Stark broadening of hydrogen lines in dense plasmas: Analysis of recent experiments

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In recent years experiments conducted by a number of different groups on line broadening of hydrogen lines, mainly H_α on dense plasmas of densities larger than or equal to 10^{18} e/cm^3 have claimed significant differences from the predictions of the standard theory. At these high densities the standard theory predictions depend on some cutoffs, necessary to preserve unitarity, the long range approximation and to ensure the validity of a semiclassical picture. Furthermore, a new, supposedly "advanced" theory based on a number of incorrect assumptions and/or approximations with extra exotic effects has claimed good agreement with these experiments. In this work we produce benchmark simulation calculations for these data to identify relevant and not relevant physics for the parameters of these experiments. In this way, we evaluate claims of electron-ion coupling, ion dynamics, electron vs ion broadening, nonimpact effects, and nonperturbative effects. At least one data set is seen to be dubious, in agreement with previous analyses.

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I. INTRODUCTION

In recent years experiments conducted by a number of different groups [1–5] on line broadening of hydrogen lines, mainly H_α on dense plasmas of densities larger than or equal to 10^{18} e/cm^3 have claimed significant differences from the predictions of the standard theory(ST) [6,7]. At these high densities the standard theory predictions depend significantly on some cutoffs, necessary to preserve unitarity, and the long range approximation to ensure the validity of a semiclassical picture [8]. Preserving unitarity and the semiclassical picture is important at low velocities, while preserving the long range approximation is important at high velocities. The resulting width has contributions from the large impact parameter phase space $\rho \geqslant \rho_{min}(v)$, presumably computed correctly by ST plus a "strong" collision contribution from impact parameters $\rho < \rho_{min}(v)$. The contribution of this later part may not be computed within ST and only unitarity-based error bounds may be given. These may be comparable to and eventually larger than the large impact parameter phase space contribution at high enough densities.

Furthermore, a new, supposedly "advanced" theory(AGT) [9] based on a number of incorrect assumptions and/or approximations with extra exotic effects [10,11] has claimed good agreement with these experiments. The numerous problems with this theory have been pointed out [8,12–15] and are summarized later on and as a result this theory is not a viable one. In addition, as a result of a debate concerning the broadening of isolated ion lines [16–19], the importance of penetration has been realized. This is a very strong effect at short impact parameters, much stronger than any assumed electron-ion coupling or other exotic effects. Indeed the reason the electronic contribution from short impact parameters is small is not some kind of electron-ion coupling [9]. In fact this contribution is small even in the absence of ions. Furthermore, because of penetration, in certain cases such collisions are quite weak, so that unitarity is often not an issue and the so-called strong collisions are actually weak or even very weak. Although this effect has now been included analytically into the ST [20], we will not deal with it here, as no other method accounts for this effect and because it is not at the heart of the controversy regarding the experimental results. Until now it is by no means clear if electron broadening or strong collisions are the dominant issue for these experiments.

In the present work we have performed simulation calculations. These calculations serve to provide benchmark results, as well as to determine important physics aspects for the line and parameters in questions. These aspects are electron-ion coupling, quasistatic vs ion dynamical issues, nonperturbative aspects, and nonimpact electron effects. In addition, only dipole interactions are considered in simulations, as well as ST. Although results quoted as ST usually contain also some estimate of quadrupole and inelastic contributions, we have not included these conbutions in our calculations labeled ST, in order to isolate the dipole contribution under study here. Finally, we should stress that in the present work we do not examine in detail the experiments, as this has been done elsewhere [5,12,14]. Since our purpose is to identify the relevant physics in the parameter range reported by the experiments, experimental issues or problems are not discussed at length here.

II. SIMULATION CALCULATIONS

For the H_α line, simulation calculations were carried out as discussed in [21]. These calculations serve a number of purposes, as already discussed: They provide benchmark theoretical results and allow the detailed investigation of a number of issues, such as dynamic vs quasistatic ions, nonimpact electron effects, and electron-ion coupling. These investigations are very important in guiding theoretical efforts as well as theory-experiment comparisons. For instance they address issues that simpler theories like ST and AGT cannot answer. In addition when, for example, nonimpact effects are important, then impact-based theories like AGT and ST are *expected* to overestimate the actual width.

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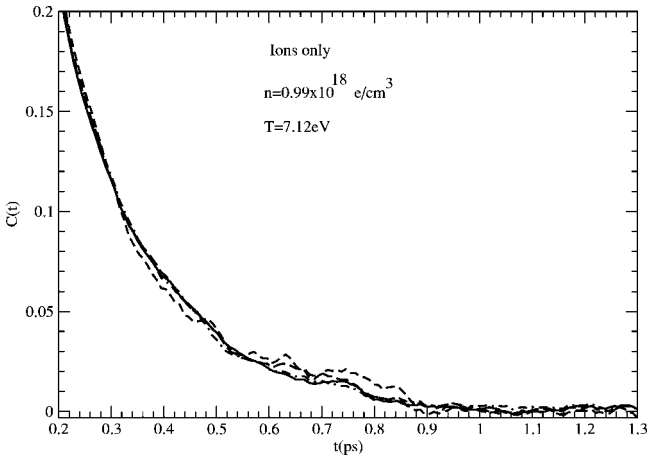

FIG. 1. Convergence for ionic autocorrelation functions.

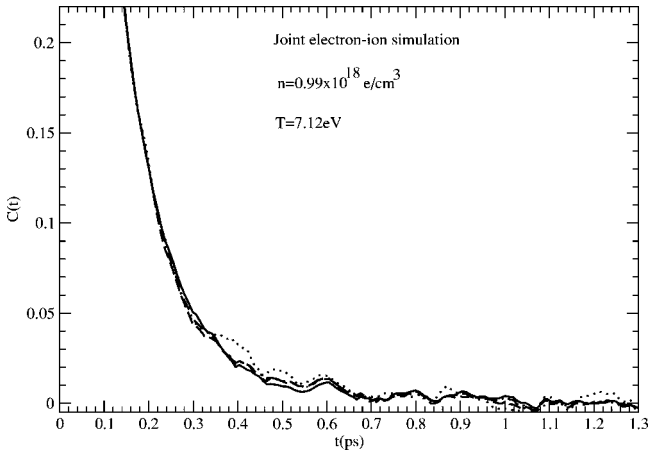

FIG. 3. Convergence for joint autocorrelation functions.

A. Description

Random positions and velocities of the plasma electron and ions are generated according to the collision-time statistics [22,23] method and for each configuration the Schrödinger equation is solved to obtain the time evolution of the atomic wave functions in the time-dependent plasma microfield. This information is used to compute the autocorrelation function $C(t)$, whose Fourier transform (FT) is the line profile. All such calculations employed 1600 configurations. Convergence was checked by comparing the 400, 800, 1200, and 1600 configuration results and was very well satisfied for all runs. In Figs. 1–3 the 400 (dotted), 800 (dashed), 1200 (dash-dotted), and 1600 (solid) configuration results are displayed for the pure ionic, the pure electronic, and the joint electronic-ionic $C(t)$, respectively. These figures focus on the fairly long times for which convergence is slower. The FT extrapolation is used for long times as soon as an impact form $[C(t) \sim e^{-\Phi t}]$ is detected to have set in.

B. Issues and shortcomings

We here discuss issues and shortcomings for the simulation calculations. First, regarding the applicability of simulations to high density plasmas, we note that the collision-time-statistics method is designed to recover the impact limit and not the quasistatic limit. Being an independent quasiparticle model, it does *not* include perturber correlations, as in the modern quasistatic distributions [24]. However, even at the strongest coupling considered, the differences are quite small. For this strongest coupling, we first computed the quasistatic autocorrelation function

$$C(t) = \int dE W(E) \Bigg[0.38812301 + 0.273736302 \cos\left(\frac{3x}{2}\right) + 0.051537645 \cos(3x) + 0.162884411 \cos\left(\frac{9x}{2}\right) + 0.118840579 \cos(6x) + 0.002262283492 \cos\left(\frac{15x}{2}\right) + 0.002545068929 \cos(9x) + 0.00007069635914 \cos(12x) \Bigg] \quad (1)$$

with $W(E)$ the APEX [24] microfield distribution and $x = eEta_0/\hbar$. This is the correct quasistatic autocorrelation function, in that all correlations are included. $C(t)$ was also computed by simulation after freezing the ions [that is using as the total ionic field $\mathbf{E}(t) = \Sigma_i \mathbf{E}_i(t=0)$, where $\mathbf{E}_i$ is the field of the ith ion]. Note that here the ions are independent quasiparticles and no account of their interaction is taken in the calculation, unlike the previous calculation where correlations appear in $W(E)$. Figure 4 shows the differences between the two calculations. Even at this strongest coupling the effect of perturber-perturber correlations are small. This means that there is no need to filter configurations so as to obtain the correct quasistatic field distribution for the parameters in question. For comparison in Fig. 5 we also show the APEX(solid) vs frozen ion $C(t)$ (dashed) at the lowest density point in [5], where agreement is excellent (the differences at long times are due to noise in the simulation).

In spite of these findings, the question of "at what plasma parameters is an independent quasiparticle approach no longer adequate and perturber-perturber interactions should

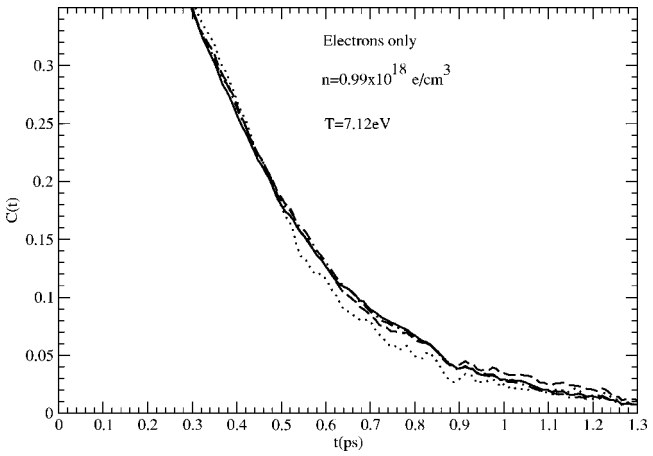

FIG. 2. Convergence for electronic autocorrelation functions.

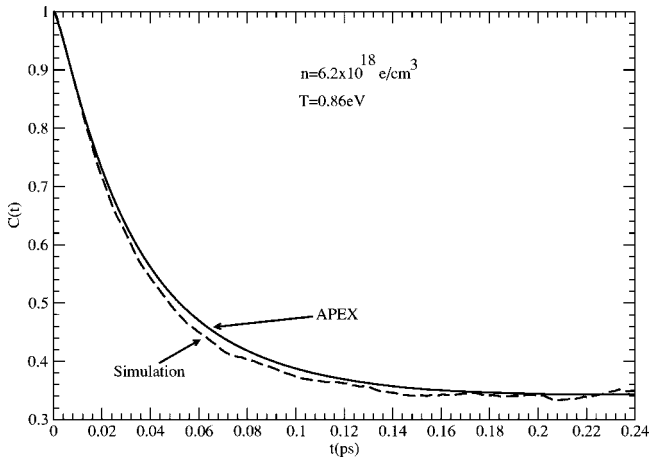

FIG. 4. APEX vs frozen ions simulation $C(t)$ for the strongest coupling.

be taken into account (by molecular dynamics in the case of simulations)" is an important one for the study of dense plasmas and should be addressed. It is not clear at this time whether the perturber-perturber interactions will be important or in which direction (i.e., broadening or narrowing the line compared to the independent quasiparticle models) their effect will be, although as Fig. 4 shows, for quasistatic broadening perturber-perturber interactions lead to a narrower line [$C(t)$ drops more slowly]. This is well-understood in the sense that APEX [or any modern distribution $W(E)$ that includes perturber-perturber interactions] is shifted towards smaller electric fields compared to the Holtsmark distribution, which does not include perturber-perturber repulsion. (There is an additional reason for the shift towards smaller fields due to the neglect of Debye shielding in the Holtsmark distribution, but this is not relevant here as our simulations use shielded fields.)

Second, we have excluded penetrating collisions from the simulation, that is particles with impact parameters $<9a_0$, the same cutoff as in Ref. [21] and ST calculations. This is not an intrisic shortcoming of simulations and is being added; the main reason for keeping this is that calculations in the dipole approximation are much faster and also on a similar basis to ST. We do not return a "strong collision" contribution from impact parameters $\rho<9a_0$ in the simulation calculations (unlike in [21]).

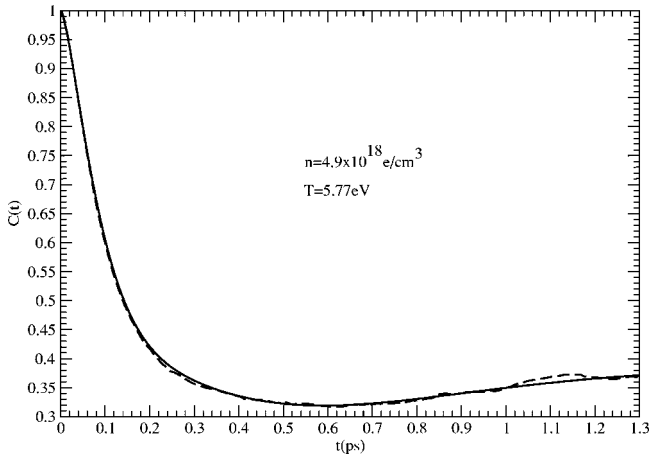

FIG. 5. APEX vs frozen ions simulation $C(t)$ for the lowest density.

C. Checks

For all experiments, extra simulation calculations have been performed. These involve computing the pure electronic and pure ionic profiles, with or without some further approximations. The goal is to judge the relative electronic and ionic contributions to the width and to check the following issues: First, it is interesting to also check a possible electron-ion coupling by comparing two different calculations, namely the simulation calculations with the joint electron-ion microfield (which retains any coupling) with the profile obtained as the convolution of the electronic and ionic profiles, each of them computed by simulation.

This is important because for many cases considered the electron and ion contributions are comparable. These calculations include exactly everything that the so-called "advanced generalized theory (AGT)" claims to do in part, namely they solve the Schrödinger equation *exactly* rather than approximately and include exactly all electron-ion coupling effects, in addition to going beyond the binary, impact, and quasistatic approximations. The only aspect these simulations do not handle correctly (though this is not an inherent shortcoming and is being added) is penetration, which the AGT does not do either.

Second, to check the static ion approximation we plot for the *weakest* coupling (i.e., smallest density/highest temperature) of each data set the autocorrelation function $C(t)$ obtained by (a) the quasistatic approximation for ions alone (solid line), (b) dynamic ions alone (no electrons, as dashed line), and (c) dynamical electrons and ions (dash-dottedline). The quasistatic approximation is valid if by the time (a) and (b) start to differ, $C(t)$ from (c) has dropped to negligibly small values. If this is the case for the weakest coupling, then there is no question that the quasistatic approximation will be valid for all experimental points, as $C(t)$ drops faster for stronger coupling.

Third, to check nonimpact electron effects, we plot $-\ln[C(t)]/t$ vs time for the pure electronic $C(t)$. Typically this quantity is scaled appropriately so that it may be plotted on the same graph as $C(t)$, i.e., so as to make it fall in (0,1). At short times the impact approximation is never valid, of course. At long times, when the impact approximation is valid, yielding $C(t)\sim\exp(-\Phi t)$, this should be flat and that constant is Φ. (This, by the way, is *the* exact nonperturbative Φ and deviations from it in simple theories are due to neglect or approximate treatment of nonperturbative effects. To the extent that the cutoffs employed are safe, the value of Φ allows one to determine the exact value of the strong collision constant.) The impact approximation is then reasonably valid if this flat regime is reached for practically all times for which $C(t)$ is important. If this is not the case, this means that short times, for which the impact approximation is not valid, are important for the bulk of the line (rather than just the wings).

TABLE I. Boeddecker [1] data.

n ($10^{18}e/\mathrm{cm}^3$)	T(eV)	FWHM	ST (FWHM)
2.44	7	153±21	0.509
3.44	7.6	182±24	0.57
4.84	8.4	187±36	0.72
7.08	9.2	228±64	0.79
9.27	10	245±54	0.91

As shown in [25–27] nonimpact electrons couple to (the slow component of) the ion field.

Last, we also computed the pure electronic contribution of impact parameters $\rho \geqslant \rho_{min}(v)$, that is the weak collision contribution, and compared this to the total electron width. This is a measure of the importance of strong collisions. Technically, in the simulation the field of an electron is zeroed if its impact parameter is less than the (unitarity-based) minimum impact parameter corresponding to its velocity. More precisely, two calculations were carried out, with $\rho_{min}(v) = 5(\hbar/mv)$ and (more correctly) $\rho_{min}(v) = 9(\hbar/mv)$ with $5 = n_a^2 - n_b^2$ and $9 = n_a^2$. This represents a measure of the relative importance of the weak vs strong collisions and hence the applicability of perturbation theory as in ST. The point is that if strong collisions are relatively important, then an accurate ST prediction strongly depends on an accurate estimate of the strong collision term.

III. THE EARLY BOCHUM EXPERIMENTS

Historically, the measurements that started this discussion were those of Böddecker *et al.* [1] produced in a helium plasma. The simulations are done for helium ions. These data (Table I) remarkably exhibited a plateau, i.e., an intermediate region of density insensitivity, followed by an increasing width with density region. As pointed out in [21] such a behavior would have been inconsistent with our understanding of Stark broadening thus far. In [21] it was suggested that although an optically thin scenario was consistent with the data, so was an optically thick scenario. Subsequently [5] it was realized that the plasma parameters diagnosed could have been in error because the diagnostics were not taken at the same time as the emission. We thus will not comment any further on agreement between theory and experiment.

It should be noted that fully nonperturbative [21] computations with the joint electron-ion microfield *agree* with the ST. These computations treat unitarity issues correctly and are able to account for nonquasistatic ions as well as for any electron-ion coupling. For the comparisons below the simulation results are not displayed, as they have already been reported in [21].

A. Electron-ion coupling

Because higher densities (favoring electron broadening) are also associated with higher temperatures (favoring ion broadening), electron and ion broadening are comparable and the independent and joint calculations in Table II show a 10% difference [25]. Also shown (EI) is the pure electron width.

TABLE II. Original Bochum [1] electron-ion coupling effects.

n ($10^{18}e/\mathrm{cm}^3$)	T(eV)	Joint(Å)	Independent(Å)	El(Å)
2.44	7	77.1	85	33.1
3.44	7.6	100	108	42.5
4.84	8.4	121.46	133	56.6
7.08	9.2	151.1	164.7	71.7
9.27	10	182	200.2	92.5

B. Nonimpact electron effects

In Fig. 6 we plot for the electronic autocorrelation function the quantity $-\ln[C(t)]/20t$ (dashed line) as well as $C(t)$ (solid line) for the joint electron-ion microfield. If the impact theory is valid, this should be (for large enough times) a constant, consistent with the impact form $C(t) \sim \exp(-\Phi t)$. Of course for short times the impact theory is never valid. As in all cases, the impact limit is initially approached fast, i.e., within 0.02 ps we are within 85% of the impact value. Subsequently, however, the impact limit is reached fairly slowly, indicating that the parameters are such that the impact theory is reaching its limits of validity. This is also discussed later in the context of Ref. [4].

C. Quasistatic vs dynamic ions

Figure 7 shows the pure quasistatic $C(t)$ (solid line), $C(t)$ obtained by dynamic ions alone (dashed), $C(t)$ obtained by quasistatic ions and dynamic electrons (dotted), and $C(t)$ obtained by dynamical electrons and ions (dash-dot) for the lowest density point. Ion dynamics does make a difference here because in the static case the decay of the ionic autocorrelation is stopped by the unshifted component while the total autocorrelation function is still appreciable. The quasistatic ion and dynamic electron profile is 43% narrower than

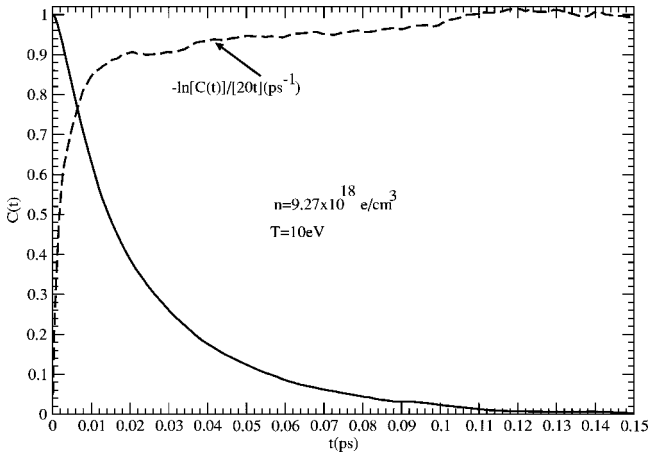

FIG. 6. Nonimpact effects at the highest density for the original Bochum experiments.

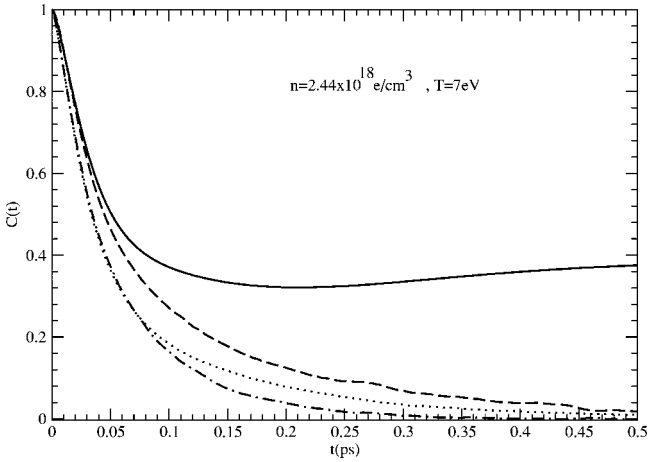

FIG. 7. Ion dynamic effects at the lowest density for the original Bochum experiments.

the convolution of the dynamic ionic and electronic profiles.

For comparison in Fig. 8 we also show the corresponding graph for the highest density point. In this case, by the time that the quasistatic and dynamic ion $C(t)$ start to differ, the autocorrelation function has decayed to smaller levels. The width obtained by multiplying the electron $C(t)$ by the analytic quasistatic ion $C(t)$ is 66% of the total width, so that ion dynamics is still important.

D. Nonperturbative aspects

The calculations have been repeated with electrons only, but this time excluding electrons with impact parameters and velocities such that $\rho v \geq 5\hbar/m$. Even at the highest density, calculations with $\rho v \geq 5\hbar/m$ and $\rho v \geq 9\hbar/m$ give a full width at half maximum (FWHM) of 85.8 and 72.14 Å, respectively, compared to the full electronic FWHM of 92.5 Å. Therefore nonperturbative effects are generally not too important for this data set.

IV. IMPROVED BOCHUM EXPERIMENTS

The previous experiments were later repeated [5] with improved diagnostics. Lower densities were reached in these experiments than the densities reported in [1]. The only density point in this new set that is comparable to the first Bochum experiment yields a width that is in agreement with the calculations in [21] and almost a factor of 2 smaller than the width reported in [1]. As in the original Bochum experiment, the perturbers are helium ions and the simulations account for this (see Table III).

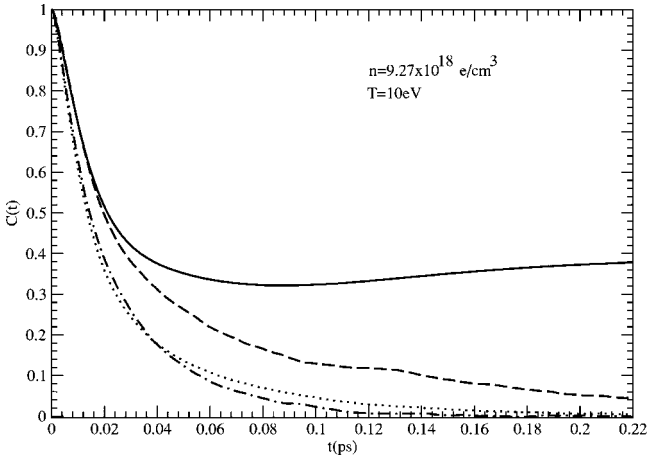

FIG. 8. Ion dynamic effects at the highest density for the original Bochum experiments.

TABLE III. Improved Bochum [5] H_α data.

n ($10^{18}e/\mathrm{cm}^3$)	T(eV)	FWHM(Å)	ST(Å)	SIM(Å)
0.49	5.77	40.3±4.3	19.47	28.1
0.53	10.46	45.4±3.8	18.8	34
0.68	6.39	47.4±6.5	25	36.47
0.99	7.12	53.1±6.5	33.47	44.65
1.35	7.82	67.8±2.5	42.5	56.33
1.96	8.4	81.9±5.6	57	69.17
2.54	8.34	96.2±9.5	70.45	81.6

A. Electron-ion coupling

Figure 9 shows the pure electron $C(t)$ (solid line), the pure ion $C(t)$ (dotted line), their product (dashed line), and the joint $C(t)$ (dash-dotted). Also shown (dash-double dot) is the pure quasistatic ion $C(t)$. It should be clear that electron-ion coupling effects are negligible and that ion dynamics is important. Already at $t=0.2$ ps the dynamic and quasistatic ion $C(t)$ are quite different; however, it is electron broadening that alleviates these differences. Table IV shows the FWHMs obtained by a joint electron-ion calculation, by independent electron and ion simulations with a subsequent profile convolution, and also the pure electronic FWHMs. It is clear that ions provide most of the broadening for all points. This could have been inferred without any calculation from the first two points, e.g., had electrons been the important contributors, then the second point should yield a width *smaller* by 25% instead of *larger* by 12%, just by virtue of the $T^{-1/2}$ electron width dependence. The ionic dominance over electrons is by a ratio of 2:1 for most points. For example, at the lowest

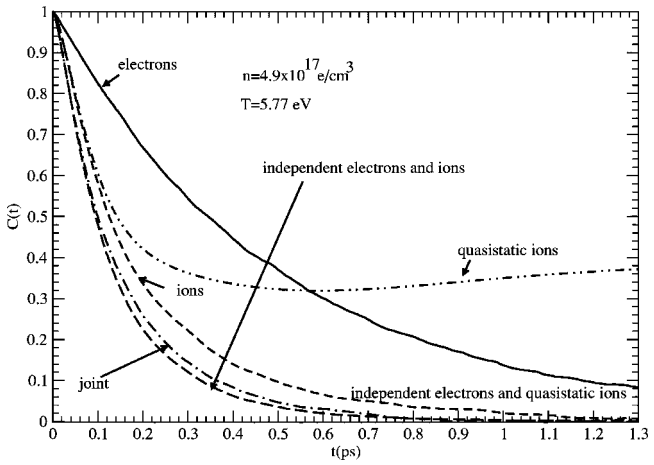

FIG. 9. Coupling effects and dynamic vs static ion behavior.

TABLE IV. Improved Bochum [5] electron-ion coupling effects.

n ($10^{18}e/\mathrm{cm}^3$)	T(eV)	Joint(Å)	Independent(Å)	El(Å)
0.49	5.77	28.1	31.95	8.93
0.53	10.46	34	35.82	8.25
0.68	6.39	36.47	38.88	11.7
0.99	7.12	44.65	50.6	15.86
1.35	7.82	56.33	59	20.3
1.96	8.4	69.17	77.37	27.6
2.54	8.34	81.6	88.16	31.77

density a pure ion (no electrons) calculation gives a FWHM of 20.28 compared to a 8.93 Å pure electron (no ions) FWHM. It is interesting to note, for example, that for the second point $T=10.46$ eV, almost twice the temperature ($T=5.77$ eV) of the first; as a result ions are more dominant and electron-ion coupling effects even weaker than the first point, as expected [25–27].

B. Nonimpact electron effects

Figure 10 plots the total autocorrelation function (solid line) versus time for the highest density point in [5]. Also shown (dashed line) is $-\ln[C(t)]/10t$ in ps^{-1} for electrons. It is seen that nonimpact effects are limited to times less than approximately 0.01 ps for which times $C(t)$ are larger than 0.9. Consequently, the use of the impact approximation for electrons is well justified.

C. Quasistatic vs dynamic ions

Figure 11 plots for the lowest density point, (a) the pure electron $C(t)$ (solid), (b) the pure dynamic ion $C(t)$ (dotted), (c) the total dynamic $C(t)$ (dashed), (d) the pure quasistatic ion $C(t)$ (dash-double dot), and (e) $C(t)$ with dynamic electrons and quasistatic ions (dash-dotted). For long times there

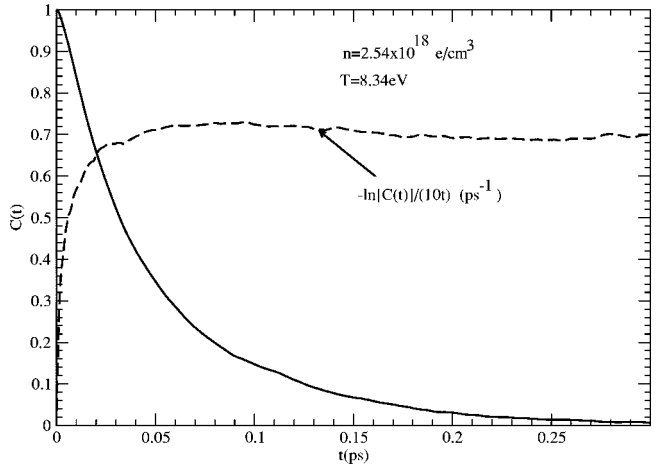

FIG. 10. Nonimpact effects at the highest density for the improved Bochum experiments.

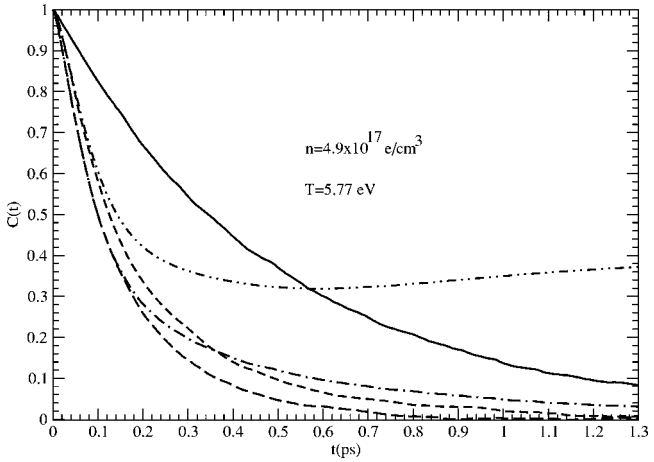

FIG. 11. Ion dynamic effects at the lowest density for the improved Bochum experiments.

are differences between (c) and (e). The widths differ by a factor of 2.5.

D. Nonperturbative aspects

The calculations have been repeated with electrons only, but this time excluding electrons with short impact parameters where unitarity is an issue. Even at the highest density, calculations with $\rho v \geq 5\hbar/m$ and $\rho v \geq 9\hbar/m$ give a FWHM of 30.6 and 27.5 Å, respectively, compared to the full electronic FWHM of 31.77 Å. Therefore nonperturbative effects are not too important for this data set.

E. Theory vs experiment

Compared to the usual excellent agreement between experiment and simulation, agreement between theory and experiment is not good, with the experimental values systematically higher than the theoretical ones. The reasons are not clear and it is not at all clear either whether they are related to similar (actually worse) discrepancies for nonhydrogenic ion lines [17–19,28–30]. It would appear that further measurements may be required to check both theoretical and experimental consistency. One way to do so is to try to make contact with established theoretical and experimental data. For instance, consider the measurement in Fig. 6 of Wiese, Kelleher, and Paquette [31]. The FWHM was measured at a density 5.7 times *lower* than the lowest density point in [5] and a temperature also lower by a factor 5.35 to be about 8.7 Å. The perturbing ions were argon instead of helium. For this case our simulation calculations obtain a FWHM of 8.2 Å, in agreement with the experimental values. At these parameters the electron and ion widths are 3.4 and about 4.8 Å, respectively. Ions are *not* static. If we extrapolate to the lowest density point in [5] using linear density scaling and inverse square root temperature dependence, we would have an electron width of about 8.4 Å, that is 2.5 times higher, consistent with our calculations in Table IV. However, for ions scaling is not that simple in this regime because in the ion-dynamic regime ions scaling is much less well-known and more complex than electron scaling. Fur-

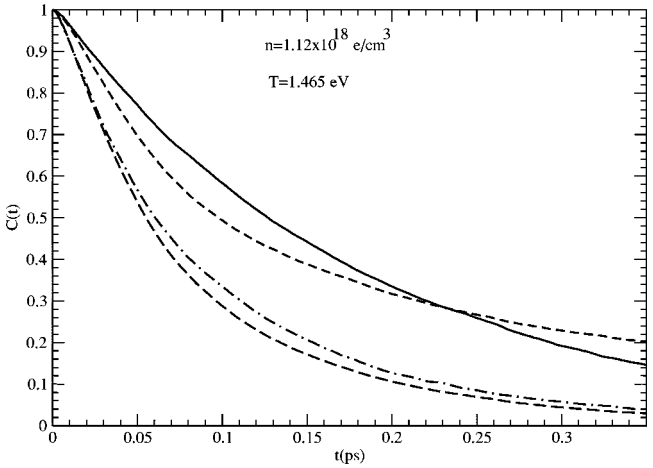

FIG. 12. Electron-ion coupling.

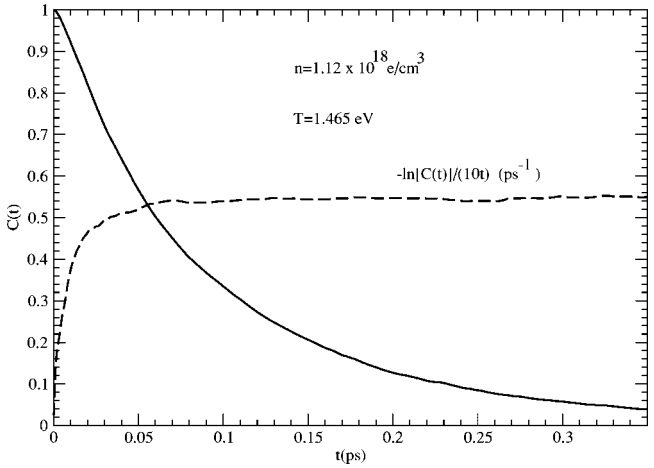

FIG. 13. Nonimpact effects for the Flih-Vitel experiments.

thermore, there is competition: the presence of lighter ions (He instead of Ar) and higher temperatures would make the ions less static, while the higher density would make them more static. Nevertheless, even if we assume that the effects of the lighter ions and higher temperature would be to produce a (maximal) linear density scaling (i.e., ion-impact regime), we *still* would not be able to produce a 32 Å ion FWHM to match the experiment. Hence the present results appear to be incompatible with established experimenal benchmarks and it might be interesting to repeat the experiments with less differences from the Ref. [31] experiments, e.g., lower densities and/or Ar driver gas, lower temperatures, etc. These could serve as small, safe steps between established experiments and the values reported in [5]. With regard to the lowest density point, it should be noted that other simulations [32] at a slightly lower temperature of about 4 eV and an electron density of $5\times10^{17}\ e/\mathrm{cm}^3$ also give a substantially lower width 30.6 Å than the one reported in [5], 40.3 Å. This behavior is also seen with the frequency fluctuation method (FFM) [5].

V. THE FLIH-VITEL EXPERIMENTS

These experiments achieve the same densities as the higher density points of the improved Bochum experiments, but at substantially lower temperatures, between 1.4 and 1.8 eV. The quasistatic ion approximation is not in doubt here.

A. Electron-ion coupling

Figure 12 shows the pure electron $C(t)$ (solid line), the pure ion $C(t)$ (dotted line), their product (dashed line), and the joint $C(t)$ (dash-dotted). The width difference is 11%. At least a part of the reason is discussed below.

B. Nonimpact electron effects

In these experiments the impact approximation is starting to be insufficient. In Fig. 13 we plot (solid line) the total $C(t)$ for the lowest density point in the set as well as the electronic $-\ln[C(t)]/10t$ in ps^{-1}. The impact limit sets in for times around 0.05 ps, at which time $C(t)$ has dropped to nearly 0.6 and is downright bad for t less than about 0.015 ps, at which time $C(t)$ has dropped to 0.8. Thus nonimpact effects might play a role for all experiments in this set. However, because in the important interval 0.02–0.05 ps the quantity $-\ln[C(t)]/t$ is close to its impact limit, nonimpact effects are not dramatic. Regarding electron-ion coupling, the nonimpact electron part couples to the ion field, thereby enhancing joint-independent calculation differences.

C. Quasistatic vs dynamic ions

Figure 14 shows the pure quasistatic autocorrelation function $C(t)$ (solid line), $C(t)$ obtained by dynamic ions alone (dashed), $C(t)$ obtained by quasistatic ions and dynamic electrons (dotted), and $C(t)$ obtained by dynamical electrons and ions (dash-dot). By the time that the quasistatic and dynamic ion $C(t)$ start to differ, $C(t)$ has decayed to very small levels, so that ion dynamics is practically not important.

D. Nonperturbative aspects

The calculations have been repeated with electrons only, but this time excluding electrons with impact parameters and

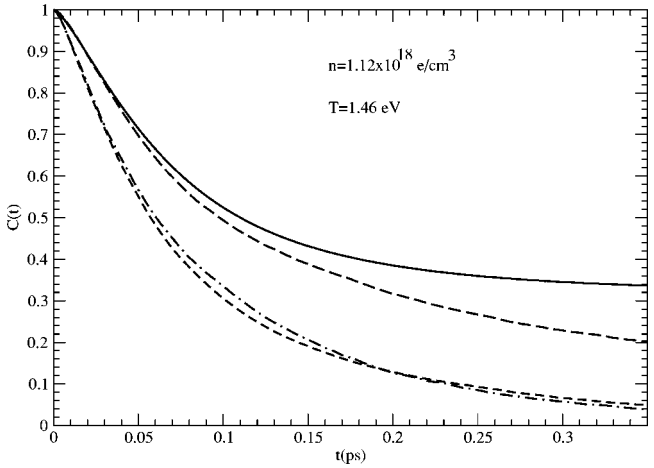

FIG. 14. Dynamic vs static ion behavior.

TABLE V. Flih and Vitel [2] H_α data.

$n(10^{18}e/\mathrm{cm}^3)$	T(eV)	FWHM (Å)	ST(Å)	SIM(Å)
1.12	1.46	49	43	43.68
1.45	1.58	58	52.16	52.84
1.6	1.67	68	56.2	56.1
2.02	1.766	81	66.73	64.52

velocities such that $\rho v \geq 5\hbar/m$. Even at the lowest density, calculations with $\rho v \geq 5\hbar/m$ and $\rho v \geq 9\hbar/m$ give a FWHM of 20.16 and 14.76 Å, respectively, compared to the full electronic FWHM of 25.2 Å. Therefore nonperturbative effects are not negligible.

E. Theory vs experiment

In spite of possible experimental problems for this data set [5], agreement with simulations is generally no worse than for the previous data set.

VI. THE UNDERWATER EXPERIMENTS

These experiments [4] are characterized by a very cold ($T<1$ eV) plasma and densities in the range $(2-6)\times 10^{18}\ e/\mathrm{cm}^3$. Griem [14] and Halenka [12] have analyzed this experiment and pointed out a number of problems. Among them the density determination is especially problematic. Nevertheless, we quote theoretical values in Tables V–VII. Agreement is poor and this has to do with the experimental problems. For instance the lowest density point agrees with the highest density point of the previous set [2]. The widths also agree, but the temperature in this experiment is smaller by a factor larger than 2. Hence this would imply a temperature insensitivity, which is at odds with the $T^{-1/2}$ temperature dependence for electron broadening. It is simple to verify that electrons dominate the broadening, as ions are quasistatic and hence cannot broaden the central component. In Fig. 5 it is demonstrated that perturber-perturber interactions might be of some importance.

A. Electron-ion coupling

Figures 15 and 16 display the pure electron $C(t)$ (solid line), the pure ion $C(t)$ (dotted line), their product (dashed line), and the joint $C(t)$ (dash-dotted). Compared to previous experiments, a deviation is now clearly visible between the independent and joint calculations. However, this is due to the fact that a substantial part of the electron distribution is

TABLE VI. Flih and Vitel [2] electron-ion coupling effects.

$n(10^{18}\ e/\mathrm{cm}^3)$	T(eV)	Joint(Å)	Independent(Å)	El(Å)
1.12	1.46495	43.68	48.87	25.2
1.45	1.58	52.84	57.04	30.25
1.6	1.67	56.1	64.9	34.72
2.02	1.766	64.52	70.9	37.72

TABLE VII. The Escarguel *et al.* [4] H_α data.

$n(10^{18}\ e/\mathrm{cm}^3)$	T(eV)	FWHM(Å)	ST(Å)	SIM(Å)
2	0.68	85.2	60.7	61.9
2.4	0.73	92	69.3	69.6
2.7	0.73	93.5	74.64	71
2.8	0.734	95.4	76.38	75.26
3.9	0.767	111.8	94.66	90.4
6.2	0.8617	147.3	128.81	118

nonimpact, as shown below. It is interesting that in spite of the stronger coupling for the higher density parameters, the difference between the joint and independent widths is roughly the same 19%.

B. Nonimpact electron effects

Defining

$$Q(t) = 4.5\sqrt{8}\frac{eE_k a_0}{4\pi\epsilon_0\hbar}, \tag{2}$$

with k corresponding to the x (solid line), y (dashed), and z (dash-dotted line) components of the total electronic electric field, in Fig. 17 we plot $Q(t)$ vs time for one configuration. $Q(t)$ figures in dU/dt for the upper level (hence the factor $4.5\sqrt{8}$ for the $l=0\rightarrow l=1$ radial matrix elements). In any case, the numerical factors are not the important thing here and what matters is the temporal variation). It may be seen that smooth features exist on a time scale that is not much less than the lifetime of $C(t)$, which is no more than 0.1 ps. According to the derivation of the impact approximation, for example in [6] or the Appendix of [33], finding an intermediate time Δt on which we can take averages becomes problematic.

In Fig. 18 we plot for the electronic autocorrelation function the quantity $-\ln[C(t)]/20t$ (dashed line) as well as the total $C(t)$ (solid line). If the impact theory is valid, this should be (for large enough times), a constant, consistent

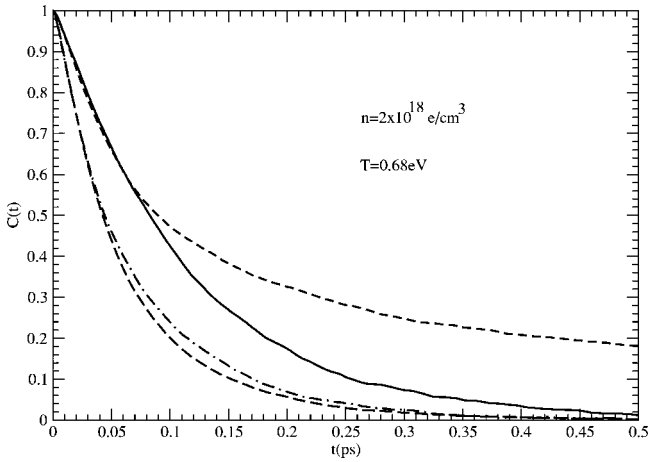

FIG. 15. Electron-ion coupling effects.

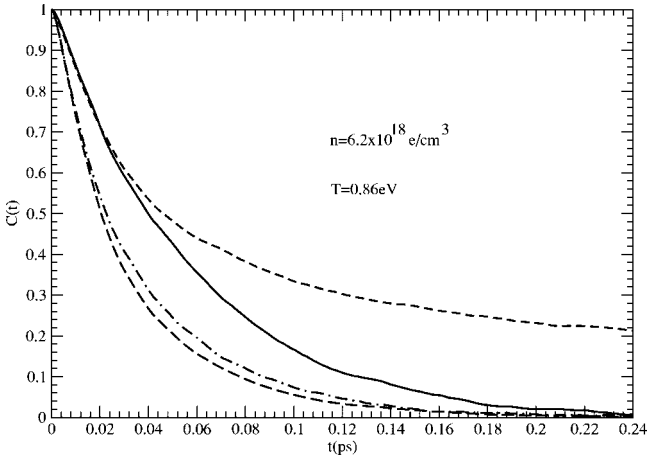

FIG. 16. Electron-ion coupling effects.

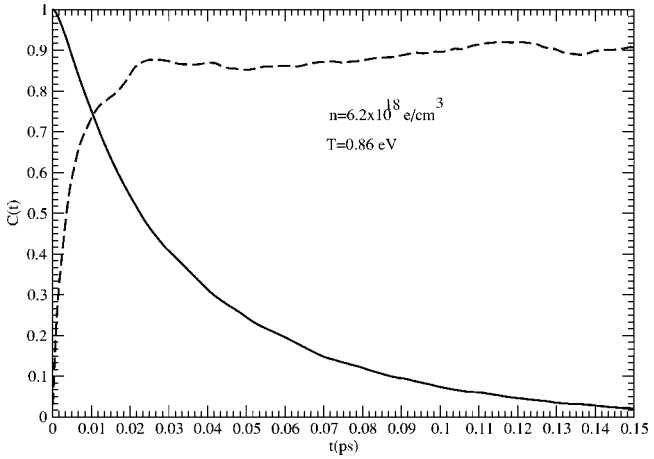

FIG. 18. Nonimpact effects at the highest density in [4].

with the impact form $C(t)=\exp(-\Phi t)$. Of course for short times the impact theory is never valid. It may be seen that this form is achieved for $t>0.02$ ps. However, from Fig. 16 we see that for $t=0.02$ ps, $C(t)$ has already decayed to 0.5. This means that nonimpact effects are important here and the impact theory needs to be dropped for the parameters in [4] (see Table VIII).

C. Quasistatic vs dynamic ions

Figure 19 plots the quasistatic pure ion $C(t)$ (solid), the dynamic pure ion $C(t)$ (dashed), and $C(t)$ with dynamic electrons and quasistatic ions (dotted) as well as $C(t)$ with dynamic electrons and ions (dash-dot). Again, for the times for which the full $C(t)$ is appreciable, the differences between the quasistatic and dynamic ions is small. The final width difference is 4% with the electrons+quasistatic ion calculation giving the larger width. This may seem strange, given that ion dynamics will not decrease the width. However, the calculation labeled electrons+quasistatic ions involved convolving the pure electronic with the APEX-integrated quasistatic ion profiles and hence is an independent electron-ion calculation, while the fully dynamic result is a joint electron-ion simulation which is narrower than the corresponding independent result.

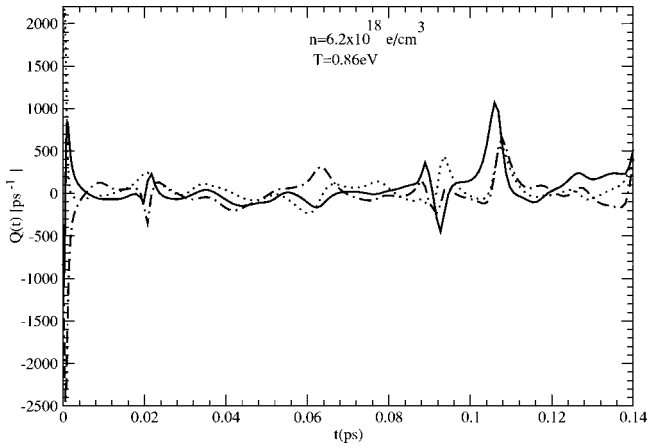

FIG. 17. Typical microfield variation for the highest density point in [4].

D. Nonperturbative aspects

The calculations have been repeated with electrons only, but this time excluding electrons with impact parameters and velocities such that $\rho v \geq 5\hbar/m$. The electronic width at the highest density is now 49.6 Å, compared to 85 Å when such collisions were not excluded. Corresponding calculations with $\rho v \geq 9\hbar/m$ gave a FWHM of 24.6 Å. Even at the lowest density calculations with $\rho v \geq 5\hbar/m$ and $\rho v \geq 9\hbar/m$ give a FWHM of 25.7 and 14.76 Å, respectively, compared to the full electronic FWHM of 40.4 Å. Therefore nonperturbative effects are quite important for this set.

VII. "ADVANCED GENERALIZED THEORY"

One theory that has claimed very good agreement with the high density experiments is the so-called "advanced generalized theory" (AGT) with various add-ons. The name would seem to be unfortunate, as it is definitely not general (for instance, since it is tied to the choice of a parabolic basis, it does not generalize to arbitrary emitters and it also is unable to handle a nonquasistatic ionic component) and it is very unclear with respect to what it should be considered "advanced," especially since there exist a number of much more advanced theories and methods than the AGT, such as

TABLE VIII. Escarguel *et al.* [4] electron-ion coupling effects.

$n(10^{18}\ e/\mathrm{cm}^3)$	T(eV)	Joint(Å)	Independent(Å)	El(Å)
2	0.68	61.9	65.1	41.3
2.4	0.73	69.6	74.5	46.1
2.7	0.73	71	79.5	48.9
2.8	0.734	75.26	81.64	51
3.9	0.767	90.4	101.87	64.6
6.2	0.8617	118	138.63	85

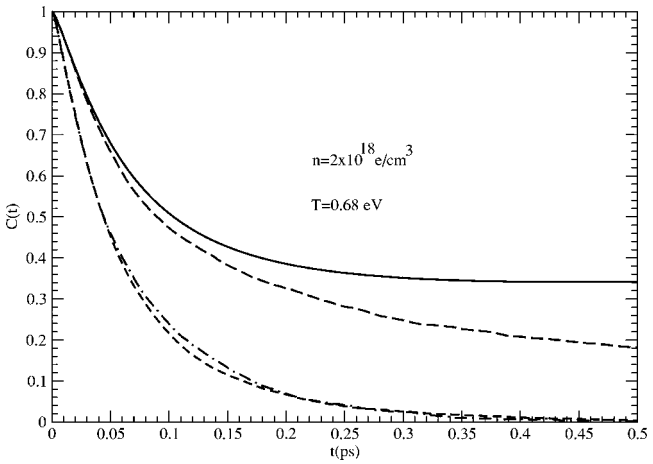

FIG. 19. Dynamic vs static ion behavior.

the well-known Pfennig-Lisitsa-Sholin(PLS) [34,35] analytical fully nonperturbative solution, the unified theory [36,37], and joint electron-ion simulations. Even the ST is at least consistent in the assumptions and approximations it uses.

The AGT essentially includes the (presumed static) ion field, taken to define the z axis, plus z component of the electronic field in the unperturbed Hamiltonian. Perturbation theory is used for the x and y components of the electronic field. This is of course not consistent in the sense of a power expansion in the emitter-electron interaction, as it keeps all orders from the dressing factor associated with the z component of the electric field and only the second order from the x and y components. Furthermore, the convergence of this theory for the lateral components (though not for the central component) was taken as an indication that one could integrate down to 0 impact parameters, neglecting the problems mentioned in the Introduction. Of course just because a theory is convergent, does not make it right: For instance the new "penetrating standard theory" (PST) [38] is also convergent, not just for the lateral components, yet it is not correct for low enough velocities, where unitarity breaks down for large enough impact parameters.

The problems with the AGT arise on many fronts: First [8,14], its application to intermediate densities has led to significant discrepancies with benchmark simulation calculations [22] with the collision-time statistics method [22,39], which treat exactly the full joint electron-ion microfield and furthermore find *no* electron-ion coupling, that is the line profile thus computed is in excellent agreement with the profile obtained by convolving the electronic and ionic profiles. In the present work we add further weight to this important point by demonstrating that the benchmark simulations show no important electron-ion coupling, that is the simulations with the joint electronic-ionic microfield produce the same width as the convolution of the independent ionic and electronic profiles, as demonstrated earlier.

In a recent publication [40] the opinion is expressed that in simulations for dense plasmas where a small number of particles is simulated the results are not statistically meaningful. This is manifestly incorrect, as the collision-time statistics method [22,23] currently employed in simulations *only simulates those particles* that will find themselves in the interaction volume (a sphere with radius of the order of the screening length) during the time of interest (a few times the inverse HWHM of the line), regardless of how far they are at $t=0$. Furthermore, it has been known for a long time [22] that statistical noise has *nothing* to do with the number of particles simulated per configuration and everything to do with the number of configurations averaged over. Consequently, such concerns about the applicability of simulations for dense plasmas are definitely unfounded. On the contrary because the relevant time scale and the shielding length shrink and less particles need to be simulated, such simulations are quite fast. Their main problem is a semiclassical treatment of electrons and also possibly perturber-perturber interactions, which require a molecular dynamics rather than an independent (quasi)particle simulation. Of course, none of the theories considered in this work and generally employed in practice includes dynamic perturber-perturber interactions. In [41] an attempt is made to argue that simulations are ill-suited for shift calculations as well as to imply a change of opinion by the present author on the reliability of shift calculations. Although Ref. [41] is too delusional to be taken seriously (for instance, it argues that a collision with a zero interaction is strong, and tries to refute a number of things that were never stated), it introduces several misconceptions that should be addressed. For instance, there has been no statement to the effect that shifts may be reliably calculated by simulations, at least by the present author. On the contrary, in recent publications the present author has repeated and documented the problems in shift calculations [13,42]. The point was simply that the argument that "because a small number of perturbers is simulated the results are not statistically meaningful" presumably is also applicable for widths, since widths and shifts arise from the same calculation, in which case it is not true. The problems with computing shifts for practical use have to do not with simulation noise (which may be reduced and/or bounded), but with effects not normally accounted for and often not known experimentally [42]. However, an easy, simple, and exact result for shifts is that in the case of hydrogen, without fine structure, with only dipole interactions and with density matrix factorization, the shift is identicaly zero, as discussed below.

Second, the theory leads to predictions of nonzero dipole shifts for hydrogen lines in the no-quenching approximation and with the usual density matrix factorization [43]. This has been shown to be in error, both numerically [12] and analytically [13]. Third, the AGT is also an impact-based theory, hence it cannot properly account for nonimpact effects which were shown to be important for Ref. [4], for instance. In Ref. [41] it is argued that the AGT is in principle able to obtain nonimpact results. This may be as true as the fact that the ST can obtain nonimpact (but still binary) results if generalized to the unified theory, but the simple point is that the *calculations in the AGT* that achieve "agreement with experiment" were done using the *impact* form of the AGT. Last, to achieve agreement with experiments, the AGT needed to introduce two more effects, i.e., a residual ion impact width [10] plus a narrowing effect due to the nearest-neighbor ion. These effects are also incorrect as has been already discussed [8,14] and as analyzed in detail elsewhere [44,45].

In short, although an electron-ion coupling may be of some theoretical interest, simulations [26] indicate that such

a coupling is negligible for the parameters of interest to the experiments in question.

VIII. COMMENTS

In general, although all experiments discussed are considered "high density," they probe *different* regimes, for instance, ions still dominate at the lowest densities considered, while electrons dominate at the higher density colder plasmas. In addition, *different* physics is important for the different experimental sets, for instance, at the cold plasmas [2,4] nonimpact effects and perturber-perturber interactions may be relevant, which is decidedly not the case for the high temperature sets [1,5]. Some of the experiments reviewed here may be viewed as scratching the surface of the exciting area of strongly correlated plasmas. At high densities, a number of ST assumptions need to be examined. Apart from penetration such effects are nonimpact effects (i.e., a part of the electron perturber phase space becomes nonimpact), quantal effects (the contributions from impact parameters of the order of or smaller than the de Broglie wavelength), and dielectric response effects. Qualitatively, since [46] the impact approximation yields the *maximum* possible width (all particles contribute in an additive manner), nonimpact effects will tend to reduce the final width. Although in general all the above effects need in general to be included in a robust theoretical framework for high density line broadening, the results of the present investigations are that exotic and incorrect "effects" are neither warranted, nor theoretically justified.

Finally, a very interesting question is "At what plasma parameters does an independent particle model become inadequate? (And molecular dynamics simulations will be necessary.)" It is not entirely clear if dynamic perturber-perturber interactions will have a significant effect on the final widths and in which direction (i.e., increase or decrease the widths) this effect will be.

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[1] S. Boddeker, S. Gunter, A. Konies, L. Hitzschke, and H. J. Kunze, Phys. Rev. E **47**, 2785 (1993).
[2] S. A. Flih, E. Oks, and Y. Vitel, J. Phys. B **36**, 283 (2003).
[3] A. Escarguel, B. Ferhat, A. Lesage, and J. Richou, J. Quant. Spectrosc. Radiat. Transf. **64**, 353 (2000).
[4] A. Escarguel, E. Oks, J. Richou, and D. Volodko, Phys. Rev. E **62**, 2667 (2000).
[5] S. Buescher *et al.*, J. Phys. B **35**, 2889 (2002).
[6] H. R. Griem, *Plasma Spectroscopy* (McGraw-Hill, New York, 1964).
[7] H. R. Griem, *Spectral Line Broadening by Plasmas* (Academic, New York, 1974).
[8] S. Alexiou, in *Spectral Line Shapes*, edited by C. Back, AIP Conf. Proc. No. 645 (AIP, Melville, NY, 2002), pp. 302–309.
[9] Y. Ispolatov and E. Oks, J. Quant. Spectrosc. Radiat. Transf. **51**, 129 (1994).
[10] E. Oks, Phys. Rev. E **60**, R2480 (1999).
[11] E. Oks, J. Quant. Spectrosc. Radiat. Transf. **65**, 405 (2000).
[12] J. Halenka, Phys. Rev. E **69**, 028401 (2004).
[13] S. Alexiou, J. Quant. Spectrosc. Radiat. Transf. **81**, 13 (2003).
[14] H. R. Griem, Contrib. Plasma Phys. **40**, 46 (2000).
[15] H. R. Griem, Phys. Rev. E **64**, 058401 (2001).
[16] S. Alexiou, Phys. Rev. Lett. **75**, 3406 (1995).
[17] H. R. Griem, Y. V. Ralchenko, and I. Bray, Phys. Rev. E **56**, 7186 (1997).
[18] S. Alexiou, S. Glenzer, and R. W. Lee, Phys. Rev. E **60**, 6238 (1999).
[19] H. R. Griem, Yu. V. Ralchenko, and I. Bray, Phys. Rev. E **60**, 6241 (1999).
[20] S. Alexiou and A. Poquérusse, in *Spectral Line Shapes*, edited by E. Leboucher (Frontier Group, Paris, 2005).
[21] S. Alexiou and E. Leboucher-Dalimier, Phys. Rev. E **60**, 3436 (1999).
[22] G. C. Hegerfeldt and V. Kesting, Phys. Rev. A **37**, 1488 (1988).
[23] J. Seidel, in *Spectral Line Shapes*, edited by L. Frommhold and J. Keto, AIP Conf. Proc. No. 216 (AIP, Melville, NY, 1990), pp. 98–99.
[24] C. A. Iglesias, J. L. Lebowitz, and D. MacGowan, Phys. Rev. A **28**, 1667 (1983).
[25] S. Alexiou, Phys. Rev. Lett. **76**, 1836 (1996).
[26] S. Alexiou *et al.*, J. Quant. Spectrosc. Radiat. Transf. **58**, 399 (1997).
[27] S. Alexiou, in *Spectral Line Shapes*, edited by M. Zoppi and L. Ulivi, AIP Conf. Proc. No. 386 (AIP, Melville, NY, 1997), p. 79.
[28] H. R. Griem and Yu. Ralchenko, J. Quant. Spectrosc. Radiat. Transf. **65**, 287 (2000).
[29] Y. V. Ralchenko, H. R. Griem, I. Bray, and D. V. Fursa, Phys. Rev. A **59**, 1890 (1999).
[30] S. Alexiou and R. W. Lee, in *Spectral Line Shapes*, edited by J. Seidel, AIP Conf. Proc. No. 559 (AIP, Melville, NY, 2001), pp. 135–143.
[31] W. L. Wiese, D. E. Kelleher, and D. R. Paquette, Phys. Rev. A **6**, 1132 (1972).
[32] M. A. Gigosos and V. Cardenoso, J. Phys. B **29**, 4795 (1996).
[33] S. Alexiou, J. Quant. Spectrosc. Radiat. Transf. **54**, 1 (1995).
[34] H. Pfennig, Z. Naturforsch. A **26A**, 1071 (1971).
[35] V. S. Lisitsa and G. V. Sholin, Sov. Phys. JETP **34**, 484 (1972).
[36] D. Voslamber, Z. Naturforsch. A **24A**, 1458 (1969).
[37] C. R. Vidal, J. Cooper, and E. W. Smith, J. Quant. Spectrosc. Radiat. Transf. **10**, 1011 (1970).
[38] S. Alexiou and A. Poquérusse (unpublished).
[39] S. Alexiou, P. Sauvan, A. Poquerusse, E. Leboucher-Dalimier, and R. W. Lee, Phys. Rev. E **59**, 3499 (1999).
[40] E. Oks, J. Phys. B **36**, 1459 (2003).
[41] E. Oks, in *Spectral Line Shapes*, edited by E. Leboucher (Fron-

tier Group, Paris, 2005).
[42] S. Alexiou, J. Quant. Spectrosc. Radiat. Transf. **81**, 461 (2003).
[43] D. B. Boercker and C. A. Iglesias, Phys. Rev. A **30**, 2771 (1984).
[44] H. R. Griem, J. Halenka, and W. Olchawa, J. Phys. B (to be published).
[45] S. Alexiou, H. R. Griem, J. Halenka, and W. Olchawa, J. Quant. Spectrosc. Radiat. Transf. (to be published).
[46] S. Alexiou, Phys. Rev. A **49**, 106 (1994).