NLTE implementation in Turbospectrum - Bertrand Plez - 06/01-2020

From Rutten 2003 (Eq. 2.105) the NLTE line source function is:

$$S_\lambda = \frac{j_\lambda}{\alpha_\lambda} = \frac{2hc^2}{\lambda^5} \frac{\psi/\varphi}{\frac{b_l}{b_u} e^{h\nu/kT} - \chi/\varphi}$$

and with complete redistribution ($\chi = \varphi = \psi$),

$$S_\lambda = \frac{2hc^2}{\lambda^5} \frac{1}{\frac{b_l}{b_u} e^{h\nu/kT} - 1} = B_\lambda \frac{e^{h\nu/kT} - 1}{\frac{b_l}{b_u} e^{h\nu/kT} - 1}$$

The bound-bound extinction is then (complete redistribution):

$$\boxed{\alpha_\lambda = \alpha^*_\lambda b_l \frac{1 - \frac{b_u}{b_l} e^{-h\nu/kT}}{1 - e^{-h\nu/kT}}}$$

From which the emissivity:

$$j_\lambda = \alpha_\lambda S_\lambda = \alpha^*_\lambda b_l \frac{1 - \frac{b_u}{b_l} e^{-h\nu/kT}}{1 - e^{-h\nu/kT}} B_\lambda \frac{e^{h\nu/kT} - 1}{\frac{b_l}{b_u} e^{h\nu/kT} - 1}$$

$$j_\lambda = \alpha^*_\lambda b_l B_\lambda \frac{1 - \frac{b_u}{b_l} e^{-h\nu/kT}}{\frac{b_l}{b_u} - e^{-h\nu/kT}}$$

and finally:

$$\boxed{j_\lambda = \alpha^*_\lambda b_u B_\lambda}$$

The total source function at a given wavelength, if more than one line contributes is:

$$\boxed{S_\lambda = \frac{\sum j_\lambda}{\sum \alpha_\lambda}}$$

Similarly for the continuum:

$$\boxed{\alpha^{bf}_\lambda = \alpha^{bf*}_\lambda b_i \frac{1 - \frac{b_c}{b_i} e^{-h\nu/kT}}{1 - e^{-h\nu/kT}}}$$

$$\boxed{j^{bf}_\lambda = \alpha^{bf*}_\lambda b_c B_\lambda}$$

and

$$\boxed{\alpha^{bf}_\lambda = \alpha^{ff*}_\lambda b_c}$$

$$\boxed{j^{ff}_\lambda = \alpha^{ff*}_\lambda b_c B_\lambda}$$

$$S^{ff}_\lambda = B_\lambda$$

In Turbospectrum the implementation can be done as follows:

- The identification of the upper and lower level is read from the line list, using two more variables at the end of the statement (eqwidt.f version, as bsyn.f does not have the obseqw and eqwerror):

  » read(lunit,*) xlb,chie,gfelog,fdamp,gu,raddmp,levlo,levup,obseqw,eqwerror

  These identifications are those of the model atom.

- The departure coefficients are read from the MULTI output file with identical level id:s.

- The absorption coefficient is corrected in bsyn.f (and eqwidt.f, if we plan to use it). Variable is called plez(). See loop: do 111 ...continue.

- The extinction coefficient is incremented: abso() only. The scattering part absos() is kept to zero. Warning: abso() is normalized by the standard opacity, and is in cm^2/gram of stellar matter. It should either be transformed to α (cm^{-1}), or the emissivity should be given in cm^2/gram as well.

- A new array is created and incremented: emissivity().

- After all lines have been scanned, and their contribution added in abso() and emissivity(), bsynb.f is called.

- In bsynb.f the continuum absocont() and absoscont() are computed, as well as the Planck function, then traneq.f is called to solve the transport equation for the continuum. SOME THINKING NEEDED HERE. Do we want to do it this way? How do we add the continuum contribution for the NLTE species?

- Then same thing is done including lines. The proper way to treat continuum here is probably to include it in the absorption (x()=x()+s()), asuming it is the way it is done in MULTI (CHECK!). The source function needs to be changed from bplan() to emissivity/alpha, i.e. emissivity/abso()*ross(). As absos() is set to zero, traneq.f will not iterate on the source function, and use the provided input, as desired.

The implementation must keep compatibility with the older line list format, and with LTE calculations, i.e.: no level identification in line list, or no MULTI outputfile, or no master model atom file, means classical LTE calculation (all departure coefficients set to one).

One uncertain issue is the treatment of bf and ff transitions for NLTE species.