Comment on "Highly nonlinear, sign-varying shift of hydrogen spectral lines in dense plasmas"

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The shift of hydrogen and hydrogenlike spectral lines in dense plasmas, calculated with the full computer simulation method, in nonquenching, classical path, dipole approximation for plasma-emitter interaction, is equal to zero. In the paper commented on, Escarguel *et al.*, Phys. Rev. E **62**, 2667 (2000) the electron concentrations N_e and the corresponding temperature values T are shown to have been determined incorrectly.

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In Ref. [1] the experimental and theoretical shifts of H_α line are reported. Escarguel *et al.* report that the theoretical shifts, calculated in Refs. [2,3], are about twice as large as the measured ones [1]. In order to explain this great discrepancy, the authors of Ref. [1] propose a theoretical model, accounting for the line shifts of the hydrogen lines in spectra of dense plasma, different from the model used in Refs. [2,3]. The leading point of this proposal is the dipole electron-impact shift d_n of a particular Stark component—the conception originally introduced by Sholin, Demura, and Lisitza [4], assuming purely binary collisions.

Griem, in his comment [5] on paper [1], pointed out that the commented values of shift d_n radically diminish and become nearly equal to zero, when one takes into account the screening effect, which in calculations [1] has been ignored. Such smallness of d_n agrees with the suggestion by the authors of Ref. [4], that in dipole approximation we indeed have, in fact, d_n about equal to zero. As a cause of differences appearing between the measurements [1] on the one hand, and the theories [2,3] on the other, Griem [5] indicates a very similar error of the electron density in experiment [1].

In Ref. [6] Oks, however, presents an opposing opinion on the importance of screening effect in d_n calculations.

In the present paper the importance of the dipole electronic shift as a reason for the observed shift of hydrogen spectral lines in dense plasmas was examined, using the full computer simulation method (FCSM). (This FCSM is described in detail in Refs. [7,8].) The actual plasma is "granular," then the FCSM is a more accurate description of the real situation than the analytical models. In the analytical models continuous velocity and impact parameter distributions are used. In addition, application of the FCSM approach has advantages over the analytical model [1] because FCSM is free of simplifications which accompany the following approximations: (i) the quasistatic approximation for ions, (ii) the impact approximation for electrons, (iii) the binary approximation for electrons, (iv) perturbation theory (as used at least in part in Ref. [6]), which are essential to the commented on paper [1].

Moreover, the case of the H_α line formed in the plasmas of the experiment [1] (high electron concentration N_e at relatively low temperature T) is especially favorable one to make use of the FCSM code. The higher the value of N_e, the greater the value of the full width at half maximum (FWHM) of the line and, consequently, the shorter the so-called time of interest in computing the autocorrelation function $C(t)$ of the line profile; the lower the temperature of the plasma, the "softer" the fluctuations of the local electric microfield. Both these circumstances are favorable to improvement of the numerical accuracy of FCSM.

The calculations were carried out in a nonquenching approximation, for isotropic plasma of the same physical conditions as in Ref. [1], within the μ^* model [9] well reproducing results of the so-called collision time statistics model [10]. Hamiltonian in a dipolar approximation for plasma-emitter interactions was used,

$$H = H_0 + \vec{d} \cdot [\vec{F}_e(t) + \vec{F}_i(t)], \tag{1}$$

where H_0 represents the Hamiltonian of the unperturbed emitter, $\vec{d}$ is the dipole moment of emitter, whereas $\vec{F}_e(t) + \vec{F}_i(t)$ is a joint electron-ion resultant electric microfield in the plasma. The corresponding Schrödinger equation was solved numerically; by this means the FCSM becomes a full nonperturbative approximation, in which the so-called *electron-ion coupling* is taken into account in a natural way [through Eq. (1)]. That type of the *electron-ion coupling* was taken into account in the quasistatic, nonperturbative (but not exact) approximation [11], on which the calculations in the paper commented on [1] are based.

The results obtained using the FCSM approach—within the stated approximations—show that the imaginary part of the autocorrelation function of the profile of H_α line is equal to zero, $\mathrm{Im}\, C(t) = 0$. In Fig. 1 the autocorrelation function for H_α is shown as an example. For this example the radius of the simulation sphere is $R_s = 9D$ (D is the Debye radius), the radius of the ball representing the dimension of the emitter is $R_{min} = 5a_0$ (a_0 is the Bohr radius), and the number of the initial perturber configurations taken for averaging is 3000. The FWHM of the profile resulting from $C(t)$ is 91.4 Å. The control calculations were carried out for different values of the parameters R_s and R_{min}, as well as for different shapes (straight and hyperbolic lines) of the perturber trajectories. In Fig. 2 the numerical values of $\mathrm{Im}\, C(t)$, calculated for two significantly different values: $R_{min} = 5a_0$ (which corresponds to the minimum Weiskopf radius for H_α in the physical conditions of the experiment [1]), and $R_{min} = 13.5a_0$ (which corresponds to the Bohr radius at $n = 3$) are compared as an example. In Fig. 2 we see that the results are the same, i.e., $\mathrm{Im}\, C(t) = 0$, independently of the numerical noise. Also, testing calculations were made in order to define

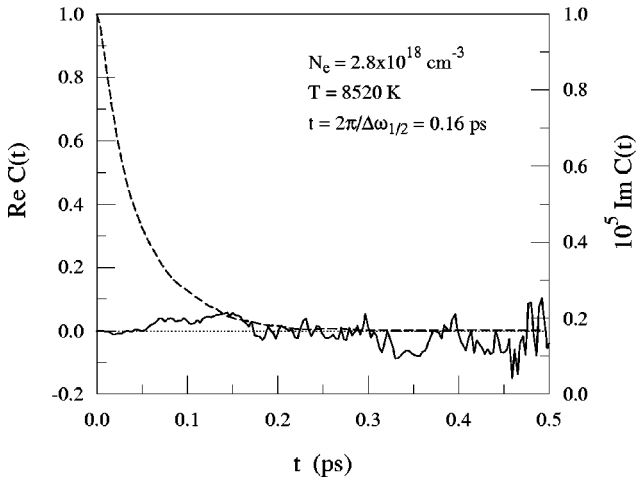

FIG. 1. The autocorrelation function for H_α as an example. The solid line represents the imaginary part $\mathrm{Im}\,C(t)$ of the autocorrelation function; the dashed line represents the real part $\mathrm{Re}\,C(t)$ of the autocorrelation function. $\Delta\omega_{1/2}$ is FWHM (in wavelength scale, FWHM=91.4 Å).

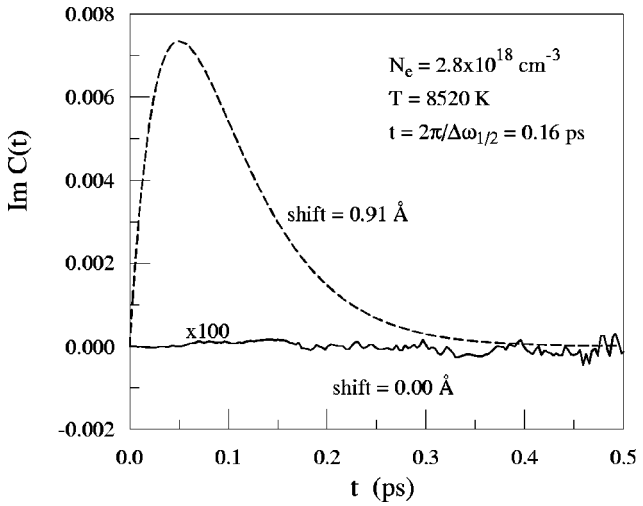

FIG. 3. Comparison of the imaginary part of the autocorrelation functions. The solid line represents the same function, $\mathrm{Im}\,C(t)$, as in Fig. 1, i.e., for an unshifted line profile; the dashed line represents $\mathrm{Im}\,C_s(t)$ for the shifted line profile (see text).

an ability of the used numerical code to ''intercept'' the ''signal'' responsible for the line shift, from the numerical noise of the calculations. For this purpose the H_α line profile, resulting from $C(t)$, was arbitrarily shifted by 1% of the FWHM value, i.e., by 0.91 Å, in other words, by an amount of one order of magnitude smaller than the supposed electronic shift reported in Ref. [1]. This shifted line profile was subsequently submitted to the Fourier transformation in order to obtain a new autocorrelation function $C_s(t)$. The imaginary part of $C_s(t)$ is presented in Fig. 3. We see that the ''signal'' predominates over the numerical noise—even at such an insignificant line shift—by about three orders of magnitude.

So, the pure dipole shift of H_α line in dense plasmas, calculated within classical path for perturbers and within the dipolar approximation for plasma-emitter interaction, with the accuracy to the first order of Stark effect (no quenching, no fine structure, and with density matrix factorization)—is equal to zero. This was also shown analytically by Alexiou [12]. One obtains the same result for each Stark broadened hydrogen line, as well as for each line of hydrogenlike ions. It should be emphasized that the result of zeroing of the line shift does not depend on the assumed radius of the simulation sphere, on the assumed radius of the ball representing the dimension of the emitter, nor the assumed shape of the trajectory of the perturbers.

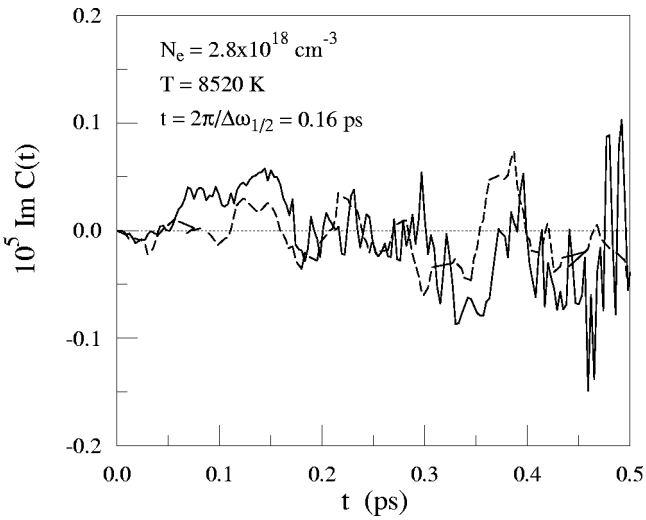

FIG. 2. Comparison of the imaginary part $\mathrm{Im}\,C(t)$ of the autocorrelation functions. The solid line corresponds to $R_{min}=5a_0$, the dashed line corresponds to $R_{min}=13.5a_0$.

The imaginary part of the autocorrelation function becomes different from zero (and consequently, the line shift becomes different from zero too) only when the inhomogeneity of the electric microfield is taken into account, and/or when the calculations are carried out with the accuracy to the second (or higher) order of the Stark effect—as is shown in Ref. [13]. The source of the electron shift different from zero, reported in papers [1,4,6,14–16], is the imperfection of the analytical models (impact, binary, perturbative, used to describe the emitter-electron collisions), but not any real physical effect.

Griem in Refs. [5,17] pointed out that the interpretation of the experiment in paper commented on [1] is doubtful as well. (The experiment [1] is described in detail in Ref. [18].) Particularly, in Refs. [1,18] the errors were made within the procedure of self-absorption correction of the measured emission coefficients. (For example, before the self-absorption correction the continuum was neglected.) In my opinion this is the main cause of the errors of the determined values N_e and T in Refs. [1,18].

For cylindrical optically thick plasmas as in Refs. [1,18], the ''*separation*'' of two procedures, self-absorption correction and Abel inversion, leads to fatal errors. In such cases the Abel inversion and the self-absorption correction have to be ''*coupled*,'' and the continuum has to be subtracted at the final step. The negligence of the continuum radiation is a

significant simplification and not justified for this experiment, because the Ca II lines are overimposed by the hydrogen quasicontinuum, while the K I line lies in the infrared region, where the absorption of radiation is expected to be relatively strong. The authors [1,18] should have applied the procedure described in Ref. [19] in Chaps. 7–4. If this had been done the emission coefficients would be larger and the half-widths narrower. Consequently, the N_e would be smaller and the T higher. Probably, the underwater plasma would appear more similar, e.g., to that in the gas-liner pinch.

I present below an indirect proof that in Refs. [1,18] the N_e and T values are determined incorrectly. For average physical conditions from Refs. [1,18], $N_e = 2.8 \times 10^{18}$ cm^{-3} and $T = 8520$ K, taken as an example, I calculated concentrations of hydrogen and oxygen atoms. I used the following assumptions: (i) Saha-Eggert law is satisfied; (ii) only singly charged ions of H II and O II occur; (iii) plasma is neutral, $N_e = N_{\mathrm{H\,II}} + N_{\mathrm{O\,II}}$; (iv) plasma composition is as that of the water, $N_{\mathrm{H\,I}} + N_{\mathrm{H\,II}} = 2 \times (N_{\mathrm{O\,I}} + N_{\mathrm{O\,II}})$.

Unsöld and/or Debye lowering of the ionization energy was used alternatively (see, e.g., Ref. [19]). For Unsöld's energy lowering, I obtained the following concentrations: $N_{\mathrm{O\,I}} = 4.18 \times 10^{22}$ cm^{-3}, $N_{\mathrm{O\,II}} = 8.3 \times 10^{17}$ cm^{-3}, $N_{\mathrm{H\,I}} = 8.36 \times 10^{22}$ cm^{-3}, $N_{\mathrm{H\,II}} = 19.7 \times 10^{17}$ cm^{-3}; the total number of atoms is $N^U = 1.25 \times 10^{23}$ cm^{-3}. For Debye's energy lowering, the total number of atoms is $N^D = 2.84 \times 10^{23}$ cm^{-3}. On this basis one can calculate the mean radius of sphere corresponding to an atom: $R^U \simeq 1.24$ Å or $R^D \simeq 0.94$ Å. At these interatomic distances the *plasma water* should be in the molecular state. It is a well-known fact that in the *normal water* we have 3.34×10^{22} cm^{-3} particles of H_2O, whereas in the *plasma water* we have at least 4.18×10^{22} cm^{-3} particles of H_2O, i.e., a greater number than in the *normal water*. Such a packing up of the plasma is physically unreal. This implies that the N_e and T values in the underwater experiment [1,18] were determined incorrectly.

I would like to point out additionally that at such concentrations as above, it is impossible for a perturbing electron to go with acceleration along the hyperbola, as this supposedly occurs from acceleration of (perturbing) electrons by the ion field (AEIF) in Refs. [20,6]

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