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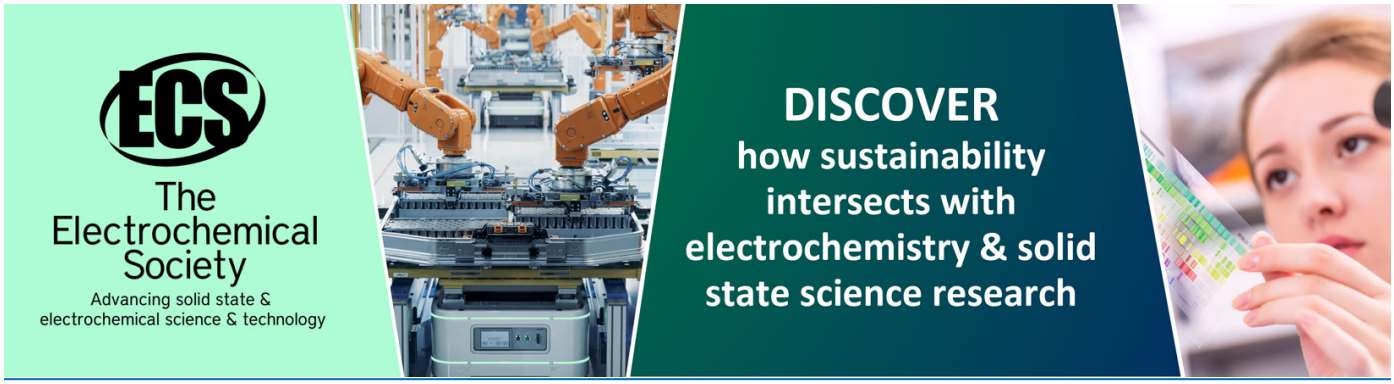

Journal of Physics: Conference Series **397** (2012) 012006 doi:10.1088/1742-6596/397/1/012006

A Stark broadening simulation using a renewal process for the electric microfield

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Abstract. Stark broadening of atomic lines in plasmas is investigated by generating the electric microfield with a renewal process. In this model, the microfield is stepwise constant, with jumping times sampled from a waiting time distribution (WTD). Our model is a true simulation of the renewal process, using random number generators for generating different probability density functions (PDF). The use of an equilibrium static microfield PDF and an exponential waiting time distribution reproduces the so called model microfield method (MMM) results. The work presented is an application to the hydrogen Lyman-α line, for which we compare our renewal process model and ab initio simulations calculations, with the aim of studying the role of non exponential waiting time distributions.

1.Introduction

Different approaches are used today for computing line profiles broadened by Stark effect. Particle based approaches have been used in early developments [1,2,3], and have recently been revisited for an inclusion of multiple simultaneous emitter-perturbers interactions [4]. Computer simulations are commonly used today with a combination of particle simulations and a numerical integration of the Schrödinger equation [5,6]. Such ab initio simulations provide useful references for developing other less computer intensive models. Using an efficient procedure for mixing Stark components, the Frequency Fluctuation Model is an example of such an approach, available as a line shape code able to compute an arbitrary atomic or ionic line [7]. This approach may be viewed as an example of a model microfield method, since it uses statistical properties of the microfield, together with a procedure for its time evolution. Model Microfield Methods (MMM) have first been proposed for Stark broadening by Brissaud and Frisch in 1971 [8], using a stochastic process. In the last decades, the MMM has been developed and applied to a large range of astrophysical conditions [9]. We report here about an alternative approach which consists of a numerical simulation for the stochastic process for the plasma microfield following a proposal made by Frerichs [10]. In section 2, we recall that the calculation is performed in the framework of the renewal process model, using stepwise constant values of the microfield. The simulation technique is described in section 3, and our first results are presented and discussed in section 4.

2.Renewal process for the electric microfield

We consider a microfield which is stepwise constant, and jumps to a new value after a waiting time following a microfield dependent Waiting Time Distribution (WTD) v(t|E) for the first step. Also for the first step, the microfield modulus E is distributed according to a Probability Density Function (PDF) P(E). We assume that the plasma is isotropic, with each new value of the microfield vector characterized by its modulus and a random direction. In the following, the average over all directions of the field will be performed analytically on the evolution operator of the atom. For a stationary renewal process, the microfield PDF for all but the first step is changed to Q(E), and the WTD is changed to w(t|E). The relations between the first step and next steps PDF and WTD is obtained by writing the stationarity conditions, i.e. imposing that a measure starting at time t=0, is identical to a measure at an arbitrary time. The following relations then hold [11]:

$$Q(E) = \frac{\nu_E P(E)}{\langle \nu_E \rangle_S}, \tag{1}$$

and

$$\mathrm{w}(t|E) = -\frac{\dot{\mathrm{v}}(t|E)}{\nu_E}. \tag{2}$$

Symbol $<..>_S$ denotes a static average taken over P(E), and ν_E is a jumping frequency equal to the inverse of the time on a step averaged over the initial WTD. It should be noted that the relations (1) and (2) are different from the corresponding relations in reference [11], since they are not expressed with the WTD at time t=0, but with the microfield dependent jumping frequency. This more general formulation is found in the work of Haus and Kerr on stochastic processes [12]. From these relations, it is clear that the statistical properties of a stationary renewal process are determined by the microfield PDF P(E) and WTD v(t|E). In the case of a Markovian process, one recovers the Kangaroo process, with a WTD:

$$\mathrm{v}(t|E) = \mathrm{w}(t|E) = \mathrm{v}(E)\exp(-\mathrm{v}(E)t). \tag{3}$$

The choice of an exponential WTD has been made for most applications of the so called model microfield method, since it allows one to write a rather simple solution for the line shape. This choice implies that the stochastic process has a jumping rate which is constant over time, and it may be interesting to investigate if this has any impact on the line shape. Renewal processes are commonly used in survival analysis (for instance in the study of lifetime of manufactured products), and the first choice for the WTD is an exponential function. For processes which are supposed to be affected by a time dependent jumping rate, an alternative WTD is often given by a Weibull function:

$$\mathrm{u}(t|E) = \nu_E \alpha \{\nu_E t\}^{\alpha-1} \exp\left[-\{\nu_E t\}^{\alpha}\right], \tag{4}$$

where the shape parameter α is a real positive number, and ν_E is a microfield dependent jumping frequency equal to the inverse of the average time on a step $<t>$ obtained with the Weibull WTD. It is now necessary to calculate the new Q(E) and w(t|E) with this WTD. One should note here by considering equation (2), that since u(t|E) and w(t|E) are non-negative probability densities, u(t|E) must be a monotonically decreasing function [11]. This restricts the use of a Weibull distribution to values of $\alpha<1$, cases for which the jumping rate decreases over time. Using equations (1) and (2), it is possible to express Q(E) and w(t|E), but we first need to write the average time on a step as:

$$\langle t \rangle = \int_0^\infty t u(t|E) dt = \frac{\Gamma(1+\frac{1}{\alpha})}{\nu_E}, \quad (5)$$

where Γ is the gamma function. Using equation 4, the WTD w(t|E) for all but the first step may be written as:

$$w(t|E) = \nu_E \alpha \{\nu_E t\}^{\alpha-2} \left[1 - \alpha + \alpha \{\nu_E t\}^{\alpha}\right] \exp - \{\nu_E t\}^{\alpha} \quad (6)$$

The survival probability of a microfield during a time interval t is obtained by the time integral of the WTD from t to infinity. Using this probability, it is then possible to write the microfield autocorrelation function for the renewal process Γ_{RP} as:

$$\Gamma_{RP}(t) = \int_0^\infty dE P(E) E^2 \exp - \{\nu_E t\}^{\alpha}. \quad (7)$$

This autocorrelation function for the renewal process should be chosen so as to reproduce the true function obtained from plasma kinetic theory. In the following , we will use the theoretical expression known from the work of Rosenbluth and Rostoker [13]:

$$C_p(\tau) = \langle \vec{\beta}(\tau).\vec{\beta}(0) \rangle = \frac{3}{\sqrt{\pi}} \left[\frac{r_0}{\lambda_D}\right] \frac{1}{\tau} \left[1 + \tau^2 - \sqrt{\pi}\,\tau \left(\tau^2 + \frac{3}{2}\right) \exp(\tau^2) erfc(\tau)\right], \quad (8)$$

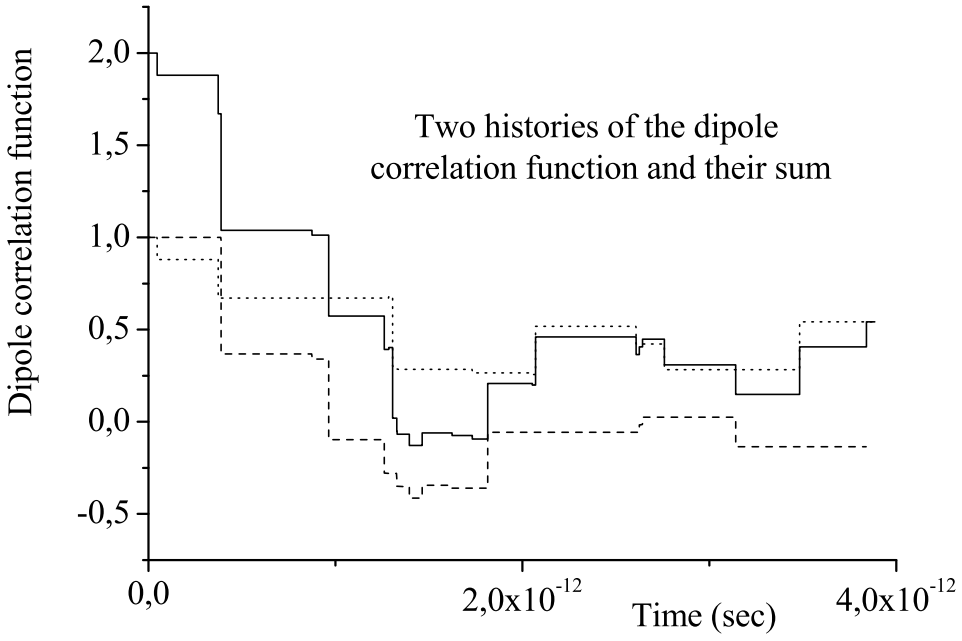

Figure 1. Sum of two histories for the dipole correlation

where $\tau=t\omega_p/2^{1/2}$ and $\omega_p=(4\pi Ne^2/m)^{1/2}$ is the plasma frequency for particles of mass m, density N and temperature T. We denoted the average distance between charged particles by r_0, and the Debye length by $\lambda_D=(kT/4\pi Ne^2)^{1/2}$. The dimensionless microfield $\beta=E/E_0$ is reduced in units of the Holtsmark field that we define as $E_0=e/r_0^2$. Equalizing equation (7) and (8) allows one to obtain the frequency ν_E as a function of the microfield.

3. Line shape calculation with a stochastic process

The line profile is obtained with a Fourier-Laplace transform of the dipole autocorrelation function $C_{dd}(t)$:

$$C_{dd}(t) = Tr\left\langle \vec{d}U^{+}(t).\vec{d}U(t)\rho \right\rangle . \tag{9}$$

In this expression, the trace is over atomic states, $\vec{d}$ is the atomic dipole operator, ρ the density matrix, and the brackets denote an average over the charged particles. The atomic evolution operator obeys to a Schrödinger equation:

$$i\hbar \frac{dU(t)}{dt} = [H_0 + V(t)]U(t), \tag{10}$$

where H_0 is the atomic Hamiltonian and $V(t) = -\vec{d}.\vec{E}(t)$ the dipolar interaction potential of the atom with the plasma microfield. As described in section 2, the microfield is assumed to follow a stepwise constant stochastic process with prescribed PDF and WTD, and we use the computer to generate microfield histories with pseudorandom numbers algorithms, associated to transformation or rejection methods. At each step, the microfield is constant, and so is the evolution operator. The evolution operator for n steps may be written as a product of constant operators in time intervals t_i-t_{i-1}:

$$U(t_n,0)=U(t_n, t_{n-1})\, U(t_{n-1}, t_{n-2}).\ldots\ldots U(t_1,0). \tag{11}$$

The evolution operator is thus obtained by an iteration from one step to the following:

$$U(t_{j+1},t_j) = \exp\left(\frac{i}{\hbar}\vec{d}.\vec{E}_j\Delta t\right)U(t_j), \tag{12}$$

where $\vec{E}_j$ is the constant microfield applied on the atom during $\Delta t = t_{j+1} - t_j$. With this approach the solution of the Schrödinger equation is obtained by multiplying matrices representing $U(t_j - t_{j-1})$, a procedure which is much more efficient on the computer than those used for ab initio simulation. Summing finally over a large number of such time histories of the microfield, it is possible to obtain a smooth averaged evolution operator, since every history has a different time grid. This calculation may be applied to both the ionic and electronic components, using for instance the joint jump approximation [10]. Our first calculations using this simulation of the stochastic process have been applied to the ionic component only. The effect of electron broadening may be retained in our calculation with an impact electronic operator.

4. Results

Calculations performed for this work have been applied to the Lyman α line of hydrogen, neglecting the fine structure. We first reproduce the calculations of the MMM, with a PDF P(E) calculated by Hooper [14], and an exponential WTD. An example of the sum of two histories is shown on figure 1. Repeating this summation procedure over several thousands microfield histories, it is possible to obtain a smooth dipole correlation function. We have first studied the angular average over the microfield angles. It is possible to generate for each field, two microfield angles, and retain the angular dependence for each $U(t_i - t_{i-1})$. After an average over a large number of field histories, we have checked that such a calculation leads

to the same averaged evolution operator as a calculation performed using an analytical angular average on each $U(t_j - t_{j-1})$. Calculating then the dipole correlation function for a density N=10^{17} cm^{-3}, and a temperature of 10^4 K, and performing a Laplace-Fourier transform, our calculation reproduces the profiles of the MMM for the Lyman α line in the case of ion broadening and impact electrons [15]. We have plotted on figure 2 the dipole autocorrelation function for Lyman α broadened by ions only and calculated with our technique (dashed line), and have compared it to an ab initio simulation (solid line). It can be seen that a standard MMM calculation applied to ions alone is significantly different from the ab initio simulation. This is a strong indication that the stochastic process may be improved for the ionic component. There is however no clear indication of how this should be done, and our proposal is to change the WTD as explained in section 2. The work underway consists in using the four functions P(E), Q(E), u(t|E) and w(t|E) in the case of a Weibull WTD, in an attempt to improve the agreement between our present technique and the ab initio simulation.

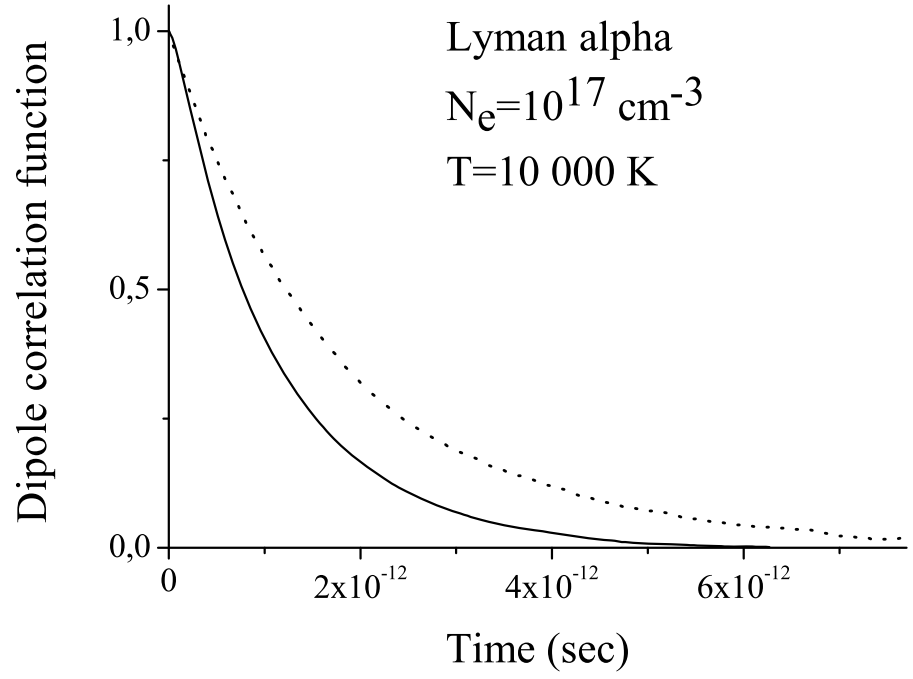

Figure 2. Lyman α dipole correlation function calculated with our simulation of the stochastic model (dotted line), and an ab initio simulation (solid line)

5.Conclusion

We have developed a simulation calculation with a renewal process for the plasma microfield, coupled to an efficient algorithm for calculating the dipole autocorrelation function of the emitter. Revisiting the basic assumptions for the stochastic process applied to Stark broadening, we have proposed the use of a Weibull WTD for the test of a time dependent jumping process. We have derived expressions for the four probability density functions required for the line shape calculation, as well as a procedure for obtaining the microfield dependence of the jumping frequency. The first calculations have shown the applicability of our model for reproducing the standard MMM calculations for the Lyman α line. Applied to

ion broadening only, and compared to ab initio simulations, our calculations are a clear indication that the stochastic process could be improved. Work is in progress for using the Weibull or other non exponential WTD

Acknowledgments
This work was carried out within the framework of the European Fusion Development Agreement and the French Research Federation for Fusion Studies. It is supported by the European Communities under the contract of Association between Euratom and CEA. The views and opinions expressed herein do not necessarily reflect those of the European Commission. We also acknowledge the support of the French National Research Agency (contract ANR-11- BS09-023, SEDIBA).

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