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Coupling and ionization effects on hydrogen spectral line shapes in dense plasmas

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Abstract. A study of hydrogen lines emitted in dense and low temperature plasmas is presented. Coupling and ionization effects in a transition from impact to quasi-static broadening for electrons are analyzed with the help of the Frequency Fluctuation Model (FFM). Electron broadening of Balmer series lines is studied for different densities and temperatures spanning a wide domain from impact to quasi-static limit. It is shown that electronic broadening makes a transition from impact to quasi-static limit depending on plasma conditions and principal quantum number. Even for the Balmer alpha line, at a density equals 10^{18} cm^{-3} and a temperature equals 1 eV, this transition occurs both in the wings and the core of the line.

PACS. 32.70.Jz Line shapes, widths, and shifts – 32.70.-n Intensities and shapes of atomic spectral lines – 32.30.-r Atomic spectra

1 Introduction

The problem of hydrogen spectral line shapes in plasmas is a subject for several years' investigations [1]. The standard approach is based on the static approximation for ions and impact approximation for electrons [2,3]. The effect of ion thermal motion was taken into account near the line centre. It was recognized also that electrons make a transition from impact to static broadening in the far wings of spectral lines. Modern state of the arts in hydrogen line broadening problems is connected with recent experimental investigations of dense plasmas with electron densities larger than or equal to 10^{18} cm^{-3} conducted by different groups [4–6]. Comparisons between experimental results and standard approach predictions having shown discrepancies, a renewed interest in hydrogen line broadening study appeared after year 2000, focusing on the Balmer alpha line emitted by dense plasmas [7–9]. The considered plasma conditions are rather close to those of Warm Dense Matter (WDM) conditions (densities near the solid density and temperature of the order of 0.1–1 eV) occurring in planetary science, in cold star physics and all plasma production devices starting from cold dense matter (pinches, laser solid matter interaction, heavy ion beam driven plasmas...). In order to have a first insight on WDM properties, a study of plasma generated by multicharged ion beams interacting with a cryogenic hydrogen sample have been proposed [10,11]. In these experiments, the electron densities may reach 10^{19} cm^{-3} at relatively low electron temperature (several eV). Diagnostic of such plasma is based on the analysis of its radiation emission and in particular the analysis of the Balmer series which has a weak opacity.

Under such nonideal plasma conditions, it may be relevant to go beyond the standard approaches of spectral line broadening and the weak coupling plasma theories. The general question related to a transition from impact to quasi-static broadening for electrons arises not only for the far wings but also for the main body of spectral lines and perturber-perturber interactions have to be taken into account properly in the description of the static and dynamic statistical properties of the plasma microfield [8–12]. Another important point in nonideal plasmas is connected with electric field ionization effects on spectral line shapes. To describe correctly the discrete-to-continuum spectrum transition, it is necessary to take into account the mechanisms which reduce the intensities of lines near the series limit and simultaneously make an allowance for continuum emission at wavelengths above the photorecombinaison limit [13,14]. Such mechanisms are related to the decay of excited atomic states in an electric field and are well known for static ion broadening [14]. Clearly, at high densities when quasi static regime is reached for electrons, a

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similar effect can become effective for electron broadening as well and models must be improved in order to account for the microfield fluctuations.

All the problems pointed above can be solved simultaneously with the help of frequency fluctuation model (FFM) [15–17]. The FFM was initially developed to account for ion dynamics effects. Electron effects on line shapes were introduced via a homogeneous broadening operator obtained within the impact approximation [2]. But, as far as the electrons can be described classically, the description of their effects on line shapes is the same one as for ions and all appropriate method developed for ions is appropriate for electrons. Then, in this work the electron and ion broadenings are determined by using the FFM in the same way. First, a line shape calculation for static electric fields of ions or electrons is performed, the ionization effects being taken into account for ion and electron broadening on the basis of the model developed in [14] and the microfield statistical properties being determined by Molecular Dynamics (MD) simulations accounting for all charge-charge correlations [18,19]. Then, the ion and electron fluctuation frequencies ν_i and ν_e are accounted for following the stochastic process implemented in the frequency fluctuation model. Finally, the total spectral line shape is obtained by means of a convolution of ion and electron profiles.

A goal of the present paper is to take into account in the frame of the FFM, the modification of spectral line shapes due to electron motional effects under conditions such that coupling and electric field ionization affect both electron and ion broadening. The results open a possibility for correct description of hydrogen line shapes in dense plasmas.

2 Calculation methods

The present calculations start with the static profiles for electron or ion perturbers accounting for ionization effects, given by the following equation:

$$I(\omega) = \sum_{i,f} \int dF W(F) I_{i,f}(\omega, F) j_i(F), \tag{1}$$

where $I_{i,f}(\omega, F) = A_{i,f}\delta(\omega - \omega_{i,f}(F))$. (i), (f) label the initial and final states of a Stark component at a frequency $\omega_{i,f}$ for a fixed value F of the electric field. The $A_{i,f}$ are the radiative decay rates. $W(F)$ is the electric field distribution function and $j_i(F)$ is a dilution factor that accounts for the field ionization effect of atomic states.

It is given by the equation:

$$j_i(F) = A_{i,f}/[A_{i,f} + \Gamma_i(F)], \tag{2}$$

$\Gamma_i(F)$ is the ionization decay rate in an electric field F, given by the equation (see [13] and references therein)

$$\Gamma_i = \left(\frac{4}{Fn^3}\right)^{2n_2+m+1} \times \exp\left[3(n_1 - n_2) - \frac{2}{3Fn^3}\right] \Big/ n^3 n_2!(n_2+m)! \tag{3}$$

where n, n_1, n_2, m are the principal and parabolic quantum numbers of the upper level (i). The Stark component frequency is given by:

$$\omega_{i,f} = \frac{3}{2} F[n(n_1 - n_2) - n'(n_1' - n_2')] \tag{4}$$

here n, n' correspond respectively to upper and lower levels.

The total intensity $I_{i,f}\ (\omega)$, normalized to the total radiative intensity of the radiative transition follows from equation (1) by multiplication with the corresponding inverse radiative transition probabilities.

The static electric field distribution function in equation (1) is obtained by molecular dynamics [18,19]. The FFM line-shape is obtained by introduction of a jumping frequency rate ν resulting in intensity exchanges between different spectral domains of the static line-shape. $\nu = N^{1/3}V_{th}$, where N is the electric charge density and V_{th} is the particle thermal velocity. $\nu(\nu_e$ or $\nu_i)$ is characteristic of the perturber (electron or ion) field fluctuations. Finally, a good approximation of the spectral line shape, taking into account both ion and electron effects, is given by convolution of ion and electron line shapes both resulting from FFM calculations.

The continuum is calculated using the general formula:

$$I_{cont}(\omega) = I^0_{cont}(\omega)\left[1 - \int_0^\infty dF W(F) j_{kn}(F)\right] \tag{5}$$

where $I^0_{cont}(\omega)$ is the intensity of recombination continuum near to the frequency of $\omega_0 = 1/2n^2 - 1/2k^2$ near a given line of the Balmer series:

$$I^0_{cont}(\omega)d\omega\left[\frac{\text{erg}}{\text{cm}^3\,\text{s}}\right] = \left(\frac{N_e}{10^{18}}\right)^2 (10^{18})^2 \frac{\hbar^2\omega}{m} \times f\left(\sqrt{2E/m}\right)\sigma^{rec}(\omega)d\omega, \tag{6}$$

where

$$E = I^i_{n=2} - \hbar\omega,$$
$$f(v) = 4\pi\left(\frac{m}{2\pi kT}\right)^{3/2} v^2 e^{-\frac{mv^2}{2kT}}dv,$$
$$\sigma^{rec}(\omega) = \frac{32\pi}{3\sqrt{3}}\alpha^3 \frac{\omega_\Gamma^2}{\omega(\omega_\Gamma/n^2 - \omega)}\frac{a_0^2}{n^3}, \quad \omega_\Gamma = Ry.$$

For the specific case of Balmer lines transitions $n' > n$, $n = 2$ and given $k \equiv \{n_1, n_2, m\}$, $k' \equiv \{n_1', n_2', m'\}$ we have

$$\omega_{nk,n'k'} = \omega_0 + \frac{3}{2}F\left[n(n_1 - n_2) - n'(n_1' - n_2')\right]$$

with $\omega_0 = 1/2n^2 - 1/2n'^2$

$$I_{cont}(\omega_{nk,n'k'}) = \int_0^\infty dF W(F) I^0_{cont}(\omega_{nk,n'k'}(F))[1 - j_{nk,n'k'}(F)] \tag{7}$$

where, $j_{nk,n'k'}(F) = A_{nk,n'k'}/(A_{nk,n'k'} + \Gamma_{nk,n'k'}(F))$.

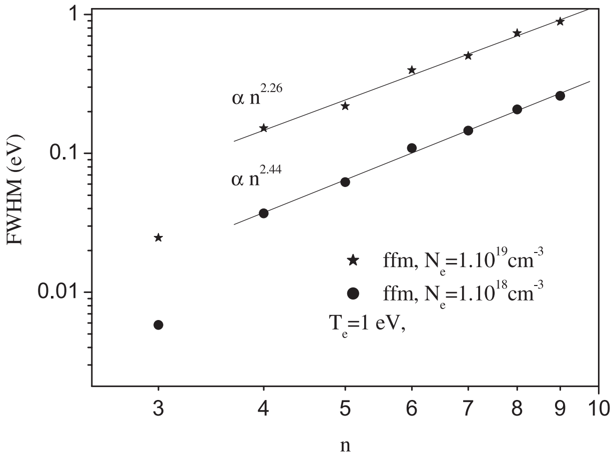


Fig. 1. Dependence of electron widths on principal quantum numbers n in the frame of FFM for $N_e = 10^{18}$ and 10^{19} cm^{-3} ($T_e = 1$ eV).

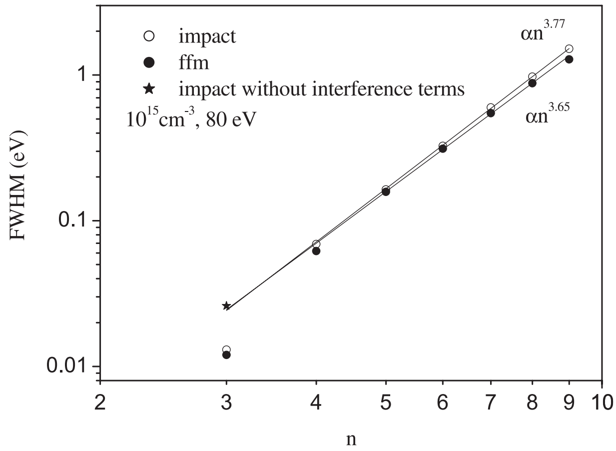


Fig. 2. Dependence of electron widths of hydrogen line profiles on principal quantum numbers n at electron densities 10^{15} cm^{-3} and temperature 80 eV in the frame of FFM and standard impact theory for electrons.

3 Results and discussion

The transition from impact to static broadening is determined by the ratio $g^{1/3}$ of typical static Stark energy levels splitting $\Delta\omega_S = CN^{2/3}$ to the jumping frequency $\nu = N^{1/3}V_{th}$. Substituting the typical value of Stark constant $C \propto n^2$ one arrives to the parameter

$$g^{1/3} = \Delta\omega_S/\nu = N^{1/3}(n^2\hbar/Mv), \tag{8}$$

where $\hbar$ is Plank constant, M is a mass of plasma particles (ions or electrons). When $g \gg 1$ the dominant broadening mechanism is static whereas for $g \ll 1$ the broadening mechanism is impact one.

For dense plasma conditions considered here the value of g is typically large for ion broadening whereas it changes from small to large values for electron broadening. In order to illustrate the FFM static and impact limits of line shapes, the FFM Balmer line width behaviours versus principal quantum number n have been investigated. Figure 1 presents the dependence of electron widths for the Balmer series as a function of principal quantum number n for plasma densities 10^{18} and 10^{19} cm^{-3}. This dependence is closer to the line width trend for the static limit which increases like n^2, than to the line width trend of impact theory which increases like n^4. It can be checked on the same figure that the density dependence is proportional to $N^{2/3}$ which is closer to static dependence of line width in contrast with impact one proportional to N.

FFM and impact widths are plotted in Figure 2 for $T = 80$ eV and low density 10^{15} cm^{-3} where the impact regime conditions are fulfilled. The good agreement found demonstrates the efficiency of FFM in describing standard impact regime for electron broadening whose trend is close to n^4.

Experimental data with three types of theory, namely impact, molecular dynamic simulation [12] and FFM are shown in Figure 3 for H_α line as a function of temperature. Discrepancies between theoretical and experimental results can be observed. Among possible reasons, they can

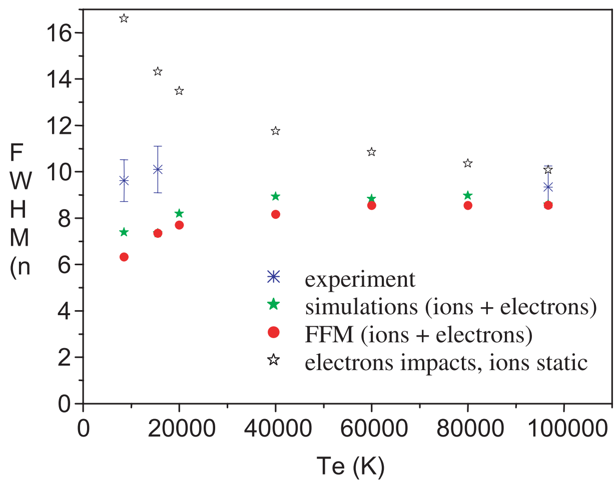
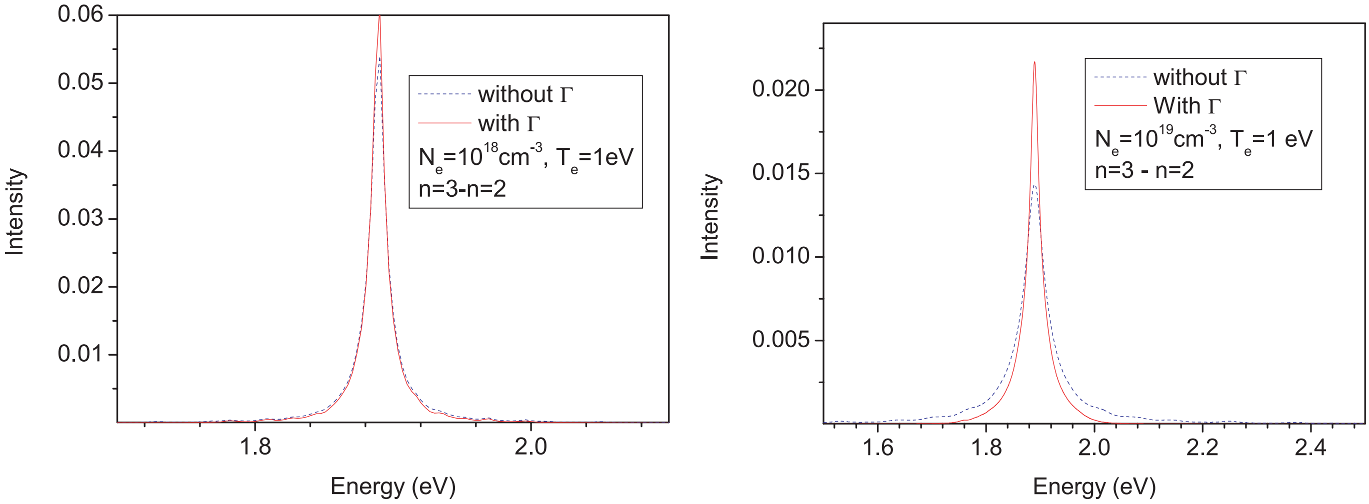


Fig. 3. Comparison of impact theory, molecular dynamic simulation and FFM with experimental data for H_α line as a function of temperature.

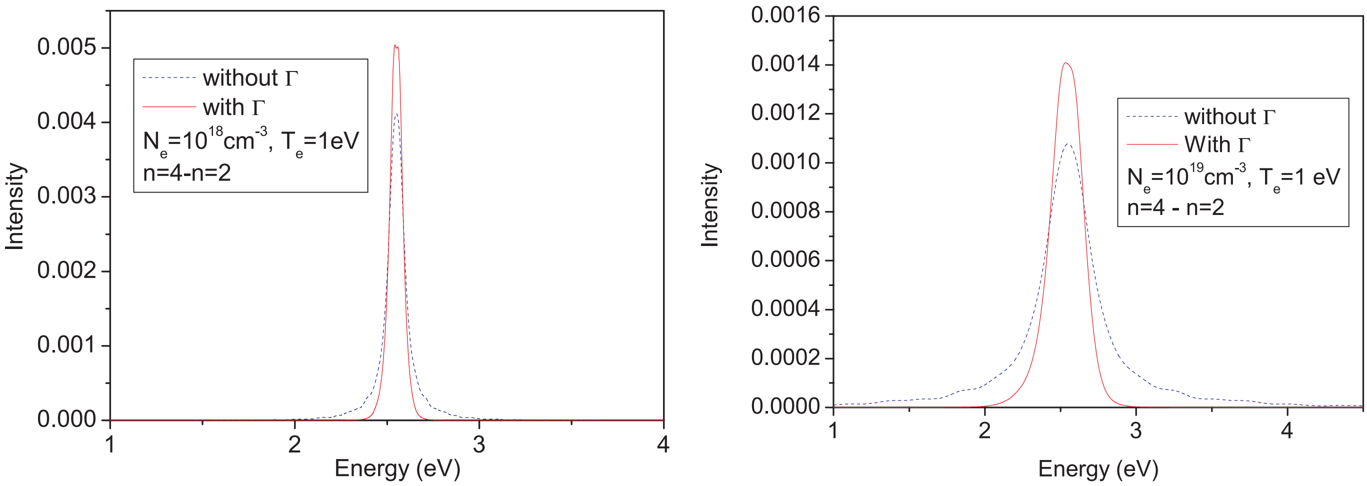
be related to uncertainties in the determination of spectral line widths in the case of high electron densities (especially for low electron temperatures) where the contribution of continuum spectra (background) is large and to the neglect of the $\Delta n \neq 0$ effects on the theoretical line widths. However, it can be pointed out that, except for standard theory, FFM, MD and experiments present the same behaviour with temperature.

The ionization effect (dilution factor Eqs. (2,3)) on spectral line intensity distribution is presented in Figures 4–6 for Balmer H_α, H_β and H_γ lines at plasma densities 10^{18} and 10^{19} cm^{-3}. The strong effect on spectral line profiles is especially evident for large plasma densities. It is clear however that higher lines can disappear in this case under large continuum radiation. It can be pointed out that for the H_α line the ionization effect results in an increase of the line intensity near its center. The effect can be understood taking into account different dilution



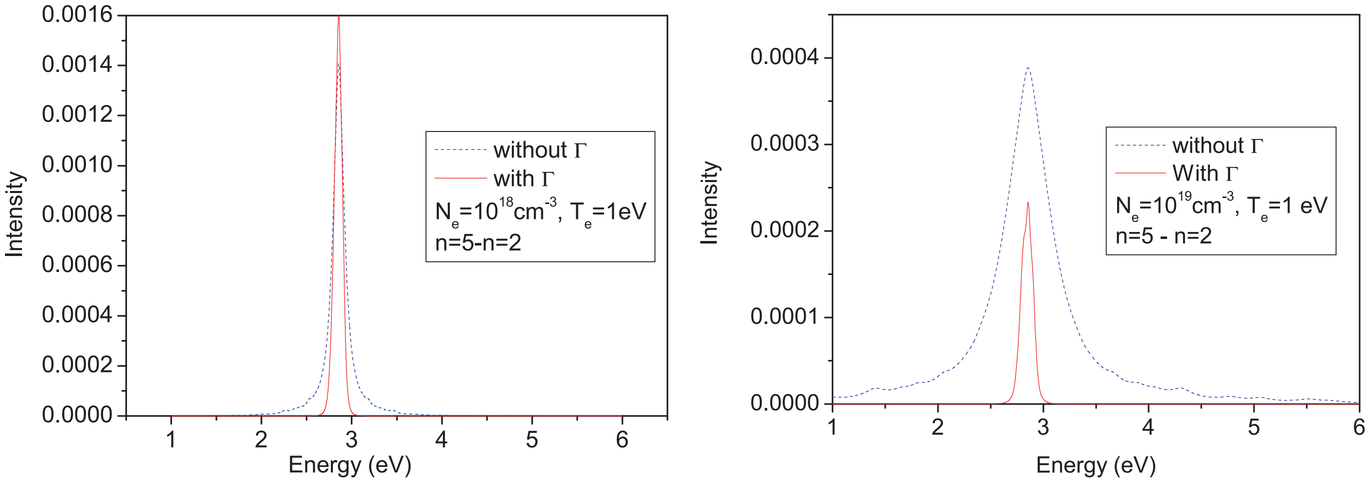
(a) (b)

Fig. 4. The effect of dilution factor on H_α line profile at electron density 10^{18} cm^{-3} (a) and 10^{19} cm^{-3} (b) and temperature 1 eV.



(a) (b)

Fig. 5. The same as in Figure 4 but for H_β line.



(a) (b)

Fig. 6. The same as in Figure 5 but for H_γ line.

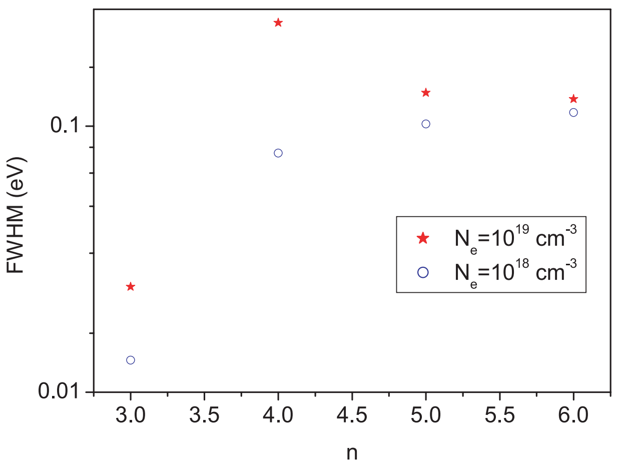


Fig. 7. The effect of dilution factor on Balmer line widths versus principal quantum numbers n for $N_e = 10^{18}$ (circles) and 10^{19} cm^{-3} (starlets).

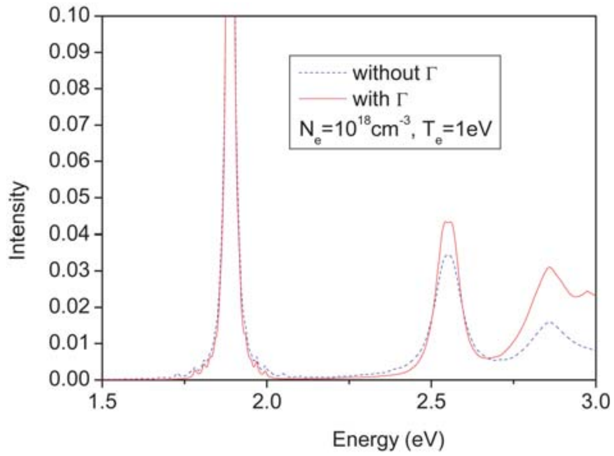


Fig. 8. Balmer series spectrum for $N_e = 10^{18}$ cm^{-3} and $T_e =$ 1 eV with (full line) and without (dash line) ionization effects.

effects for central (unshifted) and shifted components of the line.

The general overview of the ionization effect on Balmer lines widths is presented in Figure 7 for densities $10^{18}, 10^{19}$ cm^{-3}. One can see that, due to field ionization effects, for large densities (10^{19} cm^{-3}) and increasing principal quantum numbers the widths approach those obtained for smaller density (10^{18} cm^{-3}). The effect can be understood taking into account that the ionization dilution factor $j(F)$ removes strongly shifted Stark components resulting in an effective decrease of Stark constants of atomic energy levels. One can consider the effect as an effective dependence of the Stark constant of plasma density due to the ionization effect. So the spectral lines with strongly shifted components looks like lines with weakly shifted components.

Finally, total spectrum accounting for line and continuum spectra is presented in Figures 8 and 9 for the two different densities 10^{18} and 10^{19} cm^{-3} respectively. The intensities are calculated following the Saha-Boltzmann law. It can be noticed that even at the low density, taking into

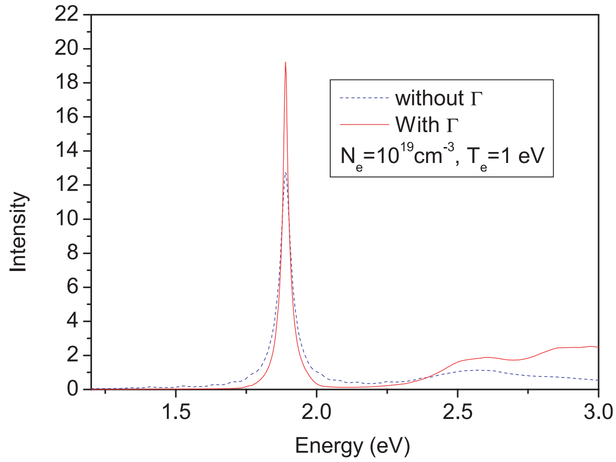


Fig. 9. The same as in Figure 8 but for $N_e = 10^{19}$ cm^{-3}.

account both the ionization effects and the static effects on the collisional broadening operator, modifies significantly the spectrum of the hydrogen Balmer series. Two trends are of a specific interest: the intensity of the continuum increases sharply with the increase of the density whereas the intensities of spectral lines decrease. At the same time the widths of spectral lines decrease in the frame of FFM as compared with the impact approximation. That means that the spectral lines become much more pronounced at the background of the continuum as compared with standard impact theory [2,3].

4 Conclusion

The general conclusion from the above considerations is that the transition of electron broadening from impact to static limit can induce changes in spectral line shapes for dense plasma conditions. Two effects are responsible for such changes: modification of electron broadening and plasma electric field ionization effect. The first effect changes dependencies of the line widths on both the density and the principal quantum number from impact scaling (proportional to Nn^4) to static scaling (proportional to $N^{2/3}n^2$). The second effect results in an effective decrease of the atomic energy levels Stark constants C due to ionization of strongly shifted Stark components in plasma microfield. The decrease influences the transition from static to impact regime but the impact line widths in the frame of FFM are also modified due to the effective decrease of line widths resulting from, first, a modification of static electric field distribution functions and, second, an effective decrease of Stark constants. So the general trend in line widths is the decrease of the line widths both in static and impact limits which is just demonstrated above.

Moreover, both effects modify the problem of interrelation between discrete and continuum spectra in dense plasmas due to the more sharp line shapes as compare with standard impact theory.

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References

1. H.R. Griem, Contrib. Plasma. Phys. **40**, 46 (2000); H.R. Griem, Contrib. Plasma. Phys. **41**, 223 (2001)
2. H.R. Griem, *Principles of Plasma Spectroscopy* (Cambridge University Press, 1997)
3. L.G. D'iachkov, G.A. Kobzev, P.M. Pankratov, J. Phys. B **21**, 1939 (1988)
4. A. Escarguel, B. Ferhat, A. Lesage, J. Richou, JQSRT **64**, 353 (2000); A. Escarguel, E. Oks, J. Richou, V. Volodko, Phys. Rev. E **62**, 2667 (2000)
5. S. Büscher et al., J. Phys. B **35**, 2889 (2002)
6. S. Flih, E. Oks, Y. Vitel, J. Phys. B **36**, 283 (2003)
7. E. Oks, J. Phys. B: At. Mol. Opt. Phys. **35**, 2251 (2002)
8. S. Alexiou, Phys. Rev. E **71**, 066403 (2005)
9. H.R. Griem, J. Halenka, W. Olchawa, J. Phys. B **38**, 975 (2005)
10. F.B. Rosmej et al., *Radiative Properties of Warm Dense Matter produced by intense heavy ion beams*, `http://www.gsi.de/phelix/Experiments/FAIR/WDM/index.htm`
11. A. Kozyreva et al., Phys. Rev. E **68**, 056406 (2003)
12. S. Ferri, A. Calisti, C. Mossé, B. Talin, M.A. González, M.A. Gigosos, AIP Conf. Proc. **874**, 142 (2006)
13. V.S. Lisitsa, *Atoms in Plasma* (Springer Berlin, 1995)
14. V.Ts. Gurovich, V.S. Engelsht, Sov. Phys.-JETP **45**, 232 (1977)
15. B. Talin et al., Phys. Rev. A **51**, 1918 (1995)
16. A. Calisti et al., J.Q.S.R.T. **65**, 109 (2000)
17. C. Mossé et al., J. Phys. B **37**, 1343 (2004)
18. B. Talin, A. Calisti, J.W. Dufty, Phys. Rev. E **65**, 056406 (2002)
19. E. Dufour et al., Phys. Rev. E **71**, 066409 (2005)