Analytical opacity formulas for low Z plasmas

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Abstract. The accurate computation of radiative opacities is basic in the ICF target physics analysis, in which the radiation is an important feature to determine in detail. For this reason, accurate analytical formulas for giving mean opacities versus temperature and density of the plasma seem to be a useful tool. In this work we analyse some analytical expressions found in the literature for the opacity low Z plasmas in a wide range of temperature and densities. The validity of these formulas for computing the opacity under NLTE conditions is investigated using the new code ABAKO.

1. Introduction

The accurate computation of radiative opacities is needed in the ICF target physics analysis, in which the radiation is an important feature to determine in detail. For these targets, 2D hydrodynamics radiation codes are necessary, and the use of thousands of multifrequency opacity points for each mesh point takes a large calculation time. The normal procedure consists of weighting these multifrequency opacities in a small number of multigroups opacities. Thus, 2D codes or even 3D codes could treat opacities in a very small number of groups, even one group, for which mean opacities, Rosseland and Planck should be very appropriate. For this reason, analytical formulas for giving mean opacities versus temperature and density of the plasma seem to be a useful tool.

In this work our goal has been to study analytical expressions found in the literature [1-5] for the opacity low Z plasmas in a wide range of temperature and densities. These formulas are obtained fitting the proposed formula to mean opacities data computed by using the new collisional-radiative steady state code ABAKO [6, 7]. This code has been successfully tested with other kinetic codes in the Fourth Kinetic Code Comparison Workshop [6] and in the last two years it has been improved introducing new features. The code has been prepared to compute the radiative properties, such as the spectrally resolved and mean opacities and emissivities and the intensity, both in LTE and NLTE conditions under the detailed-level-accounting approach. The following section is devoted to a brief explanation of the code.

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2. Method of calculation

2.1. Atomic models

The atomic data can be computed in ABAKO using and "in built" model which solves the Dirac equation using different sets of analytical potentials developed by our group. In this work we have used the analytical potential for isolated ions developed by Martel *et al,* [7]. The data thus obtained are computed in the independent particle approach. ABAKO can also work with external data. In this work we have also performed a detailed analysis of the mean opacity for Carbon plasma, using high quality data provided by the code FAC [8]. This code provides atomic magnitudes calculated into the DLA approach, using appropriate coupling schemes and including configuration interaction.

2.2. Structure of levels

Configuration average atomic physics data were calculated for all the ion stages of the element under study (Beryllium, Carbon and Oxygen). The configurations selected are shown in table 1.

Table 1. Configurations for the O-like to He-like ion stages selected for opacity calculations. The term $(n)^w$ means all the possible configurations obtained distributing the w electrons among all the relativistic orbital of the shell n. For the double or single excited configurations only transitions of one or two *s* or *p* electrons are included.

Ion stage	Configurations	Number of configurations
H-like	$n\ell$, ($n\leq10$)	100
He-like	$(1)^2$; $(1)\,n\ell$ ($n\leq10$); $(2)^2$; $(2)\,n\ell$ ($n\leq6$); $(3)^2$; $(3)\,n\ell$ ($n\leq6$)	352
Li-like	(2); $(2)\,n\ell$ ($n\leq10$);$(1)(2)^2$; $(1)(2)^2n\ell$ ($n\leq6$); $(1)(3)^2$; $(1)(3)^2\,n\ell$ ($n\leq6$);	519
Be-like	$(2)^2$; $(2)\,n\ell$ ($n\leq10$); $(3)^2$; $(3)^2\,n\ell$ ($n\leq6$); $(1)(2)^3$; $(1)(2)^2n\ell$ ($n\leq6$);	644
B-like	$(2)^3$; $(2)^2\,n\ell$ ($n\leq10$); $(2)(3)^2$; $(2)(3)^2\,n\ell$ ($n\leq6$); $(1)(2)^4$; $(1)(2)^3n\ell$ ($n\leq6$);	1299
C-like	$(2)^4$; $(2)^3\,n\ell$ ($n\leq10$); $(2)^2(3)^2$; $(2)^2(3)\,n\ell$ ($n\leq6$);	1677
N-like	$(2)^5$; $(2)^4\,n\ell$ ($n\leq10$); $(2)^3(3)^2$; $(2)^3(3)\,n\ell$ ($n\leq6$);	2072
O-like	$(2)^6$; $(2)^5\,n\ell$ ($n\leq10$); $(2)^4(3)^2$; $(2)^4(3)\,n\ell$ ($n\leq6$);	2124

2.3. Kinetics model

This module uses as input the atomic data provided by the atomic model. Then, fast calculations of ionic charge state distributions and level populations are performed by means of solving a collisional-radiative steady-state model (CRSS). The level populations are computed with a reasonable accuracy for plasmas of any element in a wide range of conditions embracing non-LTE, LTE and CE situations. In this work we have only considered optically thin plasmas. The processes included in the CRSS are the following: collisional excitation and deexcitation; spontaneous decay; collisional ionization and three body recombination; radiative recombination, autoionization and dielectronic recombination; the rate coefficients of these processes are evaluated by analytical formulas that can be found in the literature.

2.4. Computing optical properties

ABAKO is able to determine the emissivity, opacity and source function making use of the populations and the atomic data given in the previous modules being independent of how the populations and atomic data had been generated. The multifrequency opacity is obtained as a sum of the bound-bound, bound free, free-free and scattering contributions

$$\kappa(\nu) = \frac{1}{\rho}\left(\mu_{bb}(\nu) + \mu_{bf}(\nu) + \mu_{ff}(\nu) + \mu_{scatt}(\nu)\right) \tag{1}$$

where the terms are:

Bound-bound

$$\mu_{\xi_{i,j}}(\nu) = \frac{\pi}{mc}\left(\frac{e^2}{4\pi\varepsilon_0}\right) N_{\xi_i} f_{\xi_{i,j}} \phi^a_{\xi_{i,j}}(\nu)\left[1 - \frac{N_{\xi_i} g_{\xi_j}}{N_{\xi_j} g_{\xi_i}}\right] \tag{2}$$

Bound-free $$\mu_{\xi_i,\xi+1_j}(\nu) = N_{\xi_i}\sigma(\nu)_{\xi_i,\xi+1_j}\left[1-\frac{N_{\xi+1_j}g_{\xi_i}}{N_{\xi_i}g_{\xi+1_j}}\right]N_e n(\varepsilon,T) \quad (3)$$

Free-free $$\mu_{ff}(\nu) = \frac{32\pi e^4 a_0^2\alpha^3 z^2}{2\sqrt{3}(2\pi m)^{3/2}\hbar}\left(\frac{m}{2\pi kT}\right)^{1/2} N_e N_{ion} e^{-h\nu/kT} \quad (4)$$

In these equations, ξ denotes the ionic state and ij and $f_{\xi_{i,j}}$ the line transition between the configurations i and j and its oscillator strength, respectively; N_{ξ_i} and g_{ξ_j} are the level population and the statistical weight of the configuration i respectively. $\phi^a_{\xi_{i,j}}(\nu)$ is a Voigt profile for lineshape which includes Natural, Stark and Doppler widths. The scattering term is computed using the Thomson cross section. In general, the multifrequency opacity depends on density, temperature and also on radiation intensity because of photo-ionization and photo-excitation processes. These effects are neglected here and this limits the model to situations where radiation intensities are not very high. Knowing the multifrequency opacity, the Rosseland and Planck mean opacities are obtained by:

$$\frac{1}{\kappa_{Rosseland}} = \int_0^\infty d\nu B'(\nu,T)/\kappa(\nu) \quad (5)$$

$$\kappa_{Planck} = \int_0^\infty d\nu B(\nu,T)\left[\kappa(\nu) - \kappa_{scatt}(\nu)\right] \quad (6)$$

Where κ_{scatt} is the absorption coefficient contribution by scattering, and $B(\nu,T)$ and $B'(\nu,T)$ are the Planck weighting function and its derivative.

3. Results and discussion

Our main goal in this work was to analyze the range of application of analytical expressions found in the literature to model the mean opacity of low Z plasmas. The main expression used to model Rosseland and Planck mean opacities is a power law depending on temperature and density:

$$\kappa_{r,p} = e^a T^b \rho^c \quad (9)$$

Where T is the temperature (eV) and ρ the density in g/cm^{-3}.The definition of the parameter *a* can change depending on the author. These expressions are usually fitted to mach LTE plasma data and our purpose was to test if they are still valid under NLTE conditions. In a first approximation we have included the NLTE effects only for computing the populations, but we kept the LTE expressions for the Rosseland and Planck mean opacities.

To illustrate the behavior of expression (9) we have computed the Rosseland and Planck mean opacity for Beryllium, Carbon and Oxygen plasmas in a range of temperatures from 10 to 500 eV and electronic densities from 10^{-18} cm^{-3} to 10^{23} cm^{-3}. The results obtained indicated that the NLTE mean opacity is a decreasing function of the temperature. This can bee seen in figure 1 where we show the Rosseland and Planck mean opacities for Beryllium plasma computed with ABAKO as a function of the temperature .We also show two fits one taken from reference [4] and a new least-square fit. As it can be seen, the fit of reference [4] trend to overestimate the mean opacity. This behaviour has been reported in the literature [11]. The new fit shows a better behaviour but still trend overestimate at high temperatures. The parameters of the new fit for Beryllium, Carbon and Oxygen are showed in table 1

Table 1. Constants for Rosseland and Planck mean opacities.

Element	Rosseland mean			Planck mean		
	a	b	c	a	b	c
Be	11.72	-1.66	0.41	17.96	-2.83	0.284
C	10.02	-1.28	0.30	16.74	-2.38	0.063
O	9.54	-0.96	0.32	15.53	-1.80	0.023

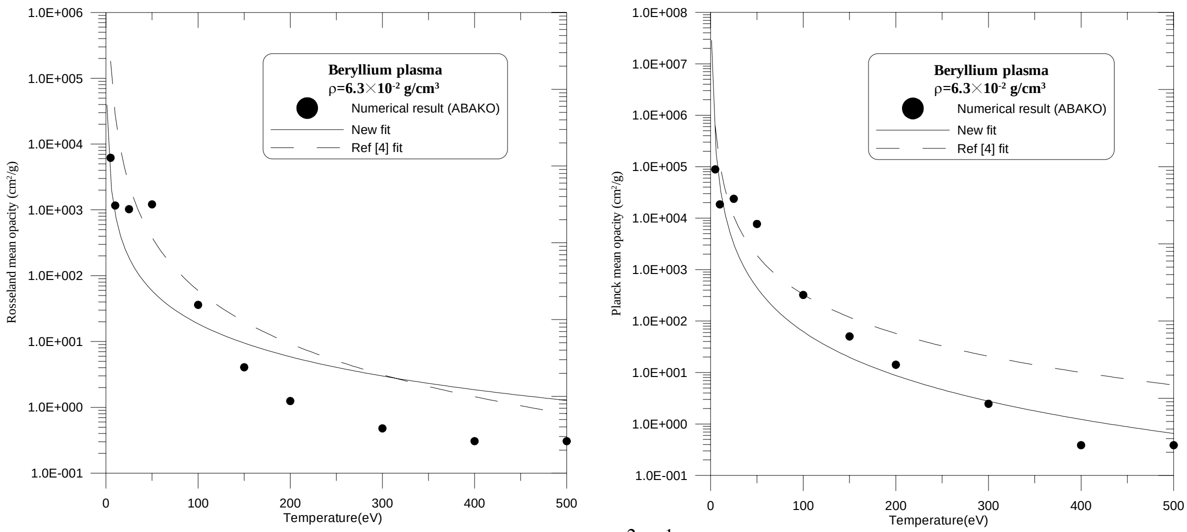

Figure 1. Rosseland and Planck mean opacities ($cm^2 \cdot g^{-1}$) for Beryllium versus temperature (eV) for a density of 6.3×10^{-2} $g \cdot cm^{-3}$.

4. Conclusions

The oscillating behaviour exhibit by the mean opacity at low temperature affects both fits and a more elaborated formula is need for a better fit of the NLTE mean opacities. We have tested a correction for low temperature based in a Gaussian fit and it show a better agreement.

$$k_{r,p} = \left(\sum_{i=1}^{n} a_i \exp\left[-\left(\frac{T - b_i}{c_i} \right)^2 \right] \right) \rho^d \quad (19)$$

An extensive testing the new expression is now under process and these results will be showed in future works. The fitting coefficients given in table are only valid for optically thin plasmas and should be used with caution for high temperature.

5. References

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