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ABAKO: A new code for population kinetics and radiative properties of plasmas under NLTE conditions

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Abstract. In this work we present ABAKO, a new computational code based on analytical models and developed to study the population kinetics of steady-state plasmas. The tool ABAKO can be applied to low-to-high Z ions under a wide range of laboratory plasma conditions: coronal, LTE or NLTE, optically thin or thick plasmas. Autoionizing states are explicitly included. The results obtained with ABAKO are competitive with more elaborated, but also time-consuming codes. Our code provides satisfactory charge state distributions (CSD) and reasonable estimations of spectroscopic observables of high-Z plasmas, as it can be seen through comparison with experimental data.

1. Introduction

Efforts continue to be made in the modeling of plasmas in non local-thermodynamic-equilibrium (NLTE). Many systematic studies have been made to assess the accuracy of such modeling attempts and detect areas needing improvements. Recent NLTE workshops [1, 2] have focused on comparisons for specific cases between collisional-radiative (CR) codes developed by diverse research groups. On the other hand, the ability to reproduce experimental data is the most valuable test for any CR model, but clean experiments are very difficult to perform and there exist only few measurements that could be used as benchmark cases for the validation of computational codes. In summary, further investigation into population kinetics of NLTE plasmas is necessary and any progress for providing a better understanding of the underlying physics will be welcomed.

In this work we present ABAKO, Analytical expressions BAsed Kinetics cOde, a new CR model to determine the population distribution of atomic levels and radiative properties of steady-state plasmas. The versatility is a remarkable characteristic in ABAKO. It can be applied to low-to-high Z ions under a wide range of laboratory plasma conditions: coronal, LTE or NLTE, optically thin or thick plasmas. On the other hand, a special care was taken during the ABAKO development to achieve an optimal equilibrium between accuracy and computational cost. ABAKO assembles a set of simple analytical models which yield a substantial saving of computational requirements, but providing satisfactory results in relation to those ones obtained from more sophisticated codes and experimental data.

2. The ABAKO features

The goal of a CR model is to determine ionization and level population distributions of a plasma for a given electron temperature T_e and density n_e, and then to assist in the analysis of spectroscopic observables. To achieve this goal the rate equations for each energy level in the plasma should be solved and this requires a complete enough set of atomic data. In order to keep the atomic data manageable and to avoid that the computation time increases, different analytical models are used to determine the atomic structure and to build the CR matrix.

2.1. The atomic structure module

ABAKO follows a relativistic detailed-configuration-accounting (DCA) scheme, which means that the state m of the ion with charge ζ and atomic number Z corresponds to a relativistic electronic configuration, i.e. $\zeta m \equiv (n_1 l_1)_{j_1}^{w_1} (n_2 l_2)_{j_2}^{w_2} \ldots (n_\lambda l_\lambda)_{j_\lambda}^{w_\lambda}$, with $\sum_{i=1}^{\lambda} w_i = Z - \zeta$. To determine the energy levels we first solve the monoelectronic Dirac equation using one of the parametric analytical potentials developed by our group [3, 4]. Then the total energy of the level ζm is evaluated by an expression taken from a density-functional-theory. When a high accuracy is required, e.g. for spectroscopic purposes, more detailed atomic structure from databases or computational codes can be used. ABAKO often runs with data generated by FAC [5], which provides a detailed-level-accounting (DLA) atomic structure. FAC also includes different coupling schemes and configuration interaction. For dense plasmas the lowering of the ionization potential is taken into account following the formulation of Stewart and Pyatt [6].

2.2. The collisional-radiative module

Let be $N_{\zeta m}$ the population density of the atomic level ζm. At the moment ABAKO works under stationary assumption. Therefore ABAKO solves the set of steady-state rate equations to find the level population distribution,

$$\sum_{\zeta' m'} N_{\zeta' m'} \mathbb{R}^+_{\zeta' m' \to \zeta m} - \sum_{\zeta' m'} N_{\zeta m} \mathbb{R}^-_{\zeta m \to \zeta' m'} = 0, \tag{1}$$

where $\mathbb{R}^+_{\zeta' m' \to \zeta m}$ and $\mathbb{R}^+_{\zeta' m' \to \zeta m}$ take into account all those processes which contribute to populate and depopulate the ζm state, respectively. Only those atomic processes whose rates are independent of the radiation field intensity are explicitly considered. These processes are enumerated in table 1. It is worth to comment that ABAKO includes the autoionizing states explicitly, since their contribution has been shown critical in determining the ionization balance.

Table 1. List of atomic processes explicitly included in ABAKO and the semiempirical formulas used to calculate the corresponding rates.

Atomic process	Rate coefficient	Expression
Spontaneous decay	$\mathcal{A}_{\zeta m' \to \zeta m}$	Einstein
Collisional excitation	$\mathcal{E}_{\zeta m' \to \zeta m}$	Van Regemorter
Collisional deexcitation	$\mathcal{D}_{\zeta m' \to \zeta m}$	detailed balance
Radiative recombination	$\mathcal{R}^r_{\zeta+1 m' \to \zeta m}$	Kramers and detailed balance
Collisional ionization	$\mathcal{I}_{\zeta-1 m' \to \zeta m}$	Lotz
Three-body recombination	$\mathcal{R}^3_{\zeta+1 m' \to \zeta m}$	detailed balance
Autoionization	$\mathcal{A}u_{\zeta-1 m' \to \zeta m}$	detailed balance
Electron capture	$\mathcal{C}_{\zeta+1 m' \to \zeta m}$	ABAKO approach

A known approximation consisting of taking the cross-section of collisional excitation to calculate the electron capture cross-section has been properly adapted to work in a DCA scheme.

The escape factor formalism [7] for the basic geometries –plane, cylindric and spherical– is used to take into account the bound-bound opacity effects. It also should be mentioned that ABAKO incorporates a new technique for the line transport [8]. This method is supported by the definition of zone-to-zone radiative coupling coefficients and it can be applied on non-uniform planar media, wherein other proposals with similar characteristics fail [9]. A full description of this formalism will be exposed in a forthcoming paper.

As a numerical issue, ABAKO uses an iterative method to carry out the matrix inversion.

The standard formulation is followed to evaluate the radiative properties like emissivity, opacity, specific intensity, source function, etc. The Kramer's semiclassical formulas are used to evaluate the photoionization and bremsstrahlung cross-sections.

3. Results
In this section we outline the main results that were obtained in the verification and validation process of ABAKO.

3.1. Internal consistency
We first performed systematic calculations to check ABAKO that exhibits the proper behaviour in the opposite limits of electron density. Effectively, in the low-density regime it converges to the Corona results and at high densities the LTE situation is reproduced.

3.2. Validation with other codes
The ABAKO results have been largely validated for many cases from NLTE-3 and NLTE-4 [1, 2] for different elements in a wide range of conditions. A sample of this is given in table 2.

3.3. Validation with experimental data
The ABAKO predictions for average ionization and CSD agree with the measurements in well-characterized experiments for high-Z plasmas. In these cases the population kinetics is governed by ion stages with a complex electronic structure. Some results are displayed in tables 3 and 4 and figures 1 and 2. Likewise ABAKO provides a reasonable estimaion of the X-ray emission spectra coming from these plasmas. It suggests that ABAKO could be a usuful tool for designing future experiments.

Table 2. Average ionization of the NLTE-4 carbon *test case* for different conditions of temperature and electron density. Results from the LANL code ATOMIC [10] for configuration-average (LA-CA) and fine-structure (LA-FS) and those provided by ABAKO using analytical potentials (AB-AP) or DLA atomic data from FAC (AB-FAC) are shown.

n_e (cm^{-3})		$T_e(eV)$					$T_e(eV)$			
		3	5	7	10		3	5	7	10
10^{13}	LA-CA	1.486	2.055	2.729	3.701	AB-AP	1.605	2.057	2.722	3.684
	LA-FS	1.730	2.165	2.887	3.723	AB-FAC	1.619	2.135	2.873	3.705
10^{15}	LA-CA	1.895	2.592	3.189	3.856	AB-AP	1.786	2.309	3.004	3.747
	LA-FS	1.923	2.514	3.185	3.862	AB-FAC	1.852	2.276	2.977	3.745
10^{19}	LA-CA	0.959	2.104	2.993	3.785	AB-AP	1.142	2.182	3.001	3.776
	LA-FS	1.004	2.076	2.987	3.786	AB-FAC	0.932	2.084	2.998	3.787

Table 3. Simulated average ionizations for the Au experiment performed in EBIT [11]. The conditions are $n_e = 10^{12}\ cm^{-3}$ and $T_e = 2500\ eV$.

experiment [11]	46.8±0.75
ABAKO	47.2
AVERROES [12]	46.4
FLYCHK [13]	48.5
RIGEL/MCXSN [11]	49.5

Table 4. Simulated average ionizations for the Xe experiment performed in LULI [14]. The conditions are $n_{ion} = 4.75 \times 10^{18}\ cm^{-3}$, $T_e = 415 \pm 40\ eV$ and $L = 100\ \mu m$ of thickness.

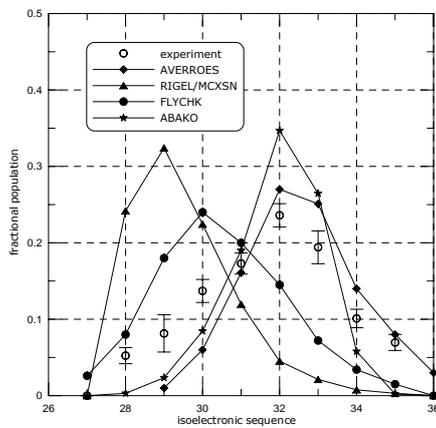|	
experiment [14]	27.4 ± 1.5
ABAKO	26.6
AVERROES [14]	26.8
SOSA [14]	26.5

Figure 1. Simulated CSDs for the Au experiment performed in EBIT.
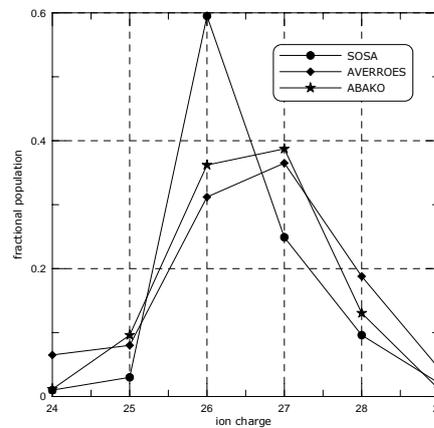
Figure 2. Simulated CSDs for the Xe experiment performed in LULI.

References
[1] Bowen C, Lee R W and Ralchenko Y 2006 *J. Quant. Spectrosc. Radiat. Transfer* **99** 102–119
[2] Rubiano J G, Florido R, Bowen C, Lee R W and Ralchenko Y 2007 *High Energy Density Phys.* **3** 225–232
[3] Martel P, Doreste L, Mínguez E and Gil J M 1995 *J. Quant. Spectrosc. Radiat. Transfer* **54** 621–636
[4] Rodríguez R, Rubiano J G, Gil J M, Martel P, Mínguez E and Florido R 2002 *J. Quant. Spectrosc. Radiat. Transfer* **75** 723–739
[5] Gu M F 2003 *Astrophys. J.* **582** 1241–1250
[6] Stewart J C and Pyatt K D 1966 *Astrophys. J.* **144** 1203–1211
[7] Mancini R C, Joyce R F and Hooper Jr C F 1987 *J. Phys. B: At. Mol. Phys.* **20** 2975–2987
[8] Florido R, Gil J M, Rodríguez R, Rubiano J G, Martel P and Mínguez E 2006 *J. Phys. IV* **133** 993–996
[9] Apruzese J P, Davis J, Duston D and Whitney K G 1980 *J. Quant. Spectrosc. Radiat. Transfer* **23** 479–487
[10] Colgan J, Fontes C J and Abdallah Jr J 2006 *High Energy Density Phys.* **2** 90–96
[11] Wong K L, May M J, Beiersdorfer P, Fournier K B, Wilson B, Brown G V and Springer P 2003 *Phys. Rev. Lett.* **90** 235001
[12] Peyrusse O, Bauche-Arnoult C and Bauche J 2005 *J. Phys. B: At. Mol. Opt. Phys.* **38** L137–L143
[13] Chung H K, Chen M H, Morgan W L, Ralchenko Y and Lee R W 2005 *High Energy Density Phys.* **1** 3–12
[14] Chenais-Popovics C, Malka V, Gauthier J C, Gary S, Peyrusse O, Rabec-Le Gloahec M, Matsushima I, Bauche-Arnoult C, Bachelier A and Bauche J 2002 *Phys. Rev. E* **65** 046418