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Opacity calculations of plasmas by using parametric potentials

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A numerical model for opacity calculations by using a family of analytical potentials for each configuration in the plasma is presented. The obtained numerical opacity results with this model are compared with those obtained by using a self-consistent potential model.

1. Introduction

In the opacity calculations of hot dense matter, it is usually necessary to consider many configurations and also thousands of line transitions. This requires the knowledge of the atomic structure of the ions in the plasma. Several computer codes are currently available to determine these atomic data, which allows improvement of the radiation opacity codes. Models using both self-consistent methods or analytical potentials have been recently tested for several elements in a short range of densities and temperatures (Rickert *et al.* 1995), and have shown important differences in the frequency-dependent opacity. Also, some of these models tried to simulate experimental results (Winhart *et al.* 1995), showing deviations from the experimental Rosseland opacity by not more than a factor of two.

For high-Z elements it is necessary to treat a large number of configurations, so that analytical potentials seem to be useful to generate the atomic physics data for opacity calculation. In a previous work we described a detailed opacity model (Mínguez & Falquina 1992) in which an average ion was first solved. Then, using the procedure reported by Goldberg *et al.* (1986), denoting and promoting electrons in turn to the average, the probability of each configuration in the plasma is determined according to Argo and Huebner (1976). Finally, for each configuration with higher probability than 10^{-5}, the radial Dirac equation is solved again using a self-consistent potential and obtaining the atomic data for opacity calculation. This procedure was tested with other models during the Third Opacity Workshop (Rickert *et al.* 1995). However, this model is large and time-consuming, essentially for high-Z elements.

Later on, we proposed a new family of parametric potentials (Martel *et al.* 1995) with three parameters in the general form, which can be reduced to two-parameter and one-parameter potentials, according to different situations. The parameters of these potentials were determined by fitting to a self-consistent potential. Also, an important feature is that the parameters of the potential were fitted by a simple function of the nuclear charge, and it is available for intermediate and highly ionized atoms from helium to uranium sequences. Transitions energies and oscillator strengths obtained with this proposed model were in good agreement with other models.

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In this work the main goal is to use this family of parametric potentials to create a numerical model useful for opacity calculations. With this model it is possible to treat a large number of configurations with a small calculation time, and to obtain results close to those obtained with the self-consistent model explained above. Numerical results of opacities for iron at several densities and temperatures are reported.

2. Opacity model using parametric potential

The first part of the numerical model to be proposed is based on the average ion model, being that the detailed configurations determined from it follow a well-known procedure. The average ion model for the given density and temperature is solved using the JIMENA computer code (Mínguez & Falquina 1992). This gives for each n subshell the occupation number N_{nlj}. Then, using the procedure of Goldberg *et al.* (1986), a set of configurations ρ in turn to the average are determined. The probability $P(\rho)$ of each configuration in the plasma is created by means of the binomial formula (Argo & Huebner 1976).

These configurations in which $P(\rho)$ is larger than 10^{-5} are now taken into account for the next phase of the calculation, where we introduce the family of parametric potentials $U(r)$ given by Martel *et al.* (1995)

$$U(r) = -\frac{1}{r}\{(N-1)\Phi(r) + Z - N + 1\}, \tag{1}$$

where the screening function, $\phi(r)$, has different values depending on N (number of bound electrons), and Z (atomic number).

We use:

$$\Phi(r) = e^{-a_1 r^{a_3}} \qquad \text{if } N \geq 12 \tag{2a}$$

or

$$\Phi(r) = (1 - a_2 r)e^{-a_1 r} \quad \text{if } 8 \leq N \leq 11 \text{ or } N = 2,3 \tag{2b}$$

or

$$\Phi(r) = e^{-a_1 r} \qquad \text{if } 4 \leq N \leq 7. \tag{2c}$$

These parameters a_1, a_2, and a_3 are determined by fitting the equation (2) to the self-consistent potential by means of a nonlinear simplex method, giving as a result a fourth-degree polynom:

$$a_k = c_{1k}Z^4 + c_{2k}Z^3 + c_{3k}Z^2 + c_{4k}Z + c_{5k} \quad (k = 1,2,3). \tag{3}$$

The coefficients, c_{ik}, of this expression were obtained for the ground state of He-like to Fe-like ions, and they can be found in Martel *et al.* (1995). Also, there are unpublished coefficients, from Co-like to U-like ions, available that follow the same procedure. These coefficients will be included in a future paper.

Using this parametric potential in the Dirac equation for each detailed configuration, the energy levels and oscillator strengths are obtained. Because the number of electrons and the parametric potential were assumed fixed, the calculation time is rather low in comparison with the self-consistent calculation, by a factor that depends on the material and the computer.

Finally, with all the atomic data generated for all the configurations, the opacity calculation is fast and simple. In this multifrequency opacity calculation, bound-bound, bound-free, free-free, and scattering processes are included, assuming that also included in the line broadening is the Moszkowski formulism (1979).

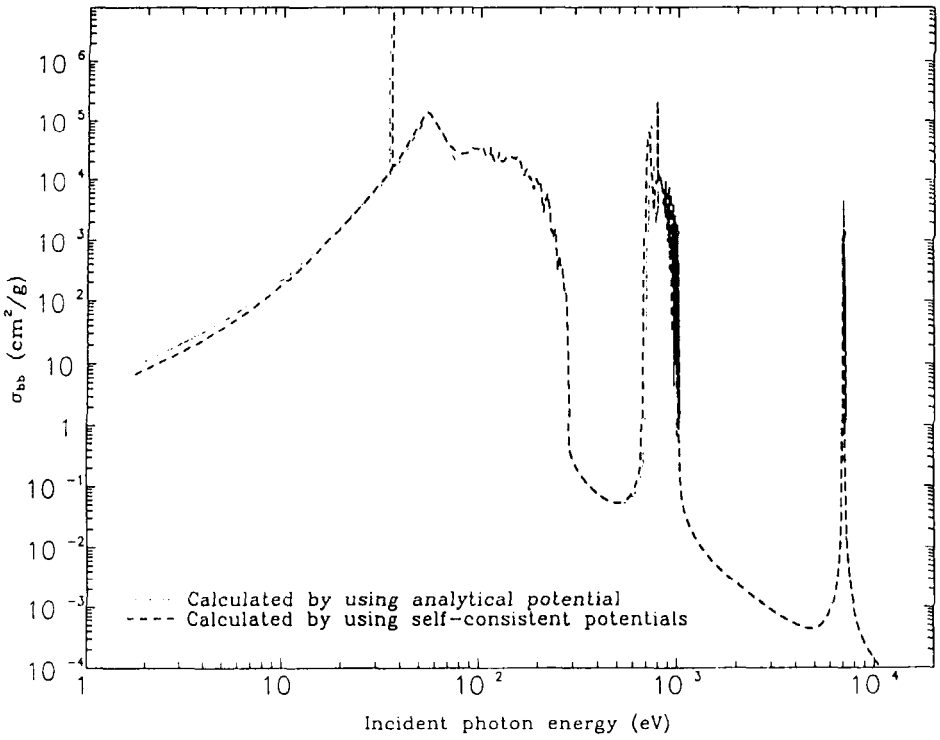

FIGURE 1. Bound-bound opacity for Fe at kT 20 eV and density 10^{-3} g cm^{-3}.

3. Analysis of numerical results for iron plasmas

Several cases of iron were simulated with this model, mainly those cases already included in previous references, such as: at 20-eV temperature and densities 10^{-3} g cm^{-3} and 10^{-2} g cm^{-3}; and higher temperatures and densities as 200 eV and 7.86 g cm^{-3}. Results were compared with those obtained with JIMENA code by using a self-consistent detailed model. The reason was that this model has already been checked with other models and with experiments, and the parametric potential was fitted with this self-consistent one.

Figures 1 through 3 show only the bound-bound opacities for iron at several temperatures and densities, obtained with the JIMENA code using a self-consistent potential, and the analytical potential given by equation (1). A similar profile is obtained with less calculation time

For the above cases, mean opacities, Planck and Rosseland, are obtained with both models, and the final results are shown in table 1, K_{Rsc} and K_{Psc} being the Rosseland and

TABLE 1. Rosseland and Planck mean opacities at several temperatures and densities with a self-consistent potential (K_{Rsc}, K_{Psc}) and the analytical potential (K_{Ra}, K_{Pa})

kT(eV)	ρ(g/cm^3)	κ_{Rsc}(cm^2/g)	κ_{Ra}(cm^2/g)	κ_{Psc}(cm^2/g)	κ_{Pa}(cm^2/g)
20	10^{-3}	2.123×10^4	2.040×10^4	4.500×10^4	5.311×10^4
20	10^{-2}	2.956×10^4	2.670×10^4	5.146×10^4	4.463×10^4
200	7.86	1.848×10^3	1.820×10^3	6.897×10^3	6.889×10^3

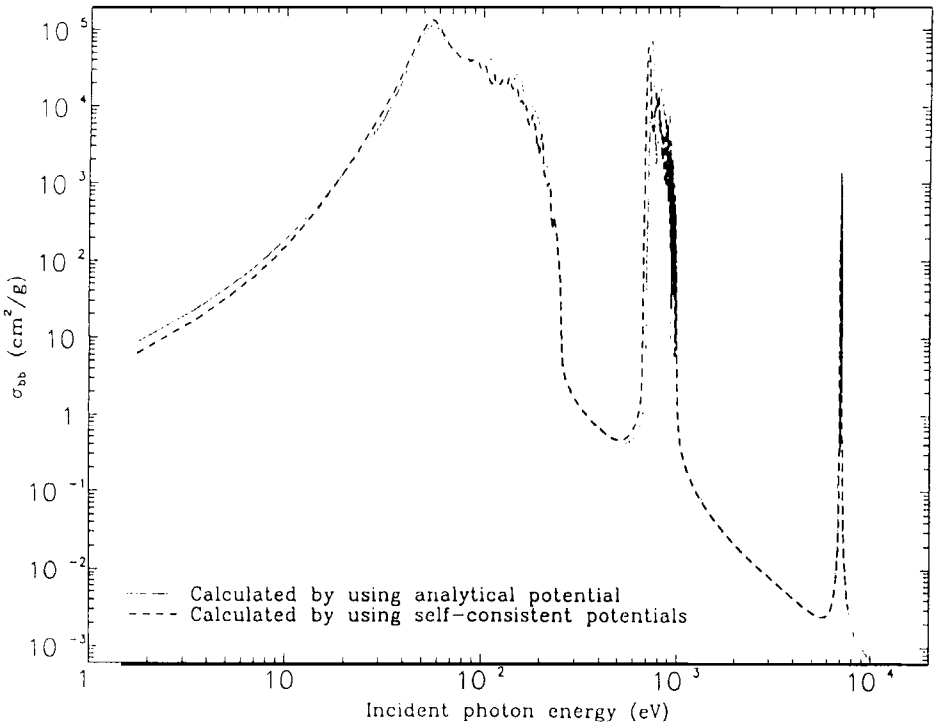

FIGURE 2. Bound-bound opacity for Fe at kT 20 eV and density 10^{-2} g cm^{-3}.

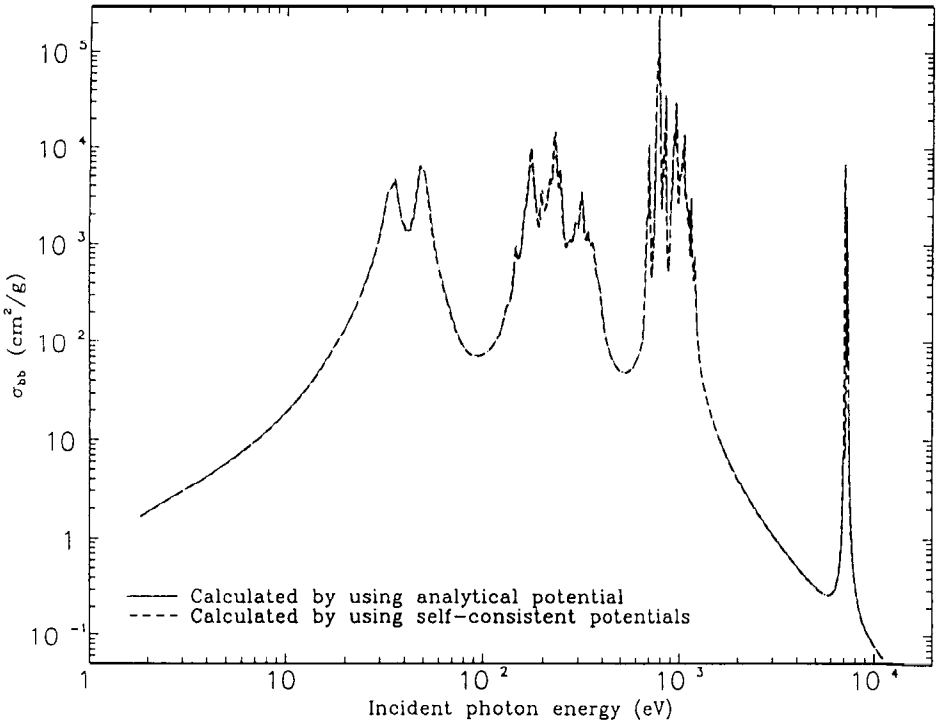

FIGURE 3. Bound-bound opacity for Fe at kT 200 eV and density 7.86 g cm^{-3}.

Planck opacities obtained with the self-consistent potential, and K_{Ra} and K_{Pa} with the analytical potential. The agreement is better at high densities, because the parameters in equation (3) fit the self-consistent potential better, as was reported by Martel *et al.* (1995).

In this work we show how the use of parametric potential allows detailed calculations of opacities to be made with considerable savings of computation time. We think that this fact could be useful in calculations of high-Z plasmas in which the large number of configurations will make a self-consistent detailed configuration calculation unapproachable. Also, this model permits one to get a set of atomic data for the analytical rate equations used in non-LTE numerical models' calculations.

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