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Advance in diagnostics for high-temperature plasmas based on the analytical result for the ion dynamical broadening of hydrogen spectral lines

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It is well known that the ion dynamics is very important for Stark broadening of spectral lines in high-T plasmas. However, it is usually assumed that with the increase of the plasma density N and/or of the principal quantum number n of the upper level of the radiator, the ionic contribution to the impact width (ICIW) tends to zero. In distinction to that paradigm, by finding an analytical result for the ion dynamical broadening of hydrogen spectral lines, we show here that with the increase of N and/or n, the ICIW does not decrease. Moreover, for practically important ranges of T, N, and n, this ''residual'' ICIW, being virtually independent of n, can be comparable to the standard electron impact width. This result leads to: (i) a substantial revision of the past of diagnostic conclusions for a variety of high-T plasma experiments; (ii) a much better possibility to deduce from experimental, Stark-broadened line profiles not only the plasma density but also the plasma temperature; (iii) a significant enhancement of the accuracy of N and T obtained from experimental line profiles; and (iv) a substantial revision of simulation models for the ion dynamical contribution that were based on a wrong assumption that the latter vanishes under increasing N and/or n. The consequences are especially important for tokamak plasmas, where the diagnostics based on experimental profiles of high Balmer and Paschen lines is frequently used. [S1063-651X(99)50209-2]

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I. INTRODUCTION

Experimental profiles of high Balmer and Paschen lines of hydrogen and deuterium are used nowadays for diagnostics of tokamak plasmas [1,2]. Up till now, the theory of Stark broadening, employed in the diagnostics for deducing the electron density N_e from the experimental profiles, was based primarily on the quasistatic treatment of the broadening by ions (while the electron broadening was calculated in the impact approximation) [1–3].

This is not to say that the role of the ion dynamics was not recognized. It is well known by now that the ion dynamics, generally speaking, is very important for Stark broadening of spectral lines in high-T plasmas. However, it was usually assumed that with the increase of the plasma density N and/or of the principal quantum number (PQN) n of the upper level of the radiator, the ion dynamics becomes less and less important and the ionic contribution to the impact width (ICIW) tends to zero. Therefore, even the application of codes based on simulation models for ion dynamics, such as the frequency fluctuation model (FFM), for calculating profiles of high Balmer lines emitted by tokamak plasmas, resulted only in minor corrections [4] to the results of the standard theories (ST). Here and below, by the ST we mean the approaches [5,6], where the ion broadening was assumed quasistatic.

In distinction to that paradigm, by finding an analytical result for the ion dynamical broadening of hydrogen lines, we show here that with the increase of N and/or n, the ICIW does not decrease. Moreover, for practically important ranges of T, $N<$ and n, this ''residual'' ICIW, being virtually independent of n, can be comparable to the standard electron impact width.

II. OUTLINE OF THE DERIVATION

The derivation proceeds from our generalized theory (GT) of Stark broadening of hydrogen lines in plasmas [7]. The GT is based on the nonperturbative treatment of one component of the field caused by charged particles passing by the radiator. Therefore, the GT is intrinsically more accurate than the fully perturbative ST [5,6]; see, e.g., [8].

Analytical results of the GT depend on the ratio of two characteristic impact parameters; Weisskopf radius $W=Z_i n^2\hbar/(m_e v)$ and mean interperturber distance $D=[3/(4\pi N)]^{1/3}$. Here v is the perturber velocity, N is the perturber density, Z_i is the perturber charge, and n is the PQN of the radiator.

Typically, for the electron broadening the ratio $D/W\gg 1$. Physically this means that most of the electrons are ''impact'' (i.e., cause the impact broadening of the particular hydrogen line). For the ion broadening, one finds usually $D/W\ll 1$, which means physically that most of the ions are not impact. However, there is a (tiny) minority of ions that cause some impact broadening of the line.

We applied the GT formalism to the ion broadening in the limit $D\ll W$, by using the following features of the GT: (i) the impact width generally consists of the adiabatic and nonadiabatic terms (as defined in [7]); however, in the limit $D\ll W$ the nonadiabatic term becomes much smaller than the adiabatic term and can be neglected; (ii) the remaining adiabatic term, obtained in [7] nonperturbatively, does not depend on any external static electric field [see Eqs. (48)–(52) from [7]]; moreover, in the limit $D\ll W$, it does not depend any more on the parabolic quantum numbers and thus becomes spherically symmetric. Therefore, in the limit $D\ll W$, the GT formalism can be applied to the ion broadening and yields the ICIW γ_i described by the following, relatively simple expression:

$$\gamma_i=(3\pi N_e/Z_i)^{1/3}[8T/(\pi\mu)]^{1/2}$$
$$\approx 3.2990\times 10^6[N_e(\mathrm{cm}^{-3})/Z_i]^{1/3}[T(\mathrm{eV})M_p/\mu]^{1/2}. \quad (1)$$

Here μ is the reduced mass of the perturber-radiator pair, M_p is the proton mass.

In the ST, with the increase of the effective PQN $n_{\rm eff} \equiv (n^2+n-n'^2-n')^{1/2}$, the ICIW reaches the maximum and then rapidly diminishes to zero (where $n_{\rm eff} \sim n$ at $n \gg n'$). In distinction to this, in the GT, as $n_{\rm eff}$ increases, the ICIW saturates at the above value γ_i independent of n and n'.

III. PHYSICAL INTERPRETATION AND JUSTIFICATION

These analytical results can be easily understood in physical terms. It is well known that the impact width can be estimated as $\gamma_i \sim N v_i \sigma$, where σ is the ''optical cross section.'' It is the effective cross-section for virtual transitions (between the states of the same multiplet) that lead to the broadening of the spectral line. In the conventional case of $W \ll D$, the cross section is determined by the Weisskopf radius $\sigma \sim W^2 \propto v_i^{-2}$, so that $\gamma_i \propto N/\not{v}_i \propto N/T^{1/2}$. However, for sufficiently high densities, the mean interperturber distance becomes smaller than the Weisskopf radius. In this case the cross section is controlled by the mean interperturber distance: $\sigma \sim D^2 \propto N^{-2/3}$. Therefore, the impact width becomes as follows: $\gamma_i \sim N v_i D^2 \propto T^{1/2} N^{1/3}$.

Let us now discuss some conceptual issues to justify the above results. The adiabatic impact term in the GT was calculated in the spirit of the ''old adiabatic theory'' (see, e.g., [9]) but with the vector summation of the contributions from the individual perturbers (in distinction to the scalar summation in the impact approximation of the old adiabatic theory). The adiabatic broadening theory reproduces in a unified fashion both the impact and the quasistatic parts of the correlation function $C(\tau)$. In our case of $D \ll W$, the impact part of $C(\tau)$ corresponds to $\tau \leqslant D/v_i$, while the quastatic part of the $C(\tau)$ corresponds to $D/v_i \leqslant \tau \leqslant W/v_i$. So the impact and quasistatic regimes are characterized by significantly different interaction volumes $V'_{\rm imp}$ and $V'_{\rm qs}$ (the interaction volume, also known as ''collision volume,'' is one of the central concepts of the adiabatic broadening theory). Indeed, in the case of $D \ll W$, we have $V'_{\rm imp} \sim D^3 \ll V'_{\rm qs} \sim W^3$.

Consequently, first quasistatic ions outnumber impact ions by the factor of $W^3/D^3 \gg 1$, so that the impact ions constitute indeed a tiny minority. Second, the number of impact ions in the corresponding interaction volume is $N_i V'_{\rm imp} \sim 1$, so that the applicability of the binary impact approximation is not violated.

Finally, to employ the impact approximation, one should be able to introduce a coarse-grain time scale dealing with time intervals Δt such that $\gamma_i < (\Delta t)^{-1} < \Omega$, where γ_i is the resultant ion impact width, Ω is the rms value of the frequency of any Cartesian component $E_{\rm comp}(t)$ of the ion-produced electric field. For an individual passage of the perturber by the radiator, we first calculated analytically the Fourier transform $\Phi(\omega)$ of the time dependence $E_{\rm comp}(t)$ and then averaged ω^2 over $\Phi(\omega)$. We have found that the even (with respect to ω) part of $\Phi(\omega)$, which controls the subsequent average, is $\Phi_{\rm even}(\omega) = |\omega| \rho^2 K_1(|\omega|\rho/v)/(\pi v^2)$, where $K_1(x)$ is the modified Bessel function. Using $\Phi_{\rm even}(\omega)$, we obtained the frequency $\Omega = \omega_{\rm rms} = 3^{1/2} v/\rho$. This result is more precise than the conventional, order of magnitude estimate of a ''typical'' frequency of the ion microfield $\sim v/\rho$. At last, we determined the cutoff $\rho_{\max}$, involved in the calculation of $\gamma_i(\rho_{\max})$, from the requirement: $\gamma_i(\rho_{\max}) < \Omega(\rho)$ for $\rho < \rho_{\max}$. Thus the result presented by Eq. (1) is derived in compliance with the physical basis of the impact approximation.

IV. DISCUSSION OF DIAGNOSTIC CONSEQUENCES

We have derived an analytical expression for the ion dynamical contribution to the width of hydrogen lines in the limit of high densities N and/or high PQN n. It should be emphasized that we have obtained a *nonperturbative* analytical result for the ion dynamical broadening.

Let us now focus at the consequences for the diagnostics of tokamak plasmas employing high Balmer and Paschen lines. The ST yields the full width at half maximum (FWHM) of a highly excited hydrogen lines in the form

$$\Delta\lambda_{1/2}^{\rm high} \approx A_e(n,n') N_e / T_e^{1/2} + B_i(n,n') N_s^{2/3}, \qquad (2)$$

where the term $A_e(n,n') N_e / T_e^{1/2} \equiv \Delta\lambda_e$ is due to electrons and the term $B_i(n,n') N_e^{2/3} \equiv \Delta\lambda_i$ is due to the ions. Here the coefficient B does not depend on the temperature or on the density, but strongly depends on the PQN [see e.g., Eq. (3) from [1] or Eq. (3) from [10]; the coefficient A has only a very weak, logarithmic dependence of N_e and T_e.

Our theory, being intrinsically more accurate than the standard theory, yields significantly different results. First, for high Balmer lines, the ICIW does not depend on the principal quantum number n, but strongly depends on the temperature ($\propto T_i^{1/2}$). Second, for highly excited hydrogen lines near the limit of the spectral series, the total (electronic plus ionic) impact width significantly exceeds the quasistatic splitting (produced by the majority of ions). Therefore, the line profiles correspond to the regime of merged (collapsed) Stark components [11] and the quasistatic contribution from ions has practically no effect on the FWHM:

$$\Delta\lambda_{1/2}^{\rm high} \approx A_e(n,n') N_e / T_e^{1/2} + C_i T_i^{1/2} N_i^{1/3}, \qquad (3)$$

where the coefficient C_i does not depend on the PQN n, as follows from Eq. (1).

It is interesting to note that for low Balmer and Paschen lines, the majority of perturbing ions produce the impact broadening. In this case, the ionic contribution to the FWHM predominates:

$$\Delta\lambda_{1/2}^{\rm low} \approx A_e(n,n') N_e / T_e^{1/2} + A_i(n,n') N_i / T_i^{1/2} \approx A_i(n,n') N_i / T_i^{1/2}, \qquad (4)$$

since $A_i/A_e \sim (m_i/m_e)^{1/2} \gg 1$. Therefore, in the reality, there is virtually no practical range of PQN where the ion quasitatic term $B_i(n,n') N_e^{2/3}$ could enter the FWHM: with the increase of n, the FWHM gradually transforms from a *linear* dependence on the density [see Eq. (4)] to a *quasilinear* dependence on the density [see Eq. (3)].

An interpolative formulas for the ionic contribution to the FWHM, that incorporates both ionic limits contained in Eqs. (3) and (4) and is therefore valid for a broad range of densities, can be expressed as follows:

$$\Delta\lambda_i=\lambda_{nn'}^2(\pi c)^{-1}\{1-\exp[-(C_iT_i)^{-1}A_i(n,n')\times(N_e/N_{\rm cr})^{2/3}]\}\gamma_i. \quad (5)$$

Here γ_i is given by Eq. (1) and the critical density $N_{\rm cr}$ has the form

$$N_{\rm cr}=(9/\pi)Z_i^{-2}n_{\rm eff}^{-6}(m_e/\hbar)^3(T_i/\mu)^{3/2}\approx 1.7309\times 10^{18}\ \ {\rm cm}^{-3}Z_i^{-2}n_{\rm eff}^{-6}[T({\rm eV})M_p/\mu]^{3/2}, \quad (6)$$

where the effective PQN $n_{\rm eff}$ is defined as

$$n_{\rm eff}\equiv(n^2+n-n'^2-n')^{1/2}. \quad (7)$$

In Eq. (5), $\lambda_{nn'}$ is the unperturbed wavelength of a hydrogen line, corresponding to the radiative transition from the upper level n to the lower level n'. At relatively low densities, keeping the first two terms of the Taylor expansion of the exponential in Eq. (5), we retrieve the primary term of Eq. (4); at relatively large densities, the exponential in Eq. (5) vanishes, and Eq. (5) reduces to the second term of Eq. (3).

The coefficient A_e in the electronic contribution to the FWHM $\Delta\lambda_e$ can be reliably obtained as follows. First, our GT [7] applied to the electron broadening produces results that are more accurate than the ST. Second, it was shown in [12] that in the regime of merged (collapsed) Stark components, the electron broadened profiles of all hydrogen lines are Lorentzian. Thus, combining the results of the GT [7,8] and of Ref. [12], the coefficient $A_e(n,n')$ can be represented in the form

$$A_e(n,n')=\lambda_{nn'}^2(\pi c)^{-1}3(2\pi)^{1/2}g_{nn'}\hbar^2m_e^{-3/2}\{1.1+\ln[T_eg_{nn'}^{-1/2}\hbar^{-1}/(4\pi e^2N_e/m_e+(6.3n\hbar Z_i^{1/3}N_e^{2/3}/m_e)^2)^{1/2}]\}, \quad (8)$$

where

$$g_{nn'}\equiv(n^2-n'^2)^2-n^2-n'^2. \quad (9)$$

Equation (8) differs from the result of Ref. [12] in two ways: first, it contains the exact value 1.1 of what the ST would call ''strong collision constant;'' second, it allows for the ion-caused Stark splitting represented by the term $6.3n\hbar Z_i^{1/3}N_e^{2/3}/m_e$. All formulas are given in the CGS units, except the second lines of Eqs. (1), (6), and Eqs. (10)–(14) below.

To enhance the accuracy of our results, we also analytically calculated the ion quasistatic correction to the FWHM, as follows. First, we calculated the correction at a fixed value of the ion microfield F. This was done by taking the well-known starting formula for the line shape of a hydrogen line subjected simultaneously to a impact broadening and to a static electric field (see, e.g., [9]) and expanding it analytically near the pure impact limit. Second, we averaged the correction over the Holtsmark distribution [13] of field F. [We note that highly excited lines can be observed only at relatively low densities, where the Holtsmark distribution is valid; see, e.g., [9].) The resulting final formula for the FWHM has the form

$$\text{FWHM(Å)}=\Delta\lambda_L(\text{Å})+[0.94761\times 10^{-19}Z_i^{3/2}N_en^6n'^6/(n^2-n'^2)^{3/2}]/[\Delta\lambda_L(\text{Å})]^{1/2}. \quad (10)$$

Here the Lorentzian contribution $\Delta\lambda_L$ to the FWHM is given by the following practical formula:

$$\Delta\lambda_L=\Delta\lambda_e+\Delta\lambda_i, \quad (11)$$

$$\Delta\lambda_e(\text{Å})=2.1200\times 10^{-20}n^4n'^4(n^2-n'^2)^{-2}g_{nn'}N_eT^{-1/2}\times\{1+\ln[1.5192\times 10^{15}Tg_{nn'}^{-1/2}(3.1826\times 10^9N_e+53.2n^2Z_i^{2/3}N_e^{4/3})^{-1/2}]\}, \quad (12)$$

$$\Delta\lambda_i(\text{Å})=f(T)(N_e/N_{\rm cr})^{1/3}\times[1-\exp(-9\pi Z_ig_{nn'}[2f(T)n_{\rm eff}^2]^{-1}\times\{1+\ln[1+6.2847\times 10^8(T/Z_i)\times(N_eg_{nn'}\mu/M_p)^{1/2}]\}(N_e/N_{\rm cr})^{2/3})], \quad (13)$$

$$f(T)=0.34941[n^4n'^4/(n^2-n'^2)^2]TM_p/[\mu Z_in_{\rm eff}^2], \quad (14)$$

where $N_{\rm cr}$, $n_{\rm eff}$, and $g_{nn'}$ are given by Eqs. (6), (7), and (9). In all of the above practical formulas, the electron density N_e is in ${\rm cm}^{-3}$, the temperature T is in eV. The validity condition of the above formulas consists of the requirement that the second term in Eq. (10) should remain smaller than the first term.

As an illustration, we apply our analytical results to the interpretation of the widths of the high-n Balmer lines measured at the tokamak Alcator C-Mod [1,2]. In Ref. [1] experimental profiles of the deuterium Balmer lines D_8, D_9, D_{10}, and D_{11} were shown in Fig. 3 and their Stark widths (FWHM) were deconvolved to be 4.9, 5.9, 7.5, and 9.6 Å,

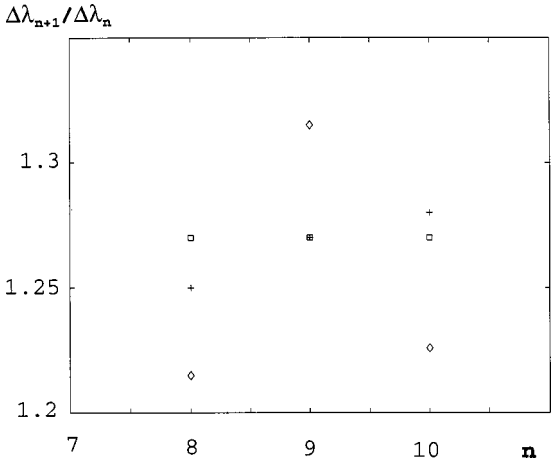

FIG. 1. The ratio of the Stark widths $\Delta\lambda_{n+1}/\Delta\lambda_n$ of the adjacent Balmer lines vs the principal quantum number n: diamonds, theoretical results based on the Kepple-Griem's code (presented in [1,2]); crosses, our theoretical results; squares, the experimental results [1,2].

respectively. Then Griem, the leading theoretical coauthor of Ref. [1], by using the Kepple-Griem's code [5], found that these Stark widths correspond to the electron densities 5.4, 5.6, 5.3, and 5.6×10^{14} cm^{-3}.

We note that the Kepple-Griem's code does not allow for the ion dynamics. Consequently, the width produced by their code have a relatively weak temperature dependence. Therefore, Griem was not able to deduce the temperature from the experimental widths based on that code. Instead, he assumed the temperature to be $T=4$ eV.

In distinction to this, our analytical results for the widths accurately incorporate the ion dynamics and, therefore, are much more sensitive to the temperature than the Kepple-Griem's code. Thus, while analyzing the same experimental widths, we were able to derive both the density $N_e=6.6\times10^{14}$ cm^{-3} and the temperature $T=7.7$ eV. It should be emphasized, that at $T=7.7$ eV we obtained the same value of $N_e=6.6\times10^{14}$ cm^{-3} from each Balmer line individually.

To further demonstrate the superior quality of our theory, we calculated the ratios of Stark widths $\Delta\lambda_{n+1}/\Delta\lambda_n$ of the adjacent Balmer lines and compared them with both the experimental results [1,2] and the Griem's theoretical results (presented in [1,2]). The idea behind calculating these ratios is that they should be less sensitive to the electron density than the widths of the individual lines. Therefore, the ratios are conventionally considered as a tool for evaluating the intrinsic self-consistency of a particular theory.

The comparison is presented in Fig. 1. It turns out that the rms deviation of our ratios from the experimental ratios is almost four times smaller than for the Griem's ratios. Thus, while a relatively small scatter of densities deduced by Griem from different lines was not alarming, the ratios of widths really demonstrate a dramatic difference in the self-consistency of the two theories.

In summary, the results presented in this paper should lead to: (a) a substantial revision of the past diagnostic conclusions for a variety of plasma experiments, especially those dealing with highly excited hydrogen lines from the edge and divertor regions of tokamaks; (b) a much better possibility to deduce from experimental line widths *not only the plasma density but also the plasma temperature*; (c) a significant enhancement of the accuracy of the density and the temperature obtained from the experimental line profiles; (d) a substantial revision of simulation models for the ion dynamical contribution that were based on a wrong assumption that the latter vanishes under increasing N and/or n.

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