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Report on the third SLSP code comparison workshop

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A R T I C L E I N F O

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A B S T R A C T

A summary of results obtained at the third Spectral Line Shape in Plasmas code comparison workshop (SLSP3) is given. As in the SLSP1 and SLSP2, a standardized set of case problems was decided on in advance and then investigated at the workshop. A presentation of these cases, together with a discussion of selected results, is provided here.

1. Introduction

The shapes of spectral lines emitted from a plasma contain information on the medium under consideration and can be used as a diagnostic tool, provided a suitable model is used. Except for limiting cases, line-shape calculations imply the use of computer codes of varying complexity and requirements of computational resources. There exist several such codes and, necessarily, limits of applicability, accuracy, and in the end, results, differ from one to another. The Spectral Line Shape in Plasmas (SLSP) code comparison workshop [1] was organized to compare the different computational and analytical methods developed and used by plasma spectroscopists. After the success of the first two workshops (SLSP1 [2] and SLSP2 [3]) in 2012 and in 2013, it was decided to continue the workshop with a focus on the most problematic issues and a deeper analysis in the numerical calculations. The SLSP3 was organized in Marseille in 2015. A total of 31 codes and models were used. We present here the list of cases considered at the workshop and we then discuss results.

2. Cases definition and code comparisons

The workshop was organized as a series of cases to be addressed using line shape codes. The cases were defined in such a way so that a given set of issues relevant to line broadening modeling could be investigated. As in the previous two SLSP workshops, a number of transitions have been selected and a grid of densities and temperatures has been defined for each case. A summary is presented here; information is also available in the SLSP3 call for submissions file (http://plasma-gate.weizmann.ac.il/projects/slsp/slsp3/).

2.1. Cases 1 and 2: slow and fast fields in ion dynamics (coordinator S. Alexiou)

These cases are classical ion dynamics tests. The hydrogen Lyman α and Lyman β lines are considered in an ideal one-component proton plasma, with straight line trajectories and assuming Debye screening with electrons but without electron broadening. A density of 10^{18} cm^{-3} and equal electron and ion temperatures of 1, 10, and 100 eV were considered. Only linear Stark effect is retained. Since a considerable spread between codes was found in the SLSP1 and SLSP2 workshops [4], it was decided here to specify fine-grained conditions. The contribution of slow- and high-velocity particles to the line broadening has been examined, using the median velocity $v_{1/2} \simeq 1.538\sqrt{k_B T/m}$ as a boundary. Seven codes have been used and compared to each other. Most of them are based on numerical simulations, where both the plasma microfield and the atomic evolution operator are evaluated numerically (for a review on this method, e.g., see [5]). The spread of results is much less significant than in the previous workshops. Fig. 1 shows a calculation of Lyman α at $N = 10^{18}$ cm^{-3} and $T = 10$ eV as an example. Good agreement between simulations is also observed in general when the contributions of $v < v_{1/2}$ and $v > v_{1/2}$ are examined individually. Discrepancies that have been observed were due to a problem specification issue in some codes, and this was made clear by looking at the separation into $v < v_{1/2}$ and $v > v_{1/2}$.

2.2. Cases 3 and 4: ion dynamics with pre-defined field histories (coordinator D. Gonzalez)

A possible cause of discrepancy between codes that was identified at SLSP1 and SLSP2 is the microfield model used. It was decided

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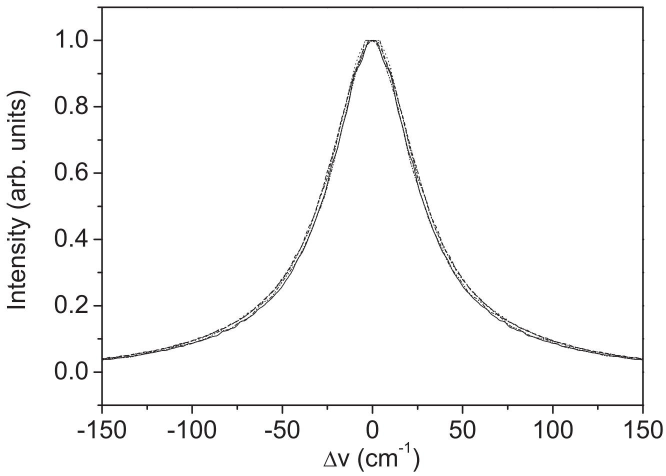

Fig. 1. Plot of H Lyman α calculated using five codes that employs the simulation technique. The codes agree well with each other. Here, a plasma density of 10^{18} cm^{-3} and a temperature of 10 eV were assumed.

to address this issue at SLSP3 using field histories generated beforehand, to be used as an input to line shape codes. Case 3 corresponds to Lyman α and case 4 corresponds to Lyman β. Four field histories have been used in each case. Four simulation codes have been tested. In general, the codes agree well with each other. Tests of the evolution operator unitarity have been performed and results indicate a small deviation only (see Fig. 2).

2.3. Case 5: convergence of line broadening in ideal plasma model (coordinator J. Rosato)

Computer simulations are considered ab initio and are commonly taken as a benchmark for line shape models, at least for hydrogen-like transitions. However, a recent study [6] has indicated that caution must be taken if an ideal plasma model with no Debye screening is used. The total microfield generated by distant particles can contribute to the line broadening in a significant manner, even though the microfield generated by each distant particle considered individually has a negligible influence. The case 5 of SLSP3 was devoted to this issue. Calculations assuming a series of spherical plasma volumes with progressively increasing radii and respectively increasing number of particles have been performed. Fig. 3 shows an example of result. The full width at half-maximum obtained from two simulation codes is plotted against the number of particles. There is a noticeable increase and the curves indicate a logarithmic trend, which is in agreement with analytical models based on collision operators. This result confirms that an artificial setting of an infinite Debye length in the numerical simulations able to work with an infinite Debye length can lead to a significant overestimate of the line broadening.

2.4. Cases 6 and 7: isolated lines (coordinator S. Sahal-Bréchot)

There have been disagreements between experiments with observations of isolated $\Delta n = 0$ lines and different theoretical calculations; e.g. see [7]. These disagreements have been noticed for many lines of different ionized atoms, the widths of which have been measured. They concern the quantum close-coupling method, which should be one of the most rigorous approaches (CCC, R-Matrix, methods based on the Schrödinger equation); it often disagrees with experiments and other methods. Here, it was decided to continue the investigations done at SLSP1 and SLSP2 and to examine in further detail the broadening of the 2s-2p Li-like series. Both line shapes and partial inelastic cross sections have been considered. Cases 6 and 7 concern Li I and B III, respectively. Calculations have been done using both analytical impact formulas and numerical simulations. For the sake of clarity in comparisons, only the 2s and 2p levels have been retained; the effect of higher levels and of Feshbach resonance on the line width are not discussed here. A detailed review of the methods and codes can be found in [8]. Fig. 4 shows the full width at half-maximum of B III 2s-2p at $N_e = 10^{18}$ cm^{-3} in terms of the energy as an example of result. Basically, the deviations observed here are due to differences in models.

2.5. Cases 8 and 9: external fields (coordinator S. Ferri)

The influence of external fields on the line broadening was investigated at SLSP3. In case 8, the C VI Lyman α is considered in conditions similar to those found in laser-driven capacitor-coil target experiments [9], with a strong external static magnetic field, of several kiloteslas. Case 9 corresponds to Ar XVIII under external harmonic perturbation, with oscillating electric and magnetic fields. The latter induces satellites on the line shape, which can be

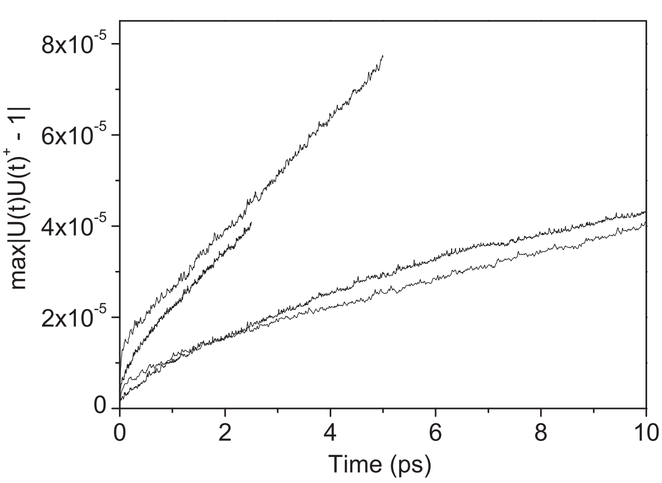

Fig. 2. Deviations to unitarity in simulation codes have been examined through an evaluation of $\max|U(t)U(t)^{\dagger} - 1|$, which provides a measure based on the matrix elements of the evolution operator $U(t)$. Here, this plot shows an example of results obtained from one code in the four Lyman α subcases. The small ($\sim 10^{-5}$–10^{-4}) values indicate that unitarity is well preserved. This trend is also present on the other simulations that were used at the workshop.

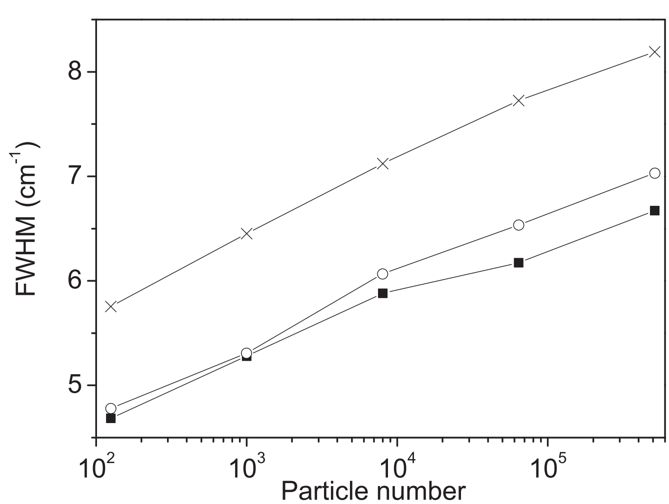

Fig. 3. Plot of the full width at half-maximum (FWHM) of Lyman α obtained using two computer simulations (squares, circles) and an analytical model based on collision operator (crosses) in terms of the number of particles present in the simulation box. The increase indicates that the field generated by distant particles contributes to the line broadening in a significant manner.