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Stochastic processes for line shapes and intensities

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Abstract

Stochastic processes provide flexible and fast calculations for modeling dynamical interactions between an atom and charged particles. We use a stochastic renewal process for the plasma microfield being the cause of Stark broadening. The accuracy and improvement possibilities of Lyman profiles calculations with a renewal process are analyzed by comparing to ab initio simulations for ion broadening only. Stochastic processes may also be applied to out of equilibrium plasmas. We present our first results for the effect of Langmuir waves on a line broadened by electrons only, and for the changes of atomic populations submitted to strong temperature fluctuations.

Keywords: Stochastic process; Stark broadening; Line shape; Atomic population; Turbulence

1. Introduction

The dynamics of atoms and ions in a plasma is often a complex phenomena which is simply described only in the cases of slow or fast interactions. This is true for transport properties as well as for the radiative properties of the neutral or charged particles. The dynamics of the particle-plasma interactions needs however to be described since it may modify the macroscopic transport or radiative observables of atoms in a plasma. Atomic radiative observables such as the line shape and intensity are essential sources of information on the environment in astrophysics and laboratory plasmas. Though being often two mutually contradictory requirements, the accuracy and a fast evaluation of the observable are essential for a convenient and reliable plasma diagnostic. Both have been sought by analytical or simulation approaches based on a particle picture. Analytical kinetic theories generally fail to solve a many body quantum problem, and numerical simulations still are a numerical challenge, reserving them for benchmarks. An alternative approach is provided by the use of a stochastic process for solving the atomic evolution equation. This has been proposed for Stark broadening using a renewal process with stepwise constant microfields (Brissaud and Frisch, 1971), and more recently for investigating the role of a fluctuating temperature on atomic populations (Catoire et al., 2011). The role of fluctuating temperatures on the transport of neutral particles in the edge plasma of fusion devices has also been recently investigated with a stochastic autoregressive process (Mekkaoui et al., 2012). Since they potentially provide many interesting possibilities for the modeling of atom-plasma dynamics, it seems very timely to assess the accuracy and open the way for their improvements in the context of various plasmas. It is the aim of this work, focused on the use of stochastic processes for calculating Stark line shapes in plasmas with temperatures close to the eV, in a large range of densities found in astrophysics or laboratory plasmas. The paper is organized as follows: after a brief review of different approaches of Stark broadening, we present in Section 3 a description of the

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stochastic renewal process adapted to line shape calculations. Our calculations of Lyman line shapes of hydrogen are presented and discussed in Section 4 for equilibrium conditions. In Section 5, first applications to out of equilibrium conditions concern a study of the effect of Langmuir waves on a line broadened by electrons, and calculations of atomic populations in a plasma with a strongly fluctuating temperature.

2. Stark broadening of spectral lines

Stark effect of line shapes is usually considered if the electronic density is high enough for becoming the dominant broadening mechanism. Detailed Stark line shapes are however also needed for low density plasmas, since they enter in the modeling of radiative transfer together with Doppler broadening. A common starting point is to present the line shape as a Fourier–Laplace transform of the dipole autocorrelation function $C(t)$ (Griem, 1964):

$$I(\omega) = \frac{1}{\pi} Re \int_0^\infty \exp(i\omega t) C(t) dt. \qquad (1)$$

This relation allows a description for this radiative process either in frequency, or in time if we use the atomic dipole autocorrelation function $C(t)$:

$$C(t) = Tr\langle \vec{D} U^+(t) \vec{D} U(t) \rho \rangle. \qquad (2)$$

The trace in this expression is over the atomic states, $\vec{D}$ and U are the atomic dipole and evolution operators, ρ is the density matrix, and the angle brackets imply an average over the charged perturbers. The atom-plasma dynamics is obtained by solving the Schrödinger equation for the evolution operator $U(t)$. This can be done easily for two limiting approximations valid when the time of interest t_i, defined as the correlation time of $C(t)$, and the collision time $\tau_c \sim r_0/v_0$, (r_0 is the mean interparticle distance $r_0 \sim N^{-1/3}$, with N the charged particle density, and v_0 is the perturber thermal velocity) verify two opposite inequalities. For plasma conditions with $t_i \ll \tau_c$, the atom does not feel the dynamics of the perturbation, and the static approximation is valid, allowing to obtain the dipole correlation C_s with an average over a probability density function (PDF) $P(E)$ for an isotropic microfield:

$$C_s(t) = \int_0^\infty dE\, P(E) C(t, E). \qquad (3)$$

The impact approximation is reached if $t_i \gg \tau_c$, and the contribution of the corresponding perturbers to the impact dipole correlation function C_i may be written as a relaxation with an impact collision operator Φ (Griem, 1964):

$$C_i(t) = e^{-\Phi t}. \qquad (4)$$

Calculations using these two approximations will be compared with approaches valid for arbitrary plasma conditions, with no particular relation between t_i and τ_c. In this respect, a useful reference is provided by an ab initio simulation of the microfield coupled to a numerical integration of the Schrödinger equation. An analysis of the Stark profiles of different models has recently been performed at the first workshop on spectral line shape in plasma (Stambulchik, 2013), and the ab initio simulation was found to provide reproducible and reliable results. Such simulations consider a large number of particles moving in a spherical or cubic cell with various boundary conditions. Straight line trajectories for the charged perturbers may be used in weakly coupled plasmas (Stamm and Voslamber, 1979; Stamm et al., 1984; Rosato et al., 2009), but also the trajectories of particles in a Coulomb interaction with molecular dynamics techniques (Stamm et al., 1986; Calisti et al., 2009), if the plasma is correlated.

3. Renewal process

The model microfield method (MMM) for Stark broadening, originally developed by Frisch and Brissaud (1971), is a particular renewal process, a type of stochastic process now being applied to a wide range of problems in physics and other fields (Cox, 1970). To illustrate the use of a renewal process in the case of Stark broadening, we consider an isotropic plasma for which the microfield modulus E is stepwise constant, with field strengths obeying to PDF $P(E)$ for the first step, and $Q(E)$ for the following (Seidel, 1977). The time duration of the first and following microfields also obey to two different PDFs, respectively $v(t|E)$ and $w(t|E)$, which are conditioned by the value of the microfield. The two latter PDFs will be called waiting time distributions (WTD) in the following, since they sample the time spend on each step. To distinguish the first step from the following is necessary if we want to have a stationary process for the microfield. Indeed the time origin for our line shape measurement is arbitrary, and thus does not generally coincide with a microfield jump. A mathematical analysis forcing a stationary process (Seidel, 1977) leads to the following relations between the PDF:

$$Q(E) = \frac{v(0|E) P(E)}{\langle v(0|E) \rangle_E}, \qquad (5)$$

and

$$w(t|E) = -\frac{\dot{v}(t|E)}{v(0|E)}, \qquad (6)$$

where the subscript E denotes a static average over the microfield with the PDF $P(E)$. From these relations, it appears that the statistical properties of the process are fixed by the functions P and v. It is obvious that the PDF $P(E)$ must be the true static microfield distribution (Hooper, 1968) used also in kinetic theory approaches. The WTD v obtained from the microfield correlation function $\Gamma_{\mathrm{RP}}(t)$ of the renewal process:

$$\Gamma_{\mathrm{RP}}(t) = \int_0^\infty dE\, E^2 P(E) \int_t^\infty ds\, v(s|E). \qquad (7)$$