Study of the Z-scaling of the $3s-3p$ line in strongly coupled plasmas through computer simulations

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Plasma diagnostics through the analysis of spectral line shapes is a widely known technique which gives very reliable values of the electron density [1]. This technique is based on the comparison of the experimental data with the theoretical calculations of the line profile, which, in many cases, is mainly due to the Stark effect.

Currently there are several theoretical models of Stark broadening which work very well and can explain many of the experimental results. However, there are some situations in which these standard theories cannot reproduce the experimental data. One of these situations is the Z-scaling of the width of the isolated lines. These lines are especially suitable for study under the impact approximation. However, even when all the requirements of this approximation are fulfilled, the dependence of the line width with the charge of the emitter that is predicted by the theory (Z^{-2}) does not correspond with the one observed in the experiments [2, 3].

To find out the reason behind the discrepancies between the theoretical calculations and the experimental data, we will study the profile of the $3s-3p$ transition from the first 4 elements of the Be isoelectronic series. We will calculate those profiles with two different computer simulation techniques and we will compare the results with the theoretical models and with some experimental results.

Computer simulations

The computer simulation can be divided into two parts. First, the calculation of the electric microfield undergone by the emitter and then the calculation Stark profile. Regarding the calculation of the field, in this work we have used two different techniques. The first one, Independent Particles (IP), is very well known and its main assumption is that the particles do not interact with one another [4]. The second technique, Molecular Dynamics (MD), is much more complicated and takes into account all the interactions between particles [5]. Despite MD simulations having been used in other fields, its application to tStark Broadening calculations is quite new. In this technique we use a cubic cell with periodic conditions, all the particles interact with

one another and the time step is small enough to avoid numerical heating. We use a regularized potential for the atractive interactions (to avoid short distance divergences) and pure Coulomb for repulsive interactions. Before starting the line calculation, the plasma has to be equilibrated. To do that, we let the plasma evolves until the kinetic and potential energy are stables. In this stage we set the ion masses equals to the electrons to speed up the equilibration process [1].

The second part, the calculation of the Stark profile, is the same in both cases: provided the electric field, the time evolution operator is calculated by solving the Schrodinger equation. Then, the correlation function of the emitter is obtained, and finally the profile shape is computed via Fourier trasform.

Theoretical models: Impact approximation

The lines of the transition $3s-3p$ are isolated lines and hence are very good candidates to be treated under the impact approximations In this approximation it is assumed that the broadening of the line is caused by "collisions" and then the statistics of the field do not have any role. Attending to the strength of the collisions (how much they disturb the emission) we can distinguish between the strong and the weak collisions approximation. In any of these cases, the width of the lines is proportional to the inverse of the square of the nuclear charge of the emitter: $\Delta\Omega \propto Z^{-2}$ [6], where $Z = Q+1$, being Q the net charge of the emitter.

These two models, which work quite well in other cases, are not able to explain the experimental meassurements of the transition $3s-3p$. Not only are the values of the widths different but also the dependence of the line width with Z does not fit [2, 3].

Results

In all the emitters studied (B II, C III, N IV and O V), the states $3s$, $3p$ and $3d$ with fine structure are included in the calculations and all of them evolve together (with quenching). The results are that there are 3 spectral lines which happen to have the same shape and width (corresponding to the fine structure of the state $3p$). In the following we will talk about the width of a single line, since the rest of them have the same behavior.

First we are going to analyze the results from the IP simulations. In this case the plasma model used is the same as the one in the theoretical models. The difference is that in the simulations there are no mathematical approximations in the profile calculations: the line shape is computed by solving numerically the evolution equation of the emitter.

[1]The details of the MD simulation technique will be explained in much more detail in other work devoted exclusively to that type of simulations. In any case the description of the simulation technique can be found in [5].

In figure 1 we can observe that the result from the Independent Particle simulations has the same trend as the one predicted by the models. This figure corresponds to a case with $N = 10^{22}\,m^{-3}$ and $T = 40000\,K$, but the same result can be observed for a wide range of densities ($10^{22}\,m^{-3} - 10^{25}\,m^{-3}$) and temperatures ($40000\,K - 100000\,K$). The agreement between the Independent Particles and the models means that the approximations done in the models are perfectly valid in those cases, since the "exact" calculations give the same result as the models. Thus, there should be something else that is not included here (either in the simulations or in the models) and which is responsible for the discrepancies between the theory and the experiments.

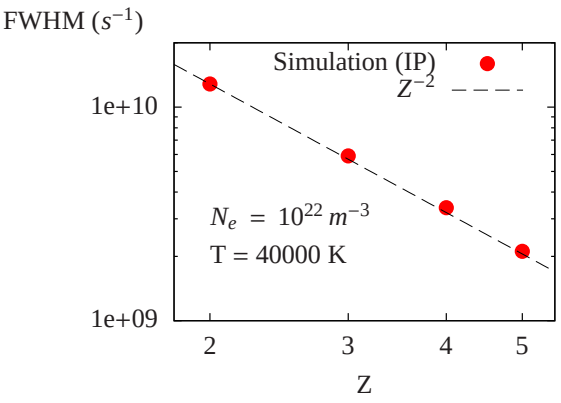

Figure 1: *Full width at half maximum (FWHM) of one of the lines from the transition* $3s-3p$ *as a function of Z (red dots) and the trend given by the models (dashed line).*

The results from Molecular Dynamics simulations are supposed to be more realistic, since all the interactions between particles are included. In this scenario, the dynamic of the field (collision frequency, correlation function, ...) depends on the charge of the ions, contrary to what happened in Independent Particles. Moreover, there is a new phenomenon that could play an important role in the broadening mechanism: the recombination process. Due to the interaction between particles, eventually the electrons can be trapped by the ions. When that happens the pair electron-ion can be seen as an ion of charge $Q-1$. Thus, the line observed is no longer visible since the emitter has changed its atomic structure completely: now it is an ion of a different species, and this is equivalent to a complete loss of coherence in the emission. This *recombination broadening*, that depends on the coupling parameter of the plasma and on the charge of the emitter, is not included in theoretical models and could play a very important role in some plasmas.

To study the Z-dependence with the Molecular Dynamics simulations it would be necessary to simulate several cases of density and temperature (as we did with Independent Particles). However, this technique is much more expensive and the computational time required for this kind of study is not affordable. Alternatively, we have performed several simulations with the conditions of some experimental cases. This way we can compare the results obtained with this technique with the experiments and with the results obtained with Independent Particles.

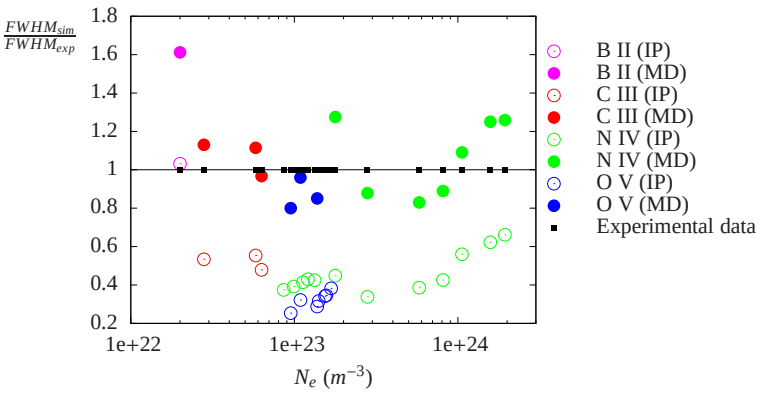

Figure 2: *Comparison of the full width at half maximum obtained form simulations ($FWHM_{sim}$) with the experimental measurements ($FWHM_{exp}$). Independed particles (IP) with hollow circles and Molecular Dynamics (MD) with dots. The experimental results have been obtained from [7], [8], [9] y [10].*

In figure 2 we can observe the comparison of the simulations results and the experimental values of the widths of the lines. The widths obtained by IP simulations are systematically smaller than the experimental values. On the contrary, the values obtained by MD simulations are in good agreement with the experimental ones. The dispersion of the results is due to the uncertainties of the density and temperature in the experiments.

As we said, the main difference between IP and MD is that in the latter the charge of the emitter affects the field dynamics and includes the recombination width. Hece, in view of the results we can conclude that the effecs of the interactions between the emitter and the perturbers actually have a non-negligible effect in the line widths, and it could be the cause of the discrepances between the experiments and the theory. Nevertheless, a more detailed study of the results of the Molecular Dynamics simulations would be very helpful to understand the phenomenon better.

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