Calculation of the radiative opacity of laser-produced plasmas using a relativistic-screened hydrogenic model for ions including plasma effects

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1. Introduction

In the study of laser – plasma interaction is necessary to deal with an enormous amount of atomic data. In particular, to study the radiative properties of hot dense matter require the knowledge of the atomic structure of different ions in the plasmas, energy levels for ground and excited states, line transitions and plasmas interactions. A detailed numerical calculation of these quantities is a very time–consuming computer task. To deal with this problem some computer codes use analytical or semi–analytical models to computed the atomic data. One model widely used in plasma physics is the screened hydrogenic model (SHM). In this work, we use a relativistic–screened hydrogenic model to compute the radiative opacity of laser-produced plasmas. The model is based a set of screening charges which allow to calculate easily atomic properties ions immersed in plasma. These screened charges are derived from an analytical potential for non isolated ions using a simple analytical iterative procedure.

2. Atomic model

In our model each bound electron moves in the individual potential

$$U_{nlj}(r) = -\frac{Q_{nlj}}{r} + A_{nlj}, \qquad (1)$$

depending on the nuclear charge and the other atomic electrons. In Eq. (1) the quantum state of the bound electron is described in a relativistic frame by the quantum numbers n, l, and j, the parameter Q_{nlj} is called the screened charge of the level and A_{nlj} is a constant term depending on the screened charge that will be referred further as the external screening constant. The screened charges are obtained following the procedure described in Rubiano, *et al.* 2002 [1] using the following screened charge function:

$$Q(r) = \left[(Z - N + 1) + (N - 1)\xi(r)\right] - \frac{4}{3}\pi r^3 N_e \qquad (2)$$

being

$$\xi(r)=\left(\phi(r)-r\phi'(r)\right)=\begin{cases}\left(1+a_1a_3r^{a_3}\right)e^{-a_1r^{a_3}} & \text{if } N\geq 12\\ \left(1+a_1r\left(1-a_2r\right)\right)e^{-a_1r} & \text{if } 8\leq N\leq 12 \text{ or } N=2,3\\ \left(1+a_1r\right)e^{-a_1r} & \text{if } 4\leq N\leq 7\end{cases} \quad (3)$$

In these expressions a_1, a_2 and a_3 are the parameters of the analytical potential proposed by Martel *et al.* (1998) [2]. The plasma environment is included in this expression through the term depending on the free electron density, N_e, which is assumed a constant for a given density and temperature [3] (Mirone *et al.* 1997)). As it has been said, the screening constant A_{nlj}, is the screening by external electrons, this parameter can be computed as a function of the screened charges Q_k.

$$A_{nlj}=Q_{nlj}\left\langle\psi_{nlj}\left(r;Q_{nlj}\right)\middle|1/r\middle|\psi_{nlj}\left(r;Q_{nlj}\right)\right\rangle-\left\langle\psi_{nlj}\left(r;Q_{nlj}\right)\middle|U_a(r)\middle|\psi_{nlj}\left(r;Q_{nlj}\right)\right\rangle \quad (4)$$

Both parameters depend on the plasma environment through the free electron density. Once these parameters have been computes, all the one electron parameter (energies, ε_{nlj}, and wave functions) are computed using relativistic hydrogenic analytical expression [4] (Nikiforov et al. 1996). The average energy of a configuration is given by:

$$E=T-\int\rho(r)\frac{Z}{r}d\mathrm{r}+\frac{1}{2}\iint\frac{\rho(r)\rho(r')}{|\mathrm{r}-\mathrm{r}'|}d\mathrm{r}\,d\mathrm{r}'+E_{xc}[\rho] \quad (5)$$

where the charge density, $\rho(r)$ is computed using relativistic hydrogenic orbitals, and the kinetic energy, T, is given by

$$T=\sum_{k=n,l,j}P_k\varepsilon_k-\sum_k P_k\int\rho_k(r)U_k(r)dr \quad (6)$$

3.- Opacity formalism

To compute the opacity of LTE plasmas we have selected a set of configurations which cover, for a given ion with atomic number Z, all the ionic species from the neutral atom to the hydrogen-like ion. The ions have been modeled using 35 relativistic single electron orbital (nlj) with principal quantum number $n\leq 10$. For an ionic stage having a number of electrons N, it has been selected the ground state configuration and all those excited configurations built by single promotion of one external electron (singly excited configurations).The abundance these configurations in the plasma for a given density and temperature is obtained by solving the Saha-Boltzmann equations.

$$\frac{N_{m+1}}{N_m}N_e=N_e e^{-\eta_e}\frac{Z_{m+1}}{Z_m}e^{-I_m/kT} \quad (7)$$

A Fermi-Dirac distribution has been assumed for the free electrons and thus in equation (7), the parameter ηe denote the degeneracy parameter of the free electrons. The opacity is then obtained by

$$\kappa(\nu) = \left[\kappa_{bb}(\nu) + \kappa_{bf}(\nu) + \kappa_{ff}(\nu)\right]\left(1 - e^{-h\nu / k_B T}\right) + \kappa_s(\nu) \tag{8}$$

Bound–bound transitions are determined using a Voigt profile for lineshape which includes natural, collisional, Doppler and UTA widths. Bound–free and free–free opacities are evaluated using the Kramer cross sections with appropriated corrections. Scattering processes are computed through the use of the Thomson formula with corrections.

4. Results

In table 1 we compare the average number of free electrons per ion for iron plasmas at several conditions of temperature and density computed by different models. The data are obtained from the Third International Opacity Workshop & Code Comparison Study final report [5] (Rickert, et al., 1995). The code LEDCOP generates the atomic data by a relativistic self-consistent Hartree-Fock code and it determines the concentration of ionic species by means of a model based on the Saha equation, including degeneracy, where the bound Rydberg sequences are cut off by plasma correction. The OPAL code computes the atomic data using parametric potentials. The LTE state occupation numbers are obtained from a renormalized expansion of the grand canonical ensemble. The CORONA code computes the energy level by the SHM with l-splitting including pressure ionization and continuum lowering effect. The ionic population is computed by using the Thomas-Fermi shell model of average ion model.

Table 1. Average ionization of iron plasmas at different conditions of temperature and density computed by different codes.

CODE	T = 200 eV ρ = 7.86 g/cc	T = 500 eV ρ = 1 g/cc	T = 1000 eV ρ = 1 g/cc
LEDCOP	14.42	22.68	23.94
OPAL	13.37	22.53	23.86
CORONA	13.22	21.96	23.67
JIMENA	14.08	22.49	23.98
ANALOP-H	15.06	23.07	23.78
This work	14.19	22.99	23.96

The JIMENA code for each temperature and density solves self-consistently the radial Dirac equation with a local spherically symmetrical potential assuming the radial density composed by both bound and free electrons. Configurations are created promoting and denoting electrons in turn to the average ion determined and the most abundant configurations are computed using a binomial distribution. The ANALOP-H code [6] (Rubiano, et al. 2004) solves for each configuration selected the Dirac equation using a relativistic hydrogenic model for isolated ions. The abundance of each ionization species is obtained by means of the Saha–Boltzmann equations with degeneracy and continuum lowering correction of Stewart and Pyatt. As it can be seen our results are in a better concordance with the rest of the codes and we concludes that this methods of including the plasma effects in the atomic potential trend to reduce the ionization in relation to the Stewart and Pyatt correction commonly used.

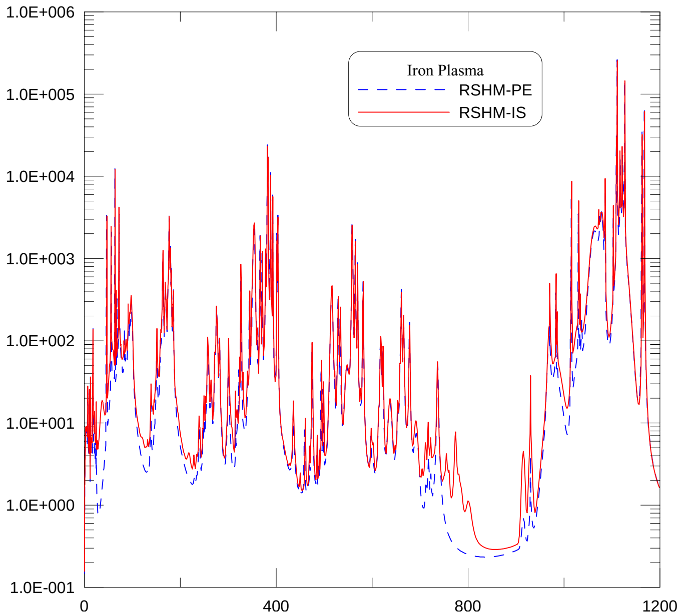

Figure 1. Iron plasma opacity (ρ = 1 1 g/cm³, T = 500 eV)

In Figure 1 we show the bound-bound multifrequency opacity of iron plasma using the relativistic screened hydrogenic model for isolated ions (RSHM-IS) and the model proposed in this work (RSHM-PE). As is can be seen both models show a similar behavior as it was expected, but some peaks have disappeared because the corresponding states have been merged into to the continuum by the atomic model.

This method appears to be more realistic than modeling the plasma with an isolated atomic model. So this model can be a proper and simple procedure to include plasma effects in the atomic structure.

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