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EXTENSION OF LTE FORMULATIONS TO NON-LTE CONDITIONS

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Abstract — LTE models cannot give a reliable description for the whole density temperature range of many types of plasmas. Among these, there are x-ray sources and ICF plasmas. We present methods for extending LTE formulations, i.e. Saha-Boltzmann and the average ion, to incorporate radiative processes so that they become able to describe Non-LTE plasmas. These new Non-LTE formulations keep their original simplicity since no additional data is required. This avoids the complex computations of a full collisional radiative model. These extended models, Saha-Boltzmann eXtension (SBX) and Non-LTE Average Ion (NAI) models may be used as standalone for example to follow trends in the physical properties of plasmas. The SBX may be incorporated in hydro codes to compute atomic populations and mean charge.

1. INTRODUCTION

The analysis of physical properties relevant to hot dense partially ionized plasmas necessitates generally Non-LTE (Non-Local Thermodynamic Equilibrium) methods. Examples of these media include x-ray lasers [1] and ICF (Inertial Confinement Fusion) targets for direct [2] or indirect [3] drives schemes. These plasmas cover large ranges of temperature and density and LTE breaks down in the low density regime where atomic processes are no more dominated by collisions. Sophisticated kinetic Collisional-Radiative (CR) models are unsuitable for routinely hydrodynamic simulations being time consuming. Saha-Boltzmann (SB) and the Fermi-Dirac based average ion models have been extensively used due to their simple formalism and to the minimal atomic data required. However they are reliable only in the high density limit. So alternative low-cost methods are needed.

This paper presents methods allowing the extension of formulations valid for the description of media in LTE to formulations that can describe media in Non-LTE. Making some simplifying assumptions help us construct an equivalent of the SB formula with the radiative processes incorporated so that it becomes usable at lower densities than can be used with the SB law. The simplicity of the model, termed SBX (Saha Boltzmann eXtension) makes it easy to implement while producing adequate quality results with short computation times. Others have developed similar extensions, either with ground states only [4], or by grouping levels into superlevels and working with two superlevels [5].

From the SBX, a Non-LTE degeneracy parameter is derived. We profit from this opportunity to insert it in the average ion model that lies on the Fermi-Dirac formula for the occupation number. This produces an average ion model that computes shell occupation numbers, energies and mean free electron numbers in Non-LTE. This extended average ion model may be applied to the computation of Planck and Rosseland opacities for low- and high- Z targets, for rapid evaluations of the optical properties.

An important quantity revealing off-equilibrium deviations is the mean charge, for this reason we focus on it in our present results. More detailed calculations will be reported elsewhere.

2. SAHA-BOLTZMANN EQUATION REVISITED

The well-known Saha (for ground state populations) and Boltzmann (for excited state populations) equations may be gathered as

$$\left[\frac{N_{z+1,1}}{N_{z,n}}\right]^{LTE} = 6.02\ \ 10^{21} \frac{g_{z+1,1}}{g_{z,n}} \frac{T_e^{3/2}}{N_e} \exp[-(I_{z,1} - E_{z,n}) / T_e] \tag{1}$$

$N_{z,n}$ is the population of an ion in charge state z with an electron in the n^{th} level, subscript 1 refers to the fundamental level of the ion, the g's are the statistical weights, $I_{z,n}$ is the ionization potential and $E_{z,n}$ the level energy. T_e and N_e are the electron temperature and density, respectively. In this study the subscript n is identified to the principal quantum number of the level, since we consider only screened hydrogenic structures [6].
Now, turning to the Quasi Steady State (QSS) approximation and considering explicit formulae for the rates of collisional ionization and excitation, collisional recombination and deexcitation and spontaneous radiative recombination and decay, we may write a similar formula gathering excitation and ionization states, expressed as a function of the above LTE formula

$$\frac{N_{z+1,1}}{N_{z,n}} = \left(\frac{N_{z+1,1}}{N_{z,n}}\right)^{LTE} \frac{1 + S_{RD}}{1 + S_{PR}} \tag{2}$$

where

$$S_{PR} = \frac{C_{RR}(z+1)\ T_e^{3/2-\eta}}{C_{SB}\ C_{CI}\ N_e} I_{z,1}^{3/2+\eta} \frac{g_{z+1,1}}{g_{z,1}} \frac{F_R}{F_I} \tag{3}$$

and

$$S_{RD} = \frac{C_{RD}}{C_{CE}}\ E_{z,n}^3\ T_e^{1/2} / (N_e G) \tag{4}$$

In the above formulae, G is the Gaunt factor of the transition between levels labeled with n and the ground state, η, C_{CI}, and C_{RR} are constants depending on the collisional ionization and recombination rate coefficients chosen, C_{RD} and C_{CE} are constants appearing in the radiative decay rate coefficient (Einstein coefficient) and collisional excitation rate coefficient, and C_{SB} comes from the Saha formula. Their values are given in section 4.
Eq. (2) includes explicit contributions from ground and excited levels. The term S_{PR} accounts for radiative recombination and the term S_{RD} accounts for spontaneous radiative decay, the collisional contributions being contained in the term identified with the superscript LTE. The functions F_I and F_R appear because we made provision for different ionization and recombination rate coefficients available in the literature. We note that for high enough densities or low enough temperatures, the collisional processes dominate over the radiative processes, and Eq. (2) recovers the LTE formulation with $S_{PR} = S_{RD} = 0$. So this form guarantees a smooth passage between LTE and Non-LTE.

3. THE AVERAGE ION REVISITED

The distribution of the electrons among the allowed energy levels obeys the statistics of Fermi-Dirac

$$P_n = \frac{D_n}{1 + \exp[E_n / T_e - \alpha]} \qquad (5)$$

As we use the same atomic structure as in the previous section, n is the principal quantum number of the energy level E_n including continuum lowering. D_n is the degeneracy of level n including pressure ionization [7], and α is the electron degeneracy parameter. At thermal equilibrium, α equals

$$\alpha_{LTE} = \mathrm{Ln}\left[\frac{T_e^{3/2}}{C_{SB}\, N_e}\right] \qquad (6)$$

Now turning back to the SBX and rewriting Eq. (2) to make appear explicitly the degeneracy parameter, we obtain a Non-LTE electron degeneracy parameter

$$\alpha_{Non-LTE} = \mathrm{Ln}\left[\frac{T_e^{3/2}}{C_{SB}\, N_e}\ \frac{1+S_{RD}}{1+S_{PR}}\right] \qquad (7)$$

Introducing this latter in Eq. (5) removes the hypothesis of LTE populations, offering the opportunity of covering a larger range of density-temperature conditions.

4. RESULTS AND DISCUSSION

Inserting in Eqs. (3) and (4) the rates of [8-10] implies the following values for the constants : $G = 0.2$, $C_{CE} = 1.58\ 10^{-5}$, $C_{RD} = 4.34\ 10^{7}$, $C_{SB} = 1.66\ 10^{-22}$, $C_{RR} = 5.2\ 10^{-14}$, $C_{CI} = 2.97\ 10^{-6}$, $\eta = 1$ and $F_R / F_I = 1$.

Figs. 1a and 1b show the degree of ionization of Molybdenum (Z=42) vs. temperature, for electron densities of 10^{20} and 10^{18} cm^{-3}, computed with the LTE, Eq. (1), and SBX, Eq. (2), models. LTE is indicated by a continuous line, SBX by a dashed line and CRE by crosses. It is clear that the LTE model overestimates the mean ionization. We note the good behavior of the SBX when compared to the CRE (Collisional Radiative Equilibrium) model, which includes the same atomic structure and the same set of rate coefficients plus dielectronic recombination and solves a set of coupled rate equations.

Figs. 2a and 2b show for Sn (Z=50), at $\rho = 0.1$ and 0.001 gr/cm^3, the mean number of free charges as a function of temperature for the average ion model. Here again the Non-LTE curves depart from the LTE ones.

In both SBX and NAI cases, the enhancements over LTE results are noticeable. The Non-LTE ion ionizes less than the LTE ion, reflecting the effect of the radiative processes that come to compete with or overwhelm the collisional processes.

Thus, LTE formulations can be simply extended to Non-LTE conditions, either for a detailed distribution of levels or for the average ion models, giving physical insights without recourse to sophisticated modeling.

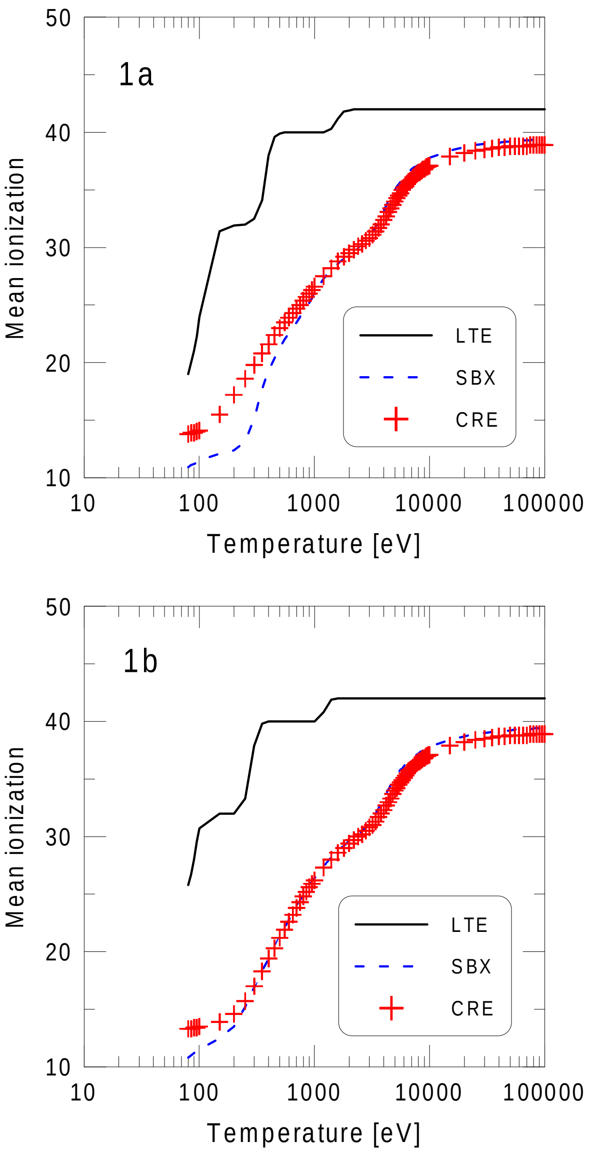

Fig. 1. Mean ionization for Mo vs. electron temperature computed with the LTE, SBX and CRE models, at an electron density of a) 10^{20} cm^{-3} and b) 10^{18} cm^{-3}.

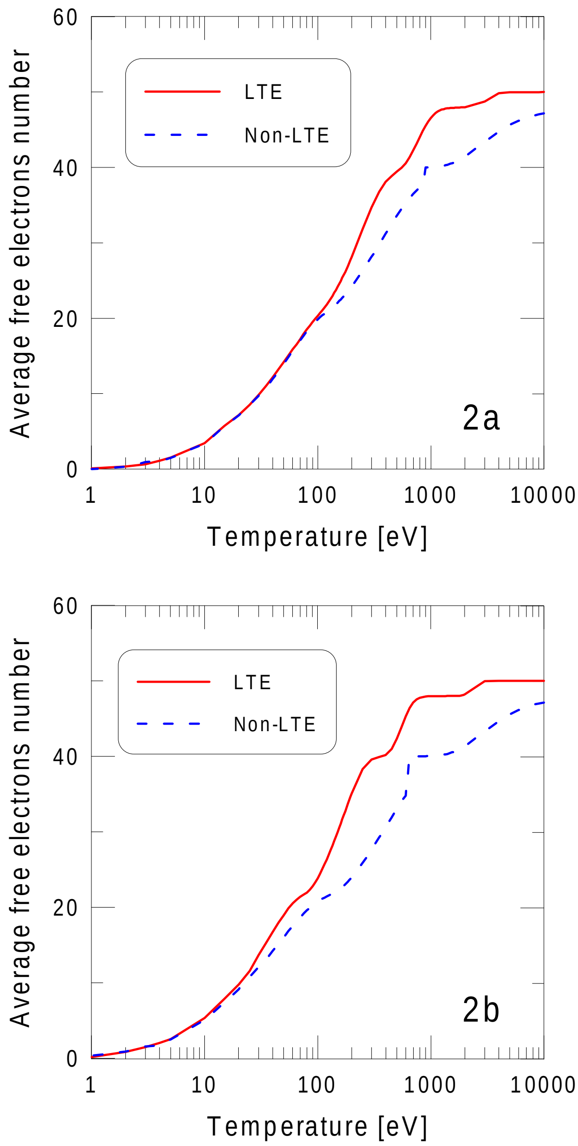

Fig. 2. Average number of free electrons computed with the LTE and Non-LTE average ion models for Sn as a function of electron temperature at a matter density of a) 0.1 gr/cm^3 and b) 0.001 gr/cm^3.

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