# Ionization Schemes and Rate Equations in Python

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November 20, 2014

**Abstract**

A summary of the ionization schemes used in Python, together with derivations.

## 1 Abbott & Lucy (1985: AL85)

**Mode:** Not used in Python directly.
**System:** Take a system in which an upper and lower ion are in ionization balance. Photoionizations are only allowed from the ground state but recombinations are allowed to excited states.
**Derivation / Discussion:** The rate equation for this can be written in terms of the photoionization rate coefficient $\gamma$ and the total recombination rate coefficient $\alpha_{tot}$ as

$$\alpha_{tot}(T_e) n_e n_{i+1} = n_i \gamma.$$

We can rewrite $\alpha_{tot}$ in terms of $\alpha$, the recombination rate coeffficient to the ground state, and $\zeta$, the fraction of recombinations which go directly to ground,

$$\alpha(T_e) n_e n_{i+1} = \zeta n_i \gamma.$$

Now assume the photoionizations are done by a dilute blackbody radiation field with a temperature $T_R$, giving

$$\alpha(T_e) n_e n_{i+1} = \zeta n_i \int \frac{W B_\nu(T_R) \sigma_\nu}{h\nu} d\nu \tag{1}$$

Now consider the same system in LTE at temperature $T_R$. We are in detailed balance, so the rate equation is

$$\alpha(T_R) n_e^* n_{i+1}^* = n_i^* \int \frac{B_\nu(T_R) \sigma_\nu}{h\nu} d\nu \tag{2}$$

We can now combine this equation with the one above to give

$$\frac{n_e n_{i+1}}{n_i} = W \zeta \frac{\alpha(T_R)}{\alpha(T_e)} \frac{n_e^* n_{i+1}^*}{n_i^*}, \tag{3}$$

and then assume that $\alpha(T) \sim T^{-1/2}$

$$\frac{n_e n_{i+1}}{n_i} = W\zeta\sqrt{\frac{T_e}{T_R}}\frac{n_e^* n_{i+1}^*}{n_i^*}, \tag{4}$$

**Assumptions:** There are a number of assumptions with this scheme, namely

- we assume the radiation field is a dilute blackbody with temperature $T_R$
- we assume that recombination rate coefficients have a $T^{-1/2}$ temperature dependence
- we neglect photoionizations from excited states

If one is constructing rate equations:

- recombination rate coefficients should be constructed from the Milne relation using the same cross sections used in the calculation
- The $\zeta$ term should be calculated from the same coefficients

# 2 Mazzali & Lucy (1993; ML93)

**Mode:** 3
**Notation:** Important!

- Starred teams really mean *the LTE value at temperature* $T_R$.
- The Ion fractions for ion $r$ are denoted $N_r$, whereas levels in said ion are denoted $n_{r,m}$.
- $\phi(T, Z_i, Z_{i+1})$ denotes 'the Saha equation', evaluated with the arguments in the brackets- if they are unstarred it means the partition functions are not LTE partition functions.

note that the papers which quote this formula tend not to be quite clear about the starred bracketed term in their equations, which here I call $\phi(T, Z_i, Z_{i+1})$. In fact, some of the papers claim it is evaluated at LTE, which is not strictly true as the partition functions are NLTE.

**Derivation / Discussion:** ML93 expand on the work of AL85 and previous papers by modifying the correction factor to account for photoionizations from excited states. We now rate the rate equation for this as

$$\alpha_{tot}(T_e) n_e n_{i+1} = n_0 \gamma_0 + n_{exc}\gamma_{exc} \tag{5}$$

my notation here is that 0 is ground state, whereas exc means a sum over excited states. We can now consider LTE at $T_R$ but focus on the excited states- recombinations an photoionizations must be in detailed balance over all these states, so

$$\alpha_{exc}(T_R) n_e^* n_{i+1}^* = \gamma_{exc}^*(T_R) n_{exc}^*$$

$$\alpha(T_R) n_e^* n_{i+1}^* = \gamma_0^*(T_R) n_0^*$$

Since, in a dilute BB field, $\gamma = W\gamma^*$,

$$\gamma_0 = W\gamma_0^* = W\alpha(T_R)\frac{n_e^* n_{i+1}^*}{n_0^*}$$

$$\gamma_{exc} = W\gamma_{exc}^* = W\alpha_{exc}(T_R)\frac{n_e^* n_{i+1}^*}{n_{exc}^*}$$

We can write

$$\alpha_{exc} = (1-\zeta)\alpha_{tot} = \frac{(1-\zeta)}{\zeta}\alpha$$

giving

$$\gamma_{exc} = W\frac{(1-\zeta)}{\zeta}\alpha(T_R)\frac{n_e^* n_{i+1}^*}{n_{exc}^*}$$

We can now substitute into (5) and do a bit of fiddling (note I have also substituted in $\alpha = \alpha_{tot}\zeta$)

$$\alpha(T_e)n_e n_{i+1,0} = \zeta W \left( n_0 \alpha(T_R)\frac{n_e^* n_{i+1,0}^*}{n_{i,0}^*} + \frac{(1-\zeta)}{\zeta}\alpha(T_R) n_{i,exc}\frac{n_e^* n_{i+1,0}^*}{n_{i,exc}^*} \right)$$

We can now divide through by $n_i$ and factorise out the alphas, then do a bit of fiddling and assume the usual $T^{-1/2}$ dependence:

$$\begin{aligned}
\frac{n_e n_{i+1,0}}{N_i} &= \zeta W \frac{\alpha(T_R)}{\alpha(T_e)}\frac{1}{N_i}\left( n_{i,0}\frac{n_e^* n_{i+1,0}^*}{n_{i,0}^*} + \frac{(1-\zeta)}{\zeta} n_{i,exc}\frac{n_e^* n_{i+1,0}^*}{n_{i,exc}^*} \right) \\
&= \zeta W \sqrt{\frac{T_e}{T_R}} \left( \frac{n_{i,0}}{N_i}\frac{n_e^* n_{i+1,0}^*}{n_{i,0}^*} + \frac{(1-\zeta)}{\zeta}\frac{n_{i,exc}}{N_i}\frac{n_e^* n_{i+1,0}^*}{n_{i,exc}^*} \right) \\
&= W \sqrt{\frac{T_e}{T_R}} \left( \zeta \frac{n_{i,0} N_i^*}{n_{i,0}^* N_i} + (1-\zeta)\frac{n_{i,exc} N_i^*}{n_{i,exc}^* N_i} \right) \frac{n_e^* n_{i+1,0}^*}{N_i^*}
\end{aligned}$$

The partition function for a given level $m$ in an ion $r$ is defined by

$$n_{r,m} = \frac{N_r g_{r,m}}{Z_r}$$

$$\frac{n_e N_{i+1}}{N_i} = \frac{Z_{i+1}}{g_{i+1,0}}\frac{n_e n_{i+1,0}}{N_i}$$

giving

$$\frac{n_e N_{i+1}}{N_i} = W \sqrt{\frac{T_e}{T_R}} \left( \zeta \frac{n_{i,0} N_i^*}{n_{i,0}^* N_i} + (1-\zeta)\frac{n_{i,exc} N_i^*}{n_{i,exc}^* N_i} \right) \frac{n_e^* N_{i+1}^*}{N_i^*}\frac{Z_{i+1}}{Z_{i+1}^*} \qquad (6)$$

To get the final equation of ML93 used in the code, one has to make an important distinction. The starred quantity in their equation, which I shall call $\phi$, is really the Saha equation evaluated at $T_R$ for NLTE partition functions, i.e.

$$\phi(T_R, Z_{i+1}, Z_i) = \frac{(2\pi m k_b T_R)^3/2}{h^3} \frac{Z_{i+1} g_e}{Z_i} \exp(-\chi_i / k_b T_R)$$

Whereas what I have written down on my RHS is, in Saha form,

$$\frac{n_e^* N_{i+1}^*}{N_i^*} = \phi(T_R, Z_{i+1}^*, Z_i^*) = \frac{(2\pi m k_b T_R)^3/2}{h^3} \frac{Z_{i+1}^* g_e}{Z_i^*} \exp(-\chi_i / k_b T_R)$$

therefore

$$\frac{n_e^* N_{i+1}^*}{N_i^*} = \phi \frac{Z_i Z_{i+1}^*}{Z_i^* Z_{i+1}}$$

substituting into (6) gives us

$$\frac{n_e N_{i+1}}{N_i} = W \sqrt{\frac{T_e}{T_R}} \left( \zeta \frac{n_{i,0} N_i^*}{n_{i,0}^* N_i} + (1-\zeta) \frac{n_{i,exc} N_i^*}{n_{i,exc}^* N_i} \right) \frac{n_e^* N_{i+1}^*}{N_i^*} \frac{Z_i^*}{Z_i} \phi(T_R, Z_{i+1}, Z_i) \tag{7}$$

...Nearly there! Now we need to assume that the excited levels are dilute, i.e.

$$n_{i,exc}/n_{i,exc}^* = W(n_{i,0}/n_{i,0}^*)$$

Giving us

$$\frac{n_e N_{i+1}}{N_i} = W \sqrt{\frac{T_e}{T_R}} (\zeta + (1-\zeta)W) \frac{n_e^* N_{i+1}^*}{N_i^*} \frac{Z_i^*}{Z_i} \frac{n_{i,0} N_i^*}{n_{i,0}^* N_i} \phi(T_R, Z_{i+1}, Z_i) \tag{8}$$

and finally, since

$$\frac{n_{i,0} N_i^*}{n_{i,0}^* N_i} = \frac{Z_i}{Z_i^*}$$

Some of the factors on the right cancel and we obtain

$$\frac{n_e N_{i+1}}{N_i} = W(\zeta + (1-\zeta)W) \sqrt{\frac{T_e}{T_R}}\ \phi(T_R, Z_{i+1}, Z_i), \tag{9}$$

**Assumptions:** Identical to AL85, except we take account of photoionizations from excited states. Note also the assumption about the upper levels being dilute.

# 3 Dilute BB Variable Temperature Solver

**Mode:** 6
**Derivation / Discussion:** For reasons of numerical stability, a 'variable temperature solver' was introduced to Python. This solver evaluates the Saha equation at a sensible temperature $T'$ which produces an abundances ratio of around 1. One then applies a correction factor to get the correct ionization abundances.

Equation:

$$\frac{n_e n_{i+1}}{n_i} = W(\zeta + (1-\zeta)W)K\left(\frac{n_e^* n_{i+1}^*}{n_i^*}\right)_{T'}, \tag{10}$$

where

$$K = \frac{\alpha(T')}{\alpha(T_e)}\frac{\int B_\nu(T_R)\sigma_\nu \nu^{-1} d\nu}{\int J_\nu(T')\sigma_\nu \nu^{-1} d\nu} = \sqrt{\frac{T_e}{T'}}\frac{\int B_\nu(T_R)\sigma_\nu \nu^{-1} d\nu}{\int B_\nu(T')\sigma_\nu \nu^{-1} d\nu}$$

**Assumptions:** The assumptions here are the same as ML93, although we apply the correction factors to a different temperature, so the results could be slightly different- they would be exactly the same if the recombination coefficients scaled as $T^{-1/2}$.

# 4 Spectral Model Variable Temperature Solver

**Mode:** 7
**Derivation / Discussion:** Higginbottom et al. (2013) claim that our ionization is calculated from:

$$\frac{n_e n_{i+1}}{n_i} = \zeta S_i \left(\frac{n_e^* n_{i+1}^*}{n_i^*}\right)_{T_e}, \tag{11}$$

where

$$S_i = \frac{\int J_\nu \sigma_\nu \nu^{-1} d\nu}{\int B_\nu(T_e)\sigma_\nu \nu^{-1} d\nu} \tag{12}$$

However, really, we evaluate the equation

$$\frac{n_e n_{i+1}}{n_i} = \zeta K \left(\frac{n_e^* n_{i+1}^*}{n_i^*}\right)_{T'}, \tag{13}$$

where

$$K = \sqrt{\frac{T_e}{T'}}\frac{\int J_\nu \sigma_\nu \nu^{-1} d\nu}{\int B_\nu(T')\sigma_\nu \nu^{-1} d\nu} \tag{14}$$

Equation 7 can be derived again by considering rate equations in much the same way as AL85, but instead of assuming a dilute blackbody the general $J_\nu$ is used.

We can write down a rate equation with a general SED as

$$\alpha(T_e) n_e n_{i+1} = n_i \int \frac{J_\nu \sigma_\nu}{h\nu} d\nu \tag{15}$$

and also note that in LTE at temperature $T_e$ we have

$$\alpha(T_e) n_e^* n_{i+1}^* = n_i^* \int \frac{B_\nu(T_e)\sigma_\nu}{h\nu} d\nu \tag{16}$$

combining these two equations gives

$$\frac{n_e n_{i+1}}{n_i} = \zeta \left( \frac{n_e^* n_{i+1}^*}{n_i^*} \right)_{T_e} \frac{\int J_\nu \sigma_\nu \nu^{-1} d\nu}{\int B_\nu(T_e) \sigma_\nu \nu^{-1} d\nu} \tag{17}$$

and substituting in the expression for $S_i$ gives (8).

**Assumptions:** We no longer make assumptions about the SED here, other than we hope we have done a good job of modelling it. We still make the assumption that the recombination coefficients scaled as $T^{-1/2}$, and we do not correct for photoionizations from excited states.