Broadening of the Lyman-α lines of hydrogen and hydrogenic ions in dense plasmas

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Theoretical estimates are proposed for the profiles of the central components of Lyman-α lines for conditions where Stark effects caused by high- and low-frequency fields are more important than fine-structure splitting. An experiment-theory discrepancy of a factor ~2 for hydrogen Lyman-α lines is removed by allowing also for electron-produced low-frequency fields.

I. INTRODUCTION

Measured widths of Stark-broadened spectral lines have yielded electron or ion densities in many laboratory plasmas,[1] up to peak densities of $N \approx 10^{19}$ cm^{-3}. For the much higher densities in laser-fusion research, the upper density limit needs to be extended by large factors ($\gtrsim 10^6$) for the Stark-broadening method to remain useful. If neon or argon is mixed with the deuterium-tritium fuel, Lyman-α lines of Ne X or Ar XVIII become promising candidates for this application.[2,3] The purpose of this paper is to point out that for such lines the usual Stark-broadening calculations[1,2] must be supplemented by a consideration of low-frequency field fluctuations associated with electrons in the Debye shielding clouds of the perturbing ions. These field fluctuations were neglected in previous calculations; a model for their inclusion proposed here resolves an experiment-theory discrepancy of a factor of ~2 in the width of the optically thin Lyman-α line of hydrogen.[4]

It has been customary to represent low-frequency fields (of strength $F \approx e/\rho_D^2 = 4\pi Ne^3/kT$) by distribution functions,[2] and to assume that the radiating atoms or ions respond instantaneously. This is the quasistatic approximation[1] which is appropriate if typical Stark effects

$$\omega_i = \frac{3\hbar}{zme} F \approx \frac{3\hbar}{zm\rho_D^2} = \frac{12\pi\hbar e^2 N}{zmkT} \quad (1)$$

for the shifted components of Lyman-α lines from ions with nuclear charge z are larger than the ion plasma frequency for the (singly charged) perturbing ions (of mass M),

$$\Omega_p = (4\pi Ne^2/M)^{1/2}. \quad (2)$$

The temperature should therefore satisfy

$$kT < \frac{3}{z}\frac{M}{m}\hbar\Omega_p = \frac{3}{z}\left(\frac{M}{m}\right)^{1/2}\hbar\omega_p, \quad (3)$$

a condition consistent with expected conditions in compressed pellets. (ω_p is the electron plasma frequency. Note that the Debye radius ρ_D and mean ion-ion separations r_0 are of the same order in these plasmas, as they were in many low-temperature plasma line-broadening experiments.[1])

These Stark displacements have to be compared, first of all, with the effects caused by high-frequency field fluctuations, which are mostly due to individual electrons passing by the perturbed ions rather rapidly. These effects may be calculated by the impact approximation,[1] which results for Lyman-α lines of one-electron ions in a half-width (from central peak to half-maximum-intensity point)

$$w_e \approx \frac{12\pi}{z^2}\left(\frac{2m}{\pi kT}\right)^{1/2} N\left(\frac{\hbar}{m}\right)^2\left(\frac{3}{2} + \frac{1}{2}\int_y^\infty e^{-x}\frac{dx}{x}\right). \quad (4)$$

The (approximate) constant $\frac{3}{2}$ in this estimate was determined[5] by calculating the elastic and inelastic scattering of electrons on one-electron oxygen and aluminum ions in $2p$ states, using the distorted-wave approximation. The exponential integral allows for contributions from large-l partial waves, i.e., distant collisions, and the parameter y is

$$y \approx \frac{4}{z^2}\frac{(\hbar\omega_p)^2}{kTE_H}, \quad (5)$$

where z^2E_H is the ionization energy of the radiating ion. It accounts for Debye screening and should not exceed[5] $y \approx 0.01$ for Eq. (4) to represent the width due to electron collisions to within ~20%. For such y values and $kT \approx 0.2z^2E_H$, Eqs. (1) and (4) give practically equal contributions. The corresponding densities are $N \approx z^4 10^{20}$ cm^{-3}, and we note that at substantially lower densities, impact widths of Lyman-α lines are relatively smaller[2,5] because ω_i is proportional to $z_{av}^{1/3}N^{2/3}$ in plasmas with $r_0 \ll \rho_D$. (The most probable field strength is then larger by a factor of $\sim\rho_D^2/r_0^2$ than assumed above, and $z_{av}^{1/3}$ accounts for the actual charge of the perturbing ions.)

II. THEORY

In the usual Stark-broadening calculations[1,2] impact and quasistatic mechanisms are assumed to be statistically independent, i.e., the corresponding profiles are convolved. Also, these Stark-broadening mechanisms are considered to be the only ones besides Doppler effects. However, while the impact broadening accounts essentially for all effects of high-frequency field fluctuations, it appears that low-frequency fluctuations are accounted for by the quasistatic profiles only to the extent that they are caused by (Debye-shielded and correlated) ions. We now show that low-frequency fluctuations caused by electrons in the Debye-shielding clouds of the ions produce a broadening comparable to the two conventional Stark-broadening mechanisms. A suitable point of departure is the second-order (in the plasma-radiator monopole-dipole interaction) expression for the line-shape operator:

$$\mathcal{L}(\omega) = -i\frac{e^2}{3\hbar^2}\sum_{i''}\vec{r}|i''\rangle\cdot\langle i''|\vec{r} \times \int_0^\infty \exp[i(\omega-\omega_{i''f})t] \times [\vec{E}(t)\cdot\vec{E}(0)]_{av}\,dt\,. \qquad (6)$$

This corresponds to Eq. (358) of Ref. 1, and the resultant line profile is

$$L(\omega) = -\pi^{-1}\,\mathrm{Im\,Tr}D[\omega - H_i + E_f - \mathcal{L}(\omega)]^{-1}\,, \qquad (7)$$

e.g., a generalized Lorentz profile. The trace is over states i, i', i'', etc., of the upper group of levels E_i described by the Hamiltonian H_i, and the lower state of energy E_f is assumed to be not perturbed. The operator D governs the strengths of the various components, $\omega_{i''f}$ corresponds to $E_{i''} - E_f$, $\vec{r}$ is the position operator of the radiating electron, and $\vec{E}(t)$ is the electric field produced by the plasma electrons, assumed to be isotropic.

The key quantity in Eq. (6) is the Laplace transform of the autocorrelation function of the field. The corresponding quantity for the electron density fluctuations is well known from the theory of light scattering and was used in Ref. 1, Eqs. (360), etc., to estimate $\mathrm{Im}\mathcal{L}(\omega)$ via Poisson's equation. Replacing the ion-cloud term in this estimate by the appropriate complex function we obtain

$$\mathcal{L}(\omega) \approx -i\frac{4\pi}{3}\left(\frac{\hbar}{m}\right)^2\left(\frac{2m}{\pi kT}\right)^{1/2} N a_0^{-2} \times \sum_{i''}\vec{r}|i''\rangle\cdot\langle i''|\vec{r}\int\frac{dk}{k}[1+(\rho_D k)^{-2}]^{-2} \times\left[1+\left(\frac{M}{m}\right)^{1/2}(\rho_D k)^{-4}w(z_{i''})\right]. \qquad (8)$$

Here a_0 is the Bohr radius, k the wave number of the fluctuations, M the ion mass, and w a tabulated function,[6] whose argument is

$$z_{i''} = (\omega - \omega_{\omega''f})\left(\frac{M}{2kT}\right)^{1/2} k^{-1}\,. \qquad (9)$$

The k integral diverges for large k. However, then the dipole approximation gives certainly an overestimate. Accounting for this fact by a cutoff[5] $k_m \approx z/4a_0$ and first neglecting the second (ion-cloud) term in Eq. (8), we therefore estimate $\mathcal{L}(\omega) \sim -i\ln(k_m\rho_D)$ for large $k_m\rho_D$. This is easily seen to correspond to Eq. (4) in the limit of small y, if we also realize that the diagonal matrix element of $-\mathrm{Im}\mathcal{L}(\omega)$ corresponds to w_e.

We now discuss the additional ion-cloud term in which as in the first term any resonances were neglected and only the largest term in the more general expression[7] for the fluctuation spectrum kept. Since displacements from the unperturbed frequency, i.e., values of $\omega - \omega_{i''f}$, are generally much larger than the ion plasma frequency and k values near ρ_D^{-1} are contributing the most to the integral, we replace $w(z)$ by its asymptotic form[6]

$$w(z) \approx i/z\sqrt{\pi} \qquad (10)$$

and obtain instead of the ion-cloud term in Eq. (8)

$$\mathcal{L}_c(\omega) \approx \frac{2\pi}{3}\left(\frac{\hbar}{m}\right)^2[\rho_D(\omega - \omega_{i''f})]^{-1} N a_0^{-2} \times \sum_{i''}\vec{r}|i''\rangle\cdot\langle i''|\vec{r}\,. \qquad (11)$$

The diagonal matrix elements of this operator are for the $2p$ states, with $2s$ as intermediate state,

$$d(\omega) \approx (6\pi/z^2)(\hbar/m)^2[\rho_D(\omega-\omega_0)]^{-1}N \qquad (12)$$

if ω_0 is the frequency of the unperturbed line. We also note that $\mathrm{Re}\mathcal{L}_c(\omega)$ is negligibly small in the frequency region $|\omega - \omega_0| \ll \Omega_p$, where Eq. (12) is invalid, so that substitution of Eq. (11), augmented by $\mathrm{Im}\mathcal{L}_c$, into Eq. (7) results in a triplet with the outer components shifted such that the condition $\omega - \omega_0 \approx d(\omega)$ is fulfilled. According to Eq. (12), this shift is

$$\omega_c \approx \left(\frac{6\pi}{\rho_D}N\right)^{1/2}\frac{\hbar}{zm} = \left(\frac{1}{2}\frac{r_0}{\rho_D}\right)^{1/2}\frac{3\hbar}{zmr_0^2}\,, \qquad (13)$$

which is for $r_0 \approx \rho_D$ close to the quasistatic shift ω_i from ion-produced fields as estimated by Eq. (1). (Since ω_i for $r_0 \ll \rho_D$ actually scales with $z_{av}^{1/3} r_0^{-2}$, this near equality extends to relatively small r_0/ρ_D values.)

III. LINEWIDTHS

We conclude that for dense plasmas all three Stark broadening mechanisms are equally important. In the absence of a complete theory, we propose to convolve all three profiles and to represent, for estimates of widths, the ion-cloud

TABLE I. Comparison of measured and calculated FWHM widths of the hydrogen Lyman-α line.

$10^{-17}N$ (cm^{-3})	$10^{-4}T$ (°K)	$\Delta\lambda_e$ [a] (Å)	$\Delta\lambda_D$ [b] (Å)	$\Delta\lambda_c$ [b] (Å)	$\Delta\lambda_{th}$ [c] (Å)	$\Delta\lambda_{ex}$ [d] (Å)
1	1.27	0.055 (0.050)	0.10	0.13	0.20 (0.14)	0.23
2	1.32	0.095 (0.089)	0.10	0.22	0.29 (0.16)	0.30
3	1.32	0.13 (0.13)	0.10	0.30	0.39 (0.19)	0.36
4	1.40	0.16 (0.16)	0.10	0.37	0.47 (0.22)	0.42

[a] From Ref. 1, p. 315 (values from Ref. 8 in parentheses). Subscripts e, D, and c designate electron impact, Doppler, and ion-cloud broadening, respectively.

[b] $1/e$ widths multiplied by $2(\ln 2)^{1/2}$.

[c] Theoretical values including the ion-cloud term (values from Ref. 8, i.e., without the ion-cloud term, in parentheses).

[d] Experimental values from Ref. 4, where nanometers were used instead of angstrom units.

profile by a Gaussian with $1/e$ width given by Eq. (13). (A Lorentz profile would be a poorer choice because the triplet components are very sharp.) For the central region of Lyman-α, for which quasistatic effects are not important, we accordingly assume a Voigt profile with a Gaussian width calculated from the Doppler width, $\omega_D = (2kT/M_r)^{1/2}\omega_0/c$, and the ion-cloud shift by geometric addition, and a Lorentzian width according to Eq. (4) or equivalent results[1,8,9] for hydrogen. The two Gaussian contributions are in the ratio

$$\frac{\omega_c}{\omega_D} \approx \frac{16(2\pi)^{3/4}}{\alpha\sqrt{6}}\left(\frac{E_H}{kT}a_0^3N\right)^{3/4}\left(\frac{M_r}{m}\right)^{1/2}z^{-3}. \qquad (14)$$

The numerical factor involving the fine-structure constant is 3.55×10^3, and for the conditions ($kT \approx 1.2$ eV, $N \lesssim 4\times10^{17}$ cm^{-3}) of the first experiment[4] in which the Stark-broadened Lyman-α line of hydrogen was observed in optically thin emission, we have $\omega_c/\omega_D \lesssim 3$. The observed profiles were found to be broader than calculated profiles,[8] which account for the usual Stark and Doppler effects but not for low-frequency electron-produced fields, by factors of ~2. This deviation seems almost quantitatively accounted for by the third Stark broadening mechanism proposed in this paper (see Table I and note that experimental errors of full widths at half maximum (FWHM) are ±0.02 Å).

IV. LINE PROFILES

A more realistic account of the third Stark broadening mechanism is obtained if one uses the fact that the triplet splitting is equivalent to an effective perturbation Hamiltonian which couples the $2p$, $m=\pm1$ states with the $2s$ state. This interaction is diagonal with respect to the set

$$|\pm\rangle = \tfrac{1}{2}|21+1\rangle \pm 2^{-1/2}|200\rangle - \tfrac{1}{2}|21-1\rangle\,,$$
$$|0\rangle = 2^{-1/2}|21+1\rangle + 2^{-1/2}|21-1\rangle\,. \qquad (15)$$

The states $|+\rangle$ and $|-\rangle$ correspond to the outer components of the triplet and the state $|0\rangle$ to the central component, which therefore carries only one half of the intensity normally associated with the $|m|=1$ states, i.e., only $\frac{1}{3}$ rather than $\frac{2}{3}$ of the total Lyman-α intensity. The Stark profile of this residual unshifted component is Lorentzian with a half-width w_e corresponding to Eq. (4) or, rather, its equivalent for hydrogen as given, e.g., in Eq. (12) of Ref. 9. (The major difference is in the so-called strong collision term, $\frac{1}{5}$ instead of $\frac{3}{2}$.) However, the electron broadening of the outer components gives rise to a generalized Lorentzian profile described by the inverse of a 2×2 matrix corresponding to, e.g., Eq. (65) of Ref. 10. For the case at hand, the diagonal matrix elements of the operator ϕ of Ref. 10 are $-2w_e$, while the off-diagonal elements are w_e. The resulting profile is

$$L(\omega) = \frac{w_e}{\pi}\,\frac{3w_e^2+\omega_c^2+3\omega^2}{(3w_e^2+\omega_c^2-\omega^2)^2+16w_e^2\omega^2}\,, \qquad (16)$$

still normalized to unit total intensity, i.e., $\int_{-\infty}^{+\infty}L(\omega)d\omega = 1$.

Strictly speaking, one should also consider the influence of the effective perturbation on the $|210\rangle$ state and include this state in the set used for Eq. (15). Instead, we note that the Stark profile of the $m=0$ states, $2^{-1/2}|210\rangle \pm 2^{-1/2}|200\rangle$, as calculated in Refs. 8 and 9, is practically flat over a frequency range corresponding to $|\omega| \lesssim 3\omega_c$. It should therefore be insensitive to low-frequency electron-produced fields. Adding together the $m=0$ profile and the two $|m|=1$ profiles calculated as described in the preceding paragraph, all with equal weight, we then obtain our total Lyman-α profile which allows for all three Stark broadening mechanisms. This profile is finally convolved with the thermal Doppler profile.

Such final profiles are compared in Fig. 1 with both the measured profiles[4] and theoretical pro-

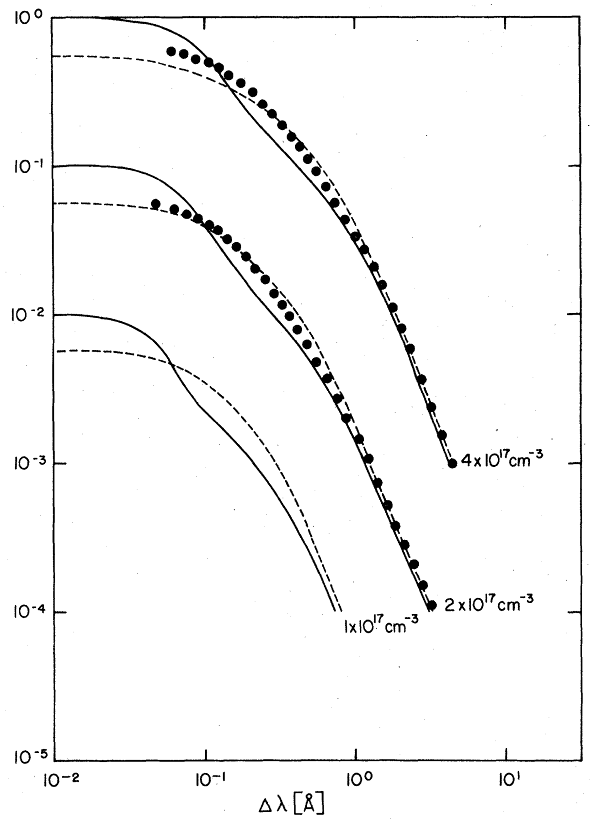

FIG. 1. Comparison of measured Lyman-α profiles (solid dots, from Ref. 4) with calculated profiles not accounting for electron-produced low-frequency fluctuations (solid lines, from Ref. 8) and with profiles calculated as described in the present paper (dashed lines). The profiles are normalized as in Ref. 4, except that the areas are normalized to 0.1 and 0.01 for the lower-density cases.

files[8] not accounting for the additional Stark broadening mechanisms proposed here. Agreement with experiment is clearly very much improved. Half-widths coincide within ~10%, although an ~20% disagreement near the line center remains at the highest density. This is to be held against an ~65% disagreement near line center when the measurement is compared with previous calculations,[1,8,9] not to mention the even larger disagreement between measured and previously calculated half-widths. An ~15% disagreement at large distances from the line center has also been removed.

V. DISCUSSION

One may ask whether or not the third Stark broadening mechanism can also explain the (much smaller) experiment-theory discrepancies for Balmer lines which were found[11] to depend on the reduced radiator (H or D)-perturbing-ion mass. Work in progress[12] suggests that this is indeed the case and that the reduced mass effect arises from Doppler shifts of low-frequency field fluctuations as seen by the radiators. To account for these Doppler shifts, the approximation made in Eq. (12) must be removed, although it remains valid for $|\omega - \omega_0| \gtrsim \max(\Omega_p, \Omega_r)$ if Ω_r is an effective ion plasma frequency calculated using the radiator mass. Conversely, the reduced mass effect is important only for $|\omega - \omega_0| \lesssim \Omega_r$. This frequency region is for the Lyman-α experiment[4] controlled by the normal (optical) Doppler effect, i.e., not important for the present calculations.

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