Heating and Cooling Estimators

Here I've tried to use Lucy's notation for macro-atom estimators. 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 communicaton pathways. bound-free transitions represent a way for radiant energy to communicate with the thermal pool and bound-bound transitions represent a way for ionization/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.

$$H_{bb,matoms} = \sum_{lines} q_{ul} n_u n_e h\nu_{ul} V \tag{1}$$

$$C_{bb,matoms} = \sum_{lines} q_{lu} n_l n_e h\nu_{ul} V \tag{2}$$

For bound-free transitions, the rate at which spontaneous recombinations convert thermal *and* ionization energy into radiant energy is $\alpha^E_{sp} h\nu_i n_\kappa n_e$, where $h\nu_i$ is the potential of the b-f transition. The amount of this energy which goes into the actual thermal pool is therefore given by

$$C_{bf,matoms} = \sum_{bf jumps} (\alpha^E_{sp} - \alpha_{sp} + \alpha^E_{st} - \alpha_{st}) n_e n_\kappa \nu_{\kappa l} \tag{3}$$

where here I have also included stimulated recombination as we do in the code. 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 $\gamma_i h\nu_{\kappa l} n_i$ goes into ionization energy, giving

$$H_{bf,matoms} = \sum_{lines} (\gamma^E_{sp} - \gamma) n_l h\nu_{\kappa l} \tag{4}$$

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

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

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

$$C_{bf,simple} = \sum_{bf jumps} \alpha_{sp} n_e n_\kappa \tag{9}$$