Fast calculation of LTE opacities for ICF plasmas

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Introduction

The accurate computation of radiative opacities is needed in several research fields such as astrophysics, magnetic fusion or ICF target physics analysis, in which the radiation transport is an important feature to determine in detail. Radiation transport plays an important role in the transport of energy in dense plasma and it is strongly influenced by the variation of plasma opacity with density and temperature, as well as, photon energy.

In this work we present some new features of the opacity code ATMED [1]. This code has been designed to compute the spectral radiative opacity as well as the Rosseland and Planck means for single element and mixture plasmas. The model presented is fast, stable and reasonably accurate into its range of application and it can be a useful tool to simulate ICF experiments in plasma laboratory.

2. Computational model

The code has been developed in the context of the average atom (AA) model approximation. The atomic data needed are computed using a Relativistic Screened Hydrogenic Model based on a new set of universal screening constants including *j*-splitting that were obtained from the fit to a wide database of atomic energies, ionization potentials and transition energies of high quality [2,3]. In this model the energy for an electronic configuration $\{P_k\}$ is given by the following expression

$$E_T = \sum_{k=1}^{k_{\max}} P_k \varepsilon_k^{Dirac} \tag{1}$$

k is a shortcut for the relativistic set of quantum numbers $\{n_k, l_k, j_k\}$ running over all the bound levels considered in the model (up to $6h_{11/2}$), ε_k^{Dirak} is he Dirac energy of the hydrogen atom replacing the nuclear charge by the screened charge defined as

$$Q_k = Z - \sum_{k'=1}^{k_{max}} \sigma_{kk'} \left(1 - \frac{\delta_{kk'}}{D_k^0}\right) P_{k'} \tag{2}$$

Being $\sigma_{kk'}$ the screening constants cited above. The fractional occupation numbers P_k are computed, minimizing, at fixed mass density ρ, electronic temperature T_e, and nuclear charge Z, the electronic Helmholtz free energy per ion of the plasma. To account for dense plasma effects, the electronic degeneracy of a subshell in the isolated ion, has been reduced using a function the prescription indicated in reference [4] adapted to our relativistic description. The chemical potential and the average ionization is determined using the condition of electroneutrality of the plasma.

The total spectral opacity of plasma $\kappa(\nu)$ is the combination of bound-bound, bound-free, free-free and scattering processes. The line absorption cross section calculation has been computed using a new analytical expression for oscillator strengths based on relativistic screened-hydrogenic wave functions. The lineshape includes natural width, Doppler line broadening and electron collisional broadening [5]. To obtain a more realistic value of the Rosseland mean opacity and additional broadening of the bound-bound transitions has been included by considering the fluctuations of the occupations numbers following a proper adaptation of the method explained in reference [6,7]. We compute the variance of each average atom line transition $i \rightarrow j$ as

$$\left(\Delta\varepsilon_{ij}\right)^2 = \sum_k P_k\left(1-P_k\right)\left(2j_k+1-\delta_{ki}-\delta_{kj}\right)\left(\varepsilon_i^k-\varepsilon_j^k\right)^2 \tag{3}$$

$$\varepsilon_i^k = \frac{\partial^2 E_T}{\partial P_k \partial P_i} \tag{4}$$

The bremsstrahlung absorption cross section has been computed with Kramer's formula and for photoionization and scattering processes expressions from reference [7] have been used.

2. Results and discussion

The accurate calculation of the Rosseland mean opacity requires accounting for all the lines presented correctly and also an accurate model of the spectral line shape, especially in the far wings. The RSHM and the Average Atom model trend to underestimate the Rosseland mean opacity due to this effect. We have corrected this behavior including the dielectronic line broadening explained above. To illustrate it, in figure 1 we compared our results for the Rosseland and Planck means for an Iron plasma at 20 eV and different densities with data obtained from the Third International Opacity Workshop & Code Comparison Study final report [8]. OPAL and

LEDCOP are DCA codes, THERMOS is a hybrid code that combines average atom with detailed configuration account and CORONA is a pure average atom code in the non-relativistic approximation.

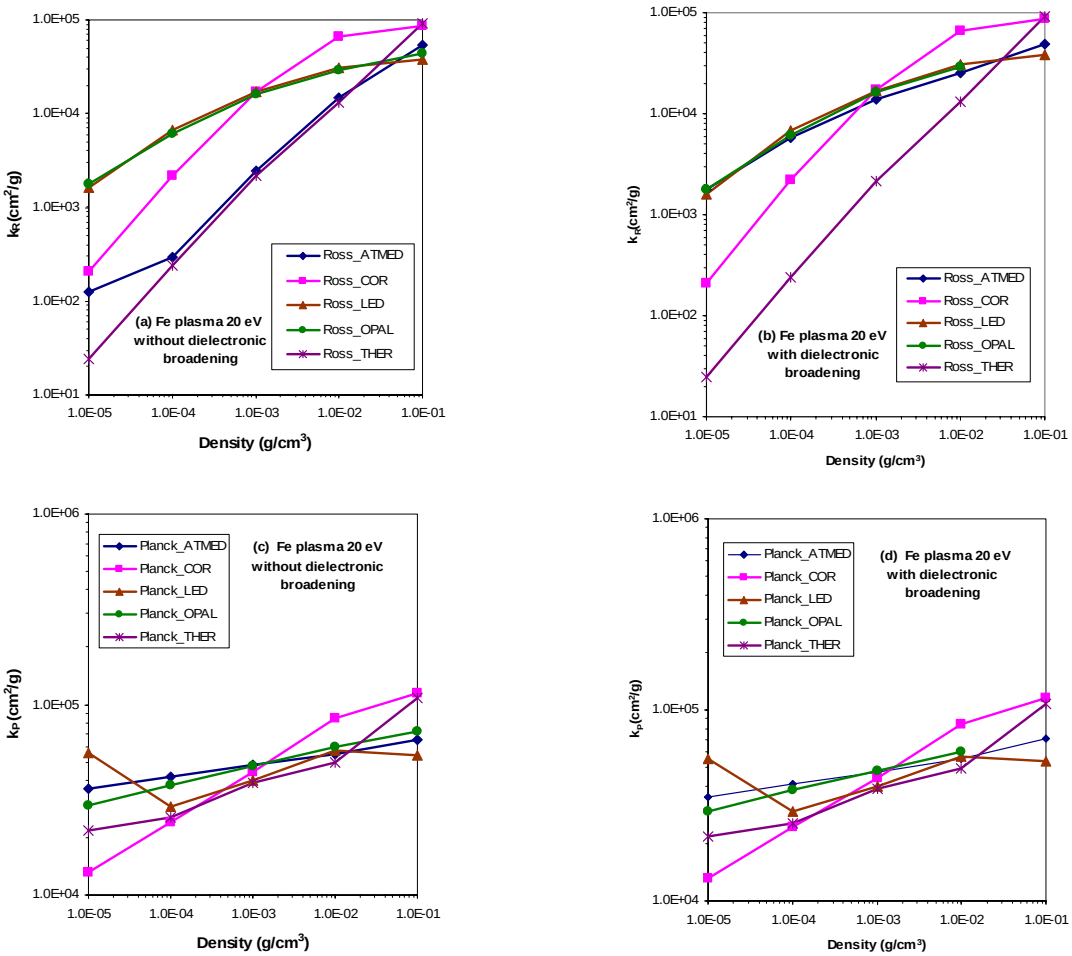

Figure 1. Rosseland and Planck mean opacities for Fe at isosecuence T = 20 eV. 1a) without dielectronic broadening 1b) including dielectronic broadening

At this temperature the bound-bound opacity dominates. We can see (fig 1a and 1b) how including the dielectronic line broadening pushes our results towards the DCA code obtaining a more realistic results a low computational cost. The Planck mean shows a little influence of the line broadening as expected.

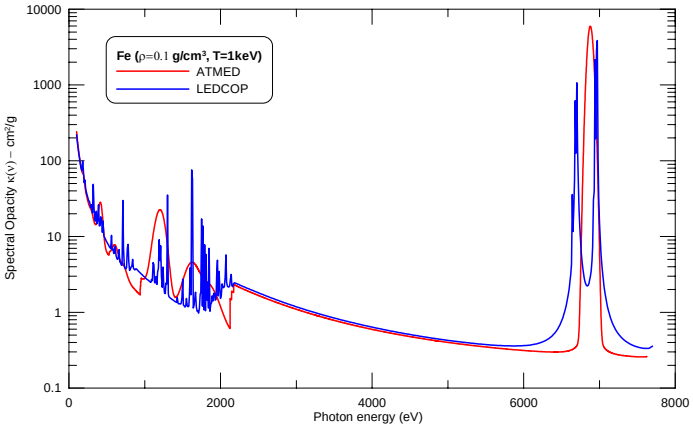

Figure 2. Spectral opacity for Fe at T = 1 keV and $\rho = 0.1$ g/cm^3

In figure 2 we plot the spectral opacity for and iron plasma computed by LEDCOP and ATMED to show the merging effect of the dilectronic broadening.

In table 1, we compare or results with experimental data provided by Avrorin et al. [9] for iron plasma with density 1 gcm^{-3} and temperature 500 eV. Looking at the results we can see that our model agrees into the experimental margins with experimental results and shows a very good behaviour in relation to more sophisticated codes.

Table 1. Rosseland mean absorption coefficient, κ_R in cm^2/g for iron.

T (keV)	0.5	0.75	1	1.25
Thomas-Fermi	62.5	7.81	2.7	1.59
THERMOS	79.6	8.37	3.14	2.29
LEDCOP	74.8		2.79	2.14
OPAL	84.2		3.48	
Experiment	82 ± 12	7.8 ± 1	2.3 ± 0.4	1.3 ± 0.2
ATMED	**79.93**	**8.31**	**2.70**	**1.75**

Conclusions

In this work we have show some features of the ATMED code, in spite of its simplicity, the model gives the magnitude order of the values correctly, so it can be used to model radiative transport phenomenon in hydrodynamic codes, and experiments in an approximate way.

Acknowledgements

This work has been partially supported by a Research Project of the Spanish Ministry of Science and Innovation (ENE2009-11208) and by a Research Project of the Government of the Canary Islands. (SOLSUBC2008000057).

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