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Line Shapes of Multiply-Charged Ions: Ion Dynamics and Concentration Effects

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Résumé. — La méthode du microchamp modèle est appliquée au calcul de l’élargissement Stark des raies émises par des ions hydrogénoides multichargés pour des plasmas à une ou plusieurs composantes ioniques. Cette étude requiert une grande précision dans le calcul de la fonction de distribution du microchamp ionique. Cet aspect est discuté dans ce papier. Nos résultats sont comparés avec les résultats théoriques existants. Les effets de structure fine sont illustrés. Ce travail confirme l’importance des effets de dynamique des ions dans les profils de raies des plasmas denses et chauds. L’influence de la dilution des espèces rayonnantes dans un plasma à deux composantes est discutée en détails.

Abstract. — The model microfield method has been applied to the broadening of spectral lines emitted by multiply charged hydrogenic ions in pure and binary mixtures. Special attention is paid to the calculation of the ionic microfield distribution function. Extensive comparisons with other theoretical results are performed. Fine structure effects are shortly discussed. This paper confirms the importance of ion dynamics effects in the line shapes and discusses in detail, in the case of mixture, the dependence of the profile on the concentration of the radiating species.

1. Introduction

In a previous paper [1] (hereafter referenced as [I]), we presented a model for the line shapes of ions in plasmas, which takes into account the effects of the ions motions. This method is an extension of the well-known model microfield method (MMM) which was originally proposed for the Stark broadening of neutral radiators, especially hydrogen [2]. The main difficulty was to fit correctly the relevant dynamical properties of the plasma, in fact the covariance of the ionic microfield. This point has been yet elucidated in the way proposed in paper I, where the model has been tested on the lines of He+ ion. By comparing the results with experimental and theoretical ones, it has been proved that this method is well-appropriated in this case.

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Moreover, the well-known impact and static limits are reached at low and high electronic densities, giving an additional proof of the validity of the theory.

In the present paper we propose to extend the method to the case of highly ionized ions, which are found in dense and hot plasmas. We shall exclude from the discussion the case of highly correlated plasmas at low temperature, where the electronic structure of the radiator is modified by the plasma environment [3] or where the formation of quasi-molecules must be carefully analyzed [4-7].

For these highly ionized ions one finds two types of approximations [8]. In the first the perturbing ions are treated in the static approximation [9-13]. This is done in terms of electric ionic microfields. These approaches may also take into account the field inhomogeneities and ionization effects which are negligible at low densities [14]. In the second kind of models, one tries to describe the ion motion effects which are important in the line centers when the line width is comparable or smaller than the ionic plasma frequency. These models have been presented in paper I and in [15-18]. All these theoretical approaches are devoted to the case of lines of heavy ions in highly correlated plasmas (\( \Gamma > 0.2 \))

We want to propose an alternative treatment which should be valid also for weakly correlated plasmas, which are frequently found in astrophysical objects and in X-rays laser studies. We shall apply this formalism to the case of pure ions (one species) and also to the case of mixtures. One example is the case of traces of radiating ions in a plasma. This case is commonly found in astrophysics and inertial confinement fusion (ICF) plasmas (impurities) and is difficult to treat in numerical simulations.

Before we present briefly the principles of the theory, we will recall some extreme limits. At high densities, the line width is large and thus the associated radiative time-scale is smaller than the typical scale of ionic motions, i.e. the inverse of the ionic plasma frequency. In this case, it is well-known that the ions can be supposed to be fixed in space during emission (or absorption). This is the static limit. At opposite, at very low densities, one has the reverse inequality, which corresponds to the (ionic) impact limit, where the ion dynamics effects are very large.

After a short description of the method, already described in paper I, we shall compare our results with those obtained by Stamm et al. [18], Boercker et al. [16, 17] on the Lyman lines of Ar\(^{17+}\), Al\(^{12+}\) and Be\(^{3+}\) and also by Oza et al. [20] for the H\(_{\alpha}\) line of C\(^{5+}\). These cases correspond mainly to physical conditions of ICF and X-ray laser plasmas. We shall also present results at higher and lower densities for a mixture of Ar\(^{17+}\) and protons. These conditions may seem unrealistic, but they allow to test the method in the limiting cases where the static and impact limits should be recovered for the ionic contribution to the intensity. We shall study also the effects of the relative concentration of argon ions and protons on the line width.

The fine structure effects are large in the case of highly ionized ions for some lines. These effects have been included in few computations [21-24], and we can include them to interpret the observed spectra. As the theoretical results mentioned above are presented without these effects, we will also neglect them, in order to obtain comparative results and to clarify the discussion. To conclude, the importance of the fine structure effects will be illustrated at the end of the paper.

2. Theory

The formalism is based on the modelling of the static and dynamic plasma statistics which we shall present now.
2.1. Model. — We consider a plasma (temperature $T$) constituted by electrons (density $N_e$) and two species of ions $t$ and $p$ with respective concentrations $(c_t, c_p)$, charges $(Z_t, Z_p)$ and masses $(m_t, m_p)$. The (t) ion will be chosen as the radiating species. Let us define the mean and mean square charges by

$$<Z> = c_t Z_t + c_p Z_p$$  
$$<Z^2> = c_t Z_t^2 + c_p Z_p^2$$  

The reduced mass for the interacting $t$-$t$ and $t$-$p$ ions are

$$\mu_t = m_t / 2$$

and

$$\mu_p = \frac{m_t m_p}{m_t + m_p}$$

The average reduced mass $\mu$ is then

$$<\mu> = c_t \mu_t + c_p \mu_p$$

The total (ionic and electronic) Debye length $\lambda_D$ is given by

$$\lambda_D = \left( \frac{kT_D}{4\pi e^2 N_e} \right)^{1/2}$$

with

$$T_D^{-1} = T^{-1} \left( 1 + \frac{<Z^2>}{<Z>} \right)$$

The electronic Debye length $\lambda_{D,e}$ is obtained by setting $T_D = T$ in the preceding expression.

We introduce two correlation parameters $\Gamma_{it}$ between the radiating $t$ and perturbing $i$ species by

$$\Gamma_{it} = \frac{Z_i Z_t e^2}{kT <r_i>}$$

where $<r_i>$ is the mean distance between ions of type $i$.

We define also a global correlation parameter $\Gamma$, relative to the mean values of the ionic species by

$$\Gamma = \frac{<Z^2> e^2}{kT <r>}$$

where $<r>$ is defined by

$$\frac{4\pi}{3 <Z>} <r>^3 N_e = 1$$

As the radiator is charged, its position is related to the field which acts on it. Moreover the ionic trajectories are influenced by simultaneous interactions with other ions. This induces a correlation between the Stark and the Doppler effects. This effect, discussed by Boercker et al. in the kinetic model [16, 17] and by Stamm et al. using molecular dynamics simulations [18], seems to be negligible in practice.

This conclusion allows us to adopt the $\mu$-ion picture, already justified in paper I. The emitter is supposed to have an infinite mass whereas the ionic perturbers are replaced by fictive ions having the masses $\mu_t$ and $\mu_p$ defined previously. The Doppler effect is included by the usual convolution between the pure Stark and Doppler profiles. In this approach we assume that these perturbers move along independent trajectories. The ions interact with the emitter by
the ionic microfield \( E(t) \). The time statistics of this microfield are modelled by the model microfield method. This method was developed by Brissaud and Frisch [2] for neutral emitters and works very well in this case. Its extension to the case of charged emitters has been proposed by Stehlé [25, 26] and tested in paper I on the He\(^+\) lines. The basic idea is to develop a model which will give the correct well-known impact or static limits when the ion dynamics effects are large or negligible respectively.

In the model, the field is supposed to vary by steps with the time. At each step its value is random. The process is supposed to be markovian. The jumping times are described by a Poisson distribution with density \( \nu(E) \). The probability to have no jump between \( t \) and \( t + \Delta t \) is equal to \( \exp(-\nu(E)\Delta t) \). The MMM field covariance \( C_{EE}(t) \) is equal to

\[
C_{EE}(t) = \left\{ E(0)E(t) \right\}_{av} \tag{11}
\]

\[
= \int_0^\infty P(E)\exp(-\nu(E)t)E^2 \, dE \tag{12}
\]

and

\[
C = \int_0^\infty C_{EE}(t) \, dt = \langle E^2 / \nu(E) \rangle \tag{13}
\]

where \( \langle ... \rangle \) denotes the average respective to the field distribution function \( P(E) \).

In this model the line shape has an analytical form, which is given in terms of the Laplace transform \( U(\omega + \nu(E)) \), of the usual time evolution operator the radiating ion \( U(t, 0) \) [1]. This operator \( U(\omega + \nu(E)) \), calculated for the fixed field value \( E \), is easily obtained. The dynamics effects are contained in the term \( \nu(E) \). The static model is formally obtained by putting \( \nu(E) \) equal to zero in the line shape expression. Thus the relevant quantities are \( P(E) \) and \( \nu(E) \).

We will discuss at first our method for calculating the jump frequency \( \nu(E) \).

2.2. Choice of \( \nu(E) \) and Calculation of \( P(E) \). — As stated before we want to have the correct impact limit at low densities. It is possible to prove that this limit is formally obtained in the model [26]. The quantity of interest is approximately equal to the time integral of the covariance \( C \) (12).

Thus we have to choose \( \nu(E) \) in this context. At first, we calculate this covariance using the independent contributions of each ion moving along the trajectory defined by the Debye screened Coulombic potential. This approach is correct at low densities. As described in paper I, we use the value derived from the case of rectilinear trajectories as a starting \( \nu(E) \) value. We adjust it in order to get the correct integral for the covariance calculated previously. We introduce to this purpose an adjustable parameter \( f \) which is close to unity when the trajectories are nearly linear, i.e. for small values of the correlation parameters (i.e. \( \Gamma_f < 1 \)).

In principle, it may differ from unity in the case of strong trajectory deflexions (i.e. \( \Gamma_f > 1 \)). This choice has been tested for the case of He\(^+\) radiator in weakly and moderate correlated plasmas. We want to demonstrate that this method is also justified for stronger correlated plasmas and highly ionized ions.

It is easy to see from expressions (11, 12) that an accurate field distribution is necessary to obtain a correct frequency jump and the MMM intensity. Many attempts have been made to include the correlations between the diverse charged particles producing the field in approximate theoretical calculations of \( P(E) \) [27-33]. However just a few of these theories provide accurate results for strongly correlated plasmas [31-33]. Moreover only the adjusted-parameter exponential approximation (APEX) method [29] or the Monte-Carlo simulations [34, 35] have
been applied to a wide range of temperature, densities and ionic species. APEX is an effective independent particle model. This technique is powerful and allows to calculate accurate microfield distributions, with almost simple numerical calculations, provided that an accurate ion-ion pair correlation function, \( g(r) \), is used to determine the exact second moment rule of \( P(E) \). Thus, in practice, the crucial quantity of APEX is \( g(r) \). The use of analytical, but too much imprecise, functions for this quantity [36] is not applicable to the present study and accurate HNC calculations of \( g(r) \) would be preferred.

Contrary to this APEX model, the MC calculations of \( P(E) \) are ab initio calculations, which in general provide reference results without too much computer time on present day computers. Hence we choose to simulate directly the microfield distributions with the MC method except in the cases of impurities \( (c = 10^{-6}) \), where MC technique can not be applied as it will imply a simulation with \( 10^6 \) particles that is impossible to handle with, with present day computers. Fortunately these situations correspond to weakly correlated plasmas and we use a Baranger-Mozer (BM) approach [39] to perform the calculations. For all the very low correlated plasmas \( (i.e. \Gamma_r < 0.6) \) the smooth BM results will be preferred to the MC ones, which present too much numerical noise. But the comparisons have always been done to validate the analytical result. In all the cases, our MC results have been smoothed carefully, if necessary. In our simulation, the ions interact with the others through Debye-Hückel (electronic) shielded potentials [34], suitable for the physical conditions of our applications. These calculations are not too computational time and storage consuming and the simulations are now routinely done with five hundred particles. In order to avoid the usual statistical fluctuations of the MC description in the tail, we performed an analytical extension for the large fields, adjusted to the MC data, which derive from the nearest neighbour approximation. The results are very close to those of Hooper [29]. This is not surprising, because large fields have an important probability only for low correlated plasmas. Otherwise, the distribution shifts towards the small fields and the extension is no more necessary for our purpose.

For one ion species plasmas, it is also possible to use an analytical description of these MC electric microfield distributions [37]. These fits reproduce the MC data with their analytical extensions, with a good accuracy. For example, the value of the most probable field, \( E_m \), is given by a simple polynomial functions of the plasmas parameters \( \Gamma \) and \( U \), as

\[
\log E_m = P_0(u) + P_1(u)(\log \Gamma) + P_2(u)(\log \Gamma)^2 + P_3(u)(\log \Gamma)^3 + \ldots \tag{14}
\]

with

\[
P_i(u) = a_{0i} + a_{1i}U + a_{2i}U^2 + \ldots + a_{5i}U^5 \tag{15}
\]

where

\[
U = \frac{<r>}{\lambda_{D,e}} \tag{16}
\]

Similar expressions have been obtained for the discrete value of the microfields \( P(E_r) \). In some applications requiring fast calculations, these fits can be applied to mixtures, using an effective charge depending on the concentration [38]. The precision of the corresponding results is not sufficient in the present plasma conditions. Thus we shall not use it.

Let us discuss now the case of a plasma mixture consisting, for example of \( \text{Ar}^{17+} \) ions and protons. We shall examine the field distribution function on the \( \text{Ar}^{17+} \) ions. The variations of \( P(E) \) with the atom concentration \( (c) \) of \( \text{Ar}^{17+} \) ions, for low correlated plasmas, have been already discussed by Hooper [28]. The MC calculations of microfields, in cases of binary ionic mixtures, are easily carried out for concentrations of radiative ions greater than 5% \( (\text{the results are not affected by the numerical noise}) \). In the Figures 1 and 2 we report the microfield distribution functions for a plasma of \( \text{Ar}^{17+} \) and protons at 862 eV, and densities of \( 1.5 \times 10^{23} \)
Fig. 1. — Field distribution function on a radiating Ar$^{17+}$ ion at $1.5 \times 10^{23}$ cm$^{-3}$ and 862 eV in a mixture of Ar$^{17+}$ and protons, for four ion concentrations $c$ of Ar$^{17+}$ ($10^{-6}$, $10^{-2}$, $10^{-1}$ and 1). The electric field is given in electronic units $\beta = E/F_0$ (where $F_0$ is the Holtsmark normal field value defined in terms of the electronic density by $F_0 = 2\pi e (4N_e/15)^{2/3}$)

Fig. 2. — Same as Figure 1 at $1.5 \times 10^{24}$ cm$^{-3}$ and 862 eV.
Fig. 3 — Convergence study of the Monte Carlo field distribution function $P(\beta)$, on a radiating $\text{Ar}^{17+}$ ion at $1.5 \times 10^{23} \text{ cm}^{-3}$ 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 each simulation is indicated in the Figure

and $1.5 \times 10^{24} \text{ cm}^{-3}$ respectively. In each figure we plot the results for four concentrations of $\text{Ar}^{17+}$ from the pure case to the impurity one. The plasma parameters and the choice of the method for the calculation of $P(E)$ are indicated at the top of Table IV. We note a strong dependence on $c$ for the lowest density and a weaker one in the second case. In practice Monte Carlo simulations are difficult to perform for small concentrations. This is illustrated for 1% of $\text{Ar}^{17+}$ at $1.5 \times 10^{23} \text{ cm}^{-3}$. Figure 3 shows the simulation results for different numbers of ions (100, 200, 400 and 500). In the first case (one $\text{Ar}^{17+}$ and 99 protons in 100 ions), one finds only one argon ion in the simulation box, and the $\text{Ar}^{17+}$-$\text{Ar}^{17+}$ interactions are taken into account only by the usual image procedure. The convergence occurs between 400 and 500 ions (i.e. with 4 $\text{Ar}^{17+}$, and 5 $\text{Ar}^{17+}$). It is clear from these results that a minimum number of 400 ions is required to obtain a reasonable result which even remains somewhat noisy. Thus an analysis of the convergence of the results must be done for simulations with a small number of $\text{Ar}^{17+}$ ions. We have carefully checked this point in the present work. The lowest reasonable limit for $c$ is 0.2%.

3. Results

At first we will present an extensive comparison with other theoretical results. These alternative treatments of ion dynamics effects are at first the molecular dynamics simulations [16-18]. Molecular dynamics (MD) simulations are usually considered as reference calculations. This is justified if the number of particles and time events are convenient to reproduce the static and time dependent plasma statistics.

The second theory is the kinetic theory of Boercker et al. [16] (KT), which treats in a coherent way the electrostatic forces and the diffusion processes. The last theoretical approach was
Table I. — Plasma composition for the test cases. The radiator t is underlined. The correlation parameters \( \Gamma \) are between t particles and t and p perturbers (7). \( \alpha \) is the ratio of the electronic Debye length to the mean distance between the electrons.

<table>
<thead>
<tr>
<th>Case</th>
<th>Plasma composition</th>
<th>( kT (\text{eV}) )</th>
<th>( N_e (\text{cm}^{-3}) )</th>
<th>( \Gamma_{tp} )</th>
<th>( \Gamma_{tt} )</th>
<th>( \alpha )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \text{Al}^{12+} )</td>
<td>233</td>
<td>( 4 \times 10^{21} )</td>
<td>1</td>
<td>0.27</td>
<td>0.22</td>
</tr>
<tr>
<td>2</td>
<td>( \text{Al}^{12+} )</td>
<td>862</td>
<td>( 4 \times 10^{21} )</td>
<td>1.6</td>
<td>0.15</td>
<td>0.11</td>
</tr>
<tr>
<td>3</td>
<td>( \text{Ar}^{17+} )</td>
<td>862</td>
<td>( 1.5 \times 10^{23} )</td>
<td>1.6</td>
<td>0.42</td>
<td>0.18</td>
</tr>
<tr>
<td>A</td>
<td>( \text{Al}^{12+} ) (50%) + ( \text{Be}^{3+} )</td>
<td>233</td>
<td>( 4 \times 10^{21} )</td>
<td>0.3</td>
<td>0.9</td>
<td>0.22</td>
</tr>
<tr>
<td>B</td>
<td>( \text{Al}^{12+} ) (50%) + ( \text{Be}^{5+} )</td>
<td>233</td>
<td>( 4 \times 10^{20} )</td>
<td>0.14</td>
<td>0.42</td>
<td>0.15</td>
</tr>
<tr>
<td>C</td>
<td>( \text{Be}^{3+} ) (5%) + ( \text{H}^+ )</td>
<td>100</td>
<td>( 1 \times 10^{20} )</td>
<td>0.032</td>
<td>0.036</td>
<td>0.18</td>
</tr>
</tbody>
</table>

formulated by Greene in 1982 [15] and applied to the H, He+ and C5+ lines [20]. This relaxation theory (RT) describes the broadening in terms of functions of time, which depend only on the plasma conditions and are thus decoupled from the atomic problem. These functions are, in this paper, obtained by a Monte Carlo simulation, where the plasma is described by independent \( \mu \) ions moving inside a reference cell, along rectilinear trajectories. This approach of linear trajectories is, in principle devoted to the case of weakly correlated plasmas and we found in paper I a very good agreement between MMM and relaxation results for the \( \text{H}_\alpha \) line of \( \text{He}^+ \) ion.

As theoretical coincidences can be fortuitous, we have performed a systematic comparison with these theoretical results. For all the cases presented in the following, the correlation between the radiator velocity and the Stark broadening are neglected. The results are given without Doppler effect.

3.1. Comparisons with Other Theoretical Results. — It is well-known that the ion dynamics effect enhances the broadening of the lines exhibiting a central component like Lyman-\( \alpha \), Lyman-\( \gamma \), H\( \alpha \), H\( \beta \). The differences between “dynamics” and static line widths can be very large. For lines which do not have a central component, like Lyman-\( \beta \) et H\( \beta \), the ion dynamics effects fill the well-known dip in the line center. In Figure 4 we plot the line shapes of Lyman-\( \beta \) of \( \text{Al}^{12+} \) and \( \text{Ar}^{17+} \) for an electronic density equal to \( 4 \times 10^{21} \text{ cm}^{-3} \) and two different temperatures corresponding to 233 and 862 eV for aluminium (Figs. 4a,b) and \( 1.5 \times 10^{23} \text{ cm}^{-3} \), 862 eV for argon (Fig. 4c). In these three cases the plasma is composed of electrons and \( \text{Al}^{12+} \) (or \( \text{Ar}^{17+} \)) ions. The differences with the results obtained with molecular dynamics simulations are relatively small. We note a good agreement with the results of Boercker et al. [16].

We have performed comparisons on the Lyman-\( \alpha \) line with the results obtained with MD and KT, in different plasma conditions (pure \( \text{Al}^{12+} \) or \( \text{Ar}^{17+} \) plasmas, mixtures of \( \text{Al}^{12+} \) and \( \text{Be}^{3+} \) or of \( \text{Be}^{3+} \) and \( \text{H}^+ \)). These conditions are reported in Table I, as are also the correlation parameters \( \Gamma_{tt} \) and the electronic screening parameter \( \alpha \) (which is the ratio of the electronic Debye length to the mean distance between the electrons, i.e. \( \alpha = \lambda_{D,e} / <r_e> \)). In the three first pure cases (\( \text{Al}^{12+} \) and \( \text{Ar}^{17+} \) plasmas), we used the field distribution function obtained by an analytical fit to the MC simulation results [37]. For the mixture A, we used MC field distribution function, and for the two last mixture cases B and C the field distribution function given by the Baranger-Mozer theory [39]. In Table II we give the halfwidth values (HWHM) compared with the other theoretical results and also the value of the adjustable parameter \( f \)
determining the field frequency jump \( \nu(E) \). We note a very good agreement between all the methods except for the low correlated case 3, where the discrepancy is reasonable. For the most correlated case C, the MMM results are closer to the results of the kinetic theory than those of MD simulation. Nevertheless the results are in good agreement between themselves. This indicates a good behaviour of MMM for weakly correlated plasmas, which was expected.

**Fig. 4 —**

- a) Normalized intensity of the Lyman-\( \beta \) of \( \text{Al}^{12+} \) in \( \text{Al}^{12+} \) in units of \( \Delta \alpha^{-1} \) versus the reduced detuning \( \Delta \alpha = \Delta \lambda / F_0 \). \( F_0 = 1.25 \times 10^{-9} N_e^{2/3} \) is the usual Holtsmark normal field value (\( \lambda \) in Å, \( N_e \) in cm\(^{-3} \), \( F_0 \) in esu). The electron kinetic temperature is 233 eV. The electronic density is \( 4 \times 10^{21} \) cm\(^{-3} \). In circles the MD results [16-18], in full curve the MMM intensity, in dashed curve the KT results [16]. Doppler effect is not included.
- b) Same as Figure 4a at 862 eV.
- c) Same as Figure 4a for the Lyman-\( \beta \) of \( \text{Ar}^{17+} \) in \( \text{Ar}^{17+} \) at 862 eV and \( 1.5 \times 10^{23} \) cm\(^{-3} \).
Table II. — HWHM (in eV) of the Lyman-\(\alpha\) line without Doppler effect (MMM). Comparison with results of the kinetic theory (KT) [16, 17] and the MD simulation [16-18]. The values of the adjustable parameter \(f\) are also given.

<table>
<thead>
<tr>
<th>Case</th>
<th>MMM</th>
<th>MD</th>
<th>KT</th>
<th>(f)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.033</td>
<td>0.031</td>
<td>0.034</td>
<td>1.07</td>
</tr>
<tr>
<td>2</td>
<td>0.040</td>
<td>0.053</td>
<td>0.056</td>
<td>1.00</td>
</tr>
<tr>
<td>3</td>
<td>0.21</td>
<td>0.21</td>
<td>0.18</td>
<td>1.19</td>
</tr>
<tr>
<td>A</td>
<td>0.032</td>
<td>0.037</td>
<td>0.030</td>
<td>1.03</td>
</tr>
<tr>
<td>B</td>
<td>0.011</td>
<td>0.011</td>
<td>0.013</td>
<td>1.16</td>
</tr>
<tr>
<td>C</td>
<td>0.014</td>
<td>0.025</td>
<td>0.012</td>
<td>1.02</td>
</tr>
</tbody>
</table>

for this theory, but also for highly correlated ones and for the cases of mixtures of ions having different or similar charges. The case of high-Z impurities in a plasma of protons, which are found in ICF confinement experiments requires special attention and will be discussed in details in Section 3.2.

As the MMM uses a simplified model for the time dependent statistical interactions between the plasma and the radiator, it allows to calculate line broadening of “complicate lines”, like \(\text{H}_\alpha\), which has up to now not been studied by MD simulations. Thus we will present results on the \(\text{H}_\alpha\) line of \(\text{C}^{5+}\) ion, which is very important in X-ray recombination laser schemes (the experimental conditions are typically \(10^{17}-10^{18}\) cm\(^{-3}\) for the electronic density, and 20 eV for \(kT\)). We have performed a systematic study of the width of the \(\text{H}_\alpha\) line for a density range from \(10^{17}\) to \(10^{20}\) cm\(^{-3}\) and three temperatures (20, 100 and 300 eV). The plasma ions are supposed to be \(\text{C}^{5+}\) ions, which can seem unrealistic for some temperatures-densities conditions, but allows to test our results with those obtained in the same conditions by Oza et al. with the relaxation theory [20] The plasma parameters \(\Gamma\) and \(\alpha\) are reported in Table III.
Table III. — Parameters \( \Gamma, a \) and \( f \) for the \( \text{C}^{5+} \) plasma and different values of \((N_e, T_e)\).

<table>
<thead>
<tr>
<th>( N_e (\text{cm}^{-3}) )</th>
<th>( T_e (\text{eV}) )</th>
<th>( \Gamma )</th>
<th>( a )</th>
<th>( f )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( 10^{17} )</td>
<td>20</td>
<td>0.079</td>
<td>0.13</td>
<td>0.96</td>
</tr>
<tr>
<td>( 10^{20} )</td>
<td>20</td>
<td>0.79</td>
<td>0.4</td>
<td>0.92</td>
</tr>
<tr>
<td>( 10^{17} )</td>
<td>300</td>
<td>0.005</td>
<td>0.03</td>
<td>0.97</td>
</tr>
<tr>
<td>( 10^{20} )</td>
<td>300</td>
<td>0.05</td>
<td>0.1</td>
<td>0.96</td>
</tr>
</tbody>
</table>

Fig. 5 — Halfwidth value in eV (HWHM) of the \( \text{H}_\alpha \) line of \( \text{C}^{5+} \) in \( \text{C}^{5+} \) at different temperatures (20, 100, 300 eV), versus the electronic density \( N_e \) in \( \text{cm}^{-3} \). In long dashed line the static limit (20 eV), in full curve the MMM results, in dashed line the KT results [20]. The cross indicates the ion impact width at \( 10^{17} \text{ cm}^{-3} \) and 20 eV.

for the extreme cases. We used MC field distribution functions at 20 eV and in the other cases BM field distribution functions. Our results are presented in Figure 5. Unfortunately we do not find a good agreement with these authors, contrary to the case of the \( \text{H}_\alpha \) line of \( \text{He}^+ \) ion presented in paper I. Hence our halfwidth values are smaller by almost a factor of two for the density - temperature range considered here. In fact the discrepancy between these results diminishes when the Doppler effect is included. The present discrepancy is difficult to interpret. In particular we do not understand the strong variations of the halfwidth observed by Oza et al., which may reach a factor of 5 between 20 and 300 eV. Hence, the results obtained for \( \text{H}^+ \) and \( \text{He}^+ \) indicate that the differences between the widths with the temperature diminish for increasing density. In the impact limit where the ion dynamics effects are maximum, the width varies roughly like \( T^{-1/2} \). Thus a difference of 4 is the upper limit for the two extreme temperatures. In Figure 5 we plotted also the (ionic) static and impact limits obtained at
20 eV. The last ones is outside its validity range, because estimations of the impact halfwidth at this temperature indicate that this limit is reached only for densities smaller than $10^{15} \text{ cm}^{-3}$, (where $\Delta \omega_{1/2} < \omega_{p1}$). At high densities we note also a disagreement with the results of Oza et al. and our static halfwidth is smaller by a factor of two. These differences may be attributed to different electronic broadenings although these authors use the same semi classical dipolar treatment (with no quenching effects) than us but they include a better description of strong collisions. Nethertheless this broadening mechanism becomes important at high densities where ion dynamics effects disappear. This point will be discussed below.

3.2. Density and Concentration Effects. — In the preceding paragraph we performed systematic comparisons with other theoretical results. The overall agreement is satisfactory except in the case of the H$_x$ transition of C$^5+$, We propose now to study the variations of the line width of the Lyman-$\alpha$ of Ar$^{17+}$ in a plasma mixture composed of Ar$^{17+}$ and protons for different Ar$^{17+}$ concentrations $c$ ($10^{-6}$, $10^{-2}$, $10^{-1}$ and 1) and electronic densities $N_e$ (from $10^{17}$ to $10^{24} \text{ cm}^{-3}$). The temperature is 862 eV. The corresponding correlation parameters $\Gamma_i$ are given in Table IV, where we mention also the method retained for the calculation of $P(E)$.

Let us discuss at first the behaviour of the line width in the static limit which should be reached at high densities. In this case, the Lyman-$\alpha$ line center is dominated by electronic broadening. Hence, this line presents an unshifted component, which is thus insensitive to the ionic microfield. For a given density and temperature, the width variations with $c$ are negligible. The relevant quantity, in the static limit, is the microfield distribution function $P(E)$. This quantity is also important in the dynamical case, owing to its role in the determination of the frequency jump

The variations of $P(E)$ with the concentration have been already discussed in Section 2.2 (Figs. 1, 2). In the static limit, they affect the intensity of the near line wings.

We will discuss now the concentrations effects in the low density case, where the ion dynamics effects are maximum, i.e. in the impact limit. The interactions between the radiator and the perturbing ions and electrons can then be described in terms of collisions. In this ideal case, the impact width is given by an analytical expression [22] composed of the additive independent contributions of ions (t) and ions (p) which are respectively proportional to

$$
c_t \ N_e \ Z_t \sqrt{\mu_t/T} \quad \text{and} \quad c_p \ N_e \ Z_p \sqrt{\mu_p/T}
$$

(17)

Thus the ratio of these two contributions is approximatively equal to

$$
\frac{c_t}{c_p} \ \frac{Z_t \sqrt{\mu_t}}{Z_p \sqrt{\mu_p}}
$$

(18)

On this limiting case, it is very easy to see the influence of the dilution effect. The impurities (t) can be considered as infinitively diluted if the preceding ratios is very small.

For example, if we consider the case of Ar$^{17+}$ radiators in a plasma of protons, the Ar$^{17+}$ can be seen as an impurity for concentrations smaller than $10^{-3}$.

These considerations indicate that the concentration effects will be larger if the ion dynamics affect the line center. This point is illustrated in Figure 6, where we have reported the halfwidth value (HWHM) on the Lyman-$\alpha$ line for the different concentrations and electronic densities mentioned above (see also Tab. IV). The low density cases have been studied in order to test the convergence of the results towards the impact limit [40]. The static limit has also been reported at higher densities for the two extreme concentrations. As expected, the impact limit is associated to broader lines for the pure case ($c = 1$). The validity condition of this limit is
Table IV. — Parameters $\Gamma$, $a$ and $f$ for mixtures of Ar$^{17+}$ (ion concentration $c$) and protons at 862 eV, for different values of $(c, N_e)$. The last column indicates the method we choose for the calculation of $P(E)$ (B.M.: Baranger-Mozer, M.C.: Monte-Carlo).

<table>
<thead>
<tr>
<th>$N_e$ (cm$^{-3}$)</th>
<th>$c$ (Ar)</th>
<th>$\Gamma_{Ar-H}$</th>
<th>$\Gamma_{Ar-Ar}$</th>
<th>$a$</th>
<th>$f$</th>
<th>$P(E)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1.5 \times 10^{24}$</td>
<td>$10^{-6}$</td>
<td>0.524</td>
<td>0.089</td>
<td>0.304</td>
<td>0.91</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
<td>$10^{-2}$</td>
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<td>4.09</td>
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<tr>
<td></td>
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<td>3.00</td>
<td>2.46</td>
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<tr>
<td></td>
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<td>3.47</td>
<td>1.62</td>
<td>M.C.</td>
<td></td>
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<tr>
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<td>0.041</td>
<td>0.207</td>
<td>0.94</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
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<td>0.848</td>
<td>2.89</td>
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<tr>
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<td>1.396</td>
<td>1.65</td>
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<tr>
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<td>1.04</td>
<td>1.19</td>
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<tr>
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<td>0.0192</td>
<td>0.141</td>
<td>0.95</td>
<td>B.M.</td>
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<tr>
<td></td>
<td>$10^{-2}$</td>
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<td>0.394</td>
<td>2.21</td>
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<tr>
<td></td>
<td>$10^{-1}$</td>
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<td>0.648</td>
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<td>M.C.</td>
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<td>1.04</td>
<td>1.07</td>
<td>M.C.</td>
<td></td>
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<tr>
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<td>0.096</td>
<td>0.95</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
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<tr>
<td></td>
<td>$10^{-1}$</td>
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<td>0.301</td>
<td>1.23</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td></td>
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<td>0.347</td>
<td>1.00</td>
<td>1.07</td>
<td>B.M.</td>
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</tr>
<tr>
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<td>$10^{-6}$</td>
<td>0.024</td>
<td>0.0041</td>
<td>0.065</td>
<td>0.96</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
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<td>0.085</td>
<td>1.50</td>
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<tr>
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<td>$10^{-1}$</td>
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<td>0.14</td>
<td>1.15</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td></td>
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<td>0.161</td>
<td>0.98</td>
<td>0.98</td>
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<td></td>
</tr>
<tr>
<td>$1.5 \times 10^{19}$</td>
<td>$10^{-6}$</td>
<td>0.0113</td>
<td>0.0019</td>
<td>0.045</td>
<td>0.96</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
<td>$10^{-2}$</td>
<td>0.0107</td>
<td>0.0394</td>
<td>1.35</td>
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<tr>
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<td>$10^{-1}$</td>
<td>0.0079</td>
<td>0.065</td>
<td>1.09</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0.075</td>
<td>0.98</td>
<td>0.98</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td>$1.5 \times 10^{18}$</td>
<td>$10^{-6}$</td>
<td>0.0052</td>
<td>$8.9 \times 10^{-3}$</td>
<td>0.030</td>
<td>0.96</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
<td>$10^{-2}$</td>
<td>0.0049</td>
<td>0.018</td>
<td>1.26</td>
<td>B.M.</td>
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</tr>
<tr>
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<td>$10^{-1}$</td>
<td>0.0037</td>
<td>0.030</td>
<td>1.06</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0.035</td>
<td>0.97</td>
<td>0.97</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td>$1.5 \times 10^{17}$</td>
<td>$10^{-6}$</td>
<td>$2.4 \times 10^{-3}$</td>
<td>$4.1 \times 10^{-4}$</td>
<td>0.024</td>
<td>0.94</td>
<td>B.M.</td>
</tr>
<tr>
<td></td>
<td>$10^{-2}$</td>
<td>$2.3 \times 10^{-3}$</td>
<td>$8.5 \times 10^{-3}$</td>
<td>1.20</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$10^{-1}$</td>
<td>$1.7 \times 10^{-3}$</td>
<td>$1.4 \times 10^{-2}$</td>
<td>1.04</td>
<td>B.M.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0.016</td>
<td>0.97</td>
<td>0.97</td>
<td>B.M.</td>
<td></td>
</tr>
</tbody>
</table>

obtained when the radiative lifetime (i.e. the inverse of the line width $\Delta \omega^{-1}_{1/2}$) is large compared to the mean time of a collision, which is given by the ratio of the total Debye length to the mean kinetic relative velocity. This typical collisional time is roughly equal to the inverse of the ionic plasma frequency. Thus the validity condition of the impact approximation for our
Fig. 6. — Halfwidth value in $\alpha$ units (HWHM) of the Lyman-$\alpha$ line of Ar$^{17+}$ in a mixture of 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 Ar$^{17+}$ ($10^{-6}$, $10^{-2}$, $10^{-1}$ and 1). The corresponding ion impact results are reported in dashed lines. The dot-dashed lines the static limit (independent of $c$). The two crosses indicate the MD results at correspond to $1.5 \times 10^{23}$ cm$^{-3}$ ($c = 10^{-2}$ and 1)

mixture is

$$
\left( \frac{4\pi e^2 N_e < Z^2 >}{<Z> \mu_p} \right)^{1/2} > \Delta \omega_{1/2}
$$

(19)

(the perturbers p are here Ar$^{17+}$ or H$^+$ ions).

This condition is more difficult to fulfill in the pure case, where the width is large, than for the impurity. This agrees with our results (Fig. 6).

At higher densities ($N_e > 10^{23}$ cm$^{-3}$), the ion dynamics effects are reduced. Heavy ions do not move significantly during the radiative process, contrary to the protons. Thus the impurity case will present more ion dynamics effects and have larger line widths. The variations with the concentration are smaller than at low densities.

In Figure 6 we report also the two MD results at $1.5 \times 10^{23}$ cm$^{-3}$ ($c = 1$ and $10^{-2}$). The simulation results are in good agreement for the pure case and differ noticeably for the case of 1% atom concentration, where we find a smaller halfwidth value. As the field distribution function has been carefully checked by convergence tests, the discrepancy can be either attributed to the choice of the frequency jump $\nu(E)$ or to insufficient description of the statistic of the Ar$^{17+}$-Ar$^{17+}$ interactions in the MD simulation. The MMM line width, for a concentration of $10^{-6}$ are closer to the preceding MD results at $10^{-2}$.

3.3. DISCUSSION. — By construction the model is specially designed to the case of weakly correlated plasmas where trajectories effects are small. According to the second order perturbation theory, the impact halfwidth expression is given in terms of the field autocorrelation function. At higher densities, this perturbative approach fails and it is not so important to
insure a correct description of $C_{EE}(t)$. Moreover the typical relevant times for the broadening (i.e. $\Delta \omega_{1/2}^{-1}$) decrease and the details of this function at larger times are useless. Our choice of the frequency jump insures a smooth interpolation between the low and the high densities limits (i.e. low and high correlations parameters $\Gamma$), providing that the field distribution function is accurately calculated. In Tables II-IV, we report the values of the adjustable parameter $f$, which enters in the calculation of the frequency jump $\nu(E)$(see paper I). They may differ from unity in the case of highly charged ions due to trajectory effects. This parameter varies with the plasma composition for mixtures of ions with very different charges. This reflects the sensitivity of $C_{EE}(t)$ to the concentration of the heaviest impurities.

The results presented in this paper indicate a good behaviour of the MMM for the lines of highly charged ions at low and moderate $\Gamma$ values. This validates our choice of the jumping frequency. We want to underline three advantages of our method. It recovers continuously the impact limit at low densities, it is by construction adapted to the case of low $Z$ and $\Gamma$ and, in the case of lines of He$^+$ ion, a very good agreement is found with experimental results [1]. Thus it may seem surprising to note disagreement with MD and relaxation theory results for moderate $Z$ and low $\Gamma$ values. But MD and MC simulations are not specially devoted to these low correlation cases (MC simulations are needed in auxiliary calculations by Oza et al. [20] in the relaxation theory). Hence the corresponding weak Debye screening requires a large number of ions for simulations. Moreover, the strong fields may play an important role at low densities for low $Z$ values (for example in the case C concerning Be$^{3+}$ ion, the fields larger than $10^4$ (electronic units) contribute to $30\%$ to $C_{EE}(t = 0)$).

The electronic contribution to the line shape is negligible in most of the cases presented in this paper. It may be important especially for lines with central component like Ly$\alpha$ and H$_\alpha$ at high densities, where ion dynamics effects are small, such as for the H$_\alpha$ line of C$^{5+}$ ion at $10^{20}$ cm$^{-3}$ (Fig. 5). Our treatment of this electronic broadening has been presented in paper I. It is based upon the dipolar, no quenching, semi-classical perturbational treatment. We used a common strong collision cutoff for its various matrix elements, assuming a zero contribution for the off diagonal ones. A more accurate treatment is given by a quantum description of the collision including short range interactions up to the octupole interaction [3, 41]. In order to check our results we have chosen the case of the H$_\alpha$ of C$^{5+}$ at $10^{20}$ cm$^{-3}$, 20 eV and 300 eV. As the two previous reference papers are devoted to the Lyman lines, we may equivalently test the validity of our semiclassical treatment upon the Lyman $\alpha$ and $\beta$ lines. The results are reported in Table V. We note a reasonable agreement with the results of Nguyen Hoe et al

Table V. — Values in units of $10^{12}$ rds.s$^{-1}$ of the matrix elements of the electronic relaxation operator $\gamma(nl)$ for the Ly$\alpha$ and Ly$\beta$ line of C$^{5+}$ at $10^{20}$ cm$^{-3}$, 20 and 300 eV. The first number refers to our semi-classical treatment, the number in parenthesis to the values obtained in quantum treatment of [3].

<table>
<thead>
<tr>
<th>$nl$</th>
<th>20 eV</th>
<th>300 eV</th>
</tr>
</thead>
<tbody>
<tr>
<td>2s</td>
<td>4.5 (5.9)</td>
<td>3.0 (2.7)</td>
</tr>
<tr>
<td>2p</td>
<td>1.5 (2.5)</td>
<td>1.0 (1.3)</td>
</tr>
<tr>
<td>3s</td>
<td>27 (34)</td>
<td>17 (15)</td>
</tr>
<tr>
<td>3p</td>
<td>20 (26)</td>
<td>13 (12)</td>
</tr>
<tr>
<td>3d</td>
<td>6.8 (12)</td>
<td>4.4 (5.7)</td>
</tr>
</tbody>
</table>
Fig. 7. — a) and b) Lyman-α line of Ar\(^{17+}\) perturbed by protons (c = 10\(^{-6}\)) at 862 eV, for two electronic densities (10\(^{24}\), Fig. 7a, and 5 \times 10\(^{24}\) cm\(^{-3}\), Fig. 7b) Fine structure effects are included. Units are eV\(^{-1}\) for the normalized intensity and eV for the detuning. The dashed curve shows the result without Doppler effect and the full one the result including Doppler broadening. Zero detuning corresponds to the unperturbed (1s1/2 - 2p3/2) transition

[3] using the Coulomb Born approximation. Our too small 2p, 3d contributions might induce an underestimation of the broadening of the H\(_{\alpha}\) central component for densities of the order of 10\(^{20}\) cm\(^{-3}\).
It is clear that in several cases presented in this paper, the fine structure effects are visible in the line center. Our model is independent of the atomic structure and is easily applicable to the case where fine structure effects are included in the practical computation. Nevertheless in order to illustrate this effect, we have performed two MMM calculations of the Ar$^{17+}$ Lyman-$\alpha$ line in a plasma of protons ($c = 10^{-6}$) at high density ($10^{24}$ and $5 \times 10^{24}$ cm$^{-3}$, 862 eV), using a BM field distribution function. The two components of the line are resolved at the lowest density and are mixed together for the densest case, leading to an asymmetry of the line (Figs. 7a and 7b). This effect of mixing has been reported earlier [23, 24] and we will not discuss it in this paper. The conclusions relative to the variations of the shape with density, temperature and concentrations are not affected by these fine structure effect.

4. Conclusions

This paper shows the importance of ion dynamics effects on the line shapes of hydrogenic multi-charged ions. This effects are enhanced in the case of heavy radiating impurities embedded in a plasma of ligh ions. This is of great importance for astrophysical applications or for laser-produced plasmas. Nevertheless other effects must be also analysed for practical studies, like radiative transfer or turbulence effects. The method presents the advantage to be easily tractable without the help of MD simulations. This allows to treat the case of line shapes in very low correlated plasmas, which is especially difficult in the impurity case. We have for the first time verified that the ion impact limit is recovered in the low density limit. We point out that accurate field distribution functions are required in all the cases. The extensive study of the variations with the plasma conditions is a test of the quality of the preceding quantity. Although this paper is devoted to the lines of hydrogenic ions, the method is easily extensible to the case of other ions. This method will represent a powerfull key to the study of line shapes in various plasma conditions, even if in some cases it might be improved by an accurate treatment of the electronic broadening.

Acknowledgments

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References