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Using sparse matrices techniques and iterative solvers in the calculation of level populations for NLTE plasmas

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1. Introduction

Calculations of populations of ion species existing in plasmas comprise an important research area for laboratory and astrophysical plasmas from low to high electron density regime. Ionic charge distribution is required for the determination of average ionizations, emissivities and opacities, both for hydro-simulations and spectroscopic diagnostics.

In this work, we present a steady-state CR model for the calculation of level population in which the sparse matrix technique is employed to store the elements of the CR matrix and we show the utility of iterative methods to solve the rate equations. This procedure allows us to determine the level populations for low-Z plasmas in a detailed level description, which is required for spectroscopic or diagnostics purposes. For intermediate and high-Z plasmas, the use of sparse matrix technique and iterative solvers is not enough to carry out a detailed level calculation, but we show that the combining use of those techniques and simple atomic models, as those based on analytical potentials, makes possible reasonable accurate calculations of average ionizations and ionic populations in a wide range of temperature and electron density conditions. Furthermore, a brief discussion about how the considered energy levels structure affects to average ionization and ionic charge distribution for different plasma conditions is also presented.

2. Model description

Our CR model [1] includes seven atomic processes which can cause both population and depopulation of the ionic states. These are: (i) collisional excitation, (ii) collisional deexcitation, (iii) spontaneous decay, (iv) collisional ionization, (v) three-body recombination, (vi) radiative recombination and (vii) dielectronic recombination. In addition, Stewart-Pyatt formalism is used as the continuum-lowering model. The rate equation for the level m of the ion with charge j can be written as $\frac{dN_{jm}}{dt} = \mathrm{R}^{+}_{jm} - \mathrm{R}^{-}_{jm}$, where N_{jm} is the

level population, R^{+}_{jm} is the populating term and R^{-}_{jm} is the depopulation one. For the determination of rate coefficients we make use of approximated analytical formulas and the detailed balance principle. Furthermore, the rate equations are solved assuming a steady-state, so it yields

$$R^{+}_{jm} - R^{-}_{jm} \equiv \sum_{k'} a_{kk'} N_{k'} = 0 \,, \ \forall\, k' \equiv jm\text{-level} \tag{1}$$

The last expression represents a system of linear equations for the N_{jm}'s. Taking into account that in our model the atomic processes only connect ionic states belonged to the considered ion and states belonged to adjacent ions, only the corresponding elements of CR matrix can be nonzero. It means that CR matrix has a high degree of sparsity and substantial savings in compute time and memory requirements can be realized by storing and operating on only the nonzero elements. On the other hand, the system dimension is given by the number of levels considered, which can easily reach the order of 10^5 for low-Z plasma in a detailed level description Therefore we handle with very large sparse matrices and the iterative methods [2] are the most appropriate choice to carry out the matrix inversion because they typically require less memory than direct methods and hence can be the only means of solution for large problems. Furthermore, an appropriate iterative technique can yield an approximation to the solution significantly faster than a direct method.

The atomic data which are necessary to calculate the non-LTE level distributions are obtained through two different ways. For a detailed level description we used the FAC code [3]. This package calculates the bound states of the atomic system with convenient specification of mixing schemes and it also includes configuration mixing. As a second and simpler way, our CR model comes with a built-in atomic model which is based on the use of analytical potentials [4, 5]. For a given ionic stage with N electrons, monoelectronic relativistic orbitals (subshells), labeled by *n,l,j* quantum numbers, are used to build an electronic configuration

$$\left(n_1 l_1 j_1\right)^{w_1} \left(n_2 l_2 j_2\right)^{w_2} \ldots \left(n_q l_q j_q\right)^{w_q} \text{ with } \sum_{i=1}^{q} w_i = N \tag{2}$$

where w_i is the number of electrons in the level $n_i l_i j_i$. Different electronic configurations are obtained by promoting one electron from one to another *nlj*-orbital. Then we assume the independent-particle approach and a Dirac equation is solved for each monoelectronic subshell, where an analytical expression is proposed for the effective radial potential.

3. Results and discussions

In this work, we are interested to show the versatility and portability of the developed code, since it can provide fast reasonable results without needing high computational requirements or sophisticated machines. Actually, all the calculations presented in this section were carried on a simple PC, with a 3.0 GHz Pentium IV processor and 1 Gb RAM memory.

Number of levels	Computation time (s)	
	Direct method	Iterative method
1000	1	<1
1500	3	<1
2000	4	1
2500	8	1
3000	14	2
3500	16	3
4000	33	4
5000	66	6
6000	84	10
7000	261	13
8000	1451	18

Table 1. Comparison between direct and iterative methods to perform the CR matrix inversion. Calculations were done for an aluminum plasma.

To illustrate the suitability of the iterative method, firstly an atomic database for aluminum with 13237 levels and 369107 bound-bound radiative transitions was generated using the FAC code and then we performed the calculation of the population distribution using two different schemes to the CR matrix inversion, traditional direct method (from LAPACK) and an iterative method. In table 1 it can be seen a comparison of computation times between two methods taking into account a different number of levels each time for aluminum at $T = 50$ eV and $n_e = 10^{20}$ cm^{-3}. We observe a substantial reduction of computation time when the iterative method is used. Besides the iterative method allows us to handle very large matrices, which means that it is feasible the determination of populations in a detailed level description for low-Z plasmas at least.

Also we have made a brief study about how the considered energy levels structure affects to average ionization and ionic charge distribution. In Fig.1 we show calculations of average ionization versus electron density at three different temperatures for an aluminum plasma. Three cases are represented, from the atomic database mentioned above we first considered the electronic configurations obtained by promoting only the outermost-shell electron, secondly we included inner-shell transitions and finally we made the calculations by means of a built-in atomic model which is based on the use of analytical potentials. As it can be seen, significant discrepancies are found between inner-shell and outermost-shell cases for all range of electron densities, although they become smaller as the temperature increases. Anyway, the consideration of outermost-shell electron transitions by itself is not an appropriate manner to simplify the calculation of atomic data. Nevertheless, if we forget the corona regime, we find a remarkable agreement between calculations with a full detailed description (≈ 13000 levels) and those made using analytical potentials (≈ 1200 levels). Therefore, the analytical potentials are a useful tool to obtain the required atomic data for the

CR model, especially if we are not interested in specific spectroscopic purposes. Besides, the analytical potentials could be an alternative way to approach the determination of average quantities, as average ionizations or ionic populations for intermediate and high-Z plasmas, where a detailed description is unpracticable.

To give an evidence of the assumption stated above, we generated using the FAC code an atomic database for Ge including the lower inner-shell states and the outermost-shell ones up to $n = 15$ for the value of the principal quantum number. The result was a set of 50600 levels and almost ten millions of radiative transitions. In Fig. 2 we compare the ionic distribution for Ge calculated with these atomic data and using analytical potentials (≈ 5000 levels). In addition, results from other known codes in the international community [6] are also presented. Small differences can be found between the detailed level (DL) description and the calculation performed with analytical potentials (AP). Furthermore, a notable concordance with sophisticated codes is also observed.

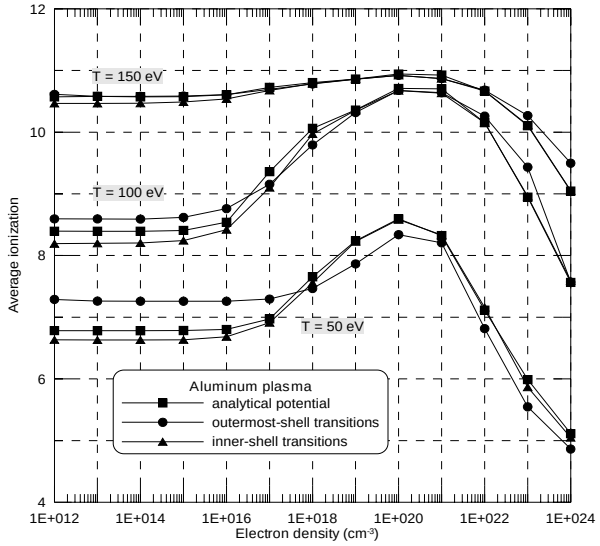

Fig. 1. Influence of energy levels structure on average ionization. Calculations were done for an aluminum plasma.

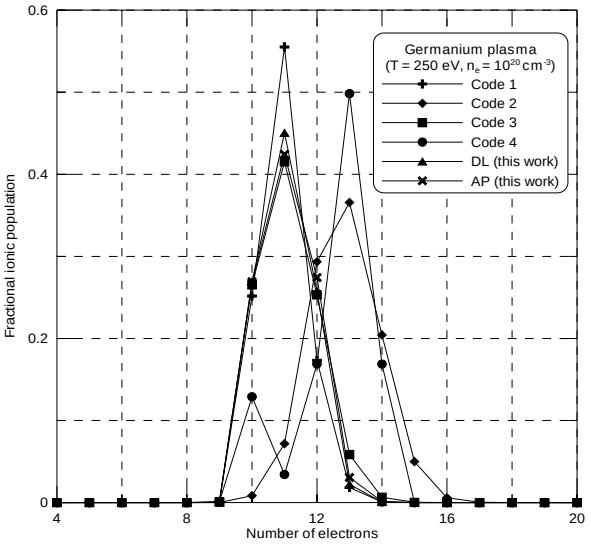

Fig. 2. Fraccional ionic distribution for a germanium plasma. Calculations with different codes are shown.

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