

# SUMMARY OF WORK DONE IN DECEMBER 2010 TO INCORPORATE A POWER LAW INTO BALANCE

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## 1. MOTIVATION

The aim of the work is to incorporate a power law spectrum into the balance code with a view to understanding how the ionisation cycle works in this new regime. Balance allows one to understand in detail how the mechanics of the ionisation cycles in Python work in a single cell. In balance, the radiation field in the cell is set using suitable parameters, rather than being defined by the geometrical relationship of the cell to a radiation source such as a disk or stellar photosphere.

## 2. THEORETICAL BACKGROUND

In order to properly model the interaction of a photon field with a gas, one needs to ensure that the gas is in the correct ionisation state. If the gas is in LTE, then the Saha equation achieves this through the assumption that the temperature of the gas uniquely specifies the energies of individual electrons via the Boltzmann distribution, and the radiation temperature of the photon field specifies the energies of individual photons via the Planck Distribution. The radiation temperature  $T_r$  and the electron temperature  $T_e$  are the same in LTE.

Previously, balance took account of departures from LTE using the formulation of Mazzali and Lucy (1993). Equation 14 in this paper is

$$\frac{n_{j+1,k}n_e}{n_{j,k}} = W[\zeta + W(1 - \zeta)] \left(\frac{T_e}{T_r}\right)^{1/2} \left(\frac{n_{j+1,k}n_e}{n_{j,k}}\right)_{T_r}^*$$

The starred term on the right hand side of the equation is the relative abundance of two adjacent ionisation states calculated from the Saha equation, and this is corrected using the dilution factor  $W$  and the additional factor  $\zeta$  which represents the proportion of ions which recombine to the ground state of the lower ionisation state relative to those recombining to all excited states. This equation provides a correction to the Saha abundances where  $T_e \neq T_r$  and the radiation field is a diluted black body distribution. In an AGN, in addition to the thermal radiation arising from the accretion disk, there is also a power law spectrum which extends into the Xray part of the spectrum. This is a radical departure from the blackbody distribution assumed by the Saha equation, and so in order to gain a correct distribution of ions we need a different correction factor. The intention is to use the correction factor  $S_i(T_e, J_\nu)$  suggested in Sim et al (2008).

$$S_i(T_e, J_\nu) = \frac{\int_{\nu_0}^{\infty} a_\nu J_\nu \nu^{-1} d\nu}{\int_{\nu_0}^{\infty} a_\nu B_\nu(T_e) \nu^{-1} d\nu}$$

Where  $a_\nu$  is the photoionisation cross section (frequency dependant),  $J_\nu$  is the mean intensity of the power law source at the cell and  $B_\nu$  is the planck spectrum at the electron temperature used to calculate the saha abundances which are being corrected. This is implemented as a correction factor as follows.

$$\frac{n_{j+1,k}n_e}{n_{j,k}} = \zeta(T_e)S_i(T_e, J_\nu) \left( \frac{n_{j+1,k}n_e}{n_{j,k}} \right)_{T_r}^*$$

In the correction factor equation, the numerator represents the ionisation rate from state  $n_{j,k}$  to state  $n_{j+1,k}$  due to the actual radiation field (represented by the mean intensity  $J_\nu$ ) and the denominator represents the ionisation rate predicted from a blackbody photon field.  $a_\nu$  is the ground state ionisation cross section. For a power law spectrum, the mean intensity is given by

$$J_\nu = W\nu^\alpha$$

and in Sim et al  $W$  and  $\alpha$  are calculated on a cell by cell basis after illuminating the entire wind structure with a power law photon field.  $W$  and  $\alpha$  therefore depend on the position in the wind and the equation for the  $S_i$  factor becomes

$$S_i(T_e, W, \alpha) = \frac{W \int_{\nu_0}^{\infty} a_\nu \nu^{\alpha-1} d\nu}{\int_{\nu_0}^{\infty} a_\nu B_\nu(T_e) \nu^{-1} d\nu}$$

In balance, the radiation field in the cell must be set using suitable parameters, since there is no physical radiation source illuminating the cell. In the black body regime, the parameters are simply the temperature of the black body, and the dilution factor, however the parameters for the power law source seem to the author to be less obvious without resorting to geometrical arguments.

### 3. SOFTWARE IMPLEMENTATION

**3.1. Summary of existing code.** The main code, Balance, allows the user to set a range of parameters like radiation temperature, electron temperature and blackbody dilution factor (weight). The main part of the code is summarised in the flow chat below. In overview, cycle first estimates the number of atoms in each possible ionisation state. This is the part of the code which is modified in this work, and will be dealt with in the next section. Next, a population of photons is produced, (more modifications here) and sent through the cell. Heating and cooling in the cell from the photons is then calculated in line\_heating, radiation, and total\_emission.

The subroutine one\_shot is now called. This attempts to balance the heating and cooling from the cell and produces a new estimate of electron temperature (the change is limited to  $0.7 \times T_e(old) \leq T_e(new) \leq 1.3 \times T_e(old)$ ). At this stage, the ionisation state of the gas is recomputed, the recombination rate is recomputed and a summary of the state of the gas is produced. There is a check for convergence and this completes one cycle. The user can then choose to rerun cycle, or if cycle is called from multicyle, it is automatically rerun a number of times as defined in the code. This allows  $T_e$  to be converged.

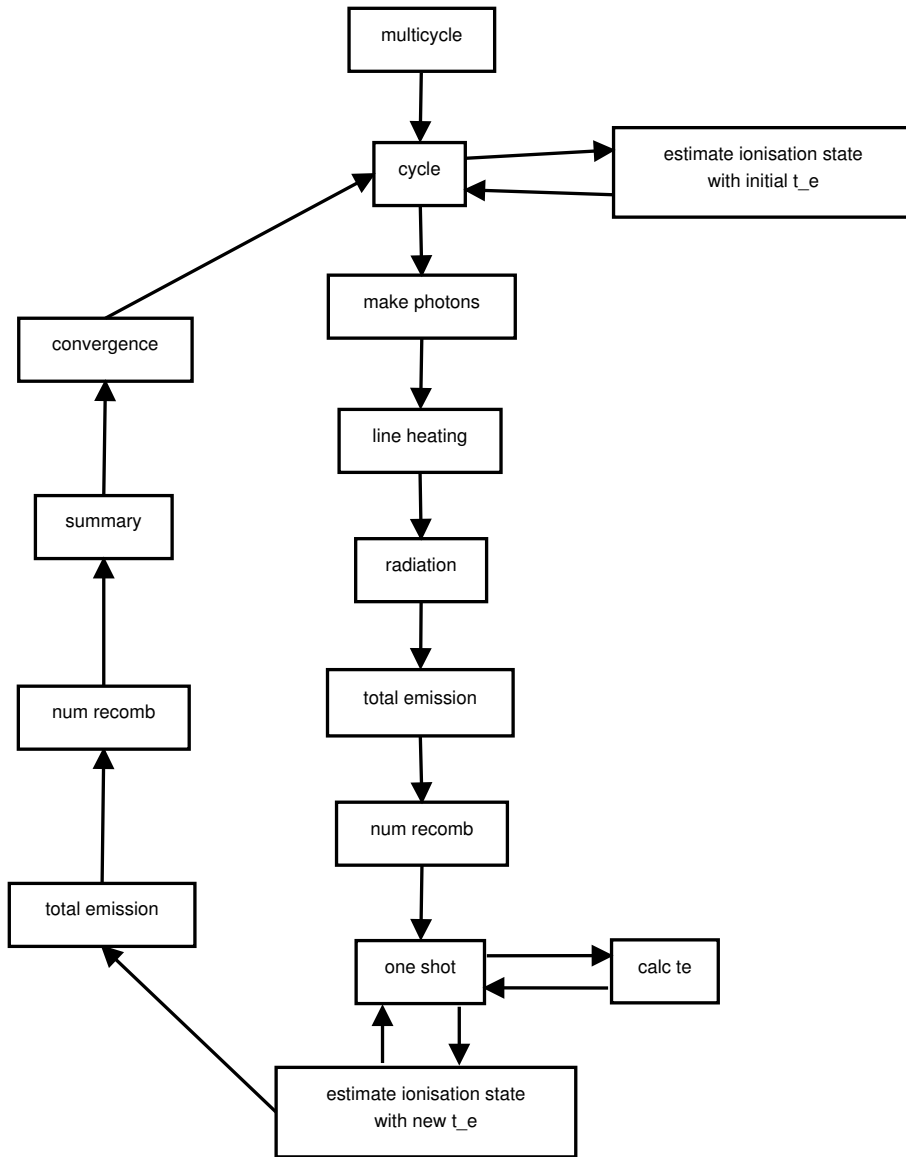


FIGURE 1. Flow chart of balance program

**3.2. Current ionization fraction calculations.** The flow chart below summarises how the current calculation of ion fractions carried out in balance. the subroutine `nebular_concentrations` is the driving routine, first making a call to `partition`. This calculates the partition functions for the ions of interest.

$$Z = \sum_j W g_j e^{-\frac{(E_j - E_1)}{k_B T}}$$

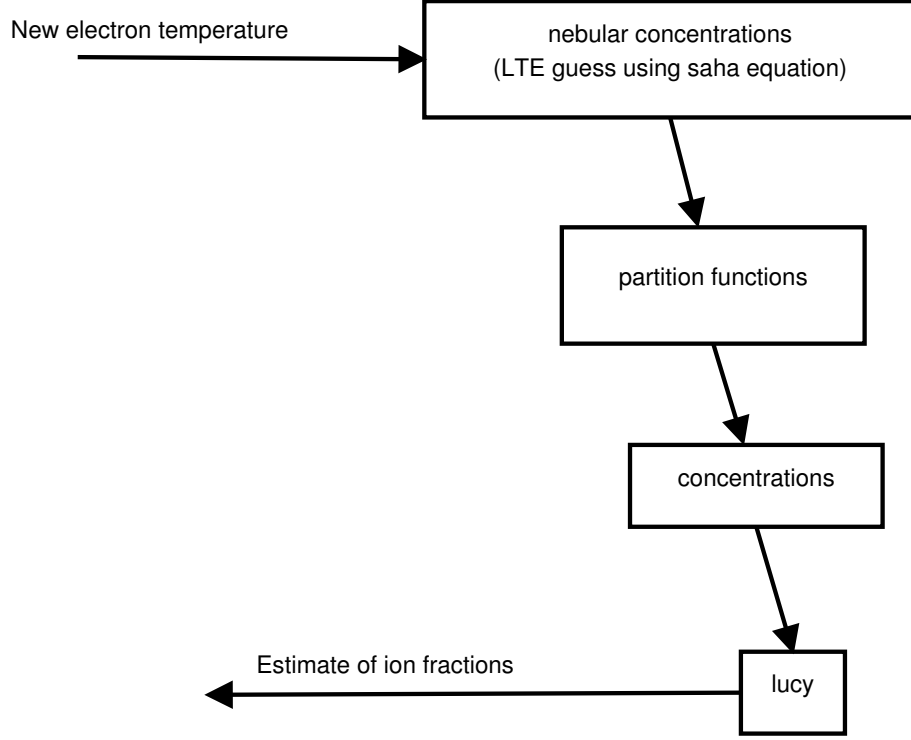


FIGURE 2. Ionisation calculation

Where  $E_j$  is the energy of state  $j$ ,  $E_1$  is the ground state energy,  $T$  can either be defined as radiation temperature or electron temperature and  $W$  is the radiative weight to allow for dilute blackbodies. In the case of a power law spectrum, the electron temperature is used and  $W$  is set to 1. Once the partition functions are calculated, concentrations is called. This simply applies the saha equation. There are two options in balance.

$$\frac{n_{j+1}n_e}{n_j} = \frac{2Z_{j+1}(T)}{Z_j(T)} \left( \frac{2\pi m_e kT}{h^2} \right)^{3/2} e^{-\chi_{j,j+1}/kT}$$

Where  $n_{j+1}$  and  $n_j$  are the number densities of the element in two adjacent ionisation states,  $n_e$  is the electron number density,  $Z_{j+1}$  and  $Z_j$  are the partition functions for the two states (the factor of 2 relates to the partition function for an electron) and  $\chi_{j,j+1}$  is the energy difference between the two states. Again, temperature is an input, and this can be either electron temperature or radiation temperature. For the power law, we use electron temperature. There is one saha equation for each pair of adjacent ionisation states for each element, and these are all linked by the number density of free electrons. A first guess at the electron density is calculated assuming a pure hydrogen plasma, and then the subroutine is rerun until this is converged.

At this point, the Lucy/Mazzali correction is applied in the current code in order to correct for a non LTE situation. We aim to apply the Sim correction factor here.

**3.3. Implementation of the Sim correction factor in Balance.** As we enter the piece of code designed to correct the saha abundances to those expected for a power law photon frequency distribution we have a current estimate of electron temperature. This starts out as a user input, but is iterated through the heating and cooling parts of balance in subsequent iterations. Recalling the equation for the correction factor

$$S_i(T_e, W, \alpha) = \frac{W \int_{\nu_0}^{\infty} a_{\nu} \nu^{\alpha-1} d\nu}{\int_{\nu_0}^{\infty} a_{\nu} B_{\nu}(T_e) \nu^{-1} d\nu}$$

we can see that we need values for  $W$  and  $\alpha$ . We set  $\alpha$  as a simple user input (set to -1.5 in the runs reported here), however  $W$  can be set in two different ways depending on whether we are running the code in automatic 'multicycle' mode or in the 'cycle' mode where the user iterates by hand. The primary aim of this work was to attempt to recreate figure 1 in Sim et al (MNRAS, 7 Feb 2010) we will concentrate on the calculations carried out in the multicycle mode.

In Sim et. al. (2010) the abscissa of figure 1 is the ionization parameter, defined in that paper as

$$\xi = \frac{L_{0.1-50}}{r^2 n_H}$$

We therefore vary the ionisation parameter and use that to calculate an input  $J_{\nu}$  into the Sim correction factor. We assume a value for  $n_H$  of  $10^{10}$  and a distance  $r$  of  $1e16$ cm (effectively the distance from the source to the cell under investigation). This allows us to calculate a  $L_{0.1-50}$  for the power law spectrum. We then make the assumption that the power law luminosity is given by the equation

$$L = \int L_{\nu} d\nu$$

where  $L_{\nu}$  is the luminosity per unit frequency interval. For a power law, we can write

$$L_{\nu} = C \nu^{\alpha}$$

and so we can write

$$L_{0.1-50} = \int_{0.1\text{eV}}^{50\text{eV}} C \nu^{\alpha} d\nu$$

and so we can simply obtain a value for  $C$ , the constant of the power law.

Following Osterbrock and Ferland,

$$J_{\nu} = \frac{L_{\nu}}{16\pi^2 r^2}$$

Therefore, our equation for the mean intensity becomes

$$J_{\nu} = \frac{C \nu^{\alpha}}{16\pi^2 r^2}$$

In the code, we split off a factor of  $1/4\pi$  and call this  $W$ , the weight. This is effectively the dilution factor for the power law radiation at a distance  $r$ , assuming a point source. We assume a starting electron temperature of  $1e6$ K, and then enter cycle to calculate the ionisation state of the cell. We calculate the partition functions as normal using the assumed electron temperature, and then the saha abundances are computed. Now we are ready to compute the sim correction factors for each pair of ions.

This calculation is simply two integrations, both involving photoionisation cross sections. In this work, we used two different sets of data for photoionisation cross sections. The cross section for most of the included ions is obtained using the parameterised approach of Verner, et al (1996) hereafter called VFXY data. This provides the frequency dependent photoionisation cross section from the ground state from the threshold frequency up to some maximum applicable frequency (by which stage the cross section has dropped to a very small number). We also have topbase data for Hydrogen, Helium, Carbon, Nitrogen and Oxygen. The topbase data contains information for excited levels of each ion, but since the correction equation contains the term  $\zeta$ , which corrects for recombinations to states other than the ground state, we will only use the ground state photoionisation data.

The actual integrations are carried out using the qromb numerical recipe, which takes as its input an equation. The integration limits are the threshold frequency up to the maximum applicable frequency. For the denominator, the integral is

$$\int_{\nu_{thresh}}^{\nu_{max}} a_{\nu} \frac{2h\nu^3}{c^2} \frac{1}{e^{\frac{h\nu}{kT}} - 1} \frac{1}{\nu}$$

For the numerator, we use the equation

$$\int_{\nu_{thresh}}^{\nu_{max}} a_{\nu} \frac{1}{4\pi} WC\nu^{\alpha-1}$$

Where C is the power law constant calculated earlier and W is the dilution factor  $1/4\pi r^2$ . Early on it became obvious that there was a problem when the frequency range of the denominator was such that the black body function was very small. This caused infinities in the sim factor, and so a kludge was introduced so that the sim factor was not allowed to be greater than 10% of the ratio between the total number density of the element under consideration and the hard wired minimum density for any ion (defined as  $1e-20$ ).

Once the full set of correction factors are computed, they are applied to the saha abundances and a new set of ionic abundances computed.

**3.4. Photon illumination.** Once the ionic abundances are computed, a flight of 100000 photons are produced and sent through the cell in order to calculate the heating and cooling effect and hence try and produce a consistent electron temperature. The frequency is randomised between  $1e14$  and  $1e19$  Hz and the weight of each photon is set to the luminosity of the power law from  $1e14$  to  $1e19$ Hz (derived from the ionisation parameter) divided by  $4\pi r^2$  and divided by 100000 where r is the distance from the power law source to the cell.

The photons propagate through the cell, and their effect on the gas is computed. A new electron temperature is derived that balances the heating from the photons with the cooling of the gas. If the code is being run in multicycle mode, this electron temperature is fed into a new saha abundance calculation and then a new Sim correction. The cycle is repeated as many times as desired.

#### 4. RESULTS

Upon running the code, the first thing that appears is that the initial electron temperature of  $1e6$  drops rapidly and finally converges at a fairly low value of some, dependant on the input ionisation parameter. The higher the ionisation parameter, the higher the final converged temperature.

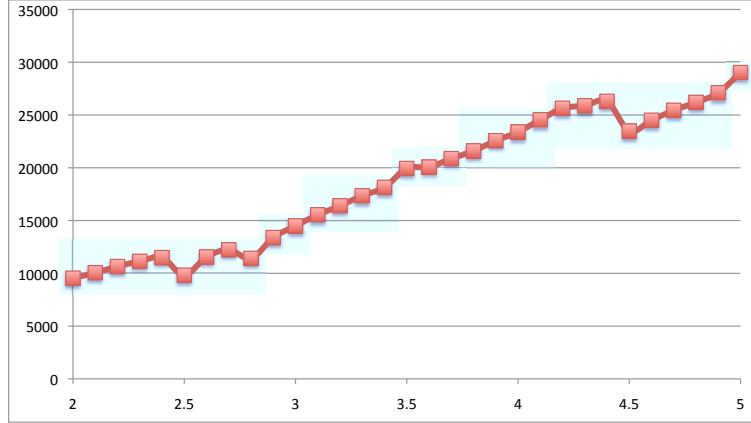


FIGURE 3. Variation of converged electron temperature with log ionisation parameter

The figure below shows the predicted abundances for Helium, Carbon, Oxygen and Iron. The X axis is ionisation parameter (after Sim et al 2010)

$$\xi = \frac{L_{0.1-50}}{r^2 n_H}$$

$n_H$  is set to  $10^{10} cm^{-3}$  and the electron temperature starts at  $10^6 K$ . The main thing to see from this figure is that each element only exists in one state at a time, not what we expect. There is also a somewhat chaotic behaviour apparent where one species can dominate, then drop off but return at a slightly different ionisation parameter. Careful examination of the behaviour of the Sim parameter as the program proceeds may provide some insight into what is happening.

#### 5. CONCLUSIONS

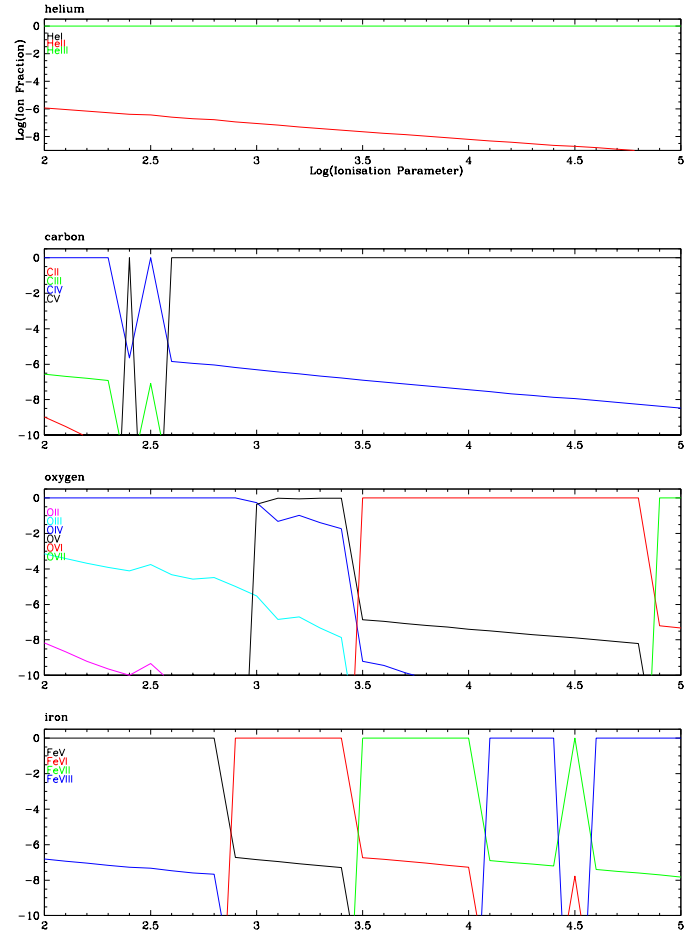


FIGURE 4. Predicted abundances of He, C, O and Fe