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Coupled electron and atomic kinetics through the solution of the Boltzmann equation for generating time-dependent X-ray spectra

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Abstract

In this work, we present a model that solves self-consistently the electron and atomic kinetics to characterize highly non-equilibrium plasmas, in particular for those systems where both the electron distribution function is far from Maxwellian and the evolution of the ion level populations are dominated by time-dependent atomic kinetics. In this model, level populations are obtained from a detailed collisional-radiative model where collision rates are computed from a time varying electron distribution function obtained from the solution of the zero-dimensional Boltzmann equation. The Boltzmann collision term includes the effects of electron–electron collisions, electron collisional ionization, excitation and de-excitation. An application for He_α spectra from a short pulse laser irradiated argon cluster target will be shown to illustrate the results of our model.

Keywords: Boltzmann equation; K-shell spectra; Time dependent kinetics; Short pulse lasers; Clusters

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1. Introduction

A rate-equation code for the description of the temporal evolution of atomic (ionic) state population densities and for the total free-electron density in Non-LTE plasmas have been developed for numerous applications, here we will use the work of Abdallah and Clark [1] and will be referred to here as ATOMIC (formally known as FINE), to discuss the standard approach. ATOMIC solves a large set of coupled differential equations for the atomic (ionic) state populations and for the total free-electron density where electron impact excitation, de-excitation, and ionization of atomic (ionic) states as well as three-body recombination, photoionization, autoionization, radiative excitation, spontaneous emission, stimulated emission and photoexcitation processes are included into the possible mechanisms that govern the dynamics of the Non-LTE plasma. In calculating the rate-coefficients for electronic collisional excitation, de-excitation, ionization and for three-body recombination processes a Maxwellian electron distribution was assumed, though ATOMIC was developed in such a way that an arbitrary electron-distribution could be accommodated. While this code is relevant in most cases, there are some situations of considerable scientific and industrial interest where the deviation of the free-electron distribution function from the Maxwellian form is sufficiently significant to require that the free-electron distribution function be solved consistently with the rate-equations for the atomic state-density populations. We have chosen to obtain temporal evolution of the free-electron distribution function by solving the Boltzmann-equation. The use of the Boltzmann-equation for such problems has a long history and detailed mathematical and numerical treatments are available in the literature [2–12]. With time discretized, and an appropriate initial description of the free-electron energy distribution function and level populations, our model propagates the free-electron kinetics from time t to $t+\delta t$ with a frozen set of level populations computed from the collisional radiative (CR) model for time t (For the rest of this paper the CR model will only refer to the following atomic processes: electron impact excitation, de-excitation and ionization; as well as spontaneous emission.) The CR model then computes the level populations from time t to $t+\delta t$ with the newly computed free-electron energy distribution for time $t+\delta t$. This stepping process is repeated until the end of the simulation.

2. The Boltzmann equation

The time evolution of the free-electron distribution function is obtained by solving the Boltzmann transport equation (BTE). This equation is written as (Ref. [13]),

$$\frac{\partial f(\vec{r},\vec{p},t)}{\partial t}+\frac{\vec{p}}{m}\cdot\nabla_r f(\vec{r},\vec{p},t)+\vec{F}\cdot\nabla_p f(\vec{r},\vec{p},t)=\left(\frac{\partial f(\vec{r},\vec{p},t)}{\partial t}\right)_{\text{coll}}, \tag{1}$$

where $f(\vec{r},\vec{p},t)$, for our case, refers to the free-electron distribution function at time t and at position and momentum coordinates $\vec{r}$ and $\vec{p}$, respectively; $\vec{F}$ refers to external forces on the system of particles; and the right hand of Eq. (1) accounts for the effects of collisional processes during the evolution of the distribution function.

Since the primary purpose of this work is to couple electron kinetics with the preexisting zero-dimensional atomic kinetic model in ATOMIC, such a detailed description of the free-electron