New Astronomy Reviews 53 (2009) 272–276

Contents lists available at ScienceDirect

New Astronomy Reviews

journal homepage: www.elsevier.com/locate/newastrev

Spectral line shapes modeling in laboratory and astrophysical plasmas

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ARTICLE INFO

Article history:
Available online 6 August 2009

Keywords:
Stark broadening
Zeeman effect
Doppler broadening
Turbulence

ABSTRACT

An overview of several spectral line shapes studies of common interest in astrophysical and laboratory plasmas is presented. For lines dominated by Stark broadening, approaches taking into account the dynamics of numerous perturbers are sometimes required. We briefly recall ab initio simulation techniques and model microfield methods used for such conditions. Together with the impact approximation, such models may also be used for studying the effects on a line profile of a magnetic field of the order of the tesla, allowing the diagnostic of stellar objects or magnetic fusion devices. The problem of the apparent spectral line emitted in a plasma affected by strong fluctuations of the plasma parameters is discussed for the case of optically thin plasmas.

1. Introduction

Astrophysicists share with laboratory plasma physicists an interest for the details of line shapes emitted in plasmas. Many studies have demonstrated that an exhaustive analysis of spectral line shapes provides invaluable information on the emitter environment (Popovic and Dimitrijevic, 2007; Stehlé, 1995). Ongoing progresses in observations drive a parallel effort in the modeling, since there can be no accurate diagnostic without a deep understanding of the emitter interaction with the plasma. Emphasizing on hydrogen emitters, we discuss in this paper the line shapes emitted by atoms perturbed by charged particles. These studies are of a particular interest for plasma diagnostic, and also provide input data for investigating plasmas with the help of numerical models. Astrophysical applications are numerous, ranging from diagnostic issues such as the knowledge of effective stellar temperature, and the surface gravity. Line shapes enter in the modeling of different regions of a star, like the stellar atmosphere and its opacity properties, stellar winds, various kinds of stellar interiors, and of many extragalactic objects. A very similar use of line shapes is found in laboratory or fusion plasmas. For instance, the modeling of edge plasmas in magnetic fusion devices requires detailed profiles for an accurate diagnostic and complete understanding of the plasma properties.

In the following, we illustrate with several examples some of the tools used in our laboratory for modeling the line shapes emitted in weakly coupled plasmas. An old problem concerns the many body dynamic interactions with the emitter which occur for a large range of plasma conditions. We will present some of the approaches which are useful, on the one hand for an accurate and ab initio description of the line shape, and on the other hand for obtaining a large amount of profiles by a computer efficient model for a real time diagnostic. Interesting application conditions for these models concern magnetized plasmas found in astrophysics or magnetic fusion plasmas. For magnetic fields of several teslas, there can be a complex interplay of Stark and Zeeman effect, and line shape models in plasma conditions of interest in astrophysics and magnetic fusion will be discussed with the help of an impact approximation. A more recently studied problem of general interest is the modeling of spectra observed in a plasma with spatially and temporally fluctuating parameters, a common situation in astrophysical conditions. Magnetic fusion plasmas and some laboratory experiments also experience strong fluctuations for instance due to drift wave turbulence. We have identified plasma conditions for which a simple statistical model can be applied for a calculation of the apparent line shape in such plasmas. Results for our model will be shown for Doppler dominated profiles.

2. Stark effect

Stark broadening may affect line shapes as the electronic density becomes significant. Hydrogen or helium lines are usually dominantly affected, but lines of all elements may be concerned in dense plasmas. In dense laboratory or astrophysical plasmas, a standard Stark broadening approach consists in a binary impact approximation for the electron perturbers, together with a static approximation for the ionic perturbers (Griem, 1964). For many laboratory or astrophysical plasma conditions, ion dynamic effects

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doi:10.1016/j.newar.2009.07.011

have to be retained since the time of interest of the transition considered (defined as the inverse of the line width) may be comparable to the ion collision time (defined for the ions as their average interparticle distance r_0 over their thermal velocity v_0). For hydrogen lines emitted from levels of a low principal quantum number n, with a plasma in the eV range, this may occur for densities as high as $N_e = 10^{17}$ cm^{-3}. On the other hand, the impact approximation for the electrons becomes more and more questionable as lines with large principal quantum numbers are considered ($n > 10$–12). In such cases the electron broadening mechanism is similar to the ion dynamics problem, since it involves many body dynamic interactions between charged particles and the emitter. Several approaches exist for a realistic description of line shapes formed during an interaction with many moving perturbers. As an external magnetic field can be present, one has in general to distinguish between the different directions of polarization for the line shape. In units of seconds/radians, the line shape $I_{\hat{e}}(\omega)$ for radiation polarized along the unit vector $\hat{e}$, is given by a one sided Fourier transform:

$$I_{\hat{e}}(\omega,\vec{B}) = \frac{1}{\pi}\mathrm{Re}\int_0^\infty C_{\hat{e}}(t,\vec{B})e^{i\omega t}\mathrm{d}t, \quad (1)$$

where the dipole autocorrelation function $C_{\hat{e}}(t,\vec{B})$ is defined by the following trace over the atomic states:

$$C_{\hat{e}}(t,\vec{B}) = \mathrm{Tr}\langle \hat{e}\cdot\vec{D}(0)\hat{e}\cdot\vec{D}(t)\rho\rangle. \quad (2)$$

In this expression $\vec{D}$ is the dipole operator, the angle brackets denote an average over all charged perturbers, and ρ is the density matrix for the atom only. Using Eqs. (1) and (2), and a kinetic model for obtaining the elements of the density matrix, non local thermodynamic equilibrium conditions may be taken into account. This point will not be considered below, where we will focus on conditions such that all the substates of the atomic levels are equally populated and both the upper and lower levels of the radiative transition are in local thermodynamic equilibrium.

For a plane wave propagating in a direction given by a vector $\vec{k}$ (direction of observation), the general state of polarization can be described by combining two independent linearly polarized plane waves with polarization vectors $\hat{e}_\lambda(\lambda = 1,2)$ orthogonal to $\vec{k}$ (Bransden and Joachain, 1983). This leads to the general expression of the Stark–Zeeman line shape for a single atom in the case of an observation with an angle θ_0 with the magnetic field:

$$I(\omega) = \cos^2\theta_0 I_{ll}(\omega) + \sin^2\theta_0 I_\perp(\omega), \quad (3)$$

where the difference between the line shape observed in directions parallel (I_{ll}) and perpendicular ($I_\perp$) to the magnetic field are due to the radiation polarization properties resulting from Eq. (2) (Nguyen-Hoe et al., 1967).

The dipole operator at time t may be expressed with the time evolution operator $U(t)$ of the emitter:

$$\vec{D}(t) = U^+(t)\vec{D}(0)U(t). \quad (4)$$

The time evolution operator $U(t)$ obeys to the following Schrödinger equation:

$$i\hbar\frac{\mathrm{d}U(t)}{\mathrm{d}t} = H(t)U(t), \quad (5)$$

where $H(t) = H_0 + V(t)$, with H_0 being the time independent atomic Hamiltonian (possibly including a static magnetic term) and $V(t) = -\vec{D}\cdot\vec{E}(t)$ the interaction potential between the emitter and the electric field of all surrounding charged particles. In order to go beyond the standard approximation of Stark broadening, numerical simulations are suitable. Basically, an ab initio technique consists in a computer simulation of the motion of a large number of charged particles, followed by a numerical solution of the Schrödinger equation for $U(t)$. This procedure is repeated a large number of times in order to perform the statistical average present in Eq. (2). With three decades of development, such computer simulations have now been used many times to benchmark studies on the effect of the emitter–perturbers dynamic on a line shape (Stamm and Voslamber, 1979; Stamm et al., 1986; Calisti et al., 1987; Gigosos and Cardenoso, 1987; Stambulchik et al., 2007). With the help of molecular dynamic techniques several other physical phenomena have been studied, like the correlation effects (Calisti et al., 2008), or the various contributions to asymmetric broadening (Wujec et al., 2002). An example of another study concerns the effect of time ordering in the evaluation of the evolution operator (Rosato et al., 2008b). In Fig. 1 we show the effect on the Lyman α dipole correlation function due to a single collision with an ion. The calculation has been performed with and without the time ordering effect, revealing the large error which would result by omitting this dynamic quantum effect. Retaining time ordering in a collision operator for the electrons, and in a numerical simulation for the ion leads to line shapes which are in a close agreement with experimental observations for this line.

In Fig. 2 we have plotted the central part of Lyman α obtained from a calculation for a density $N_e = 2\times10^{17}$ cm^{-3}, and a temperature of 15,500 K, in an argon plasma containing traces of hydrogen (Geisler et al., 1981; Stamm et al., 1984). It can also be seen in Fig. 2 that a static ion approximation leads to a profile narrower by more than a factor 2, demonstrating on this line the role of ion dynamics even for such high densities.

Other approaches are used today for retaining the dynamic effects on the profiles due to multiple collisions, and give accurate line profiles with much less computer intensive calculations. Among those, the so called model microfield approaches have proved to provide a realistic description of the line shapes by using statistical properties of the microfield, together with a procedure for the field time evolution. The Model Microfield Method, first proposed by Brissaud and Frisch (1971), has been developed and applied to a large range of astrophysical conditions by Stehlé and Hutcheon (1999). Using an efficient procedure for mixing Stark components, the Frequency Fluctuation Model, another fast approach developed in our laboratory (Talin et al., 1995), is available as a line shape code able to compute an arbitrary atomic or ionic line.

3. Effects of the magnetic field

The presence of a static magnetic field is common for many types of plasmas. Laboratory plasma experiments use a magnetic

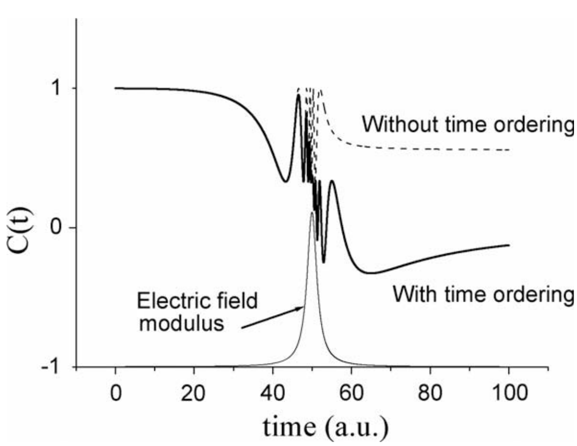

Fig. 1. Lyman alpha dipole correlation function calculated for a single collision with (solid line) and without (dashed line) time ordering effects.