Accuracy of simplified methods for ion dynamics in Stark profile calculations

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To assess the accuracy of simplified methods for the treatment of ion dynamics in Stark-broadening theory, we have compared two such methods, the relaxation theory and model microfield method, against benchmark calculations for the CVI H_α line. It is shown that both methods show poor agreement at low densities. [S1063-651X(99)12702-8]

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I. INTRODUCTION

The shape, or width, of Stark-broadened spectral lines is widely used for plasma diagnostics as the profile can be a sensitive function of the temperature and/or the density. Moreover, Stark-broadened spectral lines can provide an important testbed for analytic statistical mechanical models as experiments can directly observe line profiles. Thus the verification of an accurate treatment of the effects of the plasma electrons and ions on an emitter is important for both theoretical and experimental reasons [1]. In particular, a difficult problem that often arises for hydrogenic lines is the effect of the ion dynamics. The difficulty is due to the overlapping strong, multiparticle collisions inherent in the dynamical ion interaction. Despite these problems, we now have reliable methods of treating this problem by the collective coordinates method [2], the frequency fluctuation method (FFM) [3], and potentially the approach of Boercker, Iglesias, and Dufty [4]. Moreover, with the accessibility of computational power, numerical simulations have become the benchmark used to validate other methods [5–9]. There are also older methods, including the relaxation theory (RT) of Greene [10] and the model microfield method (MMM) [11], that have also been proposed for hydrogenic ion lines [12]. The central motivation of this work is to provide a measure of the accuracy of these two older nonsimulation techniques. Indeed, here we evaluate statements that the nonsimulation techniques are ''valid'' or '' appropriate'' [13], finding that these claims are unsubstantiated.

We present numerical simulations to test the accuracy of two nonsimulation models, the relaxation theory of Greene [10] as implemented by Oza *et al.* [14] and the MMM [12], for the H_α line of C VI. We note, incidentally, that this transition has been of importance for x-ray laser schemes [15]. To provide a straightforward comparison between the numerical simulations and the RT and MMM results we will use the halfwidth at half maximum (HWHM) as the figure of merit.

II. CALCULATIONS

The assumptions in all the calculations presented here are the same, i.e., only dipole interaction, C^{5+} perturbers, no Doppler effect, no fine structure, and no perturber-perturber interactions. Further, we have used the same screening lengths and plasma frequency as used in Ref. [13]. Moreover, since MMM and RT do not take into account perturber-perturber interactions, we have used an independent particle model, and have properly taken into account the hyperbolic trajectories of the plasma perturbing ions. That is, the perturbers are moving in hyperbolic paths, whose times of closest approach are uniformly distributed and whose asymptotic velocities and impact parameters are selected according to the collision-time statistics method [7]. However, we note that for the parameters considered, the ions and the electrons are very weakly coupled, moving essentially undeflected in straight lines.

It is worth noting that the extension of independent particle simulations to the case of charged emitters has necessitated overcoming a technical complication, since the standard parametrization of the hyperbolic trajectory requires that each perturber has its own '' time,'' corresponding to its eccentricity and velocity, while in the simulation we need the particle position for each value of real time t, and it is awkward and time-consuming to have to solve for the real time at each time step. This technical complication has been resolved with simple, highly efficient inversion formulas [16] and with these the simulations are as fast as those for neutral emitters. Although this development is important for a general code able to deal with ion perturbers, in the present case for the lowest densities considered the deviations from the straight line trajectory are quite minor.

We have also employed the Gigosos *et al.* [9] group-theoretical formulas and benchmarked the code against standard calculations [7,8,17]. Because simulations can only be carried out for a finite time interval, an extrapolation of the

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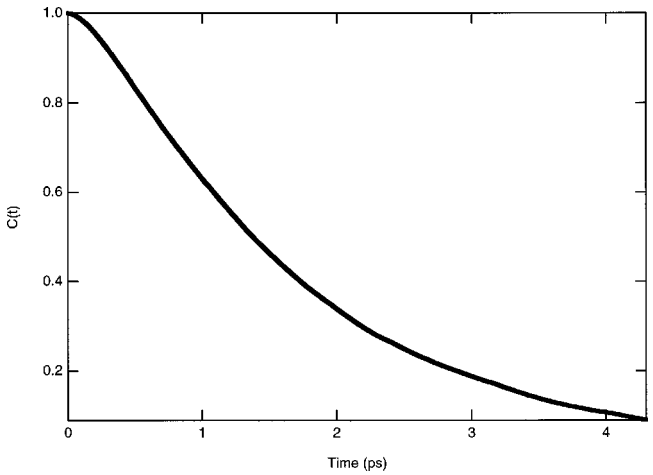

FIG. 1. Autocorrelation function $C(t)$ due to C^{5+} perturbers only. The electron density is 10^{17} cm^{-3} and the temperature is 20 eV. One thousand configurations were used.

autocorrelation function has been employed for longer times, i.e., once an exponential falloff has set in, to avoid unphysical oscillations (''ripples'') in the final profile. This exponential decay is expected at long times where the impact theory is valid, but noise is substantial for these long times so a large number of configurations would be required to smooth the computed autocorrelation function. For hydrogenlike lines this exponential decay is quite straightforward to identify. Figures 1 and 2 illustrate this point by plotting, respectively, the autocorrelation function $C(t)$ [2], which is simply the Fourier transform of the line profile, normalized to be unity at $t=0$, as a function of time and the quantity $-\ln[C(t)]/t$ as a function of time. These simulations were made at an electron density n_e of 10^{17} cm^{-3} and a temperature of 20 eV, taking into account only ion perturbers and using 1000 configurations. From Fig. 2 the exponential behavior is easily identified as the flat region. Further, using the

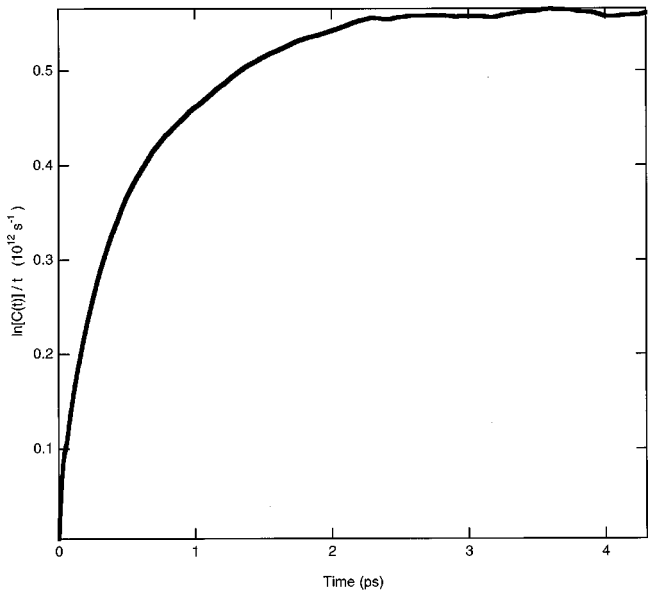

FIG. 2. Exponential behavior in the tail of $C(t)$. The parameters are the same as in Fig. 1.

TABLE I. HWHM (meV) comparison (Refs. [13,14]).

Calculation	10^{17} e/cm^3	10^{18} e/cm^3	10^{19} e/cm^3	10^{20} e/cm^3
MMM	0.28	1.05	3.5	12.7
RT	0.85	1.55	4	19
Full simulation	0.395	1.31	3.85	11.6
Ions only	0.382	1.236	2.93	5.6
Electrons only	0.013	0.109	0.803	5.97

value Φ of this flat region and extrapolating $C(t)$ as $e^{-\Phi t}$ allows us to complete the Fourier transform procedure and obtain a smooth profile.

The electron broadening is treated in the impact approximation and to avoid ambiguities in the comparison we have used the same formulas as Refs. [12,13]. [However, we have squared the right-hand side of Eq. (A2), which is incorrectly given in Ref. [12].] Although these formulas may be improved upon [18,1], we have used them to make the comparisons straightforward.

III. RESULTS

Table I summarizes the results. The temperature is taken to be 20 eV in all calculations and all the HWHMs are given in meV. In Table I the HWHM are shown as calculated in the MMM, and the RT. Also the present simulations are shown for the following two cases: with only ion perturbers (''Ions only'') and the results convolved with the electron profiles as discussed above (''full simulation''). Finally, for the purpose of discussion the electron HWHM (''electrons only'') is included. The RT clearly has a serious problem at low densities, resulting in discrepancies of up to a factor of 2. Further, it predicts a width larger than the ion impact width, which is incorrect, as the ion impact width is the maximum possible width at a given density and temperature. This is a known problem [8] that could be mitigated by the frequency separation technique (FST) [19]. It is not clear if discrepancies with the RT at high densities are due to a different electron broadening operator, since electron broadening is important at the highest density considered. Hence this comparison indicates that the RT has a serious problem in the transition to the ion impact regime.

The MMM shows best agreement at the highest density with increasing discrepancy as the density decreases. Thus the error in the MMM reaches 30% at the lowest density considered. We note that for diagnostics this could be serious, since the dependence of the width on the electron density is not linear. In fact the density dependence is close to the square root of the electron density in this regime. This is interesting, as one might have assumed, since at low density the density dependence is linear (ion impact regime) while at high density the density dependence is $n_e^{2/3}$ (quasistatic regime), that the intermediate regime would be characterized by a power law given by n_e^X with $1 \geqslant X \geqslant 2/3$. However, the results disprove this intuitive expectation, showing an $X \approx 1/2$.

As an example, MMM-based diagnostics would overestimate the density by a factor of 2 at 10^{17} cm^{-3}. That is, the

simulation results for the lowest density are reproduced by the MMM at a density roughly two times higher. For the two higher densities considered, electron broadening is significant, so the discrepancies in the HWHM, which contain both ion and electron contributions, are smaller.

IV. DISCUSSION

In review we point out that for neutral emitters, the MMM has been used for some time, as no alternative method existed. Hence, by interpolating between the impact and quasistatic limits, the MMM was able to approximately account for ion-dynamical effects. Importantly, we note that the best the MMM can achieve in terms of the impact limit is the perturbative dipole impact limit, which has been known for many years [20] to be inadequate. This is the source of the reason that the MMM does not go correctly to the impact limit as a function of the perturber density. With regard to the results presented here, the RT seriously overestimates the width at low densities, while the MMM underestimates it by 30%.

This level of inaccuracy is of importance in the context of the line broadening models, like the RT and MMM, which previously have been used to supply line profiles over a wide range of the density and temperature parameter space. Moreover, this inaccuracy is independent of experimental results and cannot be attributed to ignored effects in the simulation, as the numerical simulation is the exact solution of the model that the MMM and RT attempt to calculate. That is, the numerical simulation has solved the nonperturbative calculation, including only dipole terms and neglecting fine structure effects. In addition, it is important to understand that the cases studied here should be benign for the MMM as the trajectory effects are relatively unimportant.

With the results presented in Table I one can state that the comments made in Ref. [13] are wrong concerning the reliability of numerical simulations in the impact regime. Indeed, whether one employs molecular dynamics (MD) or an independent particle model, as is the case here, the collision-time statistics method correctly recovers the full impact theory results (and not just the perturbative impact theory results), as has been demonstrated by Seidel [8] and Hegerfeld and Kesting [7,17]. Further, the suggestions in Ref. [13] that the relaxation theory and MD simulations might be in error because they neglect strong electric fields are erroneous. The error in fact lies with the MMM due to the facts that (1) the MMM does not account for strong dynamic fields (as in the impact regime, there are no static strong fields), since these do not couple via the covariance; (2) the Monte Carlo calculations for static fields are not reliable for very strong fields, since these have a small probability density; and importantly, (3) because both the RT and MD simulations result in significantly larger widths than the MMM calculations. To elaborate on (3) it is noted that if MD neglected strong fields, corresponding to close impacts, these close impacts would, if correctly accounted for, *increase* the widths of the MD calculations, resulting in larger discrepancies with the MMM.

Finally, it should be pointed out that previous documented problems with MD simulations in the regime close to the impact limit [6] arose due to the altering of the collision frequency [7]; however, with the collision-time statistics method used here this problem does not arise. To overcome the problems of simulations close to the impact limit more particles need to be simulated and the time of interest of the simulation needs to be increased, resulting in a substantial increase in computer time. On the other hand, the computer time could be dramatically reduced if one employs the FST for those collisions that can be treated in the impact theory. Note that other methods also produce the correct impact limit if used in conjunction with the FST (e.g., the frequency fluctuation method and the collective coordinates method, which works even without the FST, but is then inefficient for low densities).

V. CONCLUSIONS

In the early 1970s the MMM held a special place for the calculation of neutral hydrogen line profiles when effects beyond the ion quasistatic regime were important. This special position lasted until competing methods appeared, starting with simulations [21], in the late 1970s, and was quickly followed by other methods—improved simulations, the method of Boercker, Iglesias, and Dufty [4], the collective coordinates method [2], and especially the frequency fluctuation method [3]. These alternative methods, when taken together with the failure of the MMM for emitters other than hydrogen, lead to the observation that the MMM should be used with extreme care.

In support of this word of warning we note that the MMM does not compare with data for hydrogenic emitters. This is manifested by discrepancies of factors of 2 from recent measurements [22] for the Paschen-α H-like helium line, e.g., at an electron density of 2.5×10^{18} cm^{-3} and temperature of 4.5 eV, with proton perturbers. Note that numerical simulations [23] give a full width at half maximum (FWHM) of 50 Å, which compares well with the data, compared to 24 Å predicted by the MMM [12]. Hence use of MMM results in, e.g., astrophysical analysis, may be problematic and lead to incorrect interpretations of the data.

The relaxation theory also does not approach the ion impact limit correctly. In particular, Oza *et al.* [14] obtain excellent agreement between the RT and ion impact results for a parameter range where the impact theory is *not* valid and realize that this agreement may be fortuitous to a certain extent. The point is that the impact theory gives, as already pointed out [24], the *maximum* possible width for a given set of plasma parameters. However, the RT overestimated the width (by a factor of roughly 2) at the lowest density considered; this problem might be partially treatable by the FST.

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