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Collisional-Radiative Calculations of Optically Thin and Thick Plasmas Using the Computational Package ABAKO/RAPCAL

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Abstract. Non-local thermodynamic equilibrium (NLTE) conditions are universal in laboratory and astrophysical plasmas and, for this reason, the theory of NLTE plasmas is nowadays a very active subject. The populations of atomic levels and radiative properties are essential magnitudes in the study of these plasmas and the calculation of those properties relies on the so-called collisional-radiative (CR) models. However, the complexity of these models has led to the development of numerous collisional-radiative codes and this is a current research topic in plasmas. In this work is presented a versatile computational package, named ABAKO/RAPCAL, to calculate the populations of atomic levels and radiative properties of optically thin and thick, low-to-high Z, NLTE plasmas. ABAKO/RAPCAL combines a set of analytical approximations which yield substantial savings in computing running time, still comparing well with more elaborated codes and experimental data. In order to show the capabilities of the code and the accuracy of its results, calculations of several relevant plasma magnitudes for various plasma situations are shown and compared.

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Key words: Collisional-radiative model, optically thin and thick NLTE plasmas.

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1 Introduction

In many research areas on plasmas and their applications such as astrophysics, X-ray laser development, inertial and magnetic confinement fusion or EUV lithography, the accurate calculation of the populations of atomic levels and radiative properties existing in the plasma is required, since they are involved, for example, in hydrodynamic simulations or spectroscopic diagnostics.

At high densities, when the plasma can be considered under local thermodynamic equilibrium (LTE) conditions the populations are calculated by means of the equations of Saha-Boltzmann. On the other hand, in the low density regime, coronal equilibrium (CE) can be assumed and, therefore, these quantities are evaluated using the CE equations. However, these limit situations are exceptions and non-LTE (NLTE) conditions are universal in laboratory and astrophysical plasmas and, for this reason, the theory of NLTE plasmas is nowadays a very active subject. In NLTE, the problem shows great complexity because there is not a priori expression for the occupation probabilities of bound states and one must find the statistical distribution of the ionic levels using a collisional-radiative (CR) model. This implies solving a set of rate equations with coupling of atomic configurations, free electrons and photons. Taking into account that for accurate simulations of the level populations and radiative properties it is essential to include as many levels as possible, the resolution of the resulting large linear equation system becomes sometimes unmanageable and approximations must be made. This fact has led to the development of numerous CR codes [1–10] since the early proposals described in [11,12].

The complexity of the CR models is mainly due to three factors. The first one is the atomic model chosen, which is still the focus of much attention and numerous discussions. The most detailed level of information that can be used in the determination of the population distributions is usually referred detailed-level-accounting (DLA) approach, in which each atomic level is explicitly included and the resolution of a level-by-level kinetic model is required. This approach is considered practical for elements with a low to medium atomic number ($Z < 30$) [13]. As the atomic number increases, the amount of atomic data involved rises considerably and the DLA approach becomes impractical and sometimes unnecessary [14]. Thus, for high-Z elements, a configuration-by-configuration kinetic model, i.e. a detailed-configuration-accounting (DCA) model, is the standard approach. In the literature there are statistical methods to reduce the level of atomic description which imply grouping of levels into configurations (resulting a DCA model) [15] or superconfigurations (SC) [16]. These methods have shown to be very efficient when they are combined with unresolved transition array (UTA/SOSA) [17, 18] and/or supertransition array (STA) [19] formalisms. In these approaches both the amount of atomic data and the number of rate equations are noticeably reduced due to the configuration or superconfiguration average. However, these models based on averages may lack the accuracy to describe isolated levels or transitions. A possible improvement lies in the definition of effective temperatures inside each statistical group (configuration or superconfiguration), where the detailed level population inside each