Incorporating dielectronic recombination into Python

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Chapter 1

Dielectronic recombination

1.1 What is dielectronic recombination?

1.1.1 The process

In dielectronic recombination, an electron recombines with an ion, but rather than immediately emitting a photon, the excess energy of the electron goes into exciting a second, bound electron into an excited state. The initial recombination is therefore radiation free. We now have a doubly excited ion, and this relaxes either by a radiative cascade, or by autoionisation where the excited electron gives its energy back to the recombining electron thereby leaving the ion in its original state.

1.2 Ionization equilibrium equations

1.2.1 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. At the end we will have an equation for the correction factor for dielectronic recombination.

Four important equations:

Boltzmann

$$\frac{N_n}{N_1} = \frac{g_n}{g_1} exp\left(-\frac{\chi_n}{kT}\right) \tag{1.1}$$

Planck

$$I_\nu = B_\nu = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/kT-1}} \tag{1.2}$$

Maxwell-Boltzman distribution of electron speeds

$$f(v) = 4\pi\left(\frac{m_e}{2\pi kT_e}\right)^{3/2}\nu^2 exp\left(-\frac{m_e v^2}{2kT_e}\right) \tag{1.3}$$

Saha equation

$$\frac{N_{m+1}n_e}{N_m} = 2\frac{Z_{m+1}}{Z_m}\left(\frac{2\pi m_e kT}{h^3}\right)^{3/2} exp\left(-\frac{\chi_m}{kT}\right) \tag{1.4}$$

1.2.2 Derivation of the SAHA equation

This derivation is from **?** although I've changed some of the nomenclature for consistency and I've started out doing the general derivation between any two ionisation stages for some reason. They start with applying Boltzmann law to a tiny volume of space containing two ions in consecutive stages of ionisation, and the electron required to go between the two stages. The equation gives the number of particles in two states in terms of the energy difference between the two states assuming thermodynamic equilibrium. Generally, this looks like this

$$\frac{N_A}{N_B} = \frac{g_A}{g_B}\exp\left[-\frac{E_A - E_B}{kt}\right]$$

If we take as our two states, an ion in ionisation stage i, and an ion in ionisation stage i+1 together with an electron of velocity in the range (u,u+du), then the energy of state B will be the sum of the electron kinetic energy and the ionisation potential between the two states, and we can write

$$\frac{dn_{r+1,0}(u)}{n_{r,0}} = \frac{g_{r+1,0}g_e}{g_{r,0}}\exp\left[-\frac{(\chi_i + \frac{1}{2}m_e u^2)}{kT}\right] \tag{1.5}$$

where $dn_{r+1,0}(u)$ is the differential number of ions in the ground state of ionisation stage r+1 with the free electron in the velocity range (u,u+du), $n_{r,0}$ is the number of ions in the ground state of ionisation stage r. The g_{r+1} and g_r terms are the statistical weights of the two ionisation stages, and χ_i is the ionisation potential between ionisation stages r and r+1. The g_e term is the differential electron statistical weight

needed because there a are a range of electron position and momenta all having the same energy. There are also two possible spin orientations, hence the factor of 2.

$$g_e = \frac{2 dx_1 dx_2 dx_3 dp_1 dp_2 dp_3}{h^3}$$

Since we are dealing with the volume containing one electron, we know that the electron must be found in the volume described by its differential positions so

$$\frac{1}{n_e} = dx_1 dx_2 dx_3$$

where n_e is the volume density of electrons. The simplification of the momenta terms is something I should understand but it goes like this

$$dp_1 dp_2 dp_3 = 4\pi m_e^3 u^3 du$$

so equation ?? becomes

$$\frac{dn_{r+1,0}(u)}{n_{r,0}} = \frac{8\pi m_e^3}{h^3} \frac{g_{r+1,0}}{n_e g_{r,0}} \exp\left[-\frac{(\chi_i + \frac{1}{2} m_e u^2)}{kT}\right] u^2 du$$

This is still a differential number of ions in state r+1, so we simply need to integrate over u. We begin by splitting up the exponential

$$\frac{dn_{r+1,0}(u)}{n_{r,0}} = \frac{8\pi m_e^3}{h^3} \frac{g_{r+1,0}}{n_e g_{r,0}} e^{-\chi_i/kT} \exp\left[-\frac{\frac{1}{2} m_e u^2}{kT}\right] u^2 du$$

We make the substitutions

$$x \equiv \left(\frac{m_e}{2kT}\right)^{\frac{1}{2}} u$$

so

$$u^2 = \left(\frac{2kT}{m_e}\right) x^2$$

and

$$\frac{dx}{du} = \left(\frac{m_e}{2kT}\right)^{\frac{1}{2}}$$

so

$$du \equiv \left(\frac{2kT}{m_e}\right)^{\frac{1}{2}} dx$$

Which gives us

$$\frac{dn_{r+1,0}(u)}{n_{r,0}} = \frac{8\pi m_e^3}{h^3} \frac{g_{r+1,0}}{n_e g_{r,0}} e^{-\chi_i/kT} \exp\left[-\frac{(\frac{1}{2} m_e \left(\frac{2kT}{m_e}\right) x^2)}{kT}\right] \left(\frac{2kT}{m_e}\right) x^2 \left(\frac{2kT}{m_e}\right)^{\frac{1}{2}} dx$$

Rearranging, integrating over x and taking the electron density over to the left hand side we get

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = \frac{8\pi m_e^3}{h^3}\frac{g_{r+1,0}}{g_{r,0}}e^{-\chi_i/kT}\left(\frac{2kT}{m_e}\right)^{\frac{3}{2}}\int_0^\infty e^{-x^2}x^2 dx$$

This is a standard integral, equal to $\pi^{1/2}/4$, and so collecting terms and simplifying we get

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

Hale Bradt does a different derivation in his online supplement to his book Astrophysical Processes (**?**). He goes via Einstein coefficients, and ends up with a more general formula linking any two excited states of any two consecutive ionisation stages. His energy term therefore includes terms for the excitation energy above ground state. Note that the statistical weight of an electron g_e is now simply 2, to take account of spin since the velocity terms have been integrated over and the volume term has gone into n_e

$$\frac{n_{r+1,j}n_e}{n_{r,k}} = \frac{(2\pi mkT)^{3/2}}{h^3}\frac{g_{r+1,j}g_e}{g_{r,k}}\exp(-(\chi_i + \epsilon_{r+1,j} - \epsilon_{r,k})/kT) \qquad (1.6)$$

This is a form of the Saha equation which links any pair of ionisation stages r and r+1 in any excitation states 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 stage r to r+1, $\epsilon_{r+1,j}$ is the energy difference between the ground state of r+1 and the excited state 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.

This equation simplifies to **??** if we write it both both ionisation stages in the ground state.

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = \frac{(2\pi mkT)^{3/2}}{h^3}\frac{g_{r+1,0}g_e}{g_{r,0}}exp-(\chi_i/kT) \qquad (1.7)$$

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 **??** slightly, including the * to designate LTE we get

$$\Phi_0^*(T) = \frac{n_{r+1,0}^* n_e^*}{n_{r,0}^*} = \frac{(2\pi mkT)^{3/2}}{h^3} \frac{g_{r+1,0} g_e}{g_{r,0}} exp - (\chi_i/kT) \tag{1.8}$$

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 **??** at the radiation temperature T_R then the recombination rate equation, which is implicitly combined in the equation, will erroneusly 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/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

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = W\Phi_0^*(T_R) \times \frac{T_R^{-1/2}}{T_E^{-1/2}} = W\Phi_0^*(T_R) \times \sqrt{\frac{T_e}{T_R}} \qquad (1.9)$$

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^*

$$\Phi_0^* = \frac{\gamma_{r,0}}{\alpha_{r+1,0\to0}}$$

Where $\alpha_{r+1,0\to r,0}$ 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

$$\zeta = \frac{\alpha_{r+1,0\to0}}{\sum_{i=1}^{\infty} \alpha_{r+1,0\to i}} \qquad (1.10)$$

where $\sum_{i=1}^{\infty} \alpha_{r+1,0\to i}$ 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

$$\frac{n_{r+1,0}n_e}{n_{r,0}} = \zeta W\sqrt{\frac{T_e}{T_R}}\Phi_0^*(T_R) \qquad (1.11)$$

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1.2.3 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

$$\gamma \propto \int_{\nu_0}^{\infty} B_\nu(T)\sigma(\nu)\nu^{-1}d\nu \tag{1.12}$$

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

$$\gamma_{pl} \propto \int_{\nu_0}^{\infty} C\nu^\alpha\sigma(\nu)\nu^{-1}d\nu \tag{1.13}$$

so a very simple correction factor is to divide $\Phi_0^*(T_e)$ by the assumed photoionization rate **??** and multiply by the actual photoionization rate **??**. 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

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

1.2.4 Dielectronic recombination

Now we understand how to work out correction factors to the saha equaion, we can derive how to implement a correction factor for dielectronic recombination. We will do this in the same way as we did above for ζ. Starting with

$$\Phi_0^* = \frac{n_{r+1,0\to0}n_e}{n_{r,0\to0}} = \frac{\gamma}{\alpha_{r+1,0\to0}}$$

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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

$$\frac{n_{r+1}n_e}{n_r} = \Phi_0^* \times \frac{\alpha_{r+1,0\to0}}{\sum_{i=1}^{\infty}\alpha_{r+1,0\to i} + \alpha_{DR}} \tag{1.14}$$

We note from equation **??** that

$$\alpha_{r+1,0\to0} = \zeta\sum_{i=1}^{\infty}\alpha_{r+1,0\to i}$$

and so we can rewrite equation **??** substituting for $\alpha_{r+1,0\to0}$

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

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.

1.3 Cooling rate

1.3.1 Introduction

If we are making the assumption that dielectronic recombination is an important factor in driving the ionization state, to b self consistent, we really need to incorporate it as a cooling mechanism. In order to see how to do this, we will first examine for normal radiative recombination cooling is dealt with in Python. Firstly, lets think about the theoretical quantity we are interested in. If the volumetric radiative recombination rate coefficient from ionisation stage r+1 into stage r of any given ion is given by α_{RR} with units of $cm^{-3}s^{-1}$ then the number of recombinations N_{RR} per unit volume per second is given by

$$N_{RR} = n_e n_{r+1}\alpha_{RR}$$

The cooling rate in python is defined as the loss of kinetic energy from the cell, so if during the recombination, a photon of frequency ν is produced, then we know that an electron of energy e was removed from the electron pool. Part of that electrons energy will go into binding energy of the recombined atom (equal to the ionisation

potential χ_i of the ion in stage r), and the remainder will be radiated as a photon. Since we do not track the potential energy of the plasma, it must offset the loss of kinetic energy so the energy lost from the plasma due to each recombination

$$e = h\nu - \chi_i = h\nu - h\nu_0$$

where ν_0 is the threshold frequency of the photoionisation from r to r+1. Therefore, the cooling rate of the cell due to recombinations of a given ion from r+1 to r is

$$C_{RR} = (h\nu - h\nu_0)n_e n_{r+1}\alpha_{RR}$$

We now need to calculate α_{RR}, the radiative recombination rate. This is done via a detailed balance argument

From **?** we start be defining $\sigma_{fb}(u)$ which is the cross section for recombination for electrons of velocity u. Therefore, the partial rate for electrons with velocity in the range (u to u+du) is

$$n_{r+1}n_e\sigma_{fb}(u)f(u)udu$$

where f(u) is the velocity distribution of the electrons - we will consider them to follow a Maxwellian velocity distribution. By detailed balance, this rate must exactly balance the photonisation rate. In order to do this, we need to make the assumption that the photon field in in equilibrium with the electrons, that is to say we are in LTE. The photon distribution is therefore given by a blackbody function B_ν and the rate is

$$\frac{4\pi}{h\nu}n_r\sigma_{bf}(1 - e^{-h\nu/kT})B\nu d\nu$$

Understand this bit a little moreThese two rates must equal in detailed balance so

$$n_{r+1}n_e\sigma_{fb}(u)f(u)udu = \frac{4\pi}{h\nu}n_r\sigma_{bf}(1 - e^{-h\nu/kT})B\nu d\nu$$

Which gives us an expression for

$$n_r\gamma(\nu) = n_e n_{r+1}\alpha_{RR}$$

where $\gamma(\nu)$ is the photoionisation rate from stage r to r+1. We can therefore rewrite equation **??** as

$$C_{RR} = (h\nu - h\nu_{thresh})n_r\gamma(\nu)$$

We can now substitute for γ, the photoionisation rate from stage r to r+1 where

$$\gamma(\nu) = \int_{\nu_0}^{\infty}$$

1.3.2 Radiative recombination cooling

Radiative recombination cooling is dealt with in total_emission (located in emission.c). The luminosity of the current cell due to free bound processes is computed through a call to total_fb (located in recomb.c)

total_fb

This subroutine calculates the total luminosity of the cell on an ion by ion basis. The actual calculation for the lumionisity of each ion r is

$$L_r = V n_e n_{r+1} \times integ\_fb(t, f1, f2, nion, 1)$$

Where V is the volume of the cell, and the operation of the subroutine integ_fb is discussed below.

integ_fb

This subroutine, when called with option 1, returns the reduced emissivity of the ion. This is the emissivity less the threshold energy, which represents the kinetic energy loss of electrons in the cell. There is some complexity in the routine to try to use stored values wherever possible (as long as the frequency range over which the integration is carried out has not changed). In this case, the code calls get_fb which simply interpolates on the array freebound.emiss which is calculated by xinteg_fb for a range of temperatures.

xinteg_fb

This subroutine does all the dirty work of calculating the specific emissivity, or the rate of radiative recombination. The fundamental equation is

$$\left(\frac{h^2}{2\pi m_e k}\right)^{3/2} \frac{8\pi}{c^2} h \frac{g_r}{2g_{r+1}} \left(\nu^2 \times T\right)^{3/2} \exp\left(-\frac{h(\nu - \nu_0)}{kT}\right) \sigma_{bf}(\nu)$$

and it is integrated from ν to some upper limit of ν. compare with equation 38 in **?**

$$4\pi\epsilon(\nu)_{jk,fb} = h\nu \left(\frac{2\pi mk}{h^2}\right)^{3/2} \left(\frac{8\pi}{c^2}\right) \frac{g_{jk}}{g_e g_{j+1}} T_e^{3/2} \nu^2 \sigma(\nu)_{jk} e^{-h(\nu-\nu_t)/kT_e}$$

clearly the same. In Hazy, this is described as the Milne relation for the state-specific radiative recombination coefficient to a level n

$$\alpha_n(T) = \left(\frac{2\pi m_e k}{h^2}\right)^{-3/2} \frac{8\pi}{c^2} \frac{g_n}{g_e g_{ion}} T^{-3/2} \int_{h\nu_0}^{\infty} \nu^2 \alpha_\nu(n) \exp(-h(\nu-\nu_0)/kT) d\nu$$

α_ν is the photoionisation cross-section (usually called σ) so, rearranging the python formula a little to make it look more like the hazy equation we can see that the python formula is equal to the radiative recombination rate coefficient weighted by $h\nu$, the energy of the photon you are currently integrating over. If xinteg_fb is called with mode 2, then this factor is removed and the result is a rate coefficient. If it is called with mode 2, then a further factor of $(\nu-\nu_0)/\nu$ is applied, which means we weight the integral by the kinetic energy removed from the gas via each recombination, which gives us a a rate in $cm^{-1}s^{-1}$ times an energy per recombination in erg, so once we get back up to total_fb, the luminosity is

$$L_r = V n_e n_r + 1 \left(\frac{h^2}{2\pi m_e k}\right)^{3/2} \frac{8\pi}{c^2} \frac{g_r}{2g_{r+1}} T^{3/2} \int_{\nu_0}^{\infty} h(\nu-\nu_0)\nu^2 \exp\left(-\frac{h(\nu-\nu_0)}{kT}\right) \sigma_{bf}(\nu)$$

And this ends up stored in the xplasma lum[nion] structure element for that cell. Next we will see how that luminosity is actually output as photons. the total luminosity of the cell is held in lum_rad.

photon_gen

This is the driver routine to generate photons. If wind photons are required, the first thing it does is call wind_luminosity, followed by

wind_luminosity

All this routine does is call total_emission once more to populate all of the fractional luminosity arrays (lum_ff, lum_rad, lum_lines, lum_fb)

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