontaneous radiative emission. Put into equations, this is:

$$J = \frac{N_2 A_{21}}{N_1} - \frac{N_2 N_e Q_{21}}{N_1}. \tag{105}$$

Eq. (105) can also be expressed as:

$$J = \frac{N_2}{N_1}(A_{21} - N_e Q_{21}) = (A_{21} - N_e Q_{21}) \frac{g_2}{g_1} \frac{e^{-\frac{h\nu_{12}}{k_B T}}}{1 + A_{21}/N_e Q_{21}}, \tag{106}$$

from which we get:

$$J = \frac{(A_{21} - N_e Q_{21})}{(A_{21} + N_e Q_{21})} N_e Q_{21} \frac{g_2}{g_1} e^{-\frac{h\nu_{21}}{k_B T}}. \tag{107}$$

The zeroes of Eq. (107) can be obtained for:

$$N_e Q_{21} = 0 \qquad N_e Q_{21} = A_{21}$$

while we get a maximum for:

$$N_e Q_{21} = 0.41 A_{21}.$$

So, for $N_e = 0.41 N_c$ we have the maximum line intensity (flash of I_ν^L). At lower densities, the line intensity decreases because the excited levels are not sufficiently populated, while, for $N_e \geq N_c$ the emission line is again suppressed, because of collisional de-population of the excited level.

Summarizing, there are 3 fundamental conditions to produce a strong forbidden emission line:

1. a temperature T high enough to provide the electrons with the required kinetic energy to populate the metastable levels
2. an electron density in the range $0.1 N_c \leq N_e \leq N_c$
3. a diluted radiation field (otherwise the metastable levels could be easily destroyed, since an optical-UV photon may be energetic enough to further ionize the excited ion).

4.5 The two-level system at radio frequencies

In the case our ion or molecule has two energy levels that are connected by a transition in the radio domain, because of the diffuse background radiation (mainly the *Cosmic Microwave Background* CMB), the radiation field comes from all directions and it has a dilution factor $W \sim 1$. Using again the Rayleigh-Jeans approximation of the black body function (holding at low frequencies), we have a thermal source with specific intensity:

$$I_\nu = 2\left(\frac{\nu}{c}\right)^2 k_B T_S, \tag{108}$$

where T_S is the radiation temperature.

In these new conditions, the general statistical equilibrium of the two levels, described by Eq. (94), becomes:

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} \frac{N'(Q_{21}/A_{21}) e^{-(h\nu_{21}/k_B T)} + W[e^{(h\nu_{21}/k_B T_s)} - 1]^{-1}}{1 + N'(Q_{21}/A_{21}) + W[e^{(h\nu_{21}/k_B T_s)} - 1]^{-1}}, \tag{109}$$

where N' is the density of the collisional partners, that, in this case, are mainly other ions and molecules. Using the approximation:

$$e^x \approx 1 + x$$

that applies when $x << 1$, we can re-arrange Eq. (109) in:

$$\frac{N_2}{N_1} = \frac{g_2}{g_1}\frac{e^{-(h\nu_{21}/k_BT)} + (A_{21}/N'Q_{21})(k_BT_S/h\nu_{21})}{1 + (A_{21}/N'Q_{21}) + (A_{21}/N'Q_{21})(k_BT_S/h\nu_{21})}. \tag{110}$$

In the limit of $A_{21}/N'Q_{21} << 1$ (dominating collisions), Eq. (110) reduces to the Boltzmann formula and we have thermodynamic equilibrium.

We can notice that Eq. (110) involves two different temperatures:

- T the kinetic temperature of the collisional partners
- T_S the radiation temperature

We introduce a third artificial definition of temperature, called the *excitation temperature* T_E, such that the population ratio is:

$$\frac{N_2}{N_1} = \frac{g_2}{g_1}e^{-(h\nu_{21}/k_BT_E)}. \tag{111}$$

Since we are in the radio regime, it turns out that

$$h\nu_{21} << k_BT_E < k_BT_S < k_BT$$

and, given that

$$e^{-(h\nu_{21}/k_BT_i)} \approx 1 - \frac{h\nu_{21}}{k_BT_i}$$

for any i, we can introduce the quantity:

$$x = \frac{A_{21}}{N'Q_{21}}\frac{k_BT_S}{h\nu_{21}}. \tag{112}$$

Combining Eq. (111) and (110), with the use of Eq. (112) and the exponential approximation, we get:

$$\frac{1}{T_E} = \frac{(x/T_S) + (1/T)}{1 + x}. \tag{113}$$

Looking at the expression of x, we see that:

$$x = \frac{(N'Q_{21})^{-1}}{(A_{21}k_BT_S/h\nu_{21})^{-1}} = \frac{t_u}{t_S}$$

i.e. x represents the ratio of the average lifetimes of the excited level against the collisional and the radiative decays. Indeed, recalling the general equation of statistical equilibrium for a two-level system (Eq. 94), we have that:

$$t_u = \frac{1}{N'Q_{21}} \tag{114}$$

is the mean lifetime in presence of collisional processes only, while:

$$t_S = \frac{1}{A_{21} + B_{21} 4\pi I_\nu / c} \tag{115}$$

is the mean lifetime in presence of radiative processes only. Using Eq. (56a) to remember that:

$$A_{21} = \frac{8\pi h \nu^3}{c^3}$$

and estimating I_ν as in Eq. (108), we can express the denominator of Eq. (115) as:

$$\begin{aligned} B_{21}\frac{4\pi}{c} I_\nu + A_{21} &= A_{21}\left(\frac{c^3}{8\pi h\nu^3}\frac{4\pi}{c} I_\nu + 1\right) = \\ &= \left(\frac{k_B T_S}{h\nu} + 1\right) A_{21} \approx \frac{k_B T_S}{h\nu} A_{21} \end{aligned} \tag{116}$$

from which Eq. (115) is justified. Eq. (113) can be, therefore, re-written in terms of mean lifetimes:

$$\frac{1}{T_E} = \frac{(t_u/T_S) + (t_S/T)}{t_u + t_S}. \tag{117}$$

We see immediately that, in the limit $t_S >> t_u$ the collisional processes dominate, then the excitation temperature coincides with the kinetic temperature of the collisional partners (*thermodynamical equilibrium*). On the other hand, if $t_u >> t_S$, radiative processes are dominating and we get $T_E \approx T_S$.

Even in the radio case, based on the lifetimes of the considered energy levels, we can determine the level population, if we assume that Eq. (111) applies, with T_E giving either an estimate of T or T_S, depending on the ratio t_u/t_S.

4.5.1 The H I 21 cm line

H I emits a very important line, arising from a hyper-fine structure transition, involving an inversion of the electron spin vector, with respect to the nuclear spin. The energy gap is $\Delta E = 5.9 \cdot 10^{-6}\,\mathrm{eV}$, corresponding to a frequency $\nu = 1420\,\mathrm{MHz}$, the excited state is the one with both the electron and nuclear spin pointing in the same direction, while the ground state is the one where the two vectors are opposed. This line is originated in H I regions (outside the border of H II regions, where all the ionizing photons have been absorbed, as we shall discuss later on), where the ionization is low. In these regions the collisional partners are other H I atoms and the following conditions apply:

$$T \sim 100\,\mathrm{K} \qquad Q_{21} \sim 10^{-10}\,\mathrm{cm^3\,s^{-1}} \qquad A_{21} \approx 2.87 \cdot 10^{-15}\mathrm{s}^{-1}$$

Measuring the energy gap in eV, it is:

$$\frac{k_B T_S}{h\nu} = \frac{T_S}{11600\Delta E}$$

and

$$x = \frac{(N_H Q_{21})^{-1}}{(A_{21} k_B T_S/h\nu)^{-1}} = 4 \cdot 10^{-4} \frac{T_S}{N_H}$$

Considering only the background radiation at $T_S \approx 3\,\mathrm{K}$, we have that $x << 1$ implies $N_H > 10^{-3}\,\mathrm{cm}^{-3}$, that, at the typical densities of an atomic cloud ($0.1\,\mathrm{cm}^{-3} \leq N_H \leq 1\,\mathrm{cm}^{-3}$) is certainly satisfied. The H I excitation temperature is called *spin temperature* and it gives a reliable estimate of the kinetic temperature of particles in the cloud.

4.5.2 The CO line at 2.6 mm

Let's now move to the case of a molecular cloud and consider the CO emission line at 2.6 mm. The most frequent collisional partners are H_2 molecules and the environmental conditions are:

$$T_K \sim 10 - 30\,\mathrm{K} \qquad Q_{21} \sim 2 \cdot 10^{-12}\,\mathrm{cm}^3\,\mathrm{s}^{-1} \qquad A_{21} \approx 6 \cdot 10^{-8}\mathrm{s}^{-1}$$

and the line corresponds to a rotational transition with $\Delta E = 4.8 \cdot 10^{-4}\,\mathrm{eV}$. Putting all the numbers together, we have that:

$$x \approx 5 \cdot 10^3 \frac{T_S}{N'}$$

In very dense clouds, we can easily reach $N' \geq 5 \cdot 10^4\,\mathrm{cm}^{-3}$ and the level population is again governed by the kinetic temperature of the collisional partners. In the intermediate cases, both the kinetic and radiation temperature affect the distribution of the level populations.

4.6 H I column densities from measurements of the 21 cm emission line

Due to the hyper-fine structure of the H I fundamental level, we can consider the term $1^2 s_{1/2}$ as a doublet with an excited stage $F = 1$ and a ground level $F = 0$. The lifetime of the level $F = 1$ is $t \approx 3.5 \cdot 10^{14}\,\mathrm{s}$ (forbidden transition). The emission coefficient is, as usual:

$$\epsilon_\nu^L = \frac{N_1}{4\pi} h\nu_{10} A_{10} \psi(\nu) \tag{118}$$

and, since H I is characterized by the spin temperature, we can assume that, within the line:

$$\frac{\epsilon_\nu^L}{k_\nu^L} = B_\nu(T_{spin}) \approx 2\left(\frac{\nu_{10}}{c}\right)^2 k_B T_{spin}, \tag{119}$$

where we used the Rayleigh-Jeans approximation, holding in the radio domain. From the observations of the radio line, we can measure the so-called *brightness temperature*:

$$I_\nu^L(T_b) = 2\left(\frac{\nu_{10}}{c}\right)^2 k_B T_b. \tag{120}$$

If the radiation is entirely produced by emission of H I along the line of sight, it is:

$$I_{\nu 0}^L = \int_0^{\tau^*} \frac{\epsilon_\nu^L}{k_\nu^L} e^{-\tau_\nu} \mathrm{d}\tau_\nu, \tag{121}$$

that, using Eq. (119) and (120), becomes

$$2\left(\frac{\nu_{10}}{c}\right)^2 k_B T_b = 2\left(\frac{\nu_{10}}{c}\right)^2 k_B T_{spin}(1 - e^{-\tau^*}),$$

which yields

$$T_b = T_{spin}(1 - e^{-\tau^*}).$$

If there is no absorption ($\tau^* << 1$) and the emission arises from atoms with constant spin temperature:

$$T_b = T_{spin}\tau^*.$$

Dividing Eq. (118) by Eq. (119), we get the line absorption coefficient:

$$k_\nu^L = \frac{N_1 \psi(\nu)}{8\pi(\nu_{10})^2}\left(\frac{h\nu_{10}}{k_B T_{spin}}\right) A_{10} c^2, \tag{122}$$

so that we can evaluate the optical depth within the line:

$$\tau_\nu^* = \int_0^{s^*} k_\nu^L \mathrm{d}s = \frac{A_{10}c^2}{8\pi\nu_{10}^2}\left(\frac{h\nu_{10}}{k_B T_{spin}}\right)\int_0^{s^*} N_1 \mathrm{d}s, \tag{123}$$

where the quantity:

$$n_1 = \int_0^{s^*} N_1 \mathrm{d}s \tag{124}$$

is called *column density* and express the number of ions which lie in a column of unit base along the line of sight and is measured in cm^{-2}. To evaluate n_1, we consider the Boltzmann equation in the form:

$$\frac{n_1}{n_0} = \frac{g_1}{g_0} e^{-(h\nu_{10}/k_B T_{spin})}$$

with the statistical weights:

$$F = 1 \rightarrow g_1 = (2F+1) = 3$$

$$F = 0 \rightarrow g_1 = (2F+1) = 1$$

so that:

$$\frac{n_1}{n_0} = 3e^{-0.07/T_{spin}} \approx 3.$$

For the total H I column density, we have:

$$n_H = n_0 + n_1 = \frac{n_1}{3} + n_1 = \frac{4}{3}n_1$$

so that, in the whole column:

$$\tau_\nu^* = \frac{A_{10}c^2}{8\pi\nu_{10}^2}\left(\frac{h\nu_{10}}{k_B T_{spin}}\right)\frac{3}{4}n_H$$

and, therefore:

$$n_H = \frac{4}{3}\tau_\nu^*\frac{8\pi\nu_{10}^2}{A_{10}c^2}\left(\frac{k_B T_{spin}}{h\nu_{10}}\right) =$$
$$= \frac{32\pi}{3}\left(\frac{k_B T_{spin}}{hc\lambda_{10}}A_{10}\right)\tau_\nu^* \approx 2.8\cdot 10^{14}\tau_\nu^* T_{spin}.$$

Since the quantity actually measured is $\tau\nu^* T_{spin} = T_b$, we can estimate the column density as:

$$n_H \approx 2.8\cdot 10^{14} T_b$$

and, given an estimate on the dimension of the cloud, we can draw a lower limit to the gas density N_H of the cloud.

4.7 Line intensity as a function of density and temperature

To determine the intensity of a line, we must solve the transport equation:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}\tau_\nu} = I_\nu - \frac{\epsilon_\nu^L}{k_\nu^L}$$

for which we need an expression of the source function:

$$S_\nu^L = \frac{\epsilon_\nu^L}{k_\nu^L} = \frac{2h\nu^3}{c^2}\left[\frac{g_n N_m}{g_m N_n} - 1\right]^{-1}$$

together with the statistical equations:

$$\underbrace{N_n \left\{ \sum_m B_{nm} \frac{4\pi}{c} I_\nu + \sum_{m<n} A_{nm} + N' \sum_m Q_{nm} \right\}}_{\text{departures from level } n} =$$

$$= \underbrace{\sum_m N_m B_{mn} \frac{4\pi}{c} I_\nu + \sum_{m>n} N_m A_{mn} + N' \sum_m N_m Q_{mn}}_{\text{arrivals to level } n}$$

If we consider the case of a diluted radiation field, we can neglect induced emission and radiative excitation and only take into account collisional excitations, collisional de-excitations and spontaneous emissions. In such circumstances we do no longer have to solve the radiative transport equation. This condition is actually verified for:

- lines arising from collisional excitation of heavy ions
- the optical recombination lines for an optically thin gaseous nebula

We recall that for the expression of the specific intensity of an emission line:

$$I_\nu^L = \int_0^{\tau_\nu^*} S_\nu^L e^{-\tau_\nu} \mathrm{d}\tau_\nu$$

since it is:

$$S_\nu^L \mathrm{d}\tau_\nu = \epsilon_\nu^L$$

in the optically thin case we can write:

$$I_\nu^L = \int_0^{r^*} \frac{h\nu_{nm}}{4\pi} N_n A_{nm} \psi(\nu) \mathrm{d}r, \tag{125}$$

where we used the line emission coefficient defined in Eq. (49). If we assume constant density and temperature and we take into account two emission lines, departing from different excited levels n and n', but with the same lower level m and the same profile $\psi(\nu)$, their intensity ratio will be:

$$\frac{I_{nm}^L}{I_{n'm}^L} = \left(\frac{\nu_{nm}^L}{\nu_{n'm}^L}\right) \left(\frac{A_{nm}^L}{A_{n'm}^L}\right) \left(\frac{N_n}{N_{n'}}\right). \tag{126}$$

Since, for optically thin lines in diluted radiation field, we can express the population ratio as in Eq. (99):

$$\frac{N_n}{N_m} = \frac{g_n}{g_m} \frac{e^{-h\nu_{nm}/k_B T}}{1 + A_{nm}/N_e Q_{nm}},$$

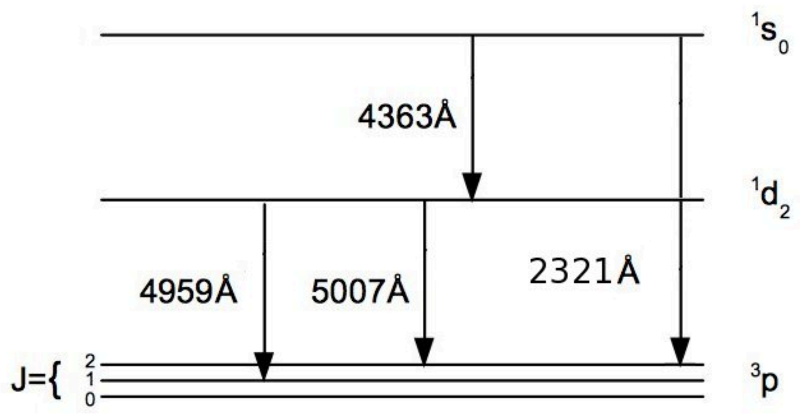

Figure 10: The transition scheme of [O III].

so that:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{g_n}{g_{n'}}\left(\frac{\nu_{nm}}{\nu_{n'm}}\right)\left(\frac{A_{nm}}{A_{n'm}}\right)\left(\frac{1+A_{nm}/N_eQ_{nm}}{1+A_{n'm}/N_eQ_{n'm}}\right)\exp\left[-\frac{h(\nu_{nm}-\nu_{n'm})}{k_BT}\right]. \tag{127}$$

4.7.1 Determination of the gas density

If we consider an emission line doublet, with the two excited levels very close in energy ($\nu_{nm} \approx \nu_{n'm}$), the exponential term of Eq. (127) is of the order of ~ 1 and the intensity ratio only depends on N_e:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{g_n}{g_{n'}}\frac{A_{nm}}{A_{n'm}}\left(\frac{1+A_{nm}/N_eQ_{nm}}{1+A_{n'm}/N_eQ_{n'm}}\right). \tag{128}$$

For the high density limit ($N_e >> 1\,\mathrm{cm}^{-3}$), Eq. (128) reduces to:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{g_n}{g_{n'}}\frac{A_{nm}}{A_{n'm}},$$

while, for the low density regime ($N_eQ << A$), we have:

$$\frac{I^L_{nm}}{I^L_{n'm}} = \frac{g_n}{g_{n'}}\frac{Q_{nm}}{Q_{n'm}} = \frac{<\Omega(n,m)>}{<\Omega(n',m)>},$$

where we made use of the general expression for the rate of the collisional processes Q_{nm} given in Eq. (84).

4.7.2 Determination of the gas temperature

In order to determine the gas temperature, we need a system of forbidden emission lines arising from two different and distant metastable levels. In this case, indeed, the dependence of the intensity ratio on temperature of Eq. (127) becomes very strong. A similar case is produced by the [O III] transition system, that we report again in Fig. 10. This is a three-level system that, in absence of radiative excitation and induced emission, has a statistical equilibrium of the form:

$$(N_1 Q_{12} + N_3 Q_{32}) N_e + N_3 A_{32} = N_2 A_{21} + N_2 N_e (Q_{21} + Q_{23}) \tag{129}$$

for level 2 ($^1d_2$) and:

$$(N_1 Q_{13} + N_2 Q_{23}) N_e = N_3 (A_{31} + A_{32}) + N_3 N_e (Q_{32} + Q_{31}) \tag{130}$$

for level 3 ($^1s_0$). Eq. (129) and (130) can be solved together, for the level occupation numbers, and they yield:

$$N_2 = \frac{N_1 N_e \{Q_1 2[A_{31} + A_{32} + N_e(Q_{31} + Q_{32})] + Q_{13}(N_e Q_{32} + A_{32})\}}{N_e Q_{23}(N_e Q32 + A_{32}) + [A_{21} + Ne(Q_{21} + Q_{23})][A_{31} + A_{32} + N_e(Q_{31} + Q_{32})]}$$

$$N_3 = \frac{N_e N_1 Q_{13} + N_e N_2 Q_{23}}{A_{31} + A_{32} + N_e(Q_{32} + Q_{31})}.$$

For this particular ion, we have:

$$A_{31}(2321) = 2.3 \cdot 10^{-1}\,\mathrm{s}^{-1}$$

$$A_{32}(4363) = 1.6\,\mathrm{s}^{-1}$$

$$A_{21}(5007) = 2.1 \cdot 10^{-2}\,\mathrm{s}^{-1}$$

$$A_{21}(4959) = 0.7 \cdot 10^{-2}\,\mathrm{s}^{-1}$$

which implies $A_{32} >> A_{31}$. In addition, due to the fact that $I_\nu^L(4363)$ is very small at low density, the 3^{rd} level is charged by collisions. However, since $Q_{13} << Q_{23}$, due to the larger energy gap, and that Q_{32} and Q_{31} do not play a major role, because level 3 decays radiatively to level 2 (and it is very rare to have collisional excitations $2 \rightarrow 3$ at low density), the the solution of the statistical equations reduces to:

$$N_2 = \frac{N_1 N_e Q_{12}}{A_{21} + N_e Q_{21}}$$

$$N_3 (A_{31} + A_{32}) = N_e N_1 Q_{13}.$$

With the appropriate substitutions,[2] it is:

$$\frac{N_3}{N_2} = \frac{\Omega_{13}}{\Omega_{12}} \frac{A_{21}}{A_{32} + A_{31}} \left(1 + 1.73 \cdot 10^{-4} x \frac{\Omega_{12}}{A_{21}} \right) e^{-\chi_{32}/k_B T_e}, \tag{131}$$

with:

$$x = 10^{-2} N_e T_e^{-1/2}.$$

5 Recombination lines

5.1 Population of the levels

The recombination lines are the lines emitted by the permitted radiative transitions, which follow the recombination of an electron with an ion. In the photoionized gas of H II regions we can realistically assume that the population of a particular level n only occurs through:

- direct recombination to n
- recombinations to higher levels, followed by a radiative transition cascade to n

In a low density environment, interacting with a diluted radiation field, this, in turn, implies that:

- there is no stimulated emission
- the level n is not populated via collisions or radiative excitations through absorptions of radiation (i. e. the nebula is optically thin)
- the neutral atoms are in their fundamental level and they are ionized from there

From the observations of H II region spectra, we know that there is statistical equilibrium (otherwise the emission lines would be subject to strong variations that are never seen) and we can, therefore, set up a system of statistical equations, accounting for the relevant processes:

$$\underbrace{N_n \sum_{m=1}^{n-1} A_{nm}}_{\text{departures from level } n} = \underbrace{\sum_{m=n+1}^{\infty} A_{mn} N_m + N_p N_e \alpha_{0n}(T_e)}_{\text{arrivals to level } n}, \tag{132}$$

[2]see appendix A for the calculation.

where $\alpha_{0n}(T_e)$ is the coefficient of direct recombination to level n as a function of the electron temperature T_e, while N_p represents the density of the most abundant ion, namely H II.

If we were in conditions of thermodynamical equilibrium, we could use the the equations of Saha and Boltzmann (Eq. 22 and 12) to describe the system:

$$\frac{N_p N_e}{N_1} = \frac{(2\pi m_e k_B T)^{3/2}}{h^3} e^{-\chi_0/k_B T}$$

$$\frac{N_n}{N_1} = \frac{2n^2}{2} e^{-\chi_{0n}/k_B T}$$

that can be combined in:

$$\frac{N_p N_e}{N_n} = \frac{(2\pi m_e k_B T)^{3/2}}{h^3} n^{-2} e^{-(\chi_0 - \chi_{0n})/k_B T}, \tag{133}$$

which would give:

$$N_n = N_p N_e n^2 \left(\frac{h^2}{2\pi m_e k_B T} \right)^{3/2} e^{(\chi_0 - \chi_{0n})/k_B T}. \tag{134}$$

Though in general we cannot assume thermodynamical equilibrium, the result of Eq. (133) can still hold by simply introducing the departure coefficient of level n:

$$N_n = b_n N_p N_e n^2 \left(\frac{h^2}{2\pi m_e k_B T} \right)^{3/2} e^{(\chi_0 - \chi_{0n})/k_B T}. \tag{135}$$

Substituting this expression of the level populations into the statistical equations Eq. (132), we have a system of equations to determine the b_n coefficients:

$$\frac{\alpha_{0n}(T_e)}{n^2} \left(\frac{2\pi m_e k_B T}{h^2} \right)^{3/2} e^{-(\chi_0 - \chi_{0n})/k_B T} + \sum_{m=n+1}^{\infty} b_m A_{mn} e^{-(\chi_0 m - \chi_{0n})/k_B T} =$$

$$= b_n \sum_{m=1}^{n-1} A_{nm}. \tag{136}$$

In this case (that we remind is an optically thin nebula), the coefficients b_n are only a function of T. This happens because at low densities the only processes that can originate the lines are captures of free electrons in the excited levels, followed by radiative cascades to the lower levels. The system of Eq. (136) is not trivial, but numerical solutions indicate that b_n increases with n, so that, when the energy level is high enough, $b_n \to 1$. This happens because the average lifetime of high excitation stages are longer and there are more probabilities to achieve thermodynamical equilibrium.

5.2 Intensity of the optical recombination lines of H I

In the optically thin case

$$I_\nu^L = \frac{h\nu_{nm}}{4\pi}\psi(\nu)A_{nm}\int_0^{r^*} N_n \mathrm{d}r. \tag{137}$$

Introducing Eq. (135) into Eq. (137) for the population of level n, we can write:

$$I_\nu^L = F_{nm}(T_e)\int_0^{r^*} N_p N_e \mathrm{d}r, \tag{138}$$

where we grouped all the characteristics of the transition into the factor $F_{nm}(T_e)$. Applying quantum mechanics considerations, that are beyond the purpose of these notes, the intensity can be expressed as:

$$I_\nu^L = 34.24\frac{g_{nm}}{n^3m^3}\frac{b_n}{T_e^{3/2}}\exp\left(\frac{15800}{n^2T_e}\right)\frac{E}{1+N(\mathrm{He}^+)/N_p}, \tag{139}$$

where we needed the *Gaunt factor* of the transition g_{nm} and we introduced the *emission degree*:

$$E = \int_0^{r^*} N_e^2 \mathrm{d}r. \tag{140}$$

Eq. (139) expresses the dependence of the intensity of a H I recombination line on the energy levels connected by the transitions and the environmental conditions.

5.3 Intensity of the radio recombination lines

In the cases with $n \sim 100$ we have a departure coefficient $b_n \sim 1$ (there is approximately thermodynamical equilibrium) and:

$$S_\nu^L = B_\nu(T_e).$$

If we again consider an optically thin medium, it is:

$$I_\nu^L = \int_0^{r^*} B_\nu(T_e)k_\nu^L \mathrm{d}r, \tag{141}$$

with (see Eq. 57):

$$k_\nu^L = \frac{h\nu_{nm}}{c}\psi(\nu)N_m B_{mn}\left(1-\frac{g_mN_n}{g_nN_m}\right). \tag{142}$$

In this expression, we can isolate the factor:

$$\left(1-\frac{g_mN_n}{g_nN_m}\right) = 1-\frac{b_n}{b_m}e^{-h\nu/k_BT_e} \approx 1-\frac{b_n}{b_m}, \tag{143}$$

where the last step applies to the low frequency regime of the radio domain. In some cases, it can happen that the factor of Eq. (143) may become negative, resulting in a negative absorption coefficient. This is the **MASER effect**, that occurs when the stimulated emission overweighs the radiation absorption, leading to an enhancement of the radiation field intensity due to the path travelled by the beam through the gas.

As opposed to the optical case, in the radio domain the continuum is strong enough to produce induced emission (due to the thickness of H II regions in radio):

$$I_{\nu 0} \geq I_\nu^L$$

and the factor:

$$B_{nm}\frac{4\pi}{c}I_\nu$$

must be included in the statistical equations (136) to determine b_n.

6 Continuous emission and absorption

6.1 Sources of continuous emission and absorption

The dominant processes that give rise to continuous absorptions and emissions in the interstellar gas are due to:

- free - free transitions (in the radio domain or in the optical and X-rays for the *thermal bremsstrahlung* of hot plasmas)
- bound - free transitions (absorption of ionizing radiation in the UV and re-emission in the optical, without significant contributions from the radio)
- acceleration of free electrons of the non-thermal cosmic radiation in interstellar magnetic fields (*synchrotron radiation* in all the frequency intervals)

It is very important to remember that the recombination cross-section is $\sigma \propto v^{-2}$ (cfr. Eq. 65), so that recombination is more likely to affect the slowest electrons of the velocity distribution. We shall later see that in ionization equilibrium, the photo-ionization processes generally produce fast electrons (depending on the average energy of the ionizing photons), that must be slowed down before recombining. The slowing process transfers the electron kinetic energy into the gas, so that ionization turns out to be a globally heating mechanism.

6.2 Free-free transitions of thermal electrons

When an electron moves close to another charged particle (most commonly a positive ion), according to the classical theory it emits a peak of radiation. If the plasma consists of *hydrogenoid ions* of charge Ze and with a Maxwellian distribution of velocity, the emission coefficient is:

$$\epsilon_\nu^k(f-f) = \frac{8}{3}\left(\frac{2\pi}{3}\right)^{1/2} \frac{Z^2 e^6}{m_e^{3/2} c^3 (k_B T)^{1/2}} g_{ff} N_e N_i \exp\left(-\frac{h\nu}{k_B T}\right), \tag{144}$$

where g_{ff} is tha Gaunt factor of the free - free transition. Numerically speaking, Eq. (144) is:

$$\epsilon_\nu^k(f-f) \approx 5.44 \cdot 10^{-39} \frac{Z^2 g_{ff}}{T^{1/2}} N_e N_i \exp\left(-\frac{h\nu}{k_B T}\right). \tag{145}$$

Due to the exponential factor, at the typical temperatures of H II regions ($T \sim 10^4$ K) the emission occurs in the radio and far IR domains.

When the radiation frequency is appreciably larger than the plasma frequency (i. e. the frequency at which plasma particles oscillate after being perturbed by an external electric field):

$$\nu >> \nu_p = \left(\frac{e^2 N_e}{\pi m_e}\right)^{1/2}$$

the Gaunt factor can be expressed as:

$$g_{ff} = \frac{\sqrt{3}}{\pi}\left[\ln \frac{(2k_B T)^{3/2}}{\pi Z e^2 m_e^{1/2} \nu} - 1.443\right] = \frac{\sqrt{3}}{\pi}\left[\ln \frac{T^{3/2}}{Z\nu} + 17.7\right] \tag{146}$$

In the radio range:

$$g_{ff} \approx T^{0.15} \nu^{-0.1}. \tag{147}$$

With these expressions, we can integrate Eq. (144) over all the frequencies and, assuming isotropy, derive the total emission coefficient:

$$4\pi\epsilon_{ff} = 4\pi \int_0^\infty \epsilon_\nu^k(f-f)\mathrm{d}\nu = 1.426 \cdot 10^{-27} Z^2 T^{-1/2} N_e N_i \overline{g_{ff}}. \tag{148}$$

For $10^4\,\mathrm{K} \leq T/Z^2 \leq 10^6\,\mathrm{K}$ we have that $1.25 \leq \overline{g_{ff}} \leq 1.45$, therefore always in the order of unity.

The absorption coefficient $k_\nu^k(f-f)$ can be computed directly from the $\epsilon_\nu^k(f-f)$ if we assume that there is thermodynamical equilibrium. From:

$$\frac{\epsilon_\nu}{k_\nu} = 2\frac{\nu^2}{c^2}k_B T,$$

we have:

$$k_\nu^k(f-f) = \frac{\epsilon_\nu^k c^2}{2\nu^2 k_B T} \propto T^{-1.35}\nu^{-2.1}, \tag{149}$$

where we used the result $\epsilon_\nu^k \propto T^{-0.35}\nu^{-0.1}$, derived combining Eq. (145) and (147).

We can now define the optical depth of the free-free process:

$$\tau_\nu^k(f-f) = \int_0^{r^*} k_\nu^k(f-f)\mathrm{d}r = 8.24\cdot 10^{-2} Z^2 T^{-1.35}\nu^{-2.1} \underbrace{\int_0^{r^*} N_e N_i \mathrm{d}r}_{\text{emission degree } E} . \tag{150}$$

We can immediately see that $\tau_\nu^k(f-f)$ is a decreasing function of T and ν, while it increases with the emission degree E. From Eq. (149) and (150) we infer that the gaseous nebulae become optically thick at low frequencies. As an example, in a H II region with

$$N_e = N_p = 10^2\,\mathrm{cm}^{-3} \qquad Z = 1 \qquad T \sim 10^4\,\mathrm{K} \qquad r^* \sim 10\,\mathrm{pc}$$

we have that $\tau_\nu^K \geq 1$ for $\nu \leq 200\,\mathrm{MHz}$.

6.2.1 The thermal radio continuum

When the particle velocity distribution is Maxwellian, in the radiative transport equation:

$$\frac{\mathrm{d}I_\nu}{\mathrm{d}s} = -I_\nu + \frac{\epsilon_\nu}{k_\nu}$$

we can apply the identity:

$$\frac{\epsilon_\nu}{k_\nu} = B_\nu(T_e),$$

with:

$$B_\nu(T_e) = 2\frac{\nu^2}{c^2}k_B T_e$$

If the source function is spatially constant (i. e. T_e is not a function of position) and there is no background source ($I_{\nu 0} = 0$), we had the solution in the form of Eq. (37):

$$I_\nu = S_\nu(1 - e^{-\tau_\nu^*}), \tag{151}$$

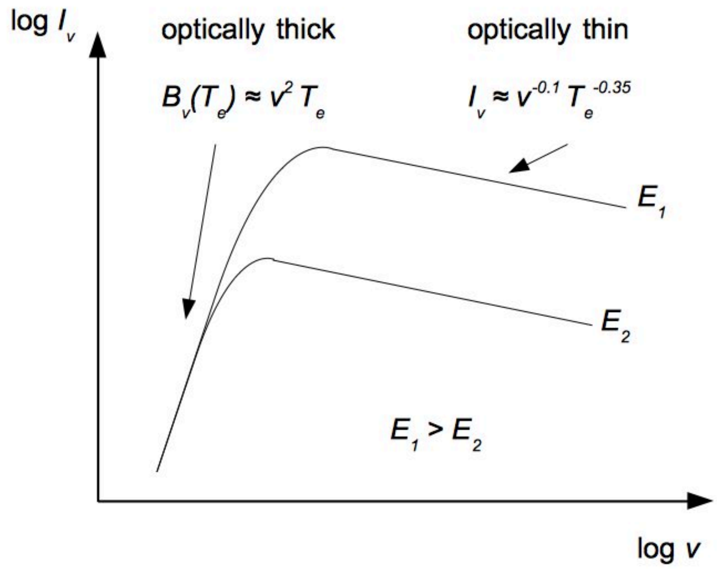

Figure 11: The thermal radio continuum in the optically thick and optically thin regimes.

with $S_\nu = B_\nu(T_e)$. Eq. (151) has two limits:

$\tau^*_\nu > 1 \quad \rightarrow \quad I_\nu = B_\nu(T_e) \quad \rightarrow \quad I_\nu \propto \nu^2 T_e$

$\tau^*_\nu << 1 \quad \rightarrow \quad I_\nu = \tau^*_\nu B_\nu(T_e) \quad \rightarrow \quad I_\nu \propto \nu^{-0.1} T_e^{-0.35}$,

where we made use of Eq. (150) to express the dependence of τ^*_ν on frequency and temperature. The two limits imply that the thermal radio continuum appears similar to the one illustrated in Fig. 11, with two different regimes. In the optically thick regime, at low frequency, the continuum reproduces the shape of a black body function and a measurement of specific intensity in this region gives the electron temperature T_e. Moving at higher frequencies, the gas becomes optically thin and the continuum is nearly independent from temperature and frequency itself. A measurement of the intensity in this region yields an estimate of the emission degree E, that, given some constraints on the size of the cloud, results in a **lower limit** on the electron density N_e.

6.3 Bound-free and free-bound transitions in the optical - UV

If we consider H and hydrogenoid atoms, we can define the free state through a continuous variable x depending on the kinetic energy of the free electron:

$$E_k = \frac{1}{2}mv^2 = \frac{RhZ^2}{x^2}, \tag{152}$$

where

$$R = \frac{2\pi e^4 m_e}{h^2} = 3.29 \cdot 10^{15}\,\mathrm{Hz}$$

is the Rydberg constant in frequency units. The absorption coefficient for a transition $n \to x$ is:

$$k_\nu^k(b-f) = \frac{64\pi^4 m_e e^1 0 Z^4}{3\sqrt{3}ch^6 n^5 \nu^3} g_{nf} N_{0n} \approx 3 \cdot 10^{29} \frac{Z^4}{n^5\nu^3} g_{nf} N_{0n}, \tag{153}$$

where g_{nf} is the Gaunt factor (~ 1 with a weak dependence on ν in the optical) and N_{0n} is the density of neutral atoms in the excitation level n. From Eq. (153) it is important to notice that absorptions are disfavored in the high excitation levels and it is inversely proportional to the 3^{rd} power of the ionizing radiation frequency. This is very important because, **provided that photons must carry enough energy to cover the ionization threshold, more energetic photons are less likely to be absorbed**.

For the recombination of a free electron with velocity in the range $v - v + \mathrm{d}v$ to a bound energy level n, we can derive an emission coefficient starting from the expression of the line emission coefficient of Eq. (49):

$$\epsilon_\nu^L = \frac{h\nu_{nm}}{4\pi}\psi(\nu)A_{nm}N_n$$

and write in analogy:

$$\epsilon_\nu^k(x-n)\mathrm{d}v = \frac{h\nu}{4\pi}N_e(v)\mathrm{d}v Q_{xn}(v)N_1, \tag{154}$$

where:

$$N_e(v)\mathrm{d}v = N_e\phi(v,T)\mathrm{d}v$$

$$Q_{xn}(v) = v\sigma_{xn}(v)$$

. If elastic collisions dominate, $\phi(v,T)$ is a Maxwellian distribution and:

$$\epsilon_\nu^k(f-b) = \frac{m_e^{1/2}h^2\nu}{(2\pi k_B T)^{3/2}} v^2 \sigma_{xn}(v) N_e N_1 \exp\left(-\frac{h\nu - \overline{x_n}}{k_B T}\right). \tag{155}$$

To express the emission coefficient, we need an estimate of the factor $v^2\sigma_{xn}(v)$.

In thermodynamic equilibrium we must have:

$$\frac{\epsilon_\nu^k}{k_\nu^k} = B_\nu(T) = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/k_BT}-1}$$

and the Saha equation between the two ionization stages:

$$\frac{N_1}{N_{0n}}p_e = 2\frac{g_{11}}{g_{0n}}\frac{(2\pi m_e)^{3/2}(k_BT)^{5/2}}{h^3}e^{-x_n/k_BT}$$

so that, taking the ratio of Eq. (154) and (153) and performing all the substitutions we get:

$$v^2\sigma_{xn}(v) = \left(\frac{h\nu}{m_ec}\right)^2\frac{g_{0n}}{g_{11}}\frac{k_\nu^k(b-f)}{N_{0n}}. \qquad (156)$$

Introducing the expression of $k_\nu^k(b-f)$ of Eq. (153), we have:

$$v^2\sigma_{xn}(v) = \frac{64\pi^4e^10Z^4g_{nf}}{3\sqrt{3}m_ec^3h^4}\frac{1}{\nu n^3}, \qquad (157)$$

that can be introduced in Eq. (155) to evaluate $\epsilon_\nu^k(f-b)$.

6.4 Continuum emission from recombination

In the visible and UV spectral ranges we have the Balmer and Paschen continua (those arising from direct recombinations to levels 2 and 3, respectively). To calculate the coefficient we can start from the effective recombination cross-sections:

$$\sigma_{xn} = \frac{64\pi^4e^10Z^4}{3\sqrt{3}m_ec^3h^3}\frac{1}{n^3}\frac{1}{v^2}\underbrace{\frac{g_{nf}}{\chi_n+m_ev^2/2}}_{h\nu}. \qquad (158)$$

For the emission coefficient, we have:

$$\epsilon_{xn}(\nu)\mathrm{d}\nu = h\nu\left(\frac{m_e}{2\pi k_BT}\right)^{3/2}\sigma_{xn}v^3e^{-m_ev^2/k_BT}N_eN_p\mathrm{d}v,$$

which becomes:

$$\epsilon_{xn}(\nu) = \frac{128\pi^4e^10m_eg_{nf}}{c^3h^2(6\pi m_ek_BT)^{3/2}}\frac{1}{n^3}\exp\left(-\frac{h\nu-\chi_n}{k_BT}\right)N_eN_p =$$

$$= 1.7\cdot10^{-33}g_{nf}T^{-3/2}n^{-3}\left(-\frac{\Delta E}{k_BT}\right)N_eN_p. \qquad (159)$$

The total energy emitted in the continuum for a recombination to the level n has a luminosity density given by:

$$4\pi\epsilon_{xn} = 4\pi\int_{\nu_n}^{\infty}\epsilon_{xn}(\nu)\mathrm{d}\nu = \frac{4.5\cdot10^{-22}}{T^{1/2}n^3}N_eN_p.$$

For the direct recombinations to the ground level $n = 1$ in a photo-ionized nebula with $T = 10^4\,\mathrm{K}$ and $1\,\mathrm{cm}^{-3} \leq N_e \leq 10^8\,\mathrm{cm}^{-3}$:

$$4\pi\epsilon_1 = 4.5 \cdot 10^{-24} - 4.5 \cdot 10^{-8}\,\mathrm{erg\,cm^{-3}\,s^{-1}}$$

and a free-free emission coefficient (Eq. 148):

$$4\pi\epsilon_{ff} = \frac{1.426 \cdot 10^{-27} Z^2 N_e N_p g_{ff}}{T^{1/2}} = 1.4 \cdot 10^{-29} - 1.4 \cdot 10^{-13}\,\mathrm{erg\,cm^{-3}\,s^{-1}},$$

therefore the recombination continuum is usually the dominant contribution.

6.5 The 2-photon emission

The transition between levels $2s \to 1s$ in H is forbidden, but it can occur through the temporary formation of a short-lived intermediate energy level and the emission of two continuum photons, provided that:

$$h\nu' + h\nu'' = h\nu_{21} = 10.2\,\mathrm{eV}.$$

The transition has a probability coefficient $A(2s \to 1s) = 8.26\,\mathrm{s}^{-1}$ and it results in the emission a a symmetric continuum peak, centered at $\lambda = 2431\,\text{Å}(\Delta E = 5.1\,\mathrm{eV})$, which becomes observable when $N_e < 10^4\,\mathrm{cm}^{-3}$.

7 Ionization equilibrium

7.1 Statistical equilibrium in ionized nebulae

We know from observations that ionized nebulae are characterized by emission line spectra. The lines are originated by a source of ionization (either a shock front or a ionizing radiation field) and by subsequent recombinations. The existence of the emission lines is possible when the ionization and recombination processes achieve an equilibrium in which the number of ionizations is balanced by the number of recombinations. Without this balance, the gas would evolve towards a state of full ionization or complete neutrality and no emission lines would be produced. In the equilibrium condition, instead, there is a constant degree of ionization, meaning that a fraction of the atoms is always ionized and the population of the free levels is constant.

If we only consider ionization and recombination processes in which only 1 electron is released or captured, the ionization equilibrium can be described as:

$$N_i(R_{i,i+1} + C_{i,i+1}) = N_{i+1}(R_{i+1,i} + C_{i+1,i}), \tag{160}$$

with:

$R_{i,i+1}$	photo-ionization rate
$C_{i,i+1}$	collisional ionization rate
$R_{i+1,i}$	radiative recombination (cooling process)
$C_{i+1,i}$	3-body recombination (recombination of an electron with energy transferred to a second electron)

It is intuitive to derive that:

$$R_{i+1,i} \propto N_e$$
$$C_{i+1,i} \propto N_e N' \quad \text{negligible at low densities}$$

7.1.1 Radiative ionization

For a nebula mainly consisting of Hydrogen atoms, Eq. (160) becomes:

$$N_0(R_{01} + C_{01}) = N_1 R_{10}. \tag{161}$$

To estimate the photo-ionization rate R_{01} we need to compute the integral:

$$N_0 R_{01} = 4\pi \int_{\nu_0}^{\infty} \underbrace{\frac{k_\nu^k(1-f)I_\nu}{h\nu}}_{\text{number of absorbed photons}} \mathrm{d}\nu, \tag{162}$$

where we assumed that ionizations occur only from the ground level. This assumption is reasonable because in interstellar conditions all neutral atoms are in their ground level (cfr. §4.3 for the case of permitted lines) and we can use $N_0 = N_{01}$. From Eq. (153) we know that the absorption coefficient is:

$$k_\nu^k(1-f) \approx 3 \cdot 10^{29} \frac{Z^4}{n^5 \nu^3} g_{nf} N_{01}$$

that, for H becomes:

$$k_\nu^k(1-f) \approx 3 \cdot 10^{29} \frac{N_{01}}{\nu^3}$$

and setting:

$$I_\nu = W B_\nu(T)$$

with $W \sim 10^{-16}$ (diluted radiation field) and $T \approx 4 \cdot 10^4$ K (ionization from hot stars), we do not need to solve the transport equation. Eq. (162) becomes:

$$N_{01}R_{01} = \frac{3 \cdot 10^{29} \cdot 4\pi N_{01} W}{h} \int_{\nu_0}^{\infty} \frac{B_\nu(T)}{\nu^4} \mathrm{d}\nu. \tag{163}$$

Using the Stefan-Boltzmann law:

$$B_\nu(T) = \frac{\sigma T^4}{4\pi}, \tag{164}$$

with $\sigma = 2\pi^5 k_B^4/15h^3c^2$ being the Stefan-Boltzmann constant, we can numerically estimate Eq. (163), obtaining:

$$R_{01} \sim 10^{-8}\mathrm{s}^{-1}.$$

This means that the typical lifetime of a neutral atom in the diluted radiation field of hot stars is $t = 10^8$ s. In H II regions all atoms are ionized from the ground level and the ionization of a neutral atom by absorption of radiation occurs every 10^8 s. Ionizations are nonetheless globally frequent, because of the large number of atoms available in the cloud.

7.1.2 Additional sources of ionization

At large distances from the hot stars the main sources of ionization are:

- the diffuse component of the cosmic radiation (mainly the X-ray background)
- the collisional ionization due to the high energy particles of the cosmic radiation

For what concerns the X-ray background, we have to recall that the absorption coefficient is $k_\nu^k(1-f) \propto \nu^{-3}$. It turns out that $R_{01} \sim 10^{-17}\,\mathrm{s}^{-1}$ for low energy photons ($0.2\,\mathrm{keV} \leq E \leq 1\,\mathrm{keV}$) while it is $R_{01} = 0$ for the high energy ones ($E \geq 1\,\mathrm{keV}$).

The collisions with particles of the cosmic radiation can be described by a collisional ionization rate C_{01} which is comparable to the low energy radiative ionization rate ($C_{01} \sim 10^{-17}\,\mathrm{s}^{-1}$) for particles with kinetic energy $E < 100\,\mathrm{MeV}$ and null above this limit.

In addition, in regions with $T >> 10^4$ K, such as the hot plasmas from which the emission lines of O IV arise (e. g. the hot intra-cluster medium, with

$T \sim 10^6 - 10^7$ K) the kinetic energy of thermal electrons can reach values as high as $E \sim 10^2 - 10^3$ eV, for which we have a rate of collisional efficiency of:

$$Q_{01} \approx 10^{-11}\sqrt{T}\,\mathrm{cm}^3\,\mathrm{s}^{-1}.$$

7.1.3 Recombination

The recombination rate with subsequent emission of photons is:

$$R_{i+1,i} = N_e \alpha_i, \tag{165}$$

where:

$$\alpha_i = \sum_n \alpha_{in}$$

is the total recombination coefficient and

$$\alpha_{in} = \int_0^\infty v\sigma_{xn}(v)\phi(v,T)\mathrm{d}v$$

is the recombination coefficient at level n. From Eq. (157) we have:

$$v^2\sigma_{xn}(v) = \frac{64\pi^4 e^1 0 Z^4}{3\sqrt{3}m_e c^3 h^4}\frac{1}{\nu}\frac{g_{nf}}{n^3}$$

and, in the case of hydrogenoid atoms with a Maxwellian distribution of velocity corresponding to the kinetic temperature of the electrons, using:

$$h\nu = \frac{1}{2}m_e v^2 + (\chi_0 - \chi_{0n})$$

we get:

$$\alpha_{0n} = \frac{2^9\pi^5 e^1 0 Z^4}{m_e^2 c^3 h^3}\left(\frac{m_e}{6\pi k_B T}\right)^{3/2} \exp\left(-\frac{\overline{\chi_n}}{k_B T}\right) F\left(\frac{\overline{\chi_n}}{k_B T}\right)\frac{g_{nf}}{n^3}, \tag{166}$$

with $\overline{\chi_n}$ representing the ionization energy from level n and

$$F(x) = \int_x^\infty \frac{e^{-t}}{t}\mathrm{d}t.$$

We define the partial recombination coefficient:

$$\alpha_0^{(j)} = \sum_{n=j}^\infty \alpha_{0n}, \tag{167}$$

so that:

$$\alpha_0^{(1)} = \alpha_0 \qquad \alpha_0^{(n)} = \alpha_0 - \sum_{i=1}^{n-1}\alpha_{0i}$$

For hydrogenoid atoms, it is:

$$\alpha_0^{(j)} = \frac{2.06 \cdot 10^{-11} Z^2}{T^{1/2}} \Phi_j \left(\frac{\chi_1}{k_B T} \right). \tag{168}$$

This coefficient is useful because nebulae are nearly transparent for recombinations to levels $n > 1$ (since all the neutral atoms are in the ground level), while recombinations to the ground level itself produce photons that can re-ionize other atoms. These are re-absorbed after traveling a certain distance, which, if smaller than a significant fraction of the cloud size, can be neglected in the so-called *on the spot approximation.*

Considering only H atoms ($Z = 1$) in a H II region with $T = 10^4\,\mathrm{K}$ and $N_e = 10^3\,\mathrm{cm}^{-3}$ we have:

$$\alpha_0^{(1)} \sim 4 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

$$\alpha_0^{(2)} \sim 2.6 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

and from the statistical equilibrium equation:

$$\frac{N_1}{N_0} = \frac{R_{01} + C_{01}}{N_e \alpha_0^1}$$

it turns out that:

$$\frac{N_1}{N_0} \sim 25.$$

In the hot component of the ISM (like the thin clouds far away from the ionizing sources detected through their O IV lines) with

$$T \sim 10^6\,\mathrm{K} \quad Q_{01} \approx 10^{-11}\sqrt{T} \quad R_{01} \sim 10^{-17}\,\mathrm{s}^{-1} \quad N_e = 4 \cdot 10^{-3}\,\mathrm{cm}^{-3}$$
$$\alpha_0^{(1)} \sim 10^{-14}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

we have:

$$\frac{N_1}{N_0} \sim 10^6$$

that is full ionization.

7.2 Ionization equilibrium in H II regions

Let's consider ionization equilibrium in the presence of a hot star. Indicating with

N_0	the number of neutral atoms
N_1	the number of ions
$N_H = N_0 + N_1$	the total H abundance

if H is much more abundant than the heavier elements it is also the only relevant source of free electrons. This implies that:

$$N_e = N_1. \tag{169}$$

Since:

$$\begin{array}{lcl} R_{01} \sim 10^{-8}\,\mathrm{s}^{-1} & \rightarrow & N_0 R_{01} = N_1 R_{10} \\ C_{01} \sim 10^{-17}\,\mathrm{s}^{-1} & & R_{10} = N_e \alpha_0^1 = N_e \alpha_0 \end{array}$$

we can neglect the ionization due to collisions (and that produced by the background radiation) and the ionization equilibrium is:

$$N_0 R_{01} = N_1 N_e \alpha_0. \tag{170}$$

From this expression, we get:

$$\frac{N_1}{N_0} = \frac{R_{01}}{N_e \alpha_0}. \tag{171}$$

Taking into account a central star belonging to the first spectral types ($T_* \sim 10^4\,\mathrm{K}$), we have:

$$R_{01} \sim 10^{-8}\,\mathrm{s}^{-1} \qquad \alpha_0 \approx 4 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

that, put into Eq. (171), gives:

$$\frac{N_1}{N_0} = \frac{2.5 \cdot 10^4\,\mathrm{cm}^{-3}}{N_e},$$

so that, using the identity of Eq. (169), we finally have:

$$N_0 = \frac{N_e^2}{2.5 \cdot 10^4\,\mathrm{cm}^{-3}}. \tag{172}$$

If we know the value of $N_0 = N_{01}$ we can evaluate the bound-free absorption coefficient. Starting again from the expression of Eq. (153), it is:

$$k_\nu^k(n - f) \approx 3 \cdot 10^{29} \frac{Z^4}{n^5 \nu^3} g_{nf} N_{0n}$$

that, for H atoms in their ground level, reduces to:

$$k_\nu^k(1 - f) \approx 3 \cdot 10^{29} \frac{N_{01}}{\nu^3}. \tag{173}$$

We recall that ionization can occur only above the threshold frequency:

$$\nu_0 = \nu(912\,\text{Å}) = 3.2895 \cdot 10^{15}\,\text{Hz},$$

so that, at the threshold frequency, we find:

$$k_\nu^k(1-f) = 8.4 \cdot 10^{-18} N_{01}.$$

Therefore, for gaseous nebulae with electron densities in the range $10^2\,\text{cm}^{-3} \leq N_e \leq 10^3\,\text{cm}^{-3}$, using Eq. (172), we get

$$3.4 \cdot 10^{-18}\,\text{cm}^{-1} \leq k_\nu^k(1-f) \leq 3.4 \cdot 10^{-16}\,\text{cm}^{-1}.$$

An optical depth of $\tau_{\nu_0} = 1$ is reached after a mean free path of the order of ${k_\nu^k}^{-1}$, which ranges approximately from 0.1 pc, for $N_e = 10^2\,\text{cm}^{-3}$, down to 0.001 pc, for $N_e = 10^2\,\text{cm}^{-3}$.[3] Since the typical dimensions of a nebula largely exceed 1 pc, this means that the ionizing photons are absorbed within a very small geometrical path, thus satisfying the *on the spot* approximation. In particular, we have demonstrated that **photo-ionized nebulae are optically thick to the Lyman continuum**.

7.3 The diffuse ionizing radiation

The optical thickness of photo-ionized nebulae to the Lyman continuum introduces some additional complications in the expression of the photo-ionization equilibrium. Indeed, we have to take into account the fact that direct recombinations to the level with $n = 1$ produce a diffuse radiation field with $\nu > \nu_0$, which contributes to the ionization. The expression of R_{01}, that we derived from Eq. (162), must be corrected for this effect, by the introduction of the diffuse radiation component in the radiation field specific intensity:

$$I_\nu = I_\nu^s + I_\nu^d.$$

We can try to estimate the fraction of direct recombinations to the ground level:

$$N_1 R_{10} = N_1 N_e \alpha_0 = N_1 N_e(\alpha_0^{(2)} - \alpha_{01}), \tag{174}$$

[3]Remember that 1 pc $\approx 3 \cdot 10^{18}$ cm.

with:

$$\alpha_{01} = 1.4 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1} \quad \alpha_0^{(2)} = 2.6 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1} \quad \alpha_0 = 4 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1}.$$

From these quantities, it turns out that the fraction of recombinations at the ground level is $\alpha_{01}/\alpha_0 = 35\%$, while the fraction of recombinations at levels with $n \geq 2$ is $\alpha_0^2/\alpha_0 = 65\%$. These ratios imply that the diffuse radiation field has a non-negligible role and we cannot neglect the contribution of ionizing photons from the environment. Introducing the distinction between the source and the diffuse radiation fields in Eq. (162), we have:

$$N_{01}R_{01} = 4\pi \int_{\nu_0}^{\infty} \frac{k_\nu^k(1-f)(I_\nu^s + I_\nu^d)}{h\nu} \mathrm{d}\nu. \tag{175}$$

Separating the contribution of direct recombinations to the ground level, the ionization equilibrium of Eq. (175) can be written as:

$$N_1 N_e \alpha_0^{(2)} + \{N_1 N_e \alpha_{01}\} = 4\pi \int_{\nu_0}^{\infty} \frac{k_\nu^k(1-f)I_\nu^s}{h\nu} \mathrm{d}\nu + \left\{4\pi \int_{\nu_0}^{\infty} \frac{k_\nu^k(1-f)I_\nu^d}{h\nu} \mathrm{d}\nu\right\}. \tag{176}$$

If the on the spot approximation holds, the two terms in curly braces of Eq. (176) are exactly balanced and cancel out.

If we define the ionization degree as:

$$x = \frac{N_1}{N_0 + N_1} \tag{177}$$

recalling that $N_H = N_0 + N_1$ it turns out that:

$$N_e = N_1 = x N_H. \tag{178}$$

The ionization equilibrium becomes then:

$$N_{01}R_{01} = N_e N_1 \alpha_0^{(2)},$$

that, in terms of x, is:

$$(1-x)N_H \cdot 4\pi \int_{\nu_0}^{\infty} \frac{k_\nu^k I_\nu^s}{h\nu} \mathrm{d}\nu = x^2 {N_H}^2 \alpha_0^{(2)}, \tag{179}$$

where we used an absorption coefficient per atom:

$$k_\nu^k = \frac{k_\nu^k(1-f)}{N_{01}}.$$

7.4 The ionization front

The transport equation expressed in polar coordinates becomes:

$$\frac{\partial I_\nu}{\partial r}\cos\theta - \frac{\partial I_\nu}{\partial \theta}\frac{\sin\theta}{r} = -k_\nu I_\nu + \epsilon_\nu, \tag{180}$$

where θ is the angle with respect to the radial coordinate. In the case of spherical symmetry, since:

$$\Phi_\nu = \int_{4\pi} I_\nu(\theta)\cos\theta \mathrm{d}\Omega, \tag{181}$$

we have:

$$\frac{\mathrm{d}\Phi_\nu}{\mathrm{d}r} + \frac{2}{r}\Phi_\nu = \frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}(r^2\Phi_\nu) = -4\pi k_\nu I_\nu + 4\pi\epsilon_\nu, \tag{182}$$

where the factor 4π arises from the fact that we define the intensity of the isotropic radiation field as:

$$4\pi I_\nu = \Omega^* I^*_\nu$$

with:

$$I^*_\nu = \frac{\Phi_\nu(r)}{\Omega^*}$$

being the average intensity of the stellar disk, that does not depend on distance. Due to the absorption along the path from the surface of the star to the distance r, we have to make the substitution $I^*_\nu \to I_\nu * e^{-\tau_\nu}$, with τ_ν determined by:

$$\mathrm{d}\tau_\nu = k^k_{\nu\, atom} N_0 \mathrm{d}r = k^k_{\nu\, a}(1-x)N_H \mathrm{d}r. \tag{183}$$

Since $k^k_\nu \propto \nu^{-3}$ (for $\nu \geq \nu_0$), the optical depth increases at low frequencies. In particular, it is:

$$\tau^*_\nu = k^k_{\nu\, atom}(1-x)N_H r^* \propto \frac{(1-x)}{\nu^3}N_H r^*.$$

Due to the pronounced dependence of the opacity on frequency, we have that the radiation at low frequency is considerably weakened and the intensity distribution appears shifted toward the higher frequencies. Another important consequence is that high energy photons penetrate deeper layers of the cloud and they are the last ones to be absorbed.

In the case of a photo-ionized nebula, we have to consider, in addition to the stellar radiation, also the diffuse radiation field, with an emission coefficient ϵ^d_ν.

With this distinction, if we divide Eq. (182) by $h\nu$, multiply by 4π and integrate over frequency, we get

$$\frac{\mathrm{d}}{\mathrm{d}r}\left[4\pi r^2\int_{\nu_0}^{\infty}\frac{\Phi_\nu^s+\Phi_\nu^d}{h\nu}\mathrm{d}\nu\right]=4\pi r^2\left[-4\pi\int_{\nu_0}^{\infty}\frac{k_\nu(I_\nu^s+I_\nu^d)}{h\nu}\mathrm{d}\nu+4\pi\int_{\nu_0}^{\infty}\frac{\epsilon_\nu^d}{h\nu}\mathrm{d}\nu\right]. \tag{184}$$

Instead of trying to solve Eq. (184) it is better to understand the meaning of its different members. For the flux of the source radiation field, we have:

$$\Phi_\nu^s=\overline{I_\nu^*}e^{-\tau_\nu}\Omega^*.$$

By definition, it is:

$$4\pi I_\nu^s=\Omega^*[\overline{I_\nu^*}e^{-\tau_\nu}]$$

and we have:

$$I_\nu^s=\overline{I_\nu^*}e^{-\tau_\nu}\frac{\Omega^*}{4\pi}=\overline{I_\nu^*}e^{-\tau_\nu}W.$$

The member in the left hand side of Eq. (184) is:

$$L_c(r)=4\pi r^2\int_{\nu_0}^{\infty}\frac{\Phi_\nu^s+\Phi_\nu^d}{h\nu}\mathrm{d}\nu, \tag{185}$$

that represents the number of ionizing photons produced by the star and by the diffuse radiation field. In the right hand side of the equation, instead, we have:

$$4\pi\int_{\nu_0}^{\infty}\frac{\epsilon_\nu^d}{h\nu}\mathrm{d}\nu=x^2N_H^2\alpha_{01},$$

meaning that the number of photons produced in the diffuse radiation field is equal to the number of direct recombinations to the ground level $n=1$. If the photons of the Lyman continuum are re-absorbed on the spot, then:

$$4\pi\int_{\nu_0}^{\infty}\frac{k_\nu I_\nu^d}{h\nu}\mathrm{d}\nu=x^2N_H^2\alpha_{01}$$

meaning that the number of absorbed photons, too, is equal to the recombinations at $n=1$ and $\Phi_\nu^d=0$. With these assumptions, we can re-define the number of ionizing photons produced by the star of Eq. (185) as:

$$L_c(r)=4\pi r^2\int_{\nu_0}^{\infty}\frac{\Phi_\nu^s}{h\nu}\mathrm{d}\nu, \tag{186}$$

and re-write Eq. (184) as:

$$\frac{\mathrm{d}}{\mathrm{d}r}L_c(r)=4\pi r^2[-x^2N_H^2\alpha_0+x^2N_H^2\alpha_{01}],$$

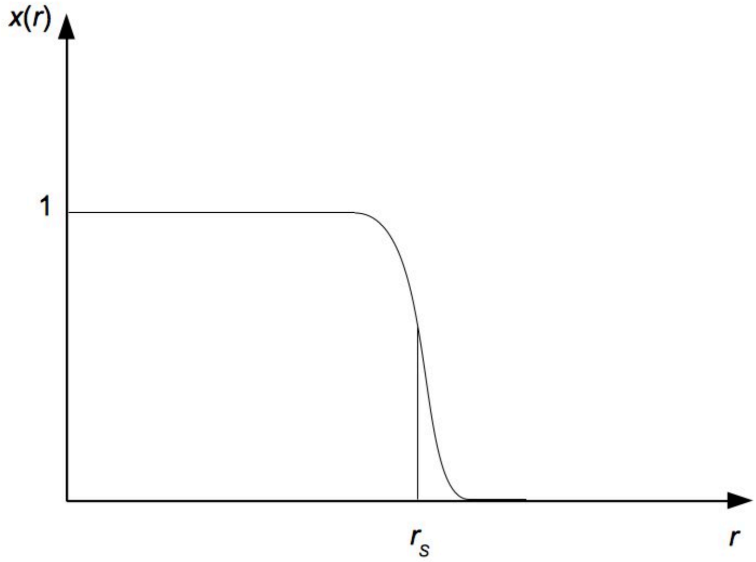

Figure 12: Ionization degree as a function of distance from the ionizing radiation source.

which, using the definition of the partial recombination coefficients of Eq. (167), becomes:

$$\frac{\mathrm{d}}{\mathrm{d}r} L_c(r) = -4\pi r^2 x^2 N_H^2 \alpha_0^{(2)}. \tag{187}$$

Eq. (187) tells us that the variation in the number of ionizing photons with distance from the source is equal to the number of recombinations at levels $n \leq 2$.

Due to the variation of the number of ionizing photons, the ionization degree itself is a function of the distance from the source $x = x(r)$. This function can be determined solving the following set of equations:

$$(1-x) N_H 4\pi \int_{\nu_0}^{\infty} \frac{k_\nu^k I_\nu^s}{h\nu} \mathrm{d}\nu = x^2 N_H^2 \alpha_0^{(2)}$$

$$I_\nu^s = \overline{I_\nu^*} e^{-\tau_\nu} \frac{R_*^2}{4r^2}$$

$$\tau_\nu(r) = k_\nu^k \cdot (1-x) N_H r.$$

If we know N_H, R_*, $\overline{I_\nu^*}$ and we use $k_\nu^k (1-f)_H = 3 \cdot 10^{29} \nu^{-3}$, it is found that $x(r)$ is nearly constant and very close to 1 (full ionization) where the ionizing photons are still available, while it quickly drops to 0 at the distance where all the ionizing photons have been absorbed, as it is shown in Fig. 12. The distance where the absorption of all the ionizing photons is carried out is called the Strömgren radius r_S and it can be obtained from integration of Eq. (187) with the condition:

$$L_c(r_S) = 0.$$

Using $x(r) = 1$ for $r < r_S$, the integral of Eq. (187) is:

$$L_c(r_S) - L_c(R_*) = -L_c(R_*) = -\frac{4\pi}{3} N_H^2 \alpha_0^{(2)} (r_S^3 - R_*^3). \tag{188}$$

Since $R_* << r_S$, it can be neglected in the right hand side of Eq. (188), obtaining:

$$L_c(R_*) = \frac{4\pi}{3} N_H^2 \alpha_0^{(2)} r_s^3. \tag{189}$$

The luminosity is given by:

$$L_c(R_*) = \int_{\nu_0}^{\infty} \frac{\Phi^s(R_*)}{h\nu} 4\pi R_*^2 \mathrm{d}\nu$$

and since:

$$\Phi^s = 4\pi \overline{I_\nu^*}$$

we can solve Eq. (189) for r_S:

$$r_S = \left[\frac{3R_*^2 \pi}{N_H^2 \alpha_0^{(2)}} \int_{\nu_0}^{\infty} \frac{\overline{I_\nu^*}}{h\nu} \mathrm{d}\nu \right]^{1/3}. \tag{190}$$

The integral:

$$N_L = \int_{\nu_0}^{\infty} \frac{\overline{I_\nu^*}}{h\nu} \mathrm{d}\nu$$

is the flux of ionizing photons at the surface of the star, and, recalling that at $T \sim 10^4\,\mathrm{K}$ it is:

$$\alpha_0^{(2)} = 2.6 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1},$$

the Strömpgren radius expressed in pc is:

$$r_S = 1.23 \cdot 10^{-7} \left(\frac{R_*}{R_\odot} \right)^{2/3} N_L^{1/3} N_H^{-2/3}. \tag{191}$$

For $x = 1$ we have:

$$N_1 >> N_0$$

$$\tau_\nu = (1 - x) N_H \frac{3 \cdot 10^{29}}{\nu^3} \approx 0.$$

Table 1: List of common element ionization potentials.

Element	1^{st} ionization potential (eV)	2^{nd} ionization potential (eV)
H	13.6	–
O	13.6	34.9
N	14.5	29.5
Ne	21.6	41.1
He	24.6	54.4

If x decreases to 0.5, the optical depth increases steeple, so that the mean free path of a photon with $\nu = \nu_0$ becomes smaller and smaller ($\ell \sim 10^{-3}$ pc for $N_H = 10^2\,\mathrm{cm}^{-3}$ and $\ell \sim 10^{-4}$ pc for $N_H = 10^3\,\mathrm{cm}^{-3}$).

As it is shown in Fig. 12, the ionization degree quickly drops to zero at a distance approximately corresponding to the Strömgren radius. In this transition region, we have an overlapping of neutral and ionized gas. For this reason, this region hosts free electrons and ion species such as H I, H II, O I and O II (the first ionization potential of O is approximately equal to that of H). This region is very important, because its the only place where a significant emission of forbidden lines from [O I] can arise. If the ionizing radiation source is non-thermal (as, for example, in the case of AGNs or other power-law spectrum sources), there is an excess of high energy photons (Fig. 4), which are absorbed at the border of the nebula, because of their smaller absorption cross-section. This results in a smoother transition from the ionized region to the neutral one, therefore producing a larger transition region. In this case the intensity of the emission lines, coming from the transition region, are enhanced and we are able to discriminate the nature of the ionizing radiation source from the emission line intensity ratios.

7.5 Stratification of ionization

In the spectra of photo-ionized nebulae we can observe emission lines produced by H and several other elements. In Table 1 we report the first ionization potentials of the elements emitting the brightest lines. The most abundant

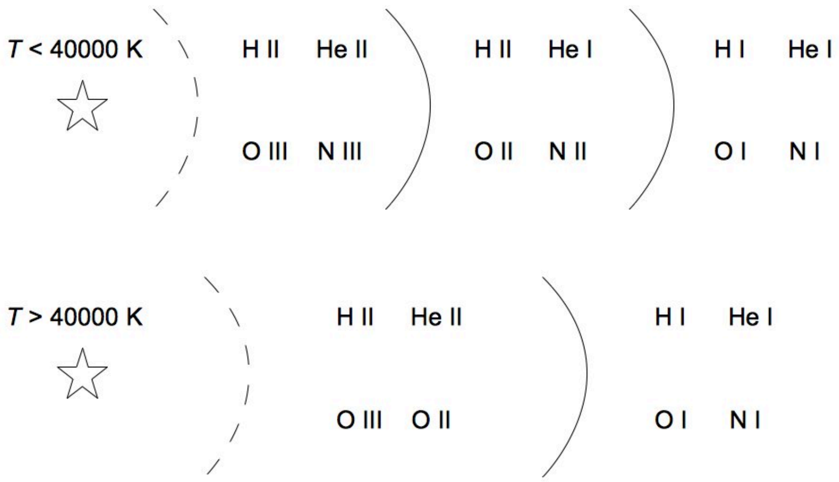

Figure 13: Ionization stratification for the cases of stars with $T \leq 40000\,\mathrm{K}$ and $T > 40000\,\mathrm{K}$.

element after H is He, with:

$$\frac{N(\mathrm{He})}{N(\mathrm{H})} \approx 0.1$$

and, since $\chi_0(\mathrm{He}) >> \chi_0(\mathrm{H})$, He can be present in H II regions either as He I or as He II. If there are not enough photons to ionize He, then there can be neither O III nor NIII. It is convenient to subdivide the UV radiation in two bands:

1. $13.6\,\mathrm{eV} \leq h\nu \leq 24.6\,\mathrm{eV}$ has photons that can only ionize H (and O)

2. $h\nu > 24.6eV$ has photons that can ionize all the elements

Though the high energy band photons can in principle ionize every element, they will rather be absorbed by heavy ions, instead of H, in spite of its higher abundance. This happens because of the photo-ionization cross-section, which, above the ionization threshold, decreases as ν^{-3}. Therefore, the H I atoms are very small targets for this kind of photons, that are much more likely to interact with an heavy element. Moreover, if there are photons in the low energy band, they can only be absorbed by H I atoms, leaving only the heavy ions with the possibility to absorb the high energy photons.

If the source of ionizing radiation is a thermal source with $T \leq 40000\,\mathrm{K}$, the ionizing photons are mainly belonging to the low energy band. A thermal source with $T > 40000\,\mathrm{K}$, instead, produces a significant number of photons with $h\nu > 24.6\,\mathrm{eV}$ and the ionization structure that is observed in the surrounding medium differs in the two cases, as it is shown in Fig. 13.

7.6 Extinction by dust grains

From observations in the IR, we know that dust is present in the densest H II regions. As a consequence, UV radiation is absorbed and the Strömgren radius becomes smaller. Since it can be assumed that the dust / gas ratio is constant, the dust content of the nebula increases with density. If we call r'_S the dust reduced Strömgren radius, we define the decrease factor as the ratio

$$\frac{r'_S}{r_S}.$$

Calling $\tau_{\nu S}$ the optical depth due to dust at the distance of r'_S and A_V the visual extinction in the H II region, there is an empirically verified relation, stating that:

$$\tau_{\nu S} = 4A_V.$$

7.7 H I regions

All the stars belonging to the O and B spectral classes are surrounded by H II regions. Photons with $h\nu > 13.6\,\mathrm{eV}$ cannot escape from these regions, but lower energy photons can still ionize heavy elements in the neutral gas, like, for example, C I ($\chi_0 = 11.26\,\mathrm{eV}$), Si I ($\chi_0 = 8.15\,\mathrm{eV}$) and Fe I ($\chi_0 = 7.87\,\mathrm{eV}$). In addition, a residual ionization of H is still possible, due to collisions with particles of the cosmic radiation ($C_{01} \sim 10^{-17}\,\mathrm{s}^{-1}$ for $E < 100\,\mathrm{MeV}$) and to interactions with the X-ray background ($R_{01} \sim 10^{-17}\,\mathrm{s}^{-1}$ for $h\nu < 1\,\mathrm{keV}$). The resultant ionization degree can be evaluated through the statistical equilibrium:

$$N_0(R_{01} + C_{01}) = N_1 R_{10}, \tag{192}$$

with $R_{10} = N_e \alpha_0^{(2)}$ (on the spot re-absorption of all the Lyman continuum photons).

In a neutral medium, we have:

$$N_1 << N_0 = N(\mathrm{H\,I}),$$

so that the electron density is:

$$N_e = N_1 + x_0 N(\mathrm{H\,I}), \tag{193}$$

where we caled x_0 the abundance of electrons coming from other sources (heavy elements) relative to H I. Eq. (192) becomes then:

$$N(\mathrm{H\,I})(R_{01} + C_{01}) = N_1[N_1 + x_0 N(\mathrm{H\,I})]\alpha_0^{(2)}$$

and:

$$(R_{01} + C_{01}) = N(\mathrm{H\,I}) \left[\left(\frac{N_1}{N(\mathrm{H\,I})} \right)^2 \alpha_0^{(2)} + x_0 \left(\frac{N_1}{N(\mathrm{H\,I})} \right) \alpha_0^{(2)} \right]. \tag{194}$$

In this case, the quantity:

$$y = \frac{N_1}{N(\mathrm{H\,I})}$$

is a measurement of the ionization degree (since it is equivalent to $x = N_1/(N_0 + N_1)$ for $N_1 << N_0$). The statistical equation Eq. (194) in terms of y is:

$$N(\mathrm{H\,I})\alpha_0^{(2)} y^2 + N(\mathrm{H\,I})\alpha_0^{(2)} y - (R_{01} + C_{01}) = 0, \tag{195}$$

that, solved for y gives:

$$y = \frac{-x_0\alpha_0^{(2)} + \sqrt{N^2(\mathrm{H\,I}) x_0^2 \alpha_0^{(2)\,2} + 4N(\mathrm{H\,I}) x_0 \alpha_0^{(2)}}}{2N(\mathrm{H\,I})\alpha_0^{(2)}},$$

that is:

$$y = \frac{N_1}{N(\mathrm{H\,I})} = \frac{x_0}{2} \left[\left(1 + 4\frac{R_{01} + C_{01}}{N(\mathrm{H\,I}) x_0^2 \alpha_0^{(2)}} \right)^{1/2} - 1 \right].$$

In the case of complete ionization of C I, Si I and Fe I, for normal chemical compositions, it is $x_0 \approx 5 \cdot 10^{-4}$.

7.7.1 Cold dense neutral cloud

We now consider, as an example, the physical conditions of a cold dense cloud of neutral gas. The typical parameters of this environment are:

$$T \sim 100\,\mathrm{K} \quad N(\mathrm{H\,I}) \approx 20\,\mathrm{cm}^{-3} \quad (R_{01} + C_{01}) \sim 10^{-17}\,\mathrm{s}^{-1}$$

$$\alpha_0^{(2)} \approx 6.8 \cdot 10^{-12}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

For the ionization degree, we get:

$$\frac{N_1}{N(\mathrm{H\,I})} \approx 1.2 \cdot 10^{-4},$$

corresponding, through Eq. (193), to an electron density of:

$$N_e = (1.2 \cdot 10^{-4} + 5 \cdot 10^{-4}) N(\mathrm{H\,I}) \approx 1.24 \cdot 10^{-2}\,\mathrm{cm}^{-3}.$$

7.7.2 Hot tenuous neutral cloud

Another set of physical conditions is found in the hot tenuous neutral regions of the gas, which surround, for example, photo-ionized clouds. Here we generally find:

$$T \approx 4000\,\mathrm{K} \quad N(\mathrm{H\,I}) \sim 1\,\mathrm{cm}^{-3} \quad (R_{01} + C_{01}) \sim 10^{-17}\,\mathrm{s}^{-1}$$
$$\alpha_0^{(2)} \approx 5.21 \cdot 10^{-13}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

It results that $y \approx 4 \cdot 10^{-3}$ and:

$$N_e \approx 4.6 \cdot 10^{-3}\,\mathrm{cm}^{-3},$$

i. e. the electron density is lower in the hot gas.

7.8 Heating and cooling mechanisms

The thermodynamical state of the interstellar gas depends on its kinetic temperature. The temperature, in its turn, is controlled by the heating rate Γ (measured in $\mathrm{erg\,cm^{-3}\,s^{-1}}$) and by the cooling rate Λ (expressed in the same units). If the system is in thermal equilibrium, the temperature must be constant and both heating and cooling have to occur with the same rate:

$$\Gamma = \Lambda.$$

Both the rates depend on gas density and temperature, though their efficiency may change, due to the different processes that are at work.

The main processes which contribute to interstellar gas heating are:

- photo-ionization
- ionization by cosmic rays
- shock waves

- heating by dust grains
- evaporation of H_2 formed on the surface of dust grains

The main cooling mechanisms, instead, are:

- collisional excitation of metastable levels, followed by radiative de-excitation (with photons that escape the nebula, because their absorption is forbidden)
- free-free emission from thermal electrons (mainly effective at very high temperatures $T \sim 10^6\,\mathrm{K}$)

The metastable cooling is very effective plasmas with $T \sim 10^4\,\mathrm{K}$, where the free electrons have the proper energy to charge the excited levels by collisions. In higher temperature plasmas, or in the case of extremely metal poor gas, cooling by excitation is not possible, because the ions are destroyed or they are not even available. In these cases, free-free becomes dominant, but equilibrium can only be achieved when it is really effective. We shall now consider some cases of interest.

7.8.1 Photo-ionization heating in H II regions

Photo-ionization is the main heating source of a H II region. The mean energy of the electrons that are released can be expressed as:

$$E_e = \frac{\int_{\nu_0}^{\infty} h(\nu - \nu_0) k_\nu^k I_\nu / h\nu \mathrm{d}\nu}{\int_{\nu_0}^{\infty} k_\nu^k I_\nu / h\nu \mathrm{d}\nu} \tag{196}$$

and it depends on the shape of the ionizing radiation spectral energy distribution, but not on its intensity. If the temperature of the source is T^* and we can assume:

$$I_\nu = W B_\nu(T),$$

then the initial temperature of the released electrons settles to:

$$T_0 = \frac{2}{3} T^*,$$

provided that $h\nu_0 > k_B T^*$.

Due to the photo-ionization cross-section ($\sigma_{ion} \propto \nu^{-3}$), the most energetic photons are absorbed far away in the nebula. For this reason, if $T^* > 40000\,\mathrm{K}$, though there are many high energy photons, the initial temperature, close to the star, is relatively low ($T_0 < T^*$), while, if $T^* \sim 10000\,\mathrm{K}$, the high energy photons are rarer, but absorptions are more frequent and the average energy of the free electrons (and, consequently, T) is higher. However, within the Strömgren radius, where all the ionizing photons have been absorbed, the average energy is larger for the hot stars.

From the emission lines of [O II] or of [S II] we can derive estimates of the gas density and try to measure T at the border of the nebula. If we are able to resolve the line emitting region, we can perform such measurements at different positions. In ionization equilibrium, it will be:

$$N_e N_1 \alpha_0 = N_e N_1 \sum_n v\sigma_{xn}, eqno(197)$$

so that we can derive the balance between the energy gain:

$$N_e N_1 \alpha_0 \overline{E_e}$$

and the energy loss:

$$\frac{1}{2} m_e N_e N_1 \sum_n \overline{v^3 \sigma_{xn}}$$

resulting in the expression of heating as:

$$\Gamma = N_e N_1 \alpha_0 \overline{E_e} - \frac{1}{2} m_e N_e N_1 \sum_n \overline{v^3 \sigma_{xn}}. \tag{198}$$

7.8.2 Cooling from metastable level transitions

To evaluate the efficiency of cooling by excitation of metastable levels, we have to balance the number of collisional excitations:

$$N_e N_{i1} Q_{1m}$$

with that of collisional de-excitations:

$$N_e N_{im} Q_{m1}$$

and consider that only the ions which, after having been collisionally excited, decay through a radiative transition actually take part to the cooling of gas. The cooling rate is, therefore:

$$\Lambda = N_e \sum_m (E_m - E_1)(N_{i1} Q_{1m} - N_{im} Q_{m1}). \tag{199}$$

If the electron density is low ($N_e < N_c$), we can neglect the collisional de-excitations and find:

$$\Lambda = N_e \sum_m (E_m - E_1) N_{i1} Q_{1m}. \tag{200}$$

In the case when no heavy ions are available, the only effective coolant is the free-free emission of thermal electrons. This implies:

$$\Lambda_{ff} = 4\pi\epsilon_{ff}$$

with:

$$\epsilon_{ff} \approx 1.43 \cdot 10^{-27} Z^2 T^{1/2} N_e N_i g_{ff}$$

and:

$$g_{ff} \propto T^{0.15} \nu^{-0.1}$$

(cfr. §6.2 Eq. 147). This mechanism is always at work, but it is far less efficient than the emission of forbidden lines, when the ions are available. If the temperature grows, the efficiency of the free-free also increases, until it eventually achieves equilibrium with the heating mechanism at some high temperature value.

7.9 Thermal equilibrium in H II regions

In H II regions the thermal balance is mainly achieved by equilibrium between photo-ionization heating and metastable level cooling, as shown in Fig. 14. The mean energy produced by photo-ionization is expressed through Eq. (196), which holds throughout the nebula. Close to the star, Eq. (196) can be evaluated in:

$$\overline{E_e} = \frac{3}{2} k_B T_0,$$

with T_0 initial temperature of the electrons. In this case, we can neglect the diffuse component of the radiation field I_ν^d and, considering $k_\nu \propto \nu^{-3}$, we can apply the Wien regime:

$$I_\nu = W B_\nu(T^*) = W \nu^3 e^{-h\nu/k_B T^*},$$

that can be integrated to get:

$$\overline{E_e} = \psi_0 T^*$$

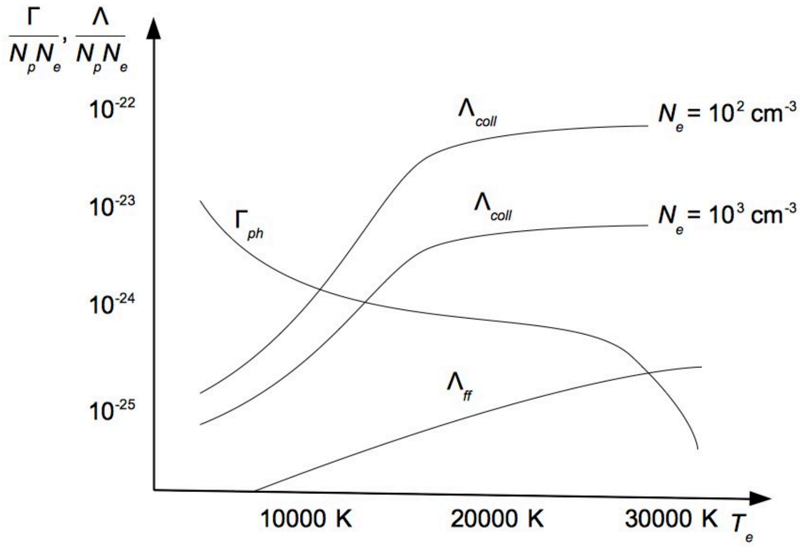

Figure 14: Thermal balance between the main heating and cooling mechanisms working in a H II region. The equilibrium temperatures correspond to the values where the efficiencies of heating and cooling processes (here expressed in $\mathrm{erg\,cm^{-3}\,s^{-1}}$) become equal.

with $\psi_0 = 0.98$ for $T^* \approx 4000\,\mathrm{K}$ and $\psi_0 \approx 0.87$ for $T^* \approx 30000\,\mathrm{K}$. For low temperature stars, we have few ionizing photons with energy very close to the ionization threshold that are absorbed immediately in the nebula. For this reason the kinetic energy of the electrons is very close to the temperature of the source.

The photo-ionization rate in photo-ionization equilibrium is:

$$\Gamma_{ph} = N_e N_1 \left(\alpha_0 \overline{E_e} - \frac{1}{2} m_e \sum_{n=1}^{\infty} < v^3 \sigma_{xn} > \right),$$

so that, close to the star, we have:

$$N_1 = N_p = N_e$$
$$\alpha_0 = \alpha_0^{(1)} = \frac{2.5}{T^{1/2}} \Phi_1 \left(\frac{\overline{\chi_1}}{k_B T} \right) \cdot 10^{-11}$$
$$\overline{E_e} = \psi_0 T^*$$

and if $\phi(v)$ is a Maxwell-Boltzmann distribution:

$$\Gamma = \frac{2.9 \cdot 10^{-27} N_e N_p}{T^{1/2}} [T^* \psi_0 \Phi_1(T) - T \psi_1(T)],$$

with:

$$\psi_1(T) = const. \sum \overline{v^3 \sigma_{xn}}.$$

Solving the transport equation in radiation dilution with the on the spot assumption, we can get $\overline{E_e}$ at each point in the nebula. If we consider the nebula as a whole, it results:

$$\overline{E_e} = \psi k_B T^*,$$

with $\psi = 1.05$ for $T^* = 4000\,\mathrm{K}$ and $\psi = 1.35$ for $T^* = 30000\,\mathrm{K}$. In this case we measure $T > T^*$ because we only see the effect of the highest energy photons.

In a pure H nebula, thermal equilibrium is achieved at a temperature $T \approx 3 \cdot 10^4\,\mathrm{K}$, while, in the presence of heavy elements, we have $T \sim 10^4\,\mathrm{K}$. However, if we increase the electron density of the gas, approaching the critical density of the forbidden lines, the temperature increases again, because the efficiency of radiative de-excitation through the emission of forbidden lines becomes smaller.

8 Extinction

The most evident effect of the interstellar dust is extinction of the light produced by faraway stars and nebulae. Extinction in the visual band is mainly due to scattering (light subtracted from our line of sight) and partially to absorption (photons re-processed and emitted at different frequencies). If we call $I_{\lambda 0}$ the intrinsic intensity of a source and I_λ its observed intensity, then we have:

$$\frac{I_\lambda}{I_{\lambda 0}} = e^{-\tau_\lambda}. \tag{201}$$

Interstellar extinction is characterized by the value of τ_λ along the path from the source to the observer. It is computed from spectro-photometric measurements of pairs of stars belonging to the same spectral type. If we label the two stars as number 1 and 2, the ratio between their fluxes is:

$$\frac{F_\lambda(1)}{F_\lambda(2)} = \frac{F_{0\lambda}(1)}{F_{0\lambda}(2)} e^{-[\tau_\lambda(1) - \tau_\lambda(2)]} = \frac{D_2^2}{D_1^2} e^{-[\tau_\lambda(1) - \tau_\lambda(2)]}, \tag{202}$$

where D_1 and D_2 are the distances to the two stars. It is convenient to choose the two stars in such a way that one is reddened and the other not. This is possible if the not reddened star is a very close one. Let's assume, for example

$\tau_\lambda(2) \sim 0$, so that Eq. (202) becomes:

$$\frac{F_\lambda(1)}{F_\lambda(2)} = \frac{D_2^2}{D_1^2} e^{-\tau_\lambda(1)}, \tag{203}$$

which yields:

$$\tau_\lambda = 2\ln\frac{D_2}{D_1} - \ln\frac{F_\lambda(1)}{F_\lambda(2)}.$$

The logarithm of the flux ratios increases with λ and it becomes approximately constant at very long wavelengths. The logarithm of the distance ratio, instead, is independent on λ and it is generally unknown, though it can be estimated from measurements of F_λ at very long wavelengths, where $\tau_\lambda \sim 0$. From measurements of the ratio F_1/F_2 taken at different wavelengths we can extract the extinction curve. It turns out that:

- τ_λ is approximately the same function of wavelength for all stars in every direction
- only the normalization of the curve is a function of direction

This result is the consequence of the fact that the dust has the same physical properties throughout the interstellar medium (at least in our own Galaxy) and that it is found approximately in the same ratio with respect to gas, except for some notable situations (such as dense molecular clouds, that are generally more dusty). We can, therefore, write:

$$\tau_\lambda = Cf(\lambda), \tag{204}$$

where C depends on the distance from the source and $f(\lambda)$ is the same in every direction. With this expression, we can evaluate Eq. (201) at two different wavelengths:

$$\frac{I(\lambda_1)}{I(\lambda_2)} = \frac{I_0(\lambda_1)}{I_0(\lambda_2)} e^{-C[f(\lambda_1)-f(\lambda_2)]}. \tag{205}$$

The effect of interstellar extinction is to change the observed intensity ratio of two lines, with respect to their intrinsic value in the original nebula.

$f(\lambda)$ is normalized in such a way that:

$$\tau_{\mathrm{H}\gamma} - \tau_{\mathrm{H}\alpha} = 0.5.$$

Setting $C = 1$ we have:

$$f(\lambda) = \frac{0.68}{\lambda} - 0.39 \quad \text{for } \lambda \geq 0.437\mu\text{m}$$

$$f(\lambda) = \frac{0.36}{\lambda} + 0.31 \quad \text{for}\, \lambda < 0.437\mu\text{m},$$

resulting in:

$$f(\text{H}\beta) = 1.$$

If we know the theoretical intensity ratios of some emission lines, like in the case of the hydrogen Balmer lines, we can calculate the value of C and apply an extinction correction to the other line intensity ratios of, for example, [O III] etc. Indeed, since it is:

$$e = 10^{0.434},$$

Eq. (205) becomes:

$$\frac{I(\lambda)}{I(\text{H}\beta)} = \frac{I_0(\lambda)}{I_0(\text{H}\beta)} 10^{-0.434(\tau_\lambda - \tau_{\text{H}\beta})} = \frac{I_0(\lambda)}{I_0(\text{H}\beta)} 10^{-c[f(\lambda) - f(\text{H}\beta)]}, \tag{206}$$

where $c = 0.434C$. Now, since we have:

$$\frac{I(\lambda)/I_0(\lambda)}{I(\text{H}\beta)/I_0(\text{H}\beta)} = \frac{10^{-cf(\lambda)}}{10^{-cf(\text{H}\beta)}} \tag{207}$$

and $f(\text{H}\beta) = 1$, taking separately the numerator and denominator of Eq. (207), we infer:

$$\log \frac{I(\text{H}\beta)}{I_0(\text{H}\beta)} = c.$$

Going to the magnitude scale:

$$A_\beta = 2.5c = 2.5 \log \frac{I(\text{H}\beta)}{I_0(\text{H}\beta)}$$

and, similarly:

$$A_\lambda = 2.5 \log \frac{I(\lambda)}{I_0(\lambda)} = 2.5cf(\lambda).$$

It is a common use to take the effective wavelength of the visual band V as a reference. It is:

$$\frac{A_V - A_\beta}{E(\text{H}\beta - \text{H}\alpha)} = \frac{f(V) - f(\text{H}\beta)}{f(\text{H}\beta) - f(\text{H}\alpha)} = \frac{f(V) - 1}{1 - f(\text{H}\alpha)} = -0.425,$$

where $E(\text{H}\beta - \text{H}\alpha)$ is the color excess at the wavelengths of Hβ and Hα, defined as:

$$E(\text{H}\beta - \text{H}\alpha) = [m(\text{H}\beta) - m_0(\text{H}\beta)] - [m(\text{H}\alpha) - m_0(\text{H}\alpha)].$$

It results:

$$A_V = A_\beta - 0.425E(\text{H}\beta - \text{H}\alpha)$$

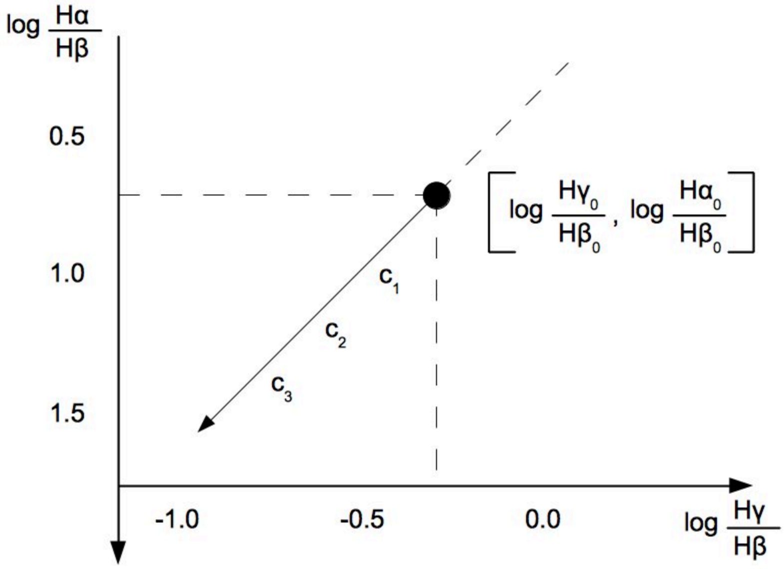

Figure 15: Effect of the extinction on the observed Balmer line intensity ratios ($c_3 > c_2 > c_1$).

and

$$\frac{E(B-V)}{E(\mathrm{H}\beta-\mathrm{H}\alpha)} = \frac{A_B - A_V}{A_\beta - A_\alpha} = \frac{f(B)-f(V)}{f(\mathrm{H}\beta)-f(\mathrm{H}\alpha)} = 0.863.$$

Therefore:

$$E(B-V) = 0.863E(\mathrm{H}\beta-\mathrm{H}\alpha).$$

The functional behavior of extinction can be obtained in the form:

$$\log\frac{I(\mathrm{H}\alpha)}{I(\mathrm{H}\beta)} = \log\frac{I_0(\mathrm{H}\alpha)}{I_0(\mathrm{H}\beta)} - c[f(\mathrm{H}\alpha)-1]$$

$$\log\frac{I(\mathrm{H}\gamma)}{I(\mathrm{H}\beta)} = \log\frac{I_0(\mathrm{H}\gamma)}{I_0(\mathrm{H}\beta)} - c[f(\mathrm{H}\gamma)-1],$$

which, putting:

$$y = \log\frac{I(\mathrm{H}\alpha)}{I(\mathrm{H}\beta)} - \log\frac{I_0(\mathrm{H}\alpha)}{I_0(\mathrm{H}\beta)}$$

$$x = \log\frac{I(\mathrm{H}\gamma)}{I(\mathrm{H}\beta)} - \log\frac{I_0(\mathrm{H}\gamma)}{I_0(\mathrm{H}\beta)},$$

yields:

$$\frac{y}{x} = \frac{f(\mathrm{H}\alpha)-1}{f(\mathrm{H}\gamma)-1},$$

meaning that the logarithms of the line intensity ratios vary along a straight line of fixed slope for different values of c (see Fig. 15). Therefore, the amount of extinction can be estimated by the distance along the line between the observed line ratio and the calculated value of the unextinguished ratio. If we estimate the Balmer line intensity ratios for different values of c, assuming that the extinction behaves in the same manner both in the Milky Way and in extra-galactic objects, we can draw maps of the extinction originated in our own Galaxy and correct the observations for this effect. Later on, reporting the object's line intensity ratios on the theoretical diagram, we can estimate the amount of residual extinction, that turns out to be the one intrinsically originated in the source itself.

A Solution of the [O III] statistical equilibrium

We start from the equation system:

$$N_e N_1 Q_{12} = N_2(A_{21} + N_e Q_{21}) \tag{A1}$$

$$N_e N_1 Q_{13} = N_3(A_{31} + A_{32}) \tag{A2}$$

Taking the ratio of Eq. (A2) and (A1):

$$\frac{Q_{13}}{Q_{12}} = \frac{N_3}{N_2}\frac{A_{32} + A_{31}}{A_{21} + N_e Q_{21}}. \tag{A3}$$

Since for this system we can assume:

$$N_1 Q_{13} = N_3 Q_{31}, \tag{A4}$$

we get:

$$Q_{13} = Q_{31}\frac{N_3}{N_1} = Q_{31}\frac{g_3}{g_1}e^{-h\nu_{31}/k_B T_e} \tag{A5}$$

and, similarly:

$$Q_{12} = Q_{21}\frac{N_2}{N_1} = Q_{21}\frac{g_2}{g_1}e^{-h\nu_{21}/k_B T_e}. \tag{A6}$$

The ratio of of Eq. (A5) and (A6) is:

$$\frac{Q_{13}}{Q_{12}} = \frac{Q_{31}}{Q_{21}}\frac{g_3}{g_2}e^{-h\nu_{32}/k_B T_e} \tag{A7}$$

We can introduce Eq. (A7) into Eq. (A3) and solve for the population ratio:

$$\frac{N_3}{N_2} = \frac{Q_{31}}{Q_{21}}\frac{g_3}{g_2}e^{-h\nu_{32}/k_B T}\frac{A_{21} + N_e Q_{21}}{A_{32} + A_{31}}, \tag{A8}$$

which, expanding the expressions of the collisional transition rates according to Eq. (84), can be evaluated as follows:

$$\frac{N_3}{N_2} = \frac{\Omega(3,1)}{\Omega(2,1)}\frac{g_2}{g_3}\frac{g_3}{g_2}e^{-h\nu_{32}/k_BT_e}\frac{A_{21}+N_eQ_{21}}{A_{32}+A_{31}} =$$

$$= \frac{\Omega(3,1)}{\Omega(2,1)}\frac{A_{21}}{A_{32}+A_{31}}\left(1+\frac{N_eQ_{21}}{A_{21}}\right)e^{-h\nu_{32}/k_BT_e} =$$

$$= \frac{\Omega(3,1)}{\Omega(2,1)}\frac{A_{21}}{A_{32}+A_{31}}\left(1+\frac{N_e}{A_{21}}\cdot 8.63\cdot 10^{-6}\frac{\Omega(2,1)}{g_2T_e^{1/2}}\right)e^{-h\nu_{32}/k_BT_e}. \qquad (A9)$$

For this ion we have:

$$g_2(^1D) = (2S+1)(2L+1) = 1 * 5 = 5$$

therefore:

$$\frac{N_3}{N_2} = \frac{\Omega(3,1)}{\Omega(2,1)}\frac{A_{21}}{A_{32}+A_{31}}\left[1+1.73\cdot 10^{-4}\frac{(10^{-2}N_eT_e^{-1/2})\Omega(2,1)}{A_{21}}\right]e^{-h\nu_{32}/k_BT_e},$$

that, after the introduction of the factor:

$$x = 10^{-2}N_eT_e^{-1/2}$$

is the result of Eq. (131).