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STOCHASTIC PROCESSES APPLIED TO LINE SHAPES

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Abstract. We present approaches using stochastic processes for the calculation of line broadening in plasmas. The derivation of model microfield methods (MMM) based on analytic formulations is recalled, as well as an approach using a simulation of the stochastic process. We discuss the possibility of an improvement of the stochastic process by comparing our first results to *ab initio* particle simulations coupled to a numerical integration of the emitters Schrödinger equation.

Key words: line shapes – Stark effect – stochastic processes

1. INTRODUCTION

Accurate line shapes are required for the diagnostic of various laboratory and astrophysical plasmas. For example, the determination of the stellar parameters is often based on hydrogen line profiles, which are also commonly used for the density diagnostic of laboratory plasmas. Detailed line shapes are also needed for an accurate calculation of the plasma opacity, a radiative property essential for the modeling of plasmas. Stark broadening calculations may be performed with a particle or a microfield point of view. A particle point of view is adopted in the impact theory (Griem 1964) and the unified theory (Smith et al. 1969; Voslamber 1969), both often used for a description of electron broadening. A standard approach of Stark broadening adopts a microfield point of view for the ionic perturbers. Neglecting ion motion then requires the knowledge of the one and only probability density function (PDF) of the static microfield P(E). For many couples of plasma condition and line transition, ion dynamics has to be retained, motivating the development of different methods: kinetic theory (Dufty 1970), Monte Carlo type simulations (Stamm et al. 1984) and stochastic processes (Brissaud & Frisch 1971; Seidel 1977; Stehlé & Hutcheon 1999). Using a procedure for mixing Stark components, the Frequency Fluctuation Model is another efficient approach developed in our laboratory (Talin et al. 1995; Calisti et al. 2010) using a stochas-

tic process. Stochastic processes represent a departure from the approaches using particles in many body problems. They present several characteristics making them interesting as alternative approaches to analytical approaches or particle simulations. Among their advantages is their flexibility allowing applications to numerous problems, the possibility for the choice of a relatively simple stochastic process, and the potential efficiency of their numerical evaluation on parallel computers.

We will discuss these approaches in the conditions of density and temperature found both in laboratory and astrophysical plasmas in which the ion perturbers can never be treated with a static approximation. We present the basic Stark broadening formalism in Section 2, where we also recall the possibility of *ab initio* simulation calculations of the line shape. Available approaches using stochastic processes in line broadening are described in Section 3, where we also present our recent contribution combining a simulation and a stochastic process. Our first calculations are presented and discussed in Section 4, followed by a conclusion and perspectives.

2. STARK LINE PROFILE

We briefly recall here the basic equations used to calculate a line profile broadened by the Stark effect. The line profile is usually presented as a Fourier-Laplace transform of the dipole autocorrelation function $C(t)$:

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

The dipole autocorrelation function may be written as a function of the emitter time evolution operator:

$$C(t) = Tr < \overrightarrow{D}.U^+(t)\overrightarrow{D}U(t)\rho > . \tag{2}$$

In this expression, the trace is over the atomic states, $\overrightarrow{D}$ is the dipole operator, ρ is the atomic density matrix, and the angle brackets denote an average over all charged perturbers. Obtaining an accurate Stark profile requires solving the Schrödinger equation for the emitter evolution operator $U(t)$:

$$i\hbar \frac{dU(t)}{dt} = [H_0 + V(t)]U(t), \tag{3}$$

where H_0 is the atomic unperturbed Hamiltonian and $V(t) = -\overrightarrow{D}\overrightarrow{E}(t)$ is the dipolar interaction potential between the emitter and the electric field created by the charged particles of the plasma. The solution for $U(t)$ has to be averaged over the effect of the ionic and electronic perturbers. For many plasma conditions the electronic collision time (defined for the electrons as their average interparticle distance r_0 over their thermal velocity v_e) is much smaller than the time of interest (defined as the inverse of the line width) of the considered transition. A binary electron impact operator appearing as a constant ϕ_e added to H_0 in the Schrödinger equation may then be used. This model first proposed by Griem et al. (1959) is known to be accurate for electron broadening. Ions may be treated by such an impact approximation only for very weak densities ($\leq 10^{12}$ cm^{-3} for

the first Lyman lines). For other conditions, the average over the ionic component involves simultaneous strong collisions. A useful reference for such a situation is provided by plasma simulations coupled to a numerical integration of the Schrödinger equation (Stamm & Voslamber 1979; Stamm et al. 1986). In its simplest version, this simulation uses ions moving along straight lines within a box with periodic boundary conditions. This *ab initio* technique uses variable time steps following as closely as possible the variations of the simulated microfield. After 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 (Calisti et al. 1987; Gigosos & Cardenoso 1987; Rosato et al. 2009; Stambulchik & Maron 2010). The drawback of such simulations is that they require large computer resources for complex atomic systems. For diagnostic requirements as encountered in astrophysics, there is thus a strong motivation to develop fast models for line shape such as those based on stochastic processes. In the next section we recall how stochastic processes have been used in Stark broadening, and propose an approach combining a simulation technique with a stochastic process.

3. STOCHASTIC PROCESSES IN LINE BROADENING

The use of a stochastic process for the emitter's perturbation was already proposed in the early work of Lorentz in 1906, in which collisions were supposed to be distributed according to the 'laws of chance' (Lorentz 1906) using a Poisson distribution $\frac{1}{\tau}\exp(-\frac{t}{\tau})$, where τ is the mean length of time during which the emitter is unperturbed. The effect of collisions distributed according to this law was then shown to lead to what we call a 'Lorentzian' line shape with a halfwidth τ^{-1}. Other early but important contributions of stochastic processes to line shape problems were proposed by Anderson and Kubo in 1954. In the work of Anderson, the line shapes of magnetic resonance spectroscopy were analyzed by assuming Markovian or Gaussian statistics for the random time property of the line frequency modulation. Using similar assumptions, Kubo obtained general properties of a spectrum perturbed by a stochastic process, and derived simple expressions of the line shape for the cases of slow and rapid transitions between the possible states of the emitters. Exactly four decades ago, in 1971, Frisch and Brissaud proposed to model Stark broadening with a stochastic electric field acting on the emitter. The model microfield method (MMM) assumes that the electric field is a stochastic process with stepwise constant values (see Figure 1). This turns Equation 3 into a linear stochastic equation which can be solved efficiently if we use the properties of renewal processes. Many results obtained in the frame of renewal processes (Cox 1962) or continuous time random walks (Montroll & Weiss 1965) can be used to construct models well suited for Stark broadening. Our process may be characterized in the following way (Seidel 1977; Frerichs 1989):

$$\overrightarrow{E}(t) = \begin{pmatrix} \overrightarrow{E}_1 & 0 \le t < t_1 \\ \overrightarrow{E}_2 & t_1 \le t < t_2 \\ \vdots & \\ \overrightarrow{E}_n & t_{n-1} \le t < t_n \\ \vdots & \end{pmatrix}, \tag{4}$$

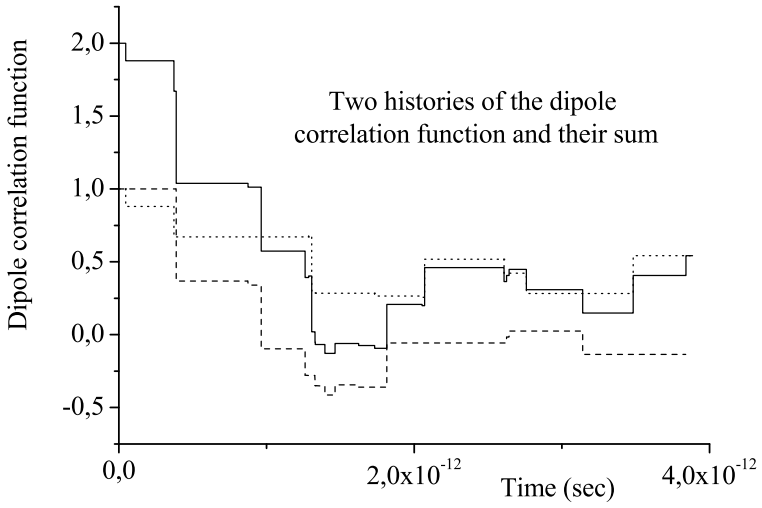

Fig. 1. Modulus of the electric field created by a stepwise constant stochastic process

where $\overrightarrow{E}_1$ is distributed according to the probability density function of the static microfield $P(\overrightarrow{E})$. This function is known from plasma kinetic theory, and we can use Hooper's (1968) microfield distribution here. The waiting time on the first step t_1 is distributed according to the PDF $v(t_1|\overrightarrow{E_1})$. It is interesting to note that the first step is a singular step in the chain of jumps. This is because our initial time does not in general coincide with a jump of the field. If we require our process to be stationary (Seidel 1974), we find that for all the steps but the first one, the microfields follow a static $Q(\overrightarrow{E})$ PDF, and have a duration distributed with a waiting time distribution $w(t_n|\overrightarrow{E_n})$. Requiring a stationary process leads to the following expressions for these PDFs:

$$Q(\overrightarrow{E}) = \frac{v(0|\overrightarrow{E})P(\overrightarrow{E})}{\langle v(0|\overrightarrow{E})\rangle_S} \tag{5}$$

and

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

where the symbol $\langle \ldots \rangle_S$ denotes a static average over the microfield with the PDF $P(\overrightarrow{E})$. Different stochastic processes may satisfy these two equations. Since the two functions P and v determine the statistical properties of the process, we need to write a relation between these two functions and the known statistical properties of the plasma. Assuming an isotropic plasma, we will use the static microfield distribution for the field modulus $P(E)$, and write the microfield autocorrelation function $\Gamma(t)$ for the renewal process as a function of $P(E)$ and $v(t|E)$:

$$\Gamma(t) =< \overrightarrow{E}(0).\overrightarrow{E}(t) >= \int_0^\infty dE E^2 P(E) \int_t^\infty dt' v(t'|E). \tag{7}$$

For several types of processes already studied, e.g. Seidel (1980), identifying Γ with the microfield autocorrelation function obtained from plasma kinetic theory (Rosenbluth & Rostoker 1962) determines $v(t|E)$. In the original work of Brissaud & Frisch (1971), the Kangaroo process (KP) has been proposed with an exponential time dependence for $v(t|E)$. The KP is a Markovian renewal process which loses all memory of its previous state at every time. This requires the equality of the v and w PDFs:

$$v(t|E) = w(t|E) = v(E)exp(-v(E)t). \tag{8}$$

In this expression $v(E)$ appears as a field dependent jumping frequency for the microfield process. The original MMM analytical solution using the KP process is then usually written in terms of $\tilde{U}(\omega)$, the Fourier-Laplace transform of $U(t)$:

$$\begin{aligned} &< \tilde{U}(\omega) >_{KP} = < \tilde{U}(\omega + iv(\overrightarrow{E})) >_S + < v(\overrightarrow{E})\tilde{U}(\omega + iv(\overrightarrow{E})) >_S \\ &(< v(\overrightarrow{E})[1 - v(\overrightarrow{E})\tilde{U}(\omega + iv(\overrightarrow{E}))] >_S)^{-1} < v(\overrightarrow{E})\tilde{U}(\omega + iv(\overrightarrow{E})) >_S . \end{aligned} \tag{9}$$

This expression includes averages over the static microfield (noted with the subscript S) and is specific for the KP process.
In the following we now propose a different evaluation of the line shape which can potentially be extended to other processes. It consists in a simulation of the stochastic process (Frerichs 1989), with a microfield sampled according to the PDF $P(E)$ and $Q(E)$, and a waiting time PDF $v(t \mid E)$ as in Equation 8. On each step of our process the electric field is constant in modulus and direction, and the evolution operator is thus a matrix whose elements remain constant until the next jump. For one microfield history, it is thus easy to obtain the value of the evolution operator at any jump time t_n, using a well-known property of evolution operators:

$$U(t_n, 0) = U(t_n, t_{n-1})U(t_{n-1}, t_{n-2}) \dots U(t_1, 0). \tag{10}$$

For each microfield history, the evolution operator appears as a stepwise constant quantity with the same time-grid as the microfield. This leads to a coarse description of the evolution for a single history, with an average time resolution equal to the inverse of the mean jumping frequency. Applying our approach to the Lyman α line, we show on Figure 2 how the dipole autocorrelation function for two different microfield histories may be added. It is clear from Figure 2 that summing the two histories of $C(t)$ increases the number of jumping times.

A usable evaluation of $C(t)$ is obtained by summing about 5000 histories, and leads to a smooth function convenient for a Fourier-Laplace transform giving the line shape (see Figure 3).

The advantage of this approach is a fast numerical evaluation, but also its flexibility with the possibility of changing the stochastic process. If the stationary conditions are satisfied, various stochastic processes using different PDFs for the field and the waiting time distributions may be used. We plan for instance to use this method for situations with out-of-equilibrium plasma conditions, such as those found in turbulent plasmas.

4. CALCULATIONS AND RESULTS

We will apply our first calculations to the Lyman α line of hydrogen. This line is very sensitive to the microfield dynamics, and allows fast calculations since the

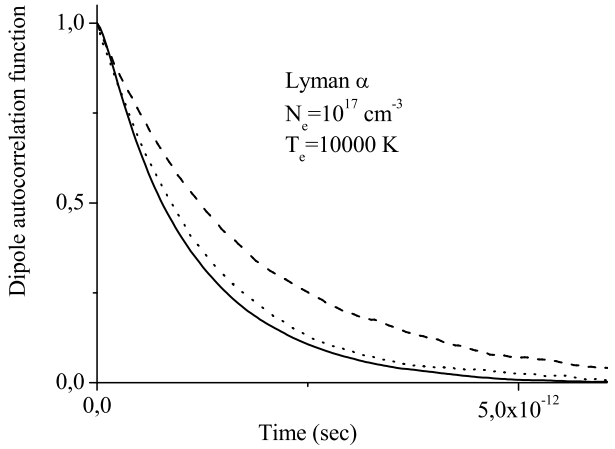

Fig. 2. Two histories (dashed and dotted lines) of the dipole autocorrelation function and their sum (solid line)

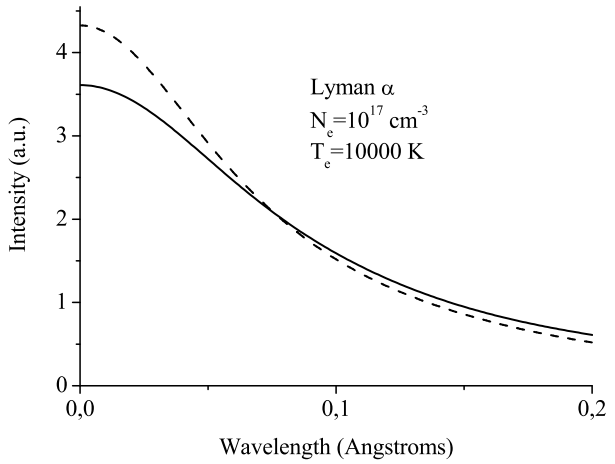

Fig. 3. Dipole autocorrelation function for ions only: comparison of an *ab initio* simulation (solid line) with our MMM calculation using the original jumping frequency $v(t|E)$ (dashed line), and this frequency times a factor 2.2 (dotted line).

lower state is not affected by the dominant linear Stark broadening. Neglecting fine structure, we use the spherical basis $\mid n, l, m >$ in subspace with principal quantum number $n = 2$. The interaction potential is thus represented by a 4x4 matrix, and so is also the evolution operator. Our following calculations have been performed for the hydrogen Lyman α line in order to compare different methods for a simple case. We present in Figure 3 the comparison of the dipole autocorrelation function for ions only, obtained with our MMM calculation and an *ab initio* numerical simulation as described in section 2, for a density $N_e = 10^{17}$ cm^{-3} and a temperature $T_e = 10000$ K. There is a significant additional decorrelation in the *ab initio* simulation (solid line), compared to our MMM calculation using the orig-

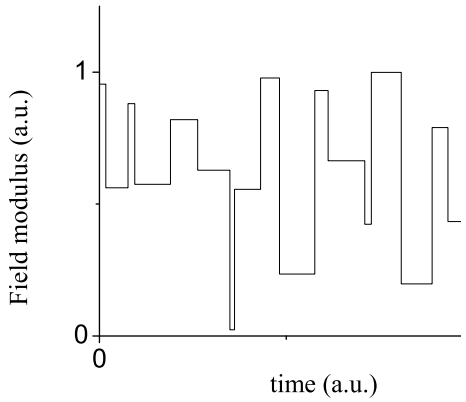

Fig. 4. Comparison of our MMM calculation (dashed line) with an *ab initio* simulation (solid line)

inal jumping frequency $v(t|\overrightarrow{E})$ (dashed line). We have also plotted a calculation which is an attempt to fit the MMM calculation to the simulation, with the mere multiplication of the jumping frequency by a constant factor. For the conditions of Figure 3, the best fit (dotted line) is obtained by multiplying $v(t|\overrightarrow{E})$ by a factor 2.2. The precise shape of the *ab initio* simulation curve can however never been reproduced by such a procedure. A modification of the stochastic process might be an alternative way for improving the agreement with the simulation. The KP process uses an exponential form for the waiting time distribution, which is just the Markovian limit of renewal processes. There are many other possible models, and we are currently investigating processes including memory effects (Capes et al. 2010). One should note however that the line profiles provided by the standard MMM (Stehlé & Hutcheon 1999) generally agree to within 20 percent with ab initio simulations. As an example, we compare in Figure 4 our MMM calculation with a simulation of the Lyman α line shape including ion and electronic broadening. It can be seen in the Figure 4 that the simulation profile is about 15 percent broader than the MMM calculation.

5. CONCLUSIONS AND PERSPECTIVES

We have reviewed the use of stochastic processes for the calculation of Stark profiles. The original model microfield method belongs to a class of renewal processes which can be calculated either by an analytic formula, or by a simulation of the stochastic process as proposed in this work. Perspectives include the possibility to further improve the stochastic process, in particular by including memory effects. This might be useful for an application of such an approach to the case of broadening by neutrals, and to non equilibrium conditions in turbulent plasmas.

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