

Ionization balance

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Chapter 1

Ionization equilibrium equations

1.1 Overview

In this chapter, we derive the standard formulae used in many papers relating to ionization balance in diffuse winds.

We will start by formally deriving the Saha equation and noting carefully the assumptions made in its derivation. By comparing these assumptions with the true conditions found in the clouds we are interested in, we will see how to correct it.

1.2 Derivation of the SAHA equation

Insert derivation here in a quiet moment...

Hale Bradts equation 30

$$\frac{n_{r+1,j}n_e}{n_{r,k}} = \frac{(2\pi mkT)^{3/2}}{h^3} \frac{g_{r+1,j}g + e}{g_{r,k}} \exp(-(\chi_i + \epsilon_{r+1,j} - \epsilon_{r,k})/kT) \quad (1.1)$$

This is a form of the Saha equation which links any pair of ionisation states r and $r+1$ in any excitation levels j and k respectively. In this equation, $g_{r+1,j}$ is the statistical weight of excitation level j of ionisation state $r+1$, χ_i is the ionisation potential to go from ionisation state r to $r+1$, $\epsilon_{r+1,j}$ is the energy difference between the ground state of $r+1$ and the excited level j of $r+1$. Bradt then goes on to show how this reduces to the more familiar form of the Saha equation by summing over all excited states. When he does this he gets the standard form of the Saha equation,

which is worth comparing because the statistical weights of individual levels become partition functions for the ionisation state. We should review this because it appears that many of the standard equations make the assumption that we are using the standard Saha equation as a basis for LTE abundances, whereas it appears that we should be using the Saha equation with ground state statistical weights, a slight difference.

There is another way of simplifying things however. We note that we can write this equation for any pair of levels, and the equation for the ground state only is

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = \frac{(2\pi mkT)^{3/2}}{h^3} \frac{g_{r+1,0}g + e}{g_{r,0}} \exp - (\chi_i/kT) \quad (1.2)$$

Clearly the ϵ terms vanish, and the statistical weights are now for the ground state. This is a useful simplification since two assumptions tend to be made in the analysis of diffuse clouds.

- Because the timescale for relaxation of an atom from an excited state to the ground state is typically much shorter than that for photoionization or recombination processes, we can assume that all ions involved in ionisation equilibrium are in the ground state. This is the NEBULAR APPROXIMATION
- The photons produced by the relaxation from excited levels to the ground state are always of less energy than that required to ionize other atoms/ions, so we can ignore their contribution to the photon field. Furthermore, the photons produced by recombination into the ground state will be quickly reabsorbed nearby, so again the photon field is unaffected by their presence. This is the ON THE SPOT APPROXIMATION

This equation therefore becomes the basis of our ionization calculations, and we will replace the whole equation by $\Phi_0^*(T)$ where the * refers to LTE, and the 0 refers to ground state only. Rewriting 1.2 slightly, including the * to designate LTE we get

$$\Phi_0^*(T) = \frac{n_{r+1,0}^*n_e^*}{n_{r,0}^*} = \frac{(2\pi mkT)^{3/2}}{h^3} \frac{g_{r+1,0}g + e}{g_{r,0}} \exp - (\chi_i/kT) \quad (1.3)$$

However, there are two problems that must be addressed. Firstly, this equation only holds in thermodynamic equilibrium, and also whilst the photoionisation process may reasonably all be considered to take place from the ground state, it is not

reasonably to assume that recombination only takes place into the ground state. The first is most simple to fix.

If we are not in LTE, we can at least assume that the photoionisation rate is governed by the local radiation field, which can be approximated by a dilute black body $J_\nu = WB_\nu(T_R)$ (more on this later for power law fields...). If we simply evaluate equation 1.3 at the radiation temperature T_R then the recombination rate equation, which is implicitly combined in the equation, will erroneously also use T_R whereas it is clear that the recombination rates depend on the electron temperature T_e . What is their dependance? The rate depends on the cross section multiplied by the velocity distribution. The Cross section goes as $1/\text{velocity squared}$, and assuming a boltzmann distribution, the velocity goes as $T^{(3/2)}$ therefore the rate is proportional to $T^{-1/2}$. Looking at the basic equation of detailed balance

$$n_{r+1}n_e\alpha = n_r\gamma$$

where α is the recombination rate coefficient, and γ is the photoionization rate coefficient. Therefore

$$\frac{n_{r+1}n_e}{n_r} = \frac{\gamma}{\alpha}$$

Since α is proportional to $T^{-1/2}$ we need to use T_R as the temperature for Φ , but multiply by $T_R^{-1/2}$ and divide by $T_e^{-1/2}$ to fix the recombination rates. The W dilution term will be applied to the photoionization rate, which is on the top, so it will be a multiplicative factor for Φ . Thus our equation for the non LTE abundances becomes

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = W\Phi_0^*(T_R) \times \frac{T_R^{-1/2}}{T_e^{-1/2}} = W\Phi_0^*(T_R) \times \sqrt{\frac{T_e}{T_R}} \quad (1.4)$$

We must now correct for the fact that Φ_0^* only accounts for recombinations to the ground state, whereas in reality there are many more possible recombinations which we must consider. They will eventually end up in the ground state, but we need to account for the increased cross section. Once again, we look at our rearranged detailed balance equation, but lets explicitly state the assumptions in each term if it is equal to Φ_0^*

$$\Phi_0^* = \frac{\gamma_{r,0}}{\alpha_{r+1,0 \rightarrow 0}}$$

Where $\alpha_{r+1,0 \rightarrow r,0}$ refers to the recombination rate coefficient from the ground state of ionization state $r+1$ to the ground state of ionization state r . In reality, we want

the recombinations to go to all states, hence we need to multiply by a factor ζ such that

$$\zeta = \frac{\alpha_{r+1,0 \rightarrow 0}}{\sum_{i=1}^{\infty} \alpha_{r+1,0 \rightarrow i}} \quad (1.5)$$

where $\sum_{i=1}^{\infty} \alpha_{r+1,0 \rightarrow i}$ is a sum of all recombination rates from the ground state of $r+1$ into all possible excited states of r . Thus our final equation for non LTE abundances becomes

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = \zeta W \sqrt{\frac{T_e}{T_R}} \Phi_0^*(T_R) \quad (1.6)$$

1.2.1 Power law input spectrum

In the special case of an incident radiation field better approximated by a power law than a black body, we require a different correction factor for the departure from LTE. We now compute Φ_0^* for the electron temperature rather than the radiation temperature. The photoionization rate γ in the equation

$$\frac{n_{r+1}n_e}{n_r} = \frac{\gamma}{\alpha}$$

depends on the mean radiation intensity, (which with the assumption of a black body (implicit in the Saha equation) is proportional to B_ν), divided by ν to get photon numbers multiplied by the cross section, or

$$\gamma \propto \int_{\nu_0}^{\infty} B_\nu(T) \sigma(\nu) \nu^{-1} d\nu \quad (1.7)$$

If we want to approximate our mean intensity by a power law, such that

$$J_\nu = C\nu^\alpha$$

where C is a constant, and α is the photon index, then our photoionization rate is

$$\gamma_{pl} \propto \int_{\nu_0}^{\infty} C\nu^\alpha \sigma(\nu) \nu^{-1} d\nu \quad (1.8)$$

so a very simple correction factor is to divide $\Phi_0^*(T_e)$ by the assumed photoionization rate 1.7 and multiply by the actual photoionization rate 1.8. We no longer need to worry about correcting for a different temperature used in the recombination rate, since we are evaluating Φ at the correct temperature T_e , however we still need to correct for ζ . Our equation is now therefore

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = \zeta \Phi_0^*(T_e) \frac{\int_{\nu_0}^{\infty} C\nu^\alpha \sigma(\nu) \nu^{-1} d\nu}{\int_{\nu_0}^{\infty} B_\nu(T) \sigma(\nu) \nu^{-1} d\nu}$$

1.2.2 Dielectronic recombination

We can derive how to implement a correction factor for this in the same way as we did above for ζ . Starting with

$$\Phi_0^* = \frac{n_{r+1,0 \rightarrow 0} n_e}{n_{r,0 \rightarrow 0}} = \frac{\gamma}{\alpha_{r+1,0 \rightarrow 0}}$$

we note that when we compute Φ_0^* we take account only of recombinations into the ground state via simple radiative recombination. We therefore also need to add in the dielectronic recombination rate at the same time as we add in the rates to all excited levels, therefore, the correction factor to Φ_0^* becomes

$$\frac{n_{r+1} n_e}{n_r} = \Phi_0^* \times \frac{\alpha_{r+1,0 \rightarrow 0}}{\sum_{i=1}^{\infty} \alpha_{r+1,0 \rightarrow i} + \alpha_{DR}} \quad (1.9)$$

We note from equation 1.5 that

$$\alpha_{r+1,0 \rightarrow 0} = \zeta \sum_{i=1}^{\infty} \alpha_{r+1,0 \rightarrow i}$$

and so we can rewrite equation 1.9 substituting for $\alpha_{r+1,0 \rightarrow 0}$

$$\frac{n_{r+1} n_e}{n_r} = \Phi_0^* \times \zeta \frac{\sum_{i=1}^{\infty} \alpha_{r+1,0 \rightarrow i}}{\sum_{i=1}^{\infty} \alpha_{r+1,0 \rightarrow i} + \alpha_{DR}}$$

The correction factor for either a diluted black body ($W(T_e/T_r)^{1/2}$) or the power law is also applied to get the correct non-LTE abundances.