COLLISIONAL-RADIATIVE MODEL FOR HIGHLY STRIPPED IONS

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E. BERTHIER, J.-F. DELPECH, and M. VUILLEMIN

Commissariat à l'Energie Atomique, Centre d'Etudes de Limeil-Valenton, B.P. n° 27, F-94190 Villeneuve-Saint-Georges, France

Résumé - Les modèles numériques Collisionnels-Radiatifs sont couramment utilisés pour concevoir ou interpréter des expériences de physique atomique des plasmas créés par laser, en particulier dans les études de laser X.

Nous décrivons notre nouveau code qui contient plusieurs options : ion moyen, configurations plus ou moins détaillées. Il est composé d'une base de données atomiques couplée à des sous-programmes qui évaluent les populations ioniques ainsi que les coefficients d'émission et d'absorption. Nous donnons des résultats numériques pour illustrer les possibilités du code et pour comparer différents modèles et types d'approximation.

Abstract - Collisional-Radiative numerical models are commonly used to design or interpret experiments in atomic physics of laser-created plasmas, including X-Ray laser studies.

We describe our new code containing several options : average ion, more or less detailed configurations. It consists of an atomic data base coupled to subroutines evaluating ionic populations and emission and absorption coefficients. Numerical results are given to illustrate the capabilities of the code and to compare different models and types of approximation.

I. INTRODUCTION

Collisional-Radiative models are useful for the design or the interpretation of experiments in atomic physics of laser created plasmas, including X-ray laser studies.

Three kinds of results are of particular interest :
- the ionization state of the plasma, i.e. the average degree of ionization Z* and the distribution of the various ionic stages,

- the populations of individual excited levels for the computation of inversions and gains,

- the X-ray emission of the plasma for confrontations with experiments.

We have developped a new highly flexible code, LASIX, and we take advantage of three of its notable features in this presentation :

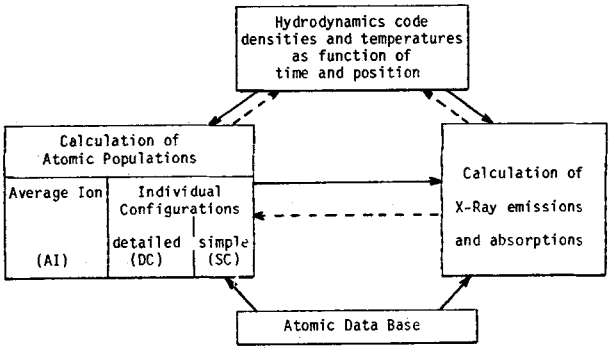
- new atomic data are easily taken into account,

- it incorporates models of varying sophistication, which may be selected according to the application,

- comparisons of atomic parameters and of various approximations are readily performed.

II. DESCRIPTION OF THE LASIX CODE

(a) Schematic organization



In this presentation, LASIX will be treated as a post-processor to the hydrodynamics code ; we shall remain within the approximation of an optically thin plasma, excluding radiative transfer problems.

(b) Average Ion Option (AI)

This option is similar to XSNQ-U (Lokke and Grasberger) with slightly more realistic evaluations of the rate coefficients and a new algorithm for solving the equations of evolution of the average occupations of the n^{th} shell : P_n.

If necessary, the ground-state population of any ionic stage may be derived from the P_n through the binomial law (this procedure is consistent with the underlying approximation of independent electrons : see for example § III. fig.5).

(c) Individual Configurations Options (DC and SC)

For each ionic stage "Detailed Configurations" (DC) and/or "Simplified Configurations" (SC) options may be used.

In the DC option, there can be as many individual excited states as are thought necessary by the user ; they can be either treated separately or averaged in groups called "superlevels". The composition of each superlevel is freely specified. In the SC option, excited levels are approximately treated by grouping together all states having the same principal quantum numbers.

In practice, the SC option is quite satisfactory for non-dominant ionic stages ; for dominant stages, the DC option is often used for lower principal quantum numbers (for example up to n = 4 or 5) ; the SC option is then restricted to higher excited levels. The highest (or the two highest) excited levels may also be maintained at Saha equilibrium with free electrons (assumed here to be non-degenerate).

(d) Atomic Data Base

In the DC (Detailed Configurations) option, we use preferentially data derived from a MCDF code (Bruneau) and from the SUPERSTRUCTURE code (see related paper by M. Cornille, J. Dubau and S. Jacquemot). Relevant data from Clark, Magee, Mann and Merts, Sampson and Parks, and Sampson and Golden are also occasionally used.

In the SC (Simplified Configurations) option, we use the relevant approximate formulas of Landshoff and Perez, Mewe, Seaton, Johnson, and Lotz, according to their ranges of validity.

Transition rates in the AI (Average Ion) case are derived from formulas used in the SC case, while energy levels are computed with the More (1981) approximation formula.

III. EXAMPLES OF NUMERICAL RESULTS

(a) Homogeneous Stationary Plasma

We have first considered the case of an iron (Z = 26) plasma of fixed mass density 10^{-2} g.cm^{-3}. Figures 1 - 3 show the average degree of ionization Z* vs. temperature with various types of approximations ; even in the DC case, detailed configurations were used only for lithium-like, helium-like and hydrogen-like ions ; the SC approximation was used for all lower ionic stages.

Fig.1

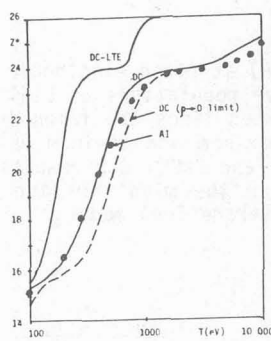


Fig.2

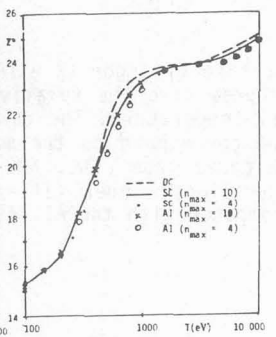


Fig.3

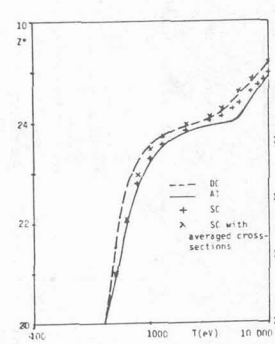


Fig.4

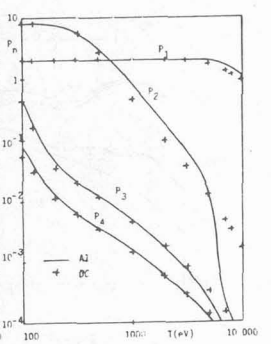


Fig. 1 Comparison of the results of DC, DC-LTE, DC (zero density limit) and AI.

Fig. 2 DC, SC (n_{max} = 10), SC (n_{max} = 4), AI (n_{max} = 10) and AI (n_{max} = 4).

Fig. 3 DC, AI, SC, and SC with averaged cross-sections ; this last approximation shows that the small observed discrepancies between the SC and DC models are mainly due to different rate coefficients.

Fig. 4 *Average shell occupations* P_n (n = 1 to 4) *with the AI and DC models* ; DC values are derived by averaging the number of electrons per shell over all the excited electronic states included in the calculation.

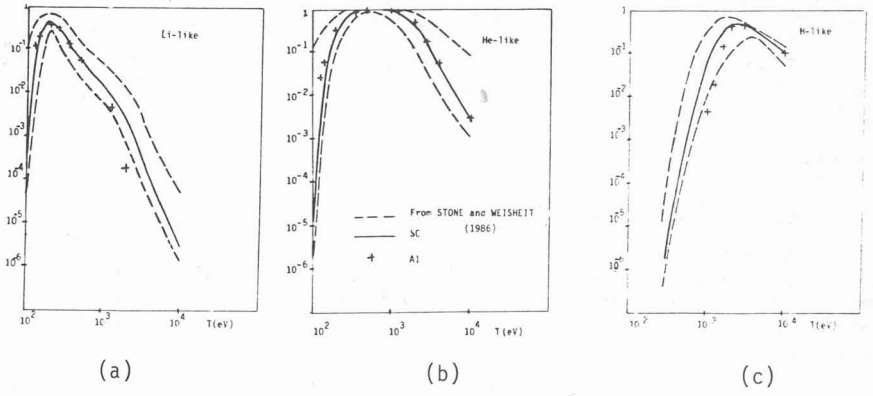


Fig. 5 (a,b and c) In the case of argon (Z = 18) at fixed electronic density ne = 10^{21} cm^{-3} these figures give the relative populations of Li-like, He-like, and H-like ions vs. temperature. The dashed lines are taken from Stone and Weisheit (1986) and correspond to the maximum and minimum values obtained using several NLTE codes from LLNL, NRL and PPPL. Our results with the SC (Simplified Configurations) model fall in the middle of the range ; also shown are values computed with the AI (Average Ion) model.

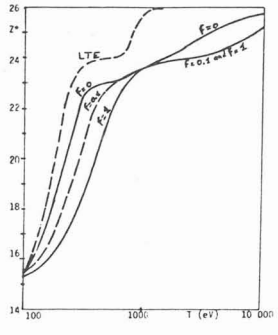


Fig.6

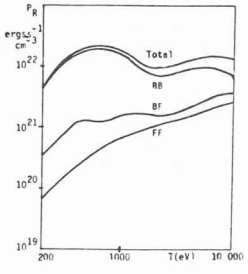


Fig.7

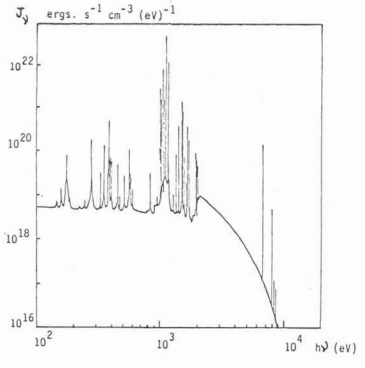


Fig.8

Fig. 6 Using again an iron plasma at a density of 10^{-2} g.cm^{-3} this figure shows the effect of non-unity escape factors f on the resonance lines in the DC (Detailed Configurations) model ; results correspond to DC - LTE, DC (f = 1), DC (f = 0.1) and DC (f = 0).

Fig. 7 Total radiated power vs. temperature ; bound-bound, bound-free and free-free contributions are shown.

Fig. 8 Example of an emissivity spectrum at a temperature of 1000 eV.

(b) Example of time-dependent problems

We consider an iron plasma (Z = 26) at a fixed ion density of 10^{-2}g.cm^{-3}; its temperature is 500 eV at t < 0. then rises linearly to 2000 eV in 20 ps, stays constant to t = 200 ps. and finally falls linearly back to 500 eV at t = 300 ps. (see figs. 9 and 10).

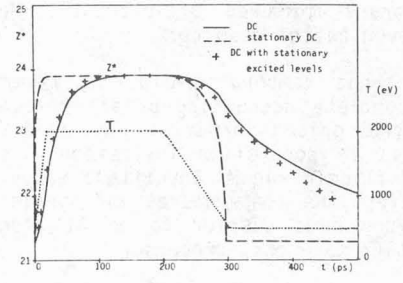


Fig. 9

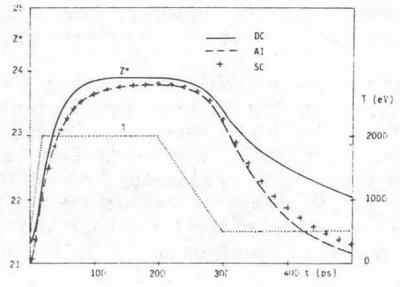


Fig.10

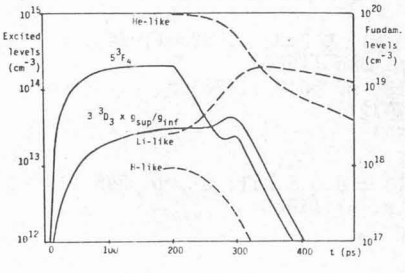


Fig.11

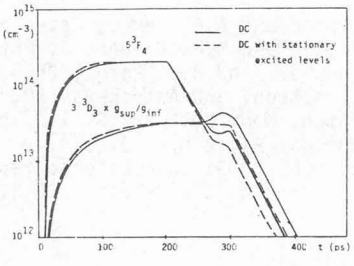


Fig.12

Fig. 9 Shows Z* as a function of time for three cases : normal DC (Detailed Configurations), stationary DC (all time derivatives set to zero ; this is the steady state case discussed previously), DC with stationary excited levels (all time derivatives set to zero for excited levels).

Fig. 10 Comparison between the DC (Detailed Configurations), SC (Simplified Configurations) and AI (Average Ion) models.

Fig. 11 When the plasma is recombining (t > 200 ps), population inversions are predicted. This example shows the inversion in the He-like ion between levels 5 $^3F_4$ and 3 $^3D_3$. H-like, He-like and Li-like ground state populations are also shown.

Fig. 12 Shows the influence of the stationarity hypothesis on predicted populations ; the dashed line was computed while keeping all time derivatives equal to zero for excited levels.

IV CONCLUSIONS

(a) Evaluations of Z* and of overall radiative losses are much more sensitive to the quality of the rate coefficients than to the complexity of the model, whether DC (Detailed Configurations), SC (Simplified Configurations) or AI (Average Ion) are used. The AI approximation, which is both simple to implement and computationally fairly efficient, is quite satisfactory over the relevant range of temperatures and densities where rapid evaluations coupled to an hydro code are of interest ; furthermore, it is readily extended to arbitrary mixtures of elements. More realistic average rate coefficients would yield even better results.

(b) For a given ionization stage, with or without temporal evolution, careful evaluations of the kinetic coefficients and a complete accounting of all relevant levels are obviously necessary if detailed spectroscopic informations are required (this is even more true when one is interested in population inversions ; see related paper by S. Jacquemot, E. Berthier, M. Vuillemin and M. Cornille). However, in many cases, temporal evolutions of the densities, the temperatures and the ionic compositions are efficiently derived from a hydro code coupled to an AI atomic model, detailed spectroscopic evaluations being left to a post-processor.

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