Application of the Model Microfield Method to the Stark broadening of ions

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(Received 10 January 1994; accepted 19 January 1994)

We have proposed an extension of the Model Microfield Method to the case of ionic radiators. Special attention is given to the accurate treatment of plasma mixtures in terms of static and dynamic statistical properties of the plasma microfield. Line shapes of one electron Carbon and Argon illustrate the influence of ion dynamic effects.

1. Introduction

Since the development of performant detectors we note a renewal of interest for the Stark broadened line shapes in laser-produced plasmas (Laser and Particle Beams, this issue). Hence, they can be used as an additive diagnostic for the electronic density. The broadening of the line is a consequence of the interactions between the radiator and the plasma constituents (Griem 1974; Lee 1992). The electronic contribution is commonly described in terms of collisions. Due to their mass, the ion contribution is often included in terms of the static microfield (Calisti et al. 1990). This approach is justified if the ions do not move significantly during the radiative process or, equivalently, when the ionic plasma frequency is smaller than the half-width of the line. Several theories have been proposed up to now to treat this problem. In molecular dynamics simulations (Stamm et al. 1986) the positions of the ions are obtained by solving numerically the equations of motion. The kinetic theory (Boercker et al. 1987) uses a modelization of the time statistics of the microfield fluctuations, in connection with the positions of the radiating ions. The relaxation theory (Oza et al. 1988) is a semi-analytical method in which the ion dynamic effects are included owing to time-dependent functions. These are obtained, in practice, by a numerical Monte Carlo simulation. An alternative method is a modelization of the ionic motion effects in the line shape expression by line component mixing. All of these approaches need in fact numerical simulations, either by molecular dynamics or by Monte Carlo simulations. This leads to practical difficulties for low correlated plasmas and also for high-Z radiating impurities.

In this article we propose an alternative treatment that takes into account the ion dynamic effects and does not present such limitations. The method is in fact the extension of the Model Microfield Method (Frisch & Brissaud 1971) already successfully applied to the broadening of hydrogen (Stehlé 1991 and references therein). Although the principles of the method are independent of the nature of the radiator, its practical application to the case of ionic radiators presents some difficulties. This point will be discussed in Section 2.2.

The method will be presented briefly in the following paragraphs. A detailed description of the theory will be presented in a subsequent paper (Stehlé 1994).
2. Theory

The emerging profile results from the Stark and Doppler effects, which are correlated in the case of ionic radiators. Nevertheless, a previous work (Stamm et al. 1986) indicates that this correlation effect is negligible. We shall also neglect it in the following and include the Doppler effect by the usual convolution procedure.

We now focus our interest on the expression of the pure Stark profile.

2.1. Line shape expression

The expression of the line intensity is given by

$$I(\omega) = \sum_{i, i', f, f'} \rho_{ii'}^{(0)} d_{f} \Theta_{i f', i' f'}(\omega) d_{i' f'}^*,$$

(1)

where \(d\) is the electronic dipole of the isolated radiator, \(\rho_{ii'}^{(0)}\) is the population of ions in state \(i\), and \(\Theta(\omega)\) denotes the Fourier transform at \(\omega\) of the radiator evolution operator \(\Theta(t, 0)\) in the Liouville space. It is simply connected to the usual time evolution operator by

$$\Theta_{i f', i' f'}(t) = T_{ii'}(t, 0) T_{f f'}^*(t, 0).$$

(2)

The effects of the interactions between the radiator and the surrounding plasma arise in the line intensity throughout this operator \(\Theta\).

We assume that the interactions between the radiator and the free electrons and between the radiator and the ions can be described independently from each other. The electronic contribution can be included in terms of a collisional damping operator \(\gamma\), which is directly connected to the usual scattering matrices. Although a quantum theory is in principle more accurate, we retain the simpler semiclassical approach, which is appropriate here due to the large temperatures involved in ICF plasmas. In this method the electronic motions are described classically (hyperbolas), whereas the interaction between the colliding electron and the ionic target is calculated within the quantum theory (Sahal-Bréchot 1969; Stehlé 1985). Using this treatment of the interactions between the radiator and the free electrons, the expression of \(\Theta(t, 0)\) is given by

$$ih \frac{d}{dt} \Theta(t, 0) = [L_0 - dE(t) - ih\gamma] \Theta(t, 0),$$

(3)

where \(E(t)\) is the ionic microfield-created by the free ions upon the radiator.

2.2. Model

This microfield constitutes a time-dependent random process. We assume that the statistical properties relevant for the line shapes are correctly described by the model microfield model. This model was developed for the case of neutral radiators (Brissaud & Frisch 1971; Frisch & Brissaud 1971) and gives good results for hydrogen. Here we extend the method to the case of ionic radiators (Stehlé 1990). The microfield is supposed to be a stepwise constant stochastic process. The jumping times \(t_i\) (figure 1) are distributed uniformly and independently in time with the density \(\rho\) (Poisson distribution), \(E\) being the field value before the jump. \(\Theta(\omega)\) then is simply given by

$$\Theta(\omega) = \langle \Theta(z) \rangle + \langle \rho \Theta(z) \rangle \langle \nu I - \nu^2 \Theta(z) \rangle^{-1} \langle \nu \Theta(z) \rangle.$$
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Figure 1. Typical time variations of the ionic microfield $E(t)$ in the MMM theory.

$$\langle \nu(E) \Theta(z,E) \rangle = \int_0^{\infty} \nu((E)) \Theta(z,E) P(E) dE. \quad (5)$$

In the high-density limit, $\nu(E)$ is small compared to $\gamma$, and the static limit is reached for the ionic contribution to the profile.

The field distribution function $P(E)$ is a key point in the computation of the profile. It depends on the composition of the plasma, in other words on the temperature $T$, the electronic density $N_e$, and also on the relative concentrations of the different ionic species. Although we assume a unique temperature, the method may be extended easily to different ionic and electronic temperatures.

In the following we shall consider only the cases of pure or binary mixtures, where the radiating ions (mass $m_r$, charge $Z_r$, concentration $c_r$) are denoted by $(r)$ and the other ions $(m_p, Z_p, c_p)$ by $(p)$. We introduce two correlation parameters:

$$\Gamma_{rp} = \frac{e^2 Z_r Z_p}{kT(r_p)} \quad \text{and} \quad \Gamma_{rr} = \frac{e^2 Z_r^2}{kT(r_r)}, \quad (6)$$

where $\langle r_i \rangle$ is the mean distance between ions $(i)$. We also introduce the screening parameter $a$ by,

$$a = \frac{\langle r_e \rangle}{\lambda_D}, \quad (7)$$

where $\langle r_e \rangle$ is the mean interelectronic distance and $\lambda_D$ the usual Debye length.

Depending on the magnitude of these parameters compared to unity, we shall use the Baranger–Mozer cluster expansion (Baranger & Mozer 1959, 1960; Demura 1988) or the Monte Carlo (MC) simulations to estimate $P(E)$ (Angelié & Gilles 1986; Gilles 1990a,b). The Baranger–Mozer (BM) approach is justified for weakly correlated plasmas ($\Gamma_{ij} < 1$, $a < 1$) where Monte Carlo simulations can be difficult to perform.

2.3. Determination of the jumping frequency

Contrary to the field distribution function $P(E)$, the frequency jump $\nu(E)$ is a free parameter that must be chosen properly. As we want to recover the impact limit that is reached for both the ions and the electrons at low densities, we decided to adjust $\nu(E)$ to fit the time variations of the field autocorrelation function:

$$C_{EE}(t) = \langle E(0) E(t) \rangle_{\text{Average}}. \quad (8)$$
Hence, it is possible to prove that the impact half-width value is nearly proportional to the
time integral of this quantity defined by

\[ C = \int_0^\infty C_{EE}(t) \, dt. \]  

Since we neglect the correlations between the field and the radiator velocity variations, we
can use the \( \mu \)-ion model to calculate \( C_{EE}(t) \).

In this \( \mu \)-ion model, the radiating ion is fixed. Each perturbing ion, with the mass \( \mu \rho = m_r m_p/(m_r + m_p) \), moves independently from the others along a trajectory corresponding
to the Debye–Hückel repulsive potential of interaction between it and the radiator. This
model is justified at low densities where the relevant times for the broadening are less than
the typical time for collective ionic motions, in other words, \( \omega_p(\text{ions})^{-1} \). It is also used in
Monte Carlo simulations (Stamm et al. 1986; Oza et al. 1988). Comparisons between molec-
ular dynamics and Monte Carlo simulations indicate that the \( \mu \)-ion approach still is valid
at higher densities, despite the increasing many-body effects for the long time variations
of \( C_{EE}(t) \). One explanation is that the ion dynamic effects are less important and also that
the relevant times for line broadening are shorter.

In this \( \mu \)-ion picture, \( C \) is always positive (note that \( C \) is equal to zero) when velocities
and fields are correlated (Pollock & Weisheit 1985). Contrary to the case of neutral radia-
tors, the expression of \( C_{EE}(t) \) in the \( \mu \)-ion picture is not analytical. Thus, we performed
in a first step the numerical evaluation of \( C \). The corresponding MMM expression is given by

\[ C = \int_0^\infty \frac{E^2(E)}{\nu(E)} \, dE. \]  

Using guess values of \( \nu(E) \) derived from the case of rectilinear trajectories, we adjust slightly
these values in order to match the numerical estimations of \( C \) using both the MMM and
the \( \mu \)-ion picture.

In the following we present results concerning the Lyman-\( \alpha \) and \( \text{H}_\alpha \) lines of hydrogenic
ions, carbon, and argon, for instance. Our purpose is to illustrate the influence of the tem-
perature, electronic density, and plasma composition on the line width. To obtain varia-
tions that are easier to interpret, we have neglected the fine structure effects. The eigenstates
belonging to the same value of the principal quantum number \( n \) are thus degenerate.

3. Results

We shall focus our attention on the cases of the broadening of the \( \text{H}_\alpha \) line of \( C^{5+} \) in a
pure carbon plasma and of the Lyman-\( \alpha \) line of \( \text{Ar}^{17+} \) in a plasma of protons.

3.1. \( \text{H}_\alpha \) line of \( C^{5+} \): Temperature and density variations

In figure 2 are reported the width variations (in eV) of this line versus the density in
cm\(^{-3}\) for different temperatures (20, 100, and 300 eV). Doppler broadening is not
included. The conditions are those of weakly correlated plasmas. At 20 eV and \( 10^{20} \) cm\(^{-3}\),
the correlation and screening parameters are, respectively, equal to 0.79 and 0.4. Thus, MC
field distribution functions are used only at 20 eV and BM in the other cases.

We note a slow convergence toward the static limit at \( 10^{20} \) cm\(^{-3}\) and a large discrepancy
with the results of the relaxation theory (Oza et al. 1988). Part of this disagreement may
be explained by the different treatments of the electronic broadening, and by the use of
linear trajectories in Oza et al.
3.2. Lyman-α line of Ar\textsuperscript{17⁺}: Concentration effects

Figure 3 shows the variations of the line width versus density at 862 eV for different concentrations \( c \) of Ar\textsuperscript{17⁺}. The other ions are protons. Doppler broadening is not included. We analyze the pure case and also the case of argon impurities. The width is reported in reduced \( \Delta \alpha \) units defined by

\[
\Delta \alpha = \Delta \lambda / F_0,
\]

where \( \Delta \lambda \) is the detuning in Angstroms and \( F_0 \) is the normal electric field value in esu,

\[
F_0 = 2\pi (4\frac{e}{13})^{2/3} eN_e^{2/3}.
\]

The density range studied here can seem unrealistic toward the low densities. This study was done in order to test the method in this domain, where the impact limit should be recovered. We also reported the ion-impact limit (Stehlé 1985) in its validity range, which is obtained when the half-width value is smaller than the detunings corresponding to the ionic plasma frequencies for H\textsuperscript{+} and Ar\textsuperscript{17⁺}. The corresponding density range depends on the concentration. As indicated by our results, this limit is nearly reached for the two lowest concentrations.

The static limit also is reported for the pure case. The value of the width, which is given by the electrons, is almost independent of the concentration. We note again a strong disagreement with this theory.

In table I we indicate the domain where MC calculations have been used for the field distribution function. The MC calculations are difficult to perform for small concentra-
Figure 3. Half-width value in $\alpha$ units (HWHM) of the Lyman-$\alpha$ line of $\text{Ar}^{17+}$ in a mixture of $\text{Ar}^{17+}$ and protons at 862 eV versus the electronic density $N_e$ in cm$^{-3}$. The results are reported for different values of the ion concentration $c$ of $\text{Ar}^{17+}$ ($10^{-6}$, $10^{-2}$, $10^{-1}$, and 1). The corresponding impact results (Stehlè 1985) are reported with dashes and the static limit (independent of $c$) with dot-dashes. The crosses indicate the MD results of Stamm et al. (1986) at $1.5 \times 10^{23}$ cm$^{-3}$ ($c = 10^{-2}$ and 1).

This is illustrated in figure 4 for $c = 10^{-2}$ and $N_e = 1.5 \times 10^{23}$ cm$^{-3}$, where we have checked the convergence of the calculation by increasing the number of particles involved in the simulation. This clearly indicates that a convergence study must be performed in MC or dynamics simulations involving small concentrations of radiating ions.

Our results at $1.5 \times 10^{23}$ cm$^{-3}$ are in good agreement with Stamm et al. (1986), using molecular dynamics simulations for the pure case. They differ in the case of small concentrations.

Table 1. Plasma parameters for the $\text{Ar}^{17+}$–$\text{H}^+$ mixture.

$c$ is the concentration (in number of ions) of $\text{Ar}^{17+}$.

| $N_e$ (cm$^{-3}$) | $c$(Ar) | $a$ | $\Gamma_{\text{Ar-H}}$ | $\Gamma_{\text{Ar-Ar}}$ |
|------------------|----------|-----|------------------------|------------------------|
| $1.5 \times 10^{24}$ | $10^{-2}$ | 0.3 | 0.497 | 1.83 |
|                  | $10^{-1}$ | 0.3 | 0.368 | 3.00 |
|                  | 1         | 0.3 |            | 3.47 |
| $1.5 \times 10^{23}$ | $10^{-2}$ | 0.2 | 0.231 | 0.848 |
|                  | $10^{-1}$ | 0.2 | 0.171 | 1.396 |
|                  | 1         | 0.2 |            | 1.609 |
| $1.5 \times 10^{22}$ | $10^{-1}$ | 0.14 | 0.079 | 0.648 |
|                  | 1         | 0.14 |        | 0.747 |
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\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig4}
\caption{Convergence of the Monte Carlo field distribution function $P(\beta)$ on a radiating $\text{Ar}^{17+}$ ion in electronic units ($\beta = F/F_0$) at $1.5 \times 10^{23}$ cm$^{-3}$ and 862 eV ($\text{Ar}^{17+}$ and protons perturbers). The $\text{Ar}^{17+}$ ion concentration is equal to $10^{-2}$. The total number of ions in the simulation is indicated on the figure.}
\end{figure}

\begin{figure}
\centering
\includegraphics[width=\textwidth]{fig5}
\caption{Lyman-$\alpha$ line of $\text{Ar}^{17+}$ perturbed by protons ($c = 10^{-6}$) at 862 eV and $5 \times 10^{24}$ cm$^{-3}$. Units are eV$^{-1}$ for the intensity and eV for the detuning. Dashes: result without Doppler; solid line: result with Doppler broadening.}
\end{figure}
trations \((c = 10^{-2})\). This disagreement can be attributed to an underestimation of dynamics effects on MMM or to convergence problems in MD.

4. Conclusion

Our results illustrate the influence of ion dynamics effects that enhance the broadening of the lines. These effects must be analyzed carefully in order to have a precise estimation of the width. This is of importance in determining the gain of lasing transitions in X-ray lasers. Our results have been presented by neglecting the fine structure effects. These effects must be included in the line shape as long as the Stark broadening is smaller than the energy level separation. This is illustrated in figure 5 for the Lyman-\(\alpha\) line of \(\text{Ar}^{17+}\) perturbed by protons at \(5 \times 10^{24} \text{ cm}^{-3}\) and 862 eV \((c = 10^{-6})\).

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