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Influence of the atomic description and configuration interaction effects on collisional-radiative calculations of low ionized carbon plasmas

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ABSTRACT

An analysis of the influence of the atomic description and the configuration interaction effects in the calculation of plasma average ionization and relevant plasma radiative properties such as the spectrally resolved emissivities and opacities, radiative power losses and mean opacities, is performed. Since the larger effects of the configuration interaction are due to the lower ionization stages, i.e. CI and CII ions, the low temperature regime is analysed. However, a wide range of plasma densities is considered, covering this way different plasma thermodynamic regimes.

1. Introduction

In several research areas, such as astrophysics or magnetic and inertial fusion confinements, the knowledge and understanding of the interaction between photons and plasma particles, i.e. plasma optical properties, are essential [1–6]. The radiation emitted from hot plasmas or short life plasmas is an important diagnostic tool since the spectrum contains information about the local instantaneous density and temperature [7]. Furthermore, modelling of the energy transport in hot dense plasmas relies on radiative opacities [8] and the spectrally integrated emissivity is used for determining the evolution of the electronic and radiation temperatures [9]. On the other hand, radiative opacities play a pivotal role in governing stellar structure and evolution [10]. For these and other reasons, plasma optical properties must be determined properly. This fact implies accurate calculations for both the atomic data and the populations of the atomic configurations or levels involved and that continuous efforts are made in the modelling of plasmas.

However, the determination of the population of the atomic configurations or levels is a complex task since the amount of levels and transitions involved is usually huge, even for low Z elements. Furthermore, the complexity is considerably increased when electron density is not large enough to ensure local thermodynamic equilibrium (LTE). In this situation, collisional-radiative (CR) models must be used which implies to solve a large set of rate equations. The most detailed level of information that can be used in radiative properties calculations is usually referred as detailed level accounting (DLA)

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approach in which each atomic level would be considered and it requires the resolution of a level-by-level kinetic model. This approach is usually only considered practical for elements with a low to medium atomic number ($Z<30$) [11]. As the atomic number increases, the amount of atomic data to handle also does and DLA approach for the calculation of radiative properties becomes impractical and, therefore, other approximations have been developed. Some of them are resorted to statistical models in which the atomic levels are grouped into configurations (detailed configuration accounting, DCA, approach) or superconfigurations (SC) [12,13]. In these approaches both the amount of atomic data and the number of rate equations required are considerably reduced due to the configuration or superconfiguration average. In this context, the absorption and emission spectra are described as unresolved transition arrays (UTA) [14], spin–orbit split arrays (SOSA) [15] or supertransition arrays (STA) [16]. However, these statistical models based on averages may lack the accuracy to describe isolated levels or transitions. Another possibility is the description of the non-LTE in terms of certain temperatures called effective temperatures inside each configuration or superconfiguration. The detailed level populations inside each of them is obtained from population of the (super)configuration and these temperatures. How the effective temperatures are determined is discussed in a series of papers [17–20]. However, the accuracy of this method is restricted to only certain configurations. Nowadays, models involving both detailed levels and configurations (called hybrid models) are being developed [11,21]. This kind of models has the advantage of retaining the fine description only for the most relevant levels in the calculations, increasing the accuracy regarding to the DCA models, whereas the rest is described into the DCA approach, reducing the amount of atomic data and rate equations involved. Given all before mentioned, it is clear that the analysis of the influence of the atomic description in plasma modelling is still an open question and new studies are always welcomed.

In this work it is accomplished a qualitatively study of the influence of the atomic description and, in particular, of the configuration interaction effects in the collisional-radiative calculations of carbon plasmas. Carbon has been chosen for two reasons. The first one is its current interest: carbon is likely to be a major plasma facing wall component in the international thermonuclear experimental reactor (ITER) [22] and it plays a major role in inertial fusion scenarios [23] and therefore, radiation rates from carbon impurities must be known. Furthermore, some laser experiments have focused on the spectrally resolved emission from hydrocarbon systems [24]. On the other hand, carbon is a highly abundant element in stars and its contribution in the opacity of the stellar mixture cannot be ignored [10]. Moreover, the analysis of certain lines of CI/II ions allows us to determine the abundance of carbon under non-LTE conditions in early type stars, which is a prerequisite for all further studies [25,26]. The second one is to show that even for low Z elements the effect of the atomic description and of the configuration interaction could be important under some plasma conditions. In recent works [27–29] it has been proved that configuration average (CA) calculations are useful for modelling carbon plasmas at temperatures higher than 10 eV. However, for lower temperatures this approach is not accurate enough and it requires the DLA approach. Furthermore, since in the low temperature regime the abundance of CI and CII ions is relevant, configuration interaction contributions must be considered. The study of this region is precisely the main objective of this work. Thus, we have accomplished an analysis of the influence of the atomic description and configuration interaction on plasma average ionization and radiative properties, such as the radiative power losses and emissivities, for low temperatures (≤ 5 eV). The analysis was carried out over a wide range of electron densities, covering non-LTE and LTE regimes. For the last regime, we have also analysed the spectrally resolved and mean opacities. The kinetics calculations have been performed using ABAKO code [30,31] which provides level populations by solving a CR model. In the resolution of the CR model opacity effects have not been included, assuming that the plasma is optically thin. ABAKO has been successfully tested with results coming from the 3th, 4th and 5th NLTE Kinetics Codes Comparison Workshops [32–34]. The radiative properties were calculated using RAPCAL code [35,36]. In the next section it is briefly explained the atomic model employed inthis work and the before mentioned codes.

2. Theoretical model

The atomic data used in this work have been generated using FAC code [37] which is designed to provide atomic data in DLA approach. The energy of the levels of an atomic ion with N electrons are obtained by diagonalizing the relativistic Hamiltonian. The basis states which are usually referred as configuration state functions (CSF) are built as anti-symmetric sums of products of N one-electron Dirac spinors. In coupling the angular momenta the standard jj-coupling scheme is used. Finally, the approximate atomic wave functions are evaluated mixing the basis states with the same symmetries with the mixing coefficients obtained from diagonalizing the total Hamiltonian. FAC can also work under DCA approach by means of configuration averages of the detailed levels.

As it is known, the level populations strongly depend on the atomic configurations included in the calculations. It is still an open question [38,21,39] which is the most suitable election of them. In this respect, the overall analysis of the large number of cases studied during the ABAKO development has led us to consider a complete enough set of configurations which allows us to obtain satisfactory results. In Table 1 are listed the atomic configurations included for the six ions of carbon. In the table $(n)^w$ contains all the possible relativistic configurations that arise from the shell with principal quantum number n and w bound electrons. The list of selected configurations has been shown to be robust for atomic kinetic modelling, since the addition of new configurations produced hardly appreciable changes in the population distributions.