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A study of ion-dynamics and correlation effects for spectral line broadening in plasma: K-shell lines

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Abstract

A method for the calculation of spectral line broadening in plasma has been developed and implemented. The method is based on a numerical simulation of the motion of the interacting plasma particles (both ions and electrons) and the use of the resulting time-dependent field to obtain the evolution of the radiator system. The Fourier transform of the resulting radiator time-dependent dipole function then gives the spectral line shape. This approach thus naturally accounts for all frequency regions of the plasma-particle fields and for the effects of the particle interactions on the fields. Due to a rather general approach used for solving the Schrödinger equation, the method is applicable to line-shape calculations of isolated and overlapping spectral lines involving both dipole-allowed and dipole-forbidden radiative transitions. In addition, line shapes under a simultaneous influence of externally-applied (constant or time-dependent) electric and magnetic fields can be calculated in a self-consistent manner, and polarization properties of the emitted light, caused by such external fields, can be investigated. Part of the method capabilities is demonstrated. Results presented are for spectral lines of H- and He-like ions of C, Si, and Ar in non-magnetized plasmas. It is found that ion dynamics contributes to the line broadening significantly, in several cases exceeding the electron impact widths by a few times. Also, the interactions between the radiator and the perturbers cause a significant reduction in the line widths, even for overall-weakly-coupled plasmas; a relation between this effect and the radiator–perturber coupling is made.

Keywords: Stark effect; Ion dynamics; Spectral line broadening

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1. Introduction

Measurements of emission and absorption spectra of atoms and ions are one of the most important tools in plasma diagnostics [1]. They allow for non-intrusive diagnostics of the properties of plasmas and electromagnetic fields in various laboratory and space plasmas. In particular, spectral line shapes may be analyzed to yield a wealth of information on the plasma parameters provided, however, that the data are compared to accurate computations of the spectral line broadening with and without externally-applied electric and magnetic fields.

The modern theory of spectral line broadening in plasmas was developed in the 1960s [2–4]. In the theory, the effects of the plasma environment on the emission spectrum is split into two parts characterized by two radically different frequency regions. The ions are essentially stationary and their effect is that of a static Stark effect, with the broadening caused by an averaging over all possible fields corresponding to the different ion configurations near the perturbed atom or ion (the quasistatic approximation). For each of the ion-field configurations, the effect of electrons has then to be calculated. The electrons, because of their high mobility, perturb the radiator by means of "collisions". These collisions cause a change of the radiator state, thus interrupting the spontaneous radiation, or alter the energy levels of the radiator, which results in a phase shift (the impact approximation). The net effect of these processes, averaged over the time and number of radiators, gives the spectral line broadening and shift.

Traditionally, ion effects in most cases were calculated within the quasistatic approximation, while the electron perturbation was believed to satisfy the impact approximation. The formal description of the method is given by the following formula:

$$I(\omega) = \frac{1}{\pi} \Re \,\mathrm{Tr} \int_0^\infty \mathrm{d}F \, W(F) \{ \varDelta_\mathrm{d} [\mathrm{i}\omega - \mathrm{i}\omega(F) + \phi(F)]^{-1} \}, \tag{1}$$

where $W(F)$ is the ion microfield distribution function, $\varDelta_\mathrm{d}$ is the dipole–dipole operator, $\omega(F)$ is the quasistatic Stark shift of the level energy, and ϕ is the so-called impact operator that, in general, depends on the ion field F. This approach to Stark line-broadening is commonly referred to as the "Standard Theory" (ST).

This separation of perturbations into ion and electron parts, in general, cannot be made without a loss of accuracy, although it is argued [5] that in many cases it is justified. A more serious problem, however, is that each of the ion and electron parts often needs to be considered beyond the limits of the quasistatic and impact approximations. In particular, the ion motion in plasma leads to the so-called ion dynamics effects. It was first shown theoretically [6,7] and soon found in experiments [8–10], that the ion dynamics can be responsible for significant corrections to the spectral line widths.

In order to advance the calculations beyond the ST, several computer simulation methods have been developed (for a comprehensive review of the development in the field since the ST foundation, see Ref. [1]). Among the first is the work described in Ref. [11], where a computer code was used to simulate the ion motion along straight paths, while the electron contribution was still calculated using the impact approximation. The method was further improved [12] by using molecular-dynamics (MD) simulations for the ions, thus accounting for interactions between the radiators and the ion perturbers. Then, more improvements were developed [13–16], where the motion of both ions and electrons was numerically simulated, resulting in a correct treatment of the intermediate time scales of the electric-field fluctuations. The particle motion was simulated