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Calculation of radiative opacity of plasma mixtures using a relativistic screened hydrogenic model

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ABSTRACT

We present the code ATMED based on an average atom model and conceived for fast computing the population distribution and radiative properties of hot and dense single and multicomponent plasmas under LTE conditions. A relativistic screened hydrogenic model (RSHM), built on a new set of universal constants considering *j*-splitting, is used to calculate the required atomic data. The opacity model includes radiative bound–bound, bound–free, free–free, and scattering processes. Bound–bound line-shape function has contributions from natural, Doppler and electron-impact broadenings. An additional dielectronic broadening to account for fluctuations in the average level populations has been included, which improves substantially the Rosseland mean opacity results. To illustrate the main features of the code and its capabilities, calculations of several fundamental quantities of one-component plasmas and mixtures are presented, and a comparison with previously published data is performed. Results are satisfactorily compared with those predicted by more elaborate codes.

1. Introduction

The accurate computation of plasma radiative hydrodynamics for the problems of high energy density physics, such as those of inertial confinement fusion (ICF) or laboratory astrophysics, needs reliable data on spectral and mean opacities of several hot, dense plasmas. The processes of emission and absorption of radiation are strongly coupled to the radiation field and to the matter, and its modeling requires a realistic description of the plasma photo-absorption spectra in a wide density and temperature range. A fundamental quantity is the ionization state distribution of plasma, which is required for the determination of radiative properties, the equation of state, thermal and electrical conductivities, and the stopping power for fast charged particles. There are several methods referenced in the literature to perform these calculations for plasmas, both in LTE [1,2] and in NLTE [3,4].

In order to solve this problem, a detailed description of all ground and excited configurations of all atomic species present in the plasma is needed. Obtaining an accurate solution is a complicate task because multielectron ions can have an extremely large number of excited states, especially for high Z plasmas, and, therefore, the amount of atomic data to compute is huge, so in practical calculations approximations have to be made. For low and intermediate Z plasmas detailed level accounting (DLA) or detailed term accounting (DTA) approaches [5,6] are commonly used. For high-Z elements, statistical approaches involving grouping of levels, such as the detailed configuration accounting

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(DCA) approach or super configuration accounting (SCA) approach [7–11], have shown to be very efficient when they are combined with unresolved transition array (UTA/SOSA) [12–14] and/or super transition array (STA) formalisms [15,16]. More recently, new hybrid models mixing detailed levels and configurations have been developed [17,18]. These methods account for all the transition lines corresponding to every ionic species in the plasma and they require a large computation time, not only for mid- and high-Z plasmas, but in the case of plasma mixtures as well. For this reason, simplified but accurate computation models are still needed to provide with low computational cost the data needed by hydrodynamics codes.

The average atom model (AAM) [19] is a fast and efficient alternative for calculation of radiative properties widely used in ICF plasma physics. The utility of the average-atom model comes about it computes the occupancies of the mono-electronic levels (or "level populations"), averaged over the distribution of ionic states, instead of computing the abundances of individual ionic states (ground or excited). As a result, the system is characterized by a fictitious atomic system with a non-integer number of electrons which are distributed among the levels in an attempt to describe the average occupation of the levels in the plasma (the average-atom). Consequently, the number of equations is greatly reduced compared to a model that accounts for individual ionic states. This kind of model runs hundred times faster than a detailed one, and a great saving of computer time is achieved. Using an average-atom model also permits us to deal with complex atomic structure problems in a manner that, although not as accurate as detailed models, is more complete regarding the number of levels involved. A fundamental approximation employed by the average-atom model that allows this simplification is that there is no statistical correlation between electrons occupying different levels. A discussion about the theoretical background of the average atom model can be found in reference [20].

Several models have been developed to obtain the radiative properties of plasma using AAM under LTE [21–23] and NLTE conditions [24–26]. The accuracy of different forms of AAM depends on the atomic model used to calculate the bound energy levels and level populations. One of the atomic models commonly used in this context is the screened hydrogenic model (SHM). This model calculates the energy levels of an ion using the analytical expressions of the hydrogenic atom the energy of a given ion being the sum of these hydrogenic one-electron energies, computed with appropriate screened nuclear charges. The SHM used in the average ion model context provides electronic populations with good accuracy and it also allows computing the opacity and the emissivity easily. There are several formulations of SHMs, with the method used to compute the screened charges being the main difference among them [27–30]. They are usually determined by an empirical adjustment, and various sets of coefficients to compute screened charges are currently available [31–35].

The ATMED code has been conceived to compute the radiative and thermodynamic properties of single element plasmas and plasma mixtures under LTE conditions in the Average Atom framework using a Relativistic Screened Hydrogenic Model (RSHM) [35]. In this paper we will focus on the presentation of the features and results of the model for the radiative properties of plasmas. In the next section we describe the average atom model, i.e. the calculation of the atomic properties such as the average ionization of the plasma, the fractional occupation numbers or the one-electron energies. Sections 3 and 4 are devoted to present in detail the opacity model for plasmas and plasma mixtures, respectively. A validation of the code is made in Section 5, where we present an extensive comparison of our results with the ones obtained with other codes, and with some experimental results available in the literature. Finally, some conclusions and general remarks are presented in Section 6.

2. Description of the average atom model

ATMED computes the atomic properties of the plasma in the average atom approximation by means of a Screened Hydrogenic Model, based on a new set of universal screening constants including *nlj*-splitting. Under this approach an electronic configuration (fundamental or excited) can be written as follows:

$$\{(n_1 l_1 j_1)^{P_1}, \ldots, (n_k l_k j_k)^{P_k}, \ldots, (n_{k_{\max}} l_{k_{\max}} j_{k_{\max}})^{P_{k\max}}\},$$

where the symbol $n_k l_k j_k$ denotes the set of quantum numbers that label the relativistic sub-shell k, and P_k is its occupation number which ranges from 0 to $2j+1$. The average energy E_T of an ion in this configuration is given as the sum of Dirac's eigenvalues ε_k for hydrogenic ions

$$E_T = \sum_k P_k \varepsilon_k, \tag{1}$$

where

$$\varepsilon_k = m_e c^2 \left[\left(1 + \left[\frac{\alpha Q_k}{n - j - 1/2 + \sqrt{(j+1/2)^2 - (\alpha Q_k)^2}} \right]^2 \right)^{-1/2} - 1 \right], \tag{2}$$

m_e being the electron mass, c the speed of light, α the fine structure constant and Q_k the screened nuclear charge experienced by an electron belonging to the k subshell, written as [34]

$$Q_k = Z - \sum_{k'} \sigma_{kk'} (P_{k'} - \delta_{kk'}). \tag{3}$$

In the latter equation, Z stands for the nuclear charge, $\delta_{kk'}$ is Kronecker's delta symbol and $\sigma_{kk'}$ is the screening constant. The set of relativistic screening constants $\{\sigma_{kk'}\}$ was obtained from the fit to an extensive database of atomic energies, which was built with both energies compiled from the *National Institute of Standards and Technology* (NIST) database of experimental atomic energy levels [36], and energies calculated with the Flexible Atomic Code (FAC) [37].

Kronecker's delta symbol in Eq. (3) was introduced to eliminate the self-screening of one electron. Since in the framework of the average atom model the occupation numbers of the atomic levels have no integer values, the