

On the nature of ion dynamics

E Stambulchik¹ and A V Demura²

¹Faculty of Physics, Weizmann Institute of Science, Rehovot 7610001, Israel

²National Research Centre “Kurchatov institute”, Moscow 123182, Russia

E-mail: Evgeny.Stambulchik@weizmann.ac.il, Demura_AV@nrcki.ru

Abstract. A study of physical mechanisms responsible for the ion dynamics effects is presented. It is shown that the effect is primarily caused by the fluctuations of ion microfield direction, which can naturally be represented as rotation of the electric-microfield vector. Various aspects of this problem are discussed.

1. Introduction

Computer simulations (CS) provided a unique tool for calculation and analysis of spectral line broadening when conventional notions of quasistatic or impact broadening were not applicable [1]. While the broadening by electrons in a rather wide range of plasma conditions is within the impact regime ($h \ll 1$), the broadening by heavy perturbers often corresponds to $h \sim 1$, where h is the number of particles in the Weisskopf sphere [2]. This means that neither quasistatic nor impact broadening approximations could be applied for the latter case. So well before appearance of CS, the deviation of broadening by ions from the results of the quasistatic approximation was thought to be attributed to effects of ion dynamics (see [3] and references therein). But although the CS technique has proved its power for variety of cases [4], there had for a long time been no serious attempts to explain its results in terms of physical mechanisms, responsible for broadening under these conditions. The experimentally observed ion dynamics effects on profiles of the hydrogen Balmer- α and Balmer- β lines, although relatively minor, allowed for discovering the dependence of ion dynamics on the temperature T and the reduced mass μ as $\propto \sqrt{T/\mu}$ [5]. The real boom in studying the ion dynamics effects began after the experimental discovery [6] of an anomalous broadening of hydrogen Ly- α , whose width was about 2.5 times larger than the value, obtained within the Standard Theory (ST) model [7, 8] (i.e., quasistatic ions + impact electrons). Seven years later it was shown, also using CS, that even larger deviations from the ST results could be observed for Ly- α profiles of highly charged hydrogen-like emitters in DT plasmas [9]. During the series of Spectral Line Shapes in Plasmas code comparison workshops held recently (2012 [10], 2013 [11], and 2015) the task of physical interpretation of CS results became again a subject of interest, including studies specifically focused on the Ly- α profiles [3, 12, 13] of hydrogen and hydrogen-like species.

2. The role of microfield rotation

Historically, the first concise study of influence of the ion microfield time dependence was limited to changes of its absolute value due to the thermal fluctuations [2]. This, as well as many other studies were done within the notion of the theory of thermal corrections (TC's) to the total profile assuming applicability of the perturbative approach, i.e., that these TC's are small enough with respect to the initial broadening profile. Several years later it was shown [14] that besides the contribution of the



fluctuations of the microfield absolute value, there was also an influence of the fluctuation of the microfield *orientation* via two effects: (i) the amplitude modulation, related to changing of dipole projection in the course of of the microfield rotation in time, and (ii) non-adiabatic effects, related to inertia in the evolution of the quantum states with respect to the rotation of the quantization axis along the microfield direction. It was shown that numerically TC's due to the fluctuation of the microfield orientation are many times larger than those related to the fluctuations of the field magnitude. However, as experiments indicated, this influence could be very significant and located in the central part of the line, so that the validity of the perturbative approach would be violated. Recently performed CS, taking into account the time evolution of only microfield magnitude or only its direction, showed explicitly that fluctuations of the microfield orientation play the dominant role in the formation of the central part of the line profile [3, 12], when the ion dynamics effects are important. This was shown for various models for weakly to moderately coupled plasmas using “rotational” and “vibrational” pseudocomponents of the total microfield $\vec{F}(t)$, defined as

$$\vec{F}_{\text{rot}}(t) = F_0 \frac{\vec{F}(t)}{F(t)} \quad (1)$$

and

$$\vec{F}_{\text{vib}}(t) = \vec{n}F(t), \quad (2)$$

respectively, where F_0 is the Holtsmark field [15] and \vec{n} is a unity vector aligned, e.g., along the z axis.

A comparison of Ly- α partial profiles of neutral hydrogen assuming the ideal one component plasma (OCP) model and the linear Stark effect interaction is presented in Fig. 1 for a few values of the reduced mass. Here and below, results of a variant of CS calculations, described in Ref. [16], are used. It is seen that the “rotational” microfield component has a significantly more pronounced effect on the total line shapes. Most notably, the width of the central component due to the rotational microfield component scales as $\propto 1/\sqrt{\mu}$, similar to the ion-dynamical effects observed experimentally [5], which is a strong indication of the rotational nature of ion dynamics.

Contrary to that, changing only the magnitude of the field while keeping its direction constant (the “vibrational” component) has only a minor effect on the shape of the lateral components (and the central component remains a δ -function, evidently). Moreover, the effect has an opposite sign, i.e., the width of the lateral component *increases* with μ . Recalling that in an ideal OCP varying μ as $s^2\mu_0$ is equivalent to varying T as T_0/s^2 , we see that the lateral component becomes slightly *narrower* due to the thermal-motion effect on the magnitude of the microfield. There is also a minor shift of the maxima of the lateral components toward the far wings of the line.

3. Rotational broadening regime

Based on rather general dimensionality considerations, it was shown [17] that in an ideal OCP, the rotational broadening of a spectral line with a central unshifted component of a hydrogen-like species must have the following dependencies:

$$w = \bar{\beta} \left(\frac{T}{\mu} \right)^{1/2} N_p^{1/3}, \quad (3)$$

where N_p is the plasma density, and $\bar{\beta}$ is a *universal* dimensionless constant, found from CS to be ≈ 1.2 . In other words, the broadening in this regime depends neither on plasma particle charges Z_p nor on *any* atomic property—including the atomic number Z and the principal quantum numbers of the initial n and final n' levels—of the radiator! The only condition required for entering this paradoxical regime is that the (quasi)static Stark broadening $w_{\text{qs}} \sim (d_i - d_j)F_0$ significantly exceeds the typical microfield frequency $w_{\text{dyn}} \sim \sqrt{T/\mu}N_p^{1/3}$, or $R \gg 1$, using the dimensionless quantity R [18]

$$R = w_{\text{qs}}/w_{\text{dyn}} \approx 7 \frac{|Z_p|(n^2 - n'^2)\mu^{1/2}N_p^{1/3}}{ZT^{1/2}}. \quad (4)$$

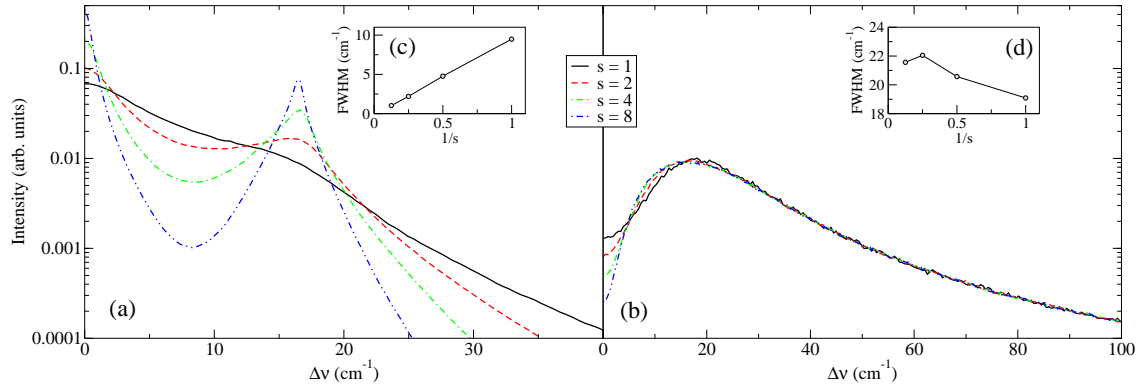


Figure 1. Ly- α profiles, broadened by (a) \vec{F}_{rot} and (b) \vec{F}_{vib} of an OCP, assuming $N = 10^{17} \text{ cm}^{-3}$ and $T = 1 \text{ eV}$. The ion radiator reduced mass $\mu = s^2 \mu_0$, where $\mu_0 = 0.5$. The FWHM's of the rotational and vibrational broadenings are shown in the insets (c) and (d), respectively. Note that in the later case, the width of a single lateral component is shown (the central component remains a δ -function, not shown here).

In spite of the counter-intuitive nature of this conclusion, it was fully confirmed using CS results [17]. Furthermore, a simple expression can be used interpolating between the impact and rotational broadening regimes, well suited to Ly- α of any H-like species:

$$w = w_{\text{qs}} \left(\frac{\bar{\alpha}}{R} + \frac{R}{\bar{\beta}} \right)^{-1} \equiv w_{\text{dyn}} \left(\frac{\bar{\alpha}}{R^2} + 1/\bar{\beta} \right)^{-1}, \quad (5)$$

where $\bar{\alpha} \approx 2$, similarly to $\bar{\beta}$, is a universal dimensionless constant. In Fig. 2 we demonstrate a good quality of this interpolation. In particular, it is seen that in the rotational regime ($R \gg 1$), the widths of both Ly- α and Balmer- α lines asymptotically approach the same value. We also show there the width of Ly- α broadened by the ‘‘rotational’’ microfield projection (1) of the same OCP. Strikingly, whether the full microfield histories or just their rotational properties are used, the results are practically indistinguishable. This is another proof of the rotational nature of ion dynamics.

We stress again that Eq. (5), interpolating between the impact and rotational broadening regimes, is universal, i.e., it is applicable to any kind of the plasma perturbors, including electrons. This allows for a straightforward generalization to the case of two-component plasma (TCP) model, assuming, as is often done in plasma line broadening, independent effects of ion and electrons. Since the lineshapes are Lorentzian in both the impact and rotational limits, the total width is approximated by an arithmetic sum of the both contributions, $w_{\text{tot}} = w_i + w_e$. As shown in Fig. 3, this simple model gives very accurate ($\sim 15\%$) results, when compared to rigorous CS calculations. We note that the effective N_p dependence of the Ly- α width in the TCP (close to $N_p^{2/3}$ over many orders of magnitude of plasma density) *coincidentally* matches that of the quasi-static

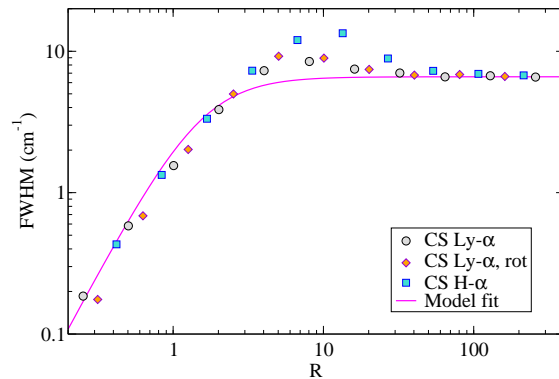


Figure 2. FWHM of Ly- α and Balmer- α in an ideal OCP with $T = 1 \text{ eV}$ and $N_p = 10^{17} \text{ cm}^{-3}$ as a function of R (4). CS results are shown, as well as a model fit according to Eq. (5).

approximation, even though each of the ion and electron contributions scales differently; the quasistatic broadening regime itself is never realized in the central part of the Ly- α shape. For similar reasons, there is practically no T dependence of the total linewidth [17]—resembling, again, the quasistatic broadening.

4. Influence of plasma coupling

The Debye screening by electrons leads to suppression of the influence of remote perturbers (i.e., lower frequencies). Therefore, a weak Debye screening (leaving fields of the perturbers at distances $\lesssim N^{-1/3}$ largely unaffected) should result in a minor *increase* of the rotational broadening. Indeed, calculations shown in Fig. 4 confirm this. For a more strongly coupled plasmas, the screening, including that due to ions, will eventually decrease the broadening. However, except for strongly coupled plasmas, these effects are relatively minor, as seen from Fig. 3 where only minor differences between results of TCP without and with the plasma coupling accounted [19] can be observed. It is important to stress that the study of partial profiles similar to presented in Fig. 1 for real plasmas of moderate coupling also demonstrate the predominance of rotational effects [12, 13].

From the ratio of the rotational width to the ion plasma frequency ω_{pi} , one can see that it is inversely proportional to the square root of the ion coupling parameter Γ_i or proportional to the cubic root of the number of particles in the ion Debye sphere N_D : $w_{rot}/\omega_{pi} \propto \Gamma_i^{-1/2} \propto N_D^{1/3}$. Therefore, it is reasonable to expect that in a strongly coupled plasma, the proportionality coefficient β in Eq. (3) might deviate significantly from that of the ideal-plasma case. At the same time, one can see that the Debye screening makes all variables interdependent, meaning the existence of some additional imposed constraints. One of these constraints stems from the fact that an infinite time is needed for the Debye screening to be fully established (see [20]).

5. Discussion

The results presented so far were obtained assuming the linear Stark effect, i.e., within the dipole-perturbation approximation, and neglecting interactions between states with different n and the fine-structure effects (the LS coupling). For hydrogen and low- Z species the latter is often justified, however, for heavier elements the LS coupling grows very fast with Z ($\propto Z^4$) and may become important. Notably, even in this case the rotational regime holds, provided the static Stark effect exceeds the fine structure. In Fig. 5 we compare Stark shapes of the Al XIII Ly- α line broadened by Al ions with $N = 10^{22} \text{ cm}^{-3}$ and $T = 240 \text{ eV}$. It is seen that the strong electric fields decrease the splitting to 2/3 of its zero-field value, and each of the component acquires width that is nearly equal to that of the central component in the calculations neglecting the LS coupling.

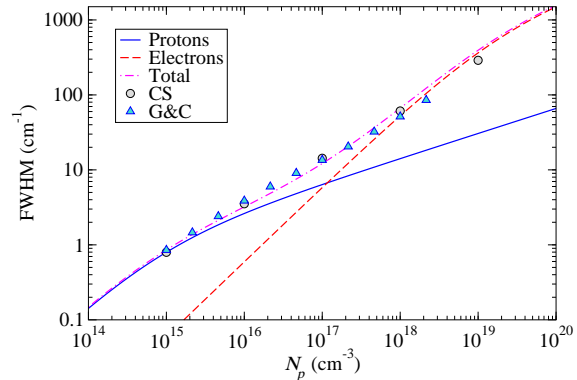


Figure 3. FWHM of Ly- α in an ideal TCP as a function of N_p : comparison of CS results with the model. $N_p = 10^{17} \text{ cm}^{-3}$ is assumed. Also shown are results for *non-ideal* hydrogen TCP from the reference diagnosis tables [19] (labeled here as “G&C”).

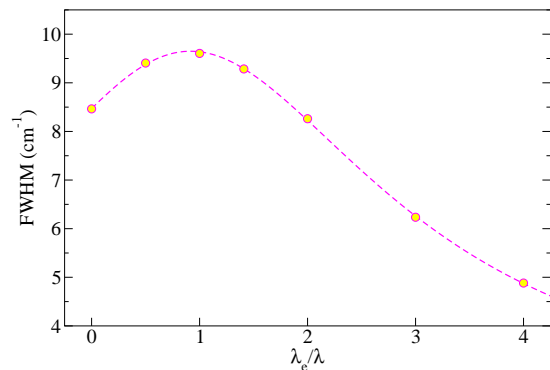


Figure 4. FWHM of Ly- α in a OCP of Debye quasiparticles with a varied screening length. $N_p = 10^{17} \text{ cm}^{-3}$ and $T = 1 \text{ eV}$.

The dipole approximation, used in most Stark broadening studies, usually suffices unless rather fine effects due to the higher members of the multipole expansions need to be described. However, transitions with unshifted Stark components, such as Ly- α , may need to be considered with the quadrupole interaction [21] accounted for. The situation is complicated, however, by the strong dipole effect of the lateral components resulting, due to the rotation of the microfield, in a complex mix of the effects of different multipoles. Therefore, a thorough study of Ly- α broadened by plasma, starting from a OCP model—while accounting for the quadrupole interactions—would be a welcome contribution to the field.

Finally, we mention that a plain field rotation leaves the central component unshifted; thus, even after averaging over a distribution of the angular frequencies, this component will remain a δ -function. Evidently, a more complicated “motion” of the microfield vector is responsible for the ion dynamical effect in general and the rotational broadening limit in particular. For example, an addition of a constant field perpendicular to the rotation plane (resulting in a cone-rotating microfield vector) removes this degeneracy. Interestingly, the effect of such a field can be described in terms of the Berry phase in an effective non-Abelian gauge potential [22].

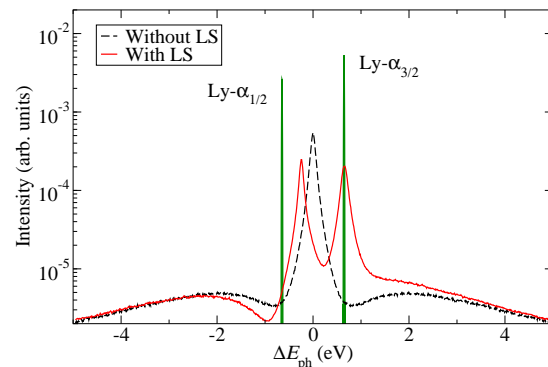


Figure 5. Al XIII Ly- α in a OCP with $N_p = 10^{22} \text{ cm}^{-3}$, $T = 240 \text{ eV}$, and $\mu = 13.5$. Compared are CS results obtained without and with fine-structure effect taken into account. Also shown are the positions of the unperturbed doublet components.

Acknowledgments

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