Heating and Cooling Estimators in Python: Macro-atoms and Simple-ions

Here I've tried to use Lucy's notation for macro-atom estimators. Take a three level system, in which l and u represent lower and upper levels, and κ represents the continuum level or upper ion. q is the 'absorption fraction' derived below, and q_{ul} and q_{lu} are the collisional rate coefficients.

1. Macro-atom estimators

In the macro-atom approach, we basically treat two communication pathways. bound-free transitions represent a way for radiant energy to communicate with the thermal pool and bound-bound transitions represent a way for excitation energy to communicate with the thermal pool.

The heating and cooling rates for macro-atom bound-bound transitions are the rates of collisional excitations and de-excitations - i.e. the rate at which thermal energy is converted into bound-bound excitation energy and vice versa.

$$C_{bb,matoms} = \sum_{lines} q_{lu} n_l n_e h\nu_{ul} V \tag{1}$$

$$H_{bb,matoms} = \sum_{lines} q_{ul} n_u n_e h\nu_{ul} V \tag{2}$$

For bound-free transitions, we define the normal photoionization and recombination rate coefficients γ and α, where α includes stimulated recombination as we do in the code. Note this differs to the approach in Lucy (2003), where it is instead included as a negative photoionization term, hence the notation $\widetilde{\gamma}$. We also need to define two 'modified rate coefficients' which are the rates at which b-f transitions add and remove energy to the radiation field. These are denoted γ^E and α^E.

The rate at which recombinations convert thermal *and* ionization energy into radiant energy is then $\alpha^E h\nu_{\kappa l} n_\kappa n_e$, where $h\nu_{\kappa l}$ is the potential of the b-f transition, or the energy difference between continuum κ and the level l we are recombining too. The amount of this energy which is removed from the actual thermal pool therefore needs a quantity $\alpha h\nu_{\kappa l} n_\kappa n_e$ subtracted from it, giving

$$C_{bf,matoms} = \sum_{bfjumps} (\alpha^E - \alpha) n_e n_\kappa \nu_{\kappa l} V \tag{3}$$

where here I have also included stimulated recombination as we do in the code. Note this differs to the approach in Lucy (2003), where it is instead included as a negative photoionization term, hence the notation $\widetilde{\gamma}$. For photoionizations, we write a similar expression. The rate of at which a level l absorbs energy by b-f transitions is given by $\gamma^E h\nu_{\kappa l} n_\kappa n_e$, but the amount $\gamma h\nu_{\kappa l} n_l$ goes into ionization energy, giving

$$H_{bf,matoms} = \sum_{bfjumps} (\gamma^E - \gamma) n_l h\nu_{\kappa l} V \tag{4}$$

as the rate at which radiant energy heats the plasma via b-f transitions.

2. Simple-ion estimators

In simple-ions it is in some ways a little more complicated. First we define q which will be different for each b-b transition, following Nick's thesis, which is given by (NB: I don't actually know how to derive this)

$$q = \frac{q_{ul} n_e (1 - e^{-h\nu/kT_e})}{\beta_{ul} A_{ul} + q_{ul} n_e (1 - e^{-h\nu/kT_e})} \tag{5}$$

where β_{ul} is the angle-averaged escape probability. q represents *the probability that an excited bound electron will collisionally de-excite*. Our b-b heating rate is computed during the photon propagation and is a sum over photons which come into resonance with each line, given by

$$H_{bb,simple} = \sum_{photons} \sum_{lines} (1 - q)(1 - e^{-\tau_S}) w_{photon} \tag{6}$$

And our bound bound cooling rate is given by

$$C_{bb,simple} = \sum_{lines} q \left(n_l \frac{g_u}{g_l} - n_u \right) q_{ul} n_e \frac{(1 - e^{-h\nu/kT_e})}{(e^{h\nu/kT_e} - 1)} h\nu_{ul} \tag{7}$$

The bound-free heating rate is given by

$$H_{bf,simple} = \sum_{photons} \sum_{bf jumps} w_{photon} e^{-\tau} \frac{\nu - \nu_0}{\nu} \tag{8}$$

where ν here is the frequency of the photon in question, and ν_0. The bound-free cooling rate is then

$$C_{bf,simple} = ?? \tag{9}$$