Ion-Dynamics Effect on Hydrogenic Stark Profiles in Hot and Dense Plasmas

R. Stamm, Y. Botzanowski, V. P. Kaftandjian, and B. Talin
Physique des Interactions Ioniques et Moléculaires, Université de Provence, 13397 Marseille Cedex 13, France

and

E. W. Smith
Ball Aerospace Systems Division, Boulder, Colorado 80306
(Received 6 February 1984)

A computer simulation has been applied to the calculation of Stark profiles of hydrogenic ions for the conditions of inertial confinement fusion. Drastic modifications of the Lyman-line profiles are observed when ion dynamics is taken into account.

PACS numbers: 32.70.Jz, 32.30.Rj, 32.60.+i

In most of the early Stark broadening theories, it was assumed that the plasma ions could be treated as stationary during the radiative lifetime of an excited atom or ion in the plasma. However, in recent years it has been shown both experimentally[1] and theoretically[2–5] that the motion of these ions can produce significant alterations near line center, particularly for low-lying series members[6] such as Lyman-α (L_α) and Lyman-β (L_β). For a plasma density of $N_e = 10^{17}$ cm^{-3}, this so-called "ion dynamics" effect can change the halfwidth by a factor of 2.[6] Since all current tabulations of Stark profiles for hydrogen[7] or hydrogenic ions[8] have employed the static-ion approximation, the use of L_α and L_β from these tables could result in serious errors in density diagnostics. The situation becomes especially unsatisfactory for the hot, dense plasmas encountered in inertial confinement fusion (ICF), because the density diagnostics rely heavily on fitting the experimental profiles with the theoretical profiles of hydrogenic ions.[9,10] Attempts have been made recently by Cauble and Griem[11] to include the effect of ion dynamics in an approximate way for the Lyman lines of Ar XVIII broadened by deuterium-tritium (DT) plasmas. For a density $N_e = 5\times 10^{23}$ cm^{-3} and a temperature $T_e = 4.6\times 10^6$ K, they found roughly a doubling in the halfwidth of L_α. In the present work, we use a computer simulation to demonstrate that in ICF conditions, the introduction of ion dynamics has a much larger effect on the profile, producing an order of magnitude increase in the halfwidth of L_α.

Our computer simulation for the ions in the plasma is based on a model of statistically independent quasiparticles moving in a spherical box,[5,12] and interacting with the radiator through a Debye shielded field,

$$\vec{\epsilon}_i = (Z_p e\, \vec{r}/r^3)(1 + r/\lambda)\exp(-r/\lambda), \qquad (1)$$

where Z_p is the charge number of the perturbing ion and λ is a screening length discussed below.

In order to evaluate the screening length λ, we first used the computer simulation to evaluate microfield distribution functions for various values of λ. We then chose the value of λ for which the computer simulation agreed with the known microfield distribution.[13,14] This fitting procedure produced better than 10% agreement between the computer simulation and the microfield distribution in Ref. 13, and it was found that λ could be given by $\lambda = [kT/4\pi e^2 N_e(1 + Z_p/2)]^{1/2}$. In these calculations, the effect of the Coulomb repulsion between the radiating ions and the perturbing ions was approximated by excluding the perturbers from a sphere of radius $r_c = Z_e Z_p e^2/\mu v^2$ where Z_e denotes the charge number of the emitting ion while μ and v are the reduced mass and relative velocity for the emitter-perturber pair. This radius r_c is the impact parameter for which an ion, moving on a hyperbolic trajectory, would experience a 90° deflection.

For the calculations reported in this paper, we have used straight-line trajectories for the ions rather than the correct hyperbolic trajectories. The deflection of the perturbers was approximated by reflecting them off a sphere of radius r_c centered on the radiator. That is, an ion approaches the radiator on a linear trajectory until it reaches the distance r_c; at that point, it is reflected away from the radiator on a new linear trajectory.

In our simulation we have treated the radiating ion as stationary so that Doppler broadening would be calculated by the usual Doppler convolution.[15,16] This procedure is adequate for heavy emitters perturbed by light ions as in the DT experiments, however, when both the emitter and the perturber have similar mass, our calculations do not properly account for changes in the emitter velocity which occur during a collision. These "velocity-changing collisions" are likely to reduce the width of the profile by the so-called "Dicke narrowing,"[17] and their effect should therefore be included in future calculations.

In our model, the time-evolution operator is expressed as a product of contributions from the electrons and the perturbing ions.[18,19] The electrons are treated with an impact theory and the ion contribution is obtained by computer simulation. The line shape is given by the Fourier transform of the emitter dipole autocorrelation function[18,19]:

$$\langle \vec{d}(t)\cdot\vec{d}(0)\rangle = \sum_{aa'} \{U_i\}_{\text{avg}} \exp(-\phi_e t)\vec{d}_{a'b}\cdot\vec{d}_{ba} e^{-i\omega_{ab}t}, \quad (2)$$

where $\vec{d}$ is the emitter dipole operator, ω_{ab} the unperturbed frequency of the transition, and $\{U_i\}$ denotes an ensemble average of the ion operator U_i. The sum is over only the upper states (a,a') of the transition because, in this paper, we are interested only in the Lyman series.

The electron-collision operator ϕ_e is taken from the calculations of Griem, Blaha, and Kepple[20] in which an ion-field cutoff procedure was employed in order to account for the influence of the ion field on the electron broadening. These calculations also contain a strong-collision term which approximates the effect of higher-order multipole interactions and inelastic collision effects.

The ion operator U_i is obtained by numerically solving the Schrödinger equation,

$$i\hbar\, \partial U_i(t)/\partial t = V_i(t)\, U_i(t), \quad (3)$$

where $V_i(t)$ denotes the interaction between the radiator and the perturbing ions. The average $\{U_i\}$ is evaluated by randomly selecting 220 different initial configurations (i.e., positions and velocities) and solving Eq. (3) for each of these; the average $\{U_i\}$ is the sum of these solutions $U_i(t)$. Noise-filtering techniques used in this procedure are discussed in Ref. 18.

In Figs. 1–4 we have plotted pure Stark profiles for low series members to illustrate the effect of ion dynamics on hydrogenic ion lines for the densities and temperatures encountered in ICF plasmas. Figures 1–3 correspond to computer simulation calculations for the L_α, L_β, and L_γ lines emitted by Ar XVIII broadened by protons for a density $N_e = 1.5\times10^{23}$ cm^{-3} and a temperature $T_e = 10^7$ K. These conditions are encountered in experiments on laser implosion of DT-filled microspheres seeded with argon. The wavelength is plotted in units of $\alpha = \Delta\lambda/\epsilon_0$ where $\epsilon_0 = 2.6eN_e^{2/3}$ and, in each figure, one curve corresponds to static ions (dashed curve) and the other corresponds to dynamic ions. In Fig. 1, dynamic-ion effects produce an order-of-magnitude increase in the halfwidth for L_α and, in Fig. 2 we see that the L_β dip is completely filled in when ion dynamics are included. The L_γ line plotted in Fig. 3 is an important line for density diagnostics because it is optically thin and, for this line, dynamic-ion effects again produce an order-of-magnitude increase in the halfwidth. Note that the Doppler effect would be negligible for this line.

Finally, in Fig. 4, we have plotted computer simulation results for the L_α line of Al XIII broadened by Al XIII perturbers for a density and temperature of $N_e = 4\times10^{21}$ cm^{-3} and $T_e = 10^7$ K which are produced by laser impact on planar tar-

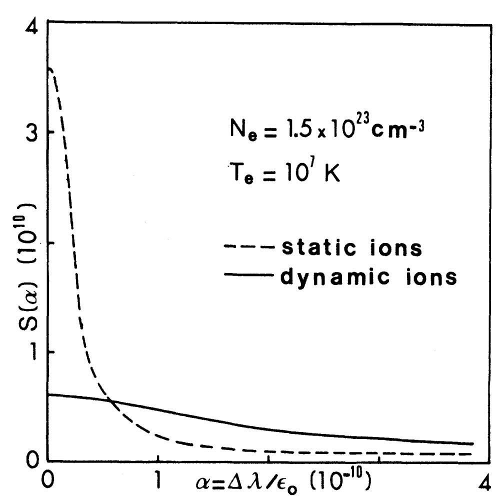

FIG. 1. Ar XVIII L_α in a DT plasma. Dashed and solid curves correspond to static and dynamic ions, respectively.

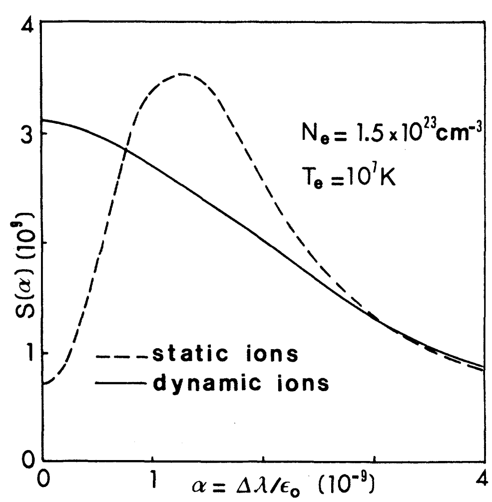

FIG. 2. Same as in Fig. 1 for L_β.

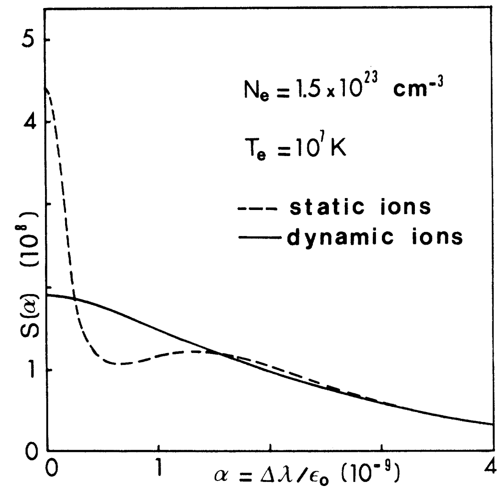

FIG. 3. Same as in Fig. 1 for L_γ.

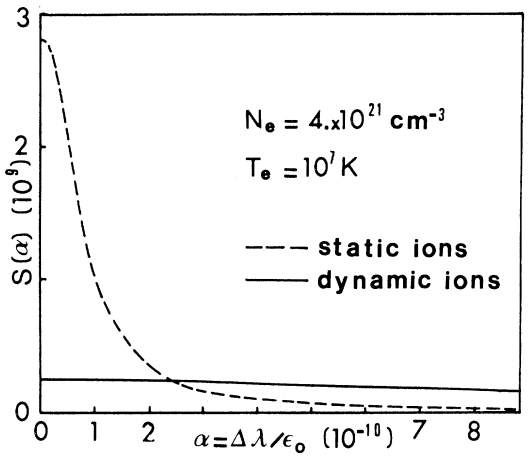

FIG. 4. Al XIII L_α perturbed by Al ions with $Z_p = 12$.

gets.[21] Again, the profile including ion dynamics is 13 times broader than the static-ion profile. The sensitivity of our results to the radius r_c has been tested on the Al XIII-L_α line by varying the size of the reflecting sphere. While minor modifications of the static and dynamic profiles were observed, the relative difference between the static and dynamic calculation was not modified.

The influence of ion dynamics is much greater for the ion lines considered in this paper than it was for the neutral lines considered previously.[18,19] To explain this difference, we use the argument presented in Sec. 4 of Ref. 18, namely that ion dynamics are important only within a frequency interval $\Delta\omega_W$ around the center of each Stark component and, outside this range, the static-ion approximation is valid. For hydrogenic-ion radiators, the Weisskopf frequency is equal to $\Delta\omega_W = Z_e \hbar v^2/1.5 n_q^2 a_0 e^2$, where n_q is the principal quantum number for the excited state and a_0 is the Bohr radius. For the L_α calculation, in the case of neutral emitters,[18,19] the ratio of $\Delta\omega_W$ to the average Stark splitting $\Delta\omega_s$ ($\Delta\omega_s \simeq \hbar^{-1} d\epsilon_0$, where d is a typical element of the dipole operator) is $\Delta\omega_W/\Delta\omega_s = \frac{1}{6}$, and the halfwidth was found to increase by a factor of 2. For the L_α line in Fig. 1 of the present paper, $\Delta\omega_W/\Delta\omega_S = 4.4$ and, for the data in Fig. 4, $\Delta\omega_W/\Delta\omega_S = 1.9$; hence the ion-dynamic effect is much more important for these lines. In addition, we expect the electron-impact broadening of the unshifted Stark components (e.g., L_α, L_γ, etc.) to be less important for ionic radiators because ϕ_e scales as $1/Z_e^2$ whereas the Weisskopf frequency increases as Z_e. That is, the region $\Delta\omega_W$ over which ion dynamics are important will now be much larger than ϕ_e whereas the opposite was true for the neutral lines considered in Ref. 18. For example, in Fig. 3, the value of α (in angströms per cgs field strength) corresponding to $\Delta\omega_W$ is $\alpha_W = 8\times 10^{-10}$ whereas ϕ_e is the order of 2×10^{-10} (i.e., the halfwidth of the static-ion profile). This figure shows that the dynamic-ion broadening of the central component greatly exceeds ϕ_e.

These calculations demonstrate that ion dynamics must be included in any calculations of the Lyman-line profiles for hydrogenic ions at the temperatures and densities encountered in laser-produced plasmas. The magnitude of these effects will obviously affect the density diagnostic of ICF plasmas. Future comparisons with experimental profiles should include a treatment of radiative transfer consistent with a dynamic-ion model, as well as other broadening mechanisms, like Doppler effects, relativistic effects, and magnetic field effects which cannot always be ignored.[22,23]

[1]D. E. Kelleher and W. L. Wiese, Phys. Rev. Lett. **31**, 1431 (1973).

[2]D. Voslamber, Phys. Lett. **61A**, 27 (1977).

[3]J. Seidel, Z. Naturforsch. **32a**, 1207 (1977).

[4]H. R. Griem, Phys. Rev. A **17**, 214 (1978).

[5]R. Stamm and D. Voslamber, J. Quant. Spectrosc. Radiat. Transfer **22**, 599 (1979).

[6]M. Geisler, K. Grützmacher, and B. Wende, in *Spectral Line Shapes,* edited by B. Wende (de Gruyter, Berlin, 1981), p. 103.

[7]C. R. Vidal, J. Cooper, and E. W. Smith, Astrophys. J. Suppl. **25**, 37 (1973).

[8]P. C. Kepple and H. R. Griem, U. S. Naval Research Laboratories Memo Report No. 3634, 1978 (unpub-

lished).

[9]B. Yaakobi, D. Steel, E. Thorsos, A. Hauer, and B. Perry, Phys. Rev. Lett. **39**, 1526 (1977).

[10]P. Jaeglé, A. Carillon, G. Jamelot, and C. Wehenkel, J. Phys. (Paris), Lett. **40**, L551 (1979).

[11]R. Cauble and H. R. Griem, Phys. Rev. A **27**, 3187 (1983).

[12]R. Stamm and E. W. Smith, Phys. Rev. A, to be published.

[13]R. J. Tighe and C. F. Hooper, Phys. Rev. A **15**, 1773 (1977).

[14]B. Held and C. Deutsch, Phys. Rev. A **24**, 540 (1981).

[15]J. Seidei, Z. Naturforsch. **34a**, 1385 (1979).

[16]J. Seidel and R. Stamm, J. Quant. Spectrosc. Radiat. Transfer **27**, 499 (1982).

[17]R. H. Dicke, Phys. Rev. **89**, 472 (1953).

[18]R. Stamm, E. W. Smith, and B. Talin, Phys. Rev. A, to be published.

[19]R. Stamm, in *Spectral Line Shapes,* edited by K. Burnett (de Gruyter, Boulder, 1983), Vol. 2, p. 3.

[20]H. R. Griem, M. Blaha, and P. C. Kepple, Phys. Rev. A **19**, 2421 (1979).

[21]R. W. Lee, J. D. Kilkenny, R. L. Kauffman, and D. L. Matthews, in *Spectral Line Shapes,* edited by K. Burnett (de Gruyter, Boulder, 1983), Vol. 2, p. 247.

[22]R. W. Lee, in *Spectral Line Shapes,* edited by B. Wende (de Gruyter, Berlin, 1981), p. 333.

[23]Nguyen Hoe, J. Grumber, M. Caby, E. Leboucher, and G. Coulaud, Phys. Rev. A **24**, 438 (1981).