Chapter 9

Astronomical Spectroscopy

In the previous chapter we looked at the energy level structure of atoms and molecules, and we looked at the probability of radiative transitions between levels. In this chapter we will look at the excitation of atoms or molecules, and the relation with radiative transfer determining the strength of the emission or absorption lines. We will also look at the processes that affect the shape of the spectral lines.

In much of this chapter we will give the relevant equations for two-level systems. Generelization to multi-level systems is straightforward but requires more complicated notation. For clarity we do not specifically discuss multi-level systems here, but all principles hold unchanged for these as well.

9.1 Excitation in thermodynamic equilibrium

9.1.1 Thermodynamic equilibrium: the Boltzmann equation

If the energy level structure of an atom (or molecule) is known, we can calculate what the likelihood is that an atom is excited to a given level. When we look at an ensemble of atoms, we can calculate what fraction is excited to a given level: we call this the *population* of the level.

If the atoms are in thermodynamic equilibrium at a temperature T, the ratio of the populations of two levels is simply given by a Boltzmann distribuion,

$$\frac{n_i}{n_j} = \frac{g_i}{g_j} e^{-\frac{E_i - E_j}{kT}}. \tag{9.1}$$

For a system with m levels we can find the populations of all levels by solving the set of $m-1$ equations (9.1) together with the boundary conditions $\sum n_i = n_{tot}$.

9.1.2 Ionization equilibrium: the Saha equation

In a very similar way we can find the ionization degree of a mixture of atoms and molecules and their ions. Let's consider two adjacent ionization stages of a species, n_j and n_{j+1}. Their ratio is given by the *Saha equation*,

$$\frac{n_{j+1} n_e}{n_j} = \frac{2U_{j+1}(T)}{U_j(T)} \Big(\frac{2\pi m_e kT}{h^2}\Big)^{3/2} e^{-\frac{\chi_{j,j+1}}{kT}}. \tag{9.2}$$

Here $\chi_{j,j+1}$ is the ionization potential for state $j \to j+1$ and U_j is the partition function for state j, $U_j \equiv g_j \exp(-E_i/kT)$.

Because electrons can be exchanged between ions of different species, we are always dealing with a mixture of species and eq. (9.2) needs to be solved together with the following boundary conditions: conservation of nuclei of species (i), $\sum_j n_j^{(i)} = n_{tot}^{(i)}$; and conservation of charge $n_e = \sum_i \sum_j Z_j n_j^{(i)}$.

9.2 Excitation out of thermodynamic equilibrium

9.2.1 Statistical equilibrium

Many systems are not in thermodynamic equilibrium, and the population of the levels cannot be described by a single temperature T. We now need to solve the detailed balance between difference excitation and de-excitation processes: collisions (both excitation and de-excitation), absorption of photons (excitation), stimulated emission (de-excitation), and spontaneous emission (de-excitation).

Let's consider a two-level system, u and l. And let's also assume that no (external) radiation field is present). In statistical equilibrium, the rate of change of the population of level u, n_u, should be zero. We find

$$\frac{dn_u}{dt} = \Big(n_c n_l q_{lu}\Big) - \Big(n_c n_u q_{ul} + n_u A_{ul}\Big) = 0, \tag{9.3}$$

where n_c is the density of collision partners and q_{lu} is the collisional excitation rate for $l \longrightarrow u$; $q_{lu} = \frac{g_l}{g_u} q_{ul} \exp(-\Delta E/kt)$. We assume here that there is only one dominant collision partner, e.g., H^+, H, or H_2. If there are more species that contribute, e.g., He or e^-, additional terms should be included, each with their appropriate collision rates. These collision rates can be found from quantum mechanical calculations.

In eq. (9.3) we have assumed (for now) that there is no appreciable radiation field present, so spontaneous emission is the only relevant radiative term to take into account. It is useful to consider a few limiting cases:

- In the limit of low n_c, $n_c q_{ul} \ll A_{ul}$, every collisional excitation if immediately followed by spontaneous emission and we have

$$\frac{n_u}{n_l} = \frac{n_c q_{ul}}{A_{ul}}. \tag{9.4}$$

- In the limit of high n_c, $n_c q_{ul} \gg A_{ul}$, the collisions dominate the excitation and de-excitation events. The system now equilibrates to the temperature of the collision partners and follows a Boltzmann distribution. In other words, the system is driven to thermodynamic equilibrium.

$$\frac{n_u}{n_l} = \frac{q_{ul}}{q_{lu}} = \frac{g_u}{g_l} e^{-\frac{\Delta E}{kT}}. \tag{9.5}$$

- A useful concept is that of *critical density*, the density above which the system reaches thermal equilibrium. We define $n_{crit} \equiv A_{ul}/q_{ul}$. Because $A_{ul} \propto \nu^3$, while q_{ul} usually does not have such a strong dependency, higher lying transitions have much higher critical densities.

  However, q_{ul} is different for different transitions. For example, the O II 3726 $^2D_{3/2}$–$^4S_{3/2}$ line has $n_{crit} = 1.6 \times 10^4$ cm^{-3}, while the O II 3729 $^2D_{5/2}$–$^4S_{3/2}$ line has $n_{crit} = 3.1 \times 10^3$ cm^{-3}. The ratio of the line strengths of these two transitions therefore can be used as a measure of density, for example in H II regions, planetary nebulae, and AGNs.

What happens if an external radiation field is present? In other words, when absorption and stimulated emission also need to be taken into account? We now get for the equation of statistical equlibrium,

$$n_l\Big(n_c q_{lu} + B_{lu}\bar{J}_\nu\Big) = n_u\Big(n_c q_{ul} + B_{ul}\bar{J}_\nu + A_{ul}\Big), \tag{9.6}$$

where the mean radiation field is given by

$$\bar{J}_\nu = \frac{1}{4\pi}\int I_\nu d\Omega. \tag{9.7}$$

Let's define a photon occupation number,

$$n_\gamma = \frac{I_\nu}{2h\nu^3/c^2} = \Big(\frac{1}{e^{h\nu/kT_r}-1}\Big), \tag{9.8}$$

where T_r is the temperature characterizing the radiation field, $I_\nu = B_\nu(T_r)$. This basically describes the number density of photons per unit of phase space.

The absorption and stimulated emission rates are now given by

$$n_l B_{lu}\bar{J} = n_l \frac{g_u}{g_l} n_\gamma A_{ul} \tag{9.9}$$

$$n_u B_{ul}\bar{J} = n_u n_\gamma A_{ul}. \tag{9.10}$$

The equation of statistical equilibrium becomes

$$n_l\Big[n_c q_{lu} + n_\gamma \frac{g_u}{g_l} A_{ul}\Big] = n_u\Big[n_c q_{ul} + A_{ul} + n_\gamma A_{ul}\Big], \tag{9.11}$$

with the equilibrium ratio of the populations becoming

$$\frac{n_u}{n_l} = \frac{n_c q_{lu} + n_\gamma \frac{g_u}{g_l} A_{ul}}{n_c q_{ul} + (n_\gamma + 1)A_{ul}}. \tag{9.12}$$

It is useful to look at the following limits

- $n_\gamma \to 0$: In this case of a negligible radiation field we recover

$$\frac{n_l}{n_u} = \frac{n_c q_{lu}}{n_c q_{ul} + A_{ul}}. \tag{9.13}$$

- $n_c \to 0$: In the limit where the collisions are negligible, we obtain

$$\frac{n_u}{n_l} = \frac{g_u}{g_l}\frac{n_\gamma}{n_\gamma + 1}. \tag{9.14}$$

If the radiation field is also negligible, $n_\gamma \to 0$, we find $n_u/n_l \to 0$. In other words, all atoms will be in the ground state. If, on the other hand, the radiation field can be characterized by a temperature T_r, i.e., $n_\gamma \to [\exp(h\nu/kT_r) - 1]^{-1}$, then

$$\frac{n_u}{n_l} = \frac{g_u}{g_l} e^{-h\nu/kT_r}. \tag{9.15}$$

In other words, the atoms will follow a thermal distribution at the temperature of the *photons*. E.g., the populations of the levels connected by the [O I] lines at 63 and 145 μm are strongly affected by the thermal continuum emitted by dust particles at 40–200 K, while the CO J=1–0, 2–1, ... lines are affected by the 2.735 K cosmic microwave background radiation.

9.2.2 Solution methods

To fully solve the problem of radiative transfer for spectral lines, we need to evaluate

$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu, \tag{9.16}$$

with

$$j_\nu = \frac{h_\nu}{4\pi} n_u A_{ul} \phi_\nu \tag{9.17}$$

$$\alpha_\nu = \frac{h_\nu}{4\pi} \Big(n_l B_{lu} - n_u B_{ul} \Big) \phi_\nu. \tag{9.18}$$

The exact form of ϕ_ν we will discuss in the next section.

Through the definitions of α_ν and j_ν, eq. (9.16) depends on n_u and n_l. These populations in turn are given by the equation for statistical equilibrium, eq. (9.11),

$$n_l \Big(n_c q_{lu} + B_{lu} \bar{J}_\nu \Big) = n_u \Big(n_c q_{ul} + B_{ul} \bar{J}_\nu + A_{ul} \Big), \tag{9.19}$$

where

$$\bar{J}_\nu = \frac{1}{4\pi} \int I_\nu d\Omega. \tag{9.20}$$

All these equtions are coupled: the radiation field is found by integrating over the absorption and emission of photons by the atoms; the absorption and emission properties of the atoms depend on their excitation; and these in turn depend on the strength of the radiation field.

Such problems can usually only be solved *iterively*: starting with a trial solution for, e.g., the populations, the radiation field is calculated; new populations are derived; a new radiation field is calculated; etc. until subsequent solutions no longer change.

In general this can be a very time consuming affair, especially because the equation of radiative transfer needs to be evaluated along – in principle – an infinite number of directions.

In special cases, one can simplify the problem. Obvious simplifications include: the atomic excitation is in thermal equilibrium, and therefore will not change from iteration to iteration; or the medium is optically thin, so that only a (constant) external radiation field needs to be taken into account, and emission or absorption events by the atoms are negligible.

Sometimes, a good solution can be found if the *local* excitation can be decoupled from the *global* radiative transfer problem. This happens if there are significant velocity shifts in the medium: photons emitted by an atom in one region will be Doppler-shifted outside the range where atoms in other regions of the medium can absorb them. This method is used in the so-called *Sobolev* and *Large Velocity Gradient* methods.

In more complex cases, one has no alternative but to calculate the full solution. Numerical techniques and clever use of symmetries (spherical, cylindrical) can keep the amount of calculation time under control, by reducing the number of directions over which to evaluate eq. (9.16) to a finite number.

9.3 Spectral line formation

9.3.1 Line broadening

Radiative transfer in spectral lines is a strong function of frquency (or velocity, by evaluating the corresponding Doppler shift). The expressions for α_ν and j_ν (eqs. 9.17 and 9.18) contain the *line profile function* ϕ_ν. What is this function?

- In a gas, atoms or molecules will have a velocity distribution in correspondence with their temperature, characterized by a Maxwellian form, $\exp(-mv/2kT)$. This results in small Doppler shifts of the emision or absorption with repsect to the rest frequency ν_0, and a Gaussian line profile function

$$\phi(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} e^{-(\nu-\nu_0)/\Delta\nu_D^2}, \tag{9.21}$$

where the Doppler width is given by

$$\Delta\nu_D \equiv \frac{\nu_0}{c}\sqrt{\frac{2kT}{m}} \tag{9.22}$$

and m is the mass of the atom or molecule. Heavier species will therefore produce narrower lines, and vice versa.

- In addition to these random thermal motions, additional turbulence is often present in astrophysical media. Assuming that these also are distributed as a Gaussian with a width ξ, these can be incorporated by defining

$$\Delta\nu_D \equiv \frac{\nu_0}{c}\sqrt{\frac{2kT}{m} + \xi^2}. \tag{9.23}$$

- Because of the uncertainty principle, no exact frequency can be defined for a given transition. For an ensemble of atoms this results in a broadening of the line. This so-called *natural broadening* is given by

$$\phi(\nu) = \frac{\gamma/4\pi^2}{(\nu-\nu_0)^2 + (\gamma/4\pi)^2}, \tag{9.24}$$

where the factor γ is defined by $\gamma \equiv \sum_{n'} A_{nn'}$, the sum of the Einstein A-coefficients over all lower levels n'. Note that this profile does not have a Gaussian shape but a *Lorentz* shape (sharper peak and wider wings).

- In systems with high pressures such as planetary and stellar atmospheres, collisions are frequent, and they also cause frequency shifts of the photons, and a broadening of the lines. This so-called *collisional* or *pressure broadening* is given by

$$\phi(\nu) = \frac{\Gamma/4\pi^2}{(\nu-\nu_0)^2 + (\Gamma/4\pi)^2}, \tag{9.25}$$

where $\Gamma = \gamma + 2\nu_{col}$, with ν_{col} the frequency of the collisions. This mechanism is only relevant when many collisions occur within the typical time the system spends before undergoing spontaneous emission of a photon.

- Putting the above Gaussian and Lorentzian effects together results in a so-called *Voigt* profile, given by

$$\phi(\nu) = \frac{1}{\Delta\nu_D\sqrt{\pi}} H(a,u), \tag{9.26}$$

where

$$H(a,u) \equiv \frac{a}{\pi}\int_{-\infty}^{+\infty} \frac{e^{-y^2}dy}{a^2+(u-y)^2}, \tag{9.27}$$

$$a \equiv \frac{\Gamma}{4\pi\Delta\nu_D}, \tag{9.28}$$

$$u \equiv \frac{\nu-\nu_0}{\Delta\nu_0}. \tag{9.29}$$

This profile has a Gaussian core but more extended line wings characteristic for a Lorentz profile.

9.3.2 Velocity patterns

The previous section discusses the processes that affect the line shape (width) on a microscopic level. Macroscopic velocity fields also determine the shape of spectral lines, and are often the dominant factor. For example, the emission lines from interstellar gas in a spiral galaxy are broadened by the rotation of the galaxy to widths of 200–300 km s^{-1}. If the observations resolve the galaxy spatially, velocity shifts will be detectable from one side of the galaxy to the other, revealing the rotation curve of the galaxy. Similarly, emission lines from molecular gas in disks around nbewly formed stars are widened to a few km s^{-1} and often show a doubnle-peaked profile.

Even more complex line profiles with peaks and dips are created when the medium is optically thick in the spectral line, but exhibits significant motions. At some wavelengths, bright emission may be able to escape unhindered; at others, absorption by low excitation material may absorb much of this emission, and reduce the emission to low values. In the special problem set in Appendix E we look at how expanding shells of gas give rise to a characteristics spectral line shaped called the P Cygni profile.