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Perturber's charge effect on Stark broadened hydrogen lines in helium plasmas

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Abstract

The Stark line profiles for hydrogen Ly_α, Ly_β, H_α, and H_β are calculated using the computer simulation method for helium plasmas in the range of electron concentration from 10^{18} to $10^{19}\,cm^{-3}$ at increasing temperature values kT from 7 to 10 eV, according to the experimental measurements in dense plasmas (Bochum experiment). The calculation was carried out at two limiting assumptions about the perturbers: (a) in the helium plasma only singly ionized helium ions occur, and (b) in the plasma the doubly ionized ions exclusively exist. In the paper the ratio of the calculated full half-widths, $FWHM(b)/FWHM(a)$, for these lines are presented. The ratio equals about to 1.1 for Ly_β and H_β lines, about 1.0 for H_α, and about 0.9 for Ly_α line.

Keywords: Hydrogen line shape; Microfield distribution function

1. Introduction

Results of the experimental as well as theoretical investigations of the H_α spectral line, formed in very dense helium plasma with trace hydrogen impurity, were presented in the paper by Böddeker et al. [1]. In that plasma the electron concentration N_e reached almost $10^{19}\,cm^{-3}$ at temperature kT to about 10 eV. The theoretical FWHM-values, calculated in the quoted paper within the quasi-static approximation for ions, were definitely smaller than the corresponding experimental values. In the case of earlier experiments, at $N_e < 10^{18}\,cm^{-3}$, such discrepancies were efficiently removed taking into account the ion dynamics effects within calculations. The best agreement of the theory and experiment for hydrogen line profiles have been attained using the computer simulation technique

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(e.g. [2–6]). However, in the case of the quoted experiment [1], it is the first instance, where the results of the simulation calculations do not agree with recent experimental data [7].

These disagreements between theory and experiment cause great amplification of the research activity in this field, in both theoretical and experimental investigations [8–14]. Griem [14], in a review article, presented the earlier measurements and calculations of the Stark broadening of the Balmer-α line in plasmas of a wide range of electron concentrations from 10^8 up to 10^{19} cm^{-3}. The author paid special attention to papers, which concerned the range of the electron concentrations above $N_e > 10^{18}$ cm^{-3}.

Alexiou and Leboucher-Dailimier [7] performed a joint simulation of electrons and ions. In that simulation: (i) the dipole approximation for emitter–plasma interactions was used; (ii) the perturbing ions were taken to be singly ionized helium ions. In both these assumptions one can introduce important physical improvements. In the matter of (i) the importance of the higher-order corrections (i.e. the quadrupolar and the quadratic Stark effect corrections) was shown by Olchawa in paper [8]. In order to check the correctness of the assumption (ii), we estimated—on the basis of the Saha-Eggert law—the ratio of concentrations of doubly and singly ionized helium ions. (The relevant internal atomic partition functions for helium were calculated according to the new procedure [15].) For the range of the physical conditions of plasma, as reported in paper [1], we obtained the concentration's ratio of the doubly to singly ionized helium ions, which assumes values from about 7 to about 10. In the light of these results, assumption (ii) appears to be unfounded; what is more: the assumption reversed, i.e. that the only doubly ionized helium ions occur in plasma, is more justifiable.

The effect of the doubly ionized helium ions on the half-widths of the hydrogen spectral lines, was preliminarily examined by the authors in the earlier paper [16]. In that earlier paper, the perturbing electrons were described within the impact approximation, and the ion dynamics effects were taken into account through the so-called small correction, similarly as in papers [17,18].

The aim of the present paper is to take into account the influence of the doubly ionized, perturbing helium ions on the Stark profiles of two beginning lines of the hydrogen Lyman and Balmer series, using the computer simulation method for perturbing both electrons and ions of plasma.

2. Microfield distribution function

For calculations of the Stark broadened line profiles, it is necessary to know the probability distribution function $W_\rho(\beta)$ of the electric microfield strength, in the scalar reduced scale $\beta = F/F_0$. The quantity F_0 is the normal field, $F_0 = e_0/R_0^2$, where R_0 is the distance defined by the relationship $(\frac{4}{15})(2\pi)^{3/2}R_0^3 N_e$. The quantity ρ is the screening parameter, $\rho = R_0/D$, where $D = (kT/4\pi e_0 N_e)^{1/2}$ is the electronic Debye radius. We wish to calculate the function $W_\rho(\beta)$ at a neutral point for the plasma consisting of electrons, and of two kinds of ions: of concentrations N_{p1} with the charge number Z_{p1}, and N_{p2} with Z_{p2}.

For isotropic plasmas, the function $W_\rho(\beta)$ can be written [19–22]

$$W_\rho(\beta) = \frac{2\beta}{\pi}\int_0^\infty \mathrm{d}x\, xF(x)\sin(\beta x), \tag{1}$$

where $A(x)$ is the Fourier transform which, after using Mayer–Mayer cluster expansion method [23], for multicomponent plasmas, has the form [22]

$$A(x)=\sum_{l=1}^{\infty}\frac{1}{l!}[N_{p1}^{l}h_{l}^{(p1)}(x)+N_{p2}^{l}h_{l}^{(p2)}(x)+N_{p1}^{l}N_{p2}^{l}h_{2l}^{(p1,\,p2)}(x)]. \tag{2}$$

For weakly coupled plasmas, the ion–ion coupling parameter $\Gamma_{\rm ii}$ fulfils the relation

$$\Gamma_{\rm ii}=\langle V_{\rm i}\rangle/kT=\tfrac{1}{3}Z_{p}^{4/3}\rho^{2}\ll 1. \tag{3}$$

For the experiment [1] the maximum value of the parameter $\Gamma_{\rm ii}$ amounts to about 0.16. In that case it is possible to restrict the summation in Eq. (2) to one-body h_1 and two-body h_2 functions (Mozer–Baranger limit [19,22]). Proceeding similarly as in [19,22], we can write the functions $h_l(x)$ as follows:

- one-body functions

$$h_{1}^{(p)}(x)=-x^{3/2}/N_{\rm e}\frac{15}{(8\pi)^{1/2}}\int_{0}^{\infty}{\rm d}y\,y^{2}[1-j_{0}(\varepsilon)], \tag{4}$$

- two-body functions

$$h_{2}^{(p1,\,p2)}(x)=-x^{3/2}/N_{\rm e}^{2}Z_{p1}Z_{p2}R_{D}v^{3}(I_{p1,\,p2}+I_{p2,\,p1}), \tag{5}$$

  where integrals $I_{p,\,p'}$ are

$$I_{pp'}=\sum_{l=0}^{\infty}(-1)^{l}(2l+1)\int_{y_1=0}^{\infty}{\rm d}y_{1}y_{1}^{2}\int_{y_2=0}^{y_1}y_{2}^{2}\,{\rm d}y_{2}$$

$$[j_{l}(\varepsilon_{1})-\delta_{l,0}][j_{l}(\varepsilon_{2})-\delta_{l,0}]f_{l}>(u_{1})f_{l}<(u_{2}), \tag{6}$$

  where $j_l(\varepsilon)$ is the *Spherical Bessel Function* of order l, and $f_l>(u)$ and, $f_l<(u)$, defined according to [20], are given by

$$f_{l}>(u)=(-1)^{l}u^{l}\left(\frac{\rm d}{u\,{\rm d}u}\right)^{l}\left(\frac{{\rm e}^{-u}}{u}\right), \tag{7}$$

  and

$$f_{l}<(u)=i^{-l}j_{l}(iu)=u^{l}\left(\frac{\rm d}{u\,{\rm d}u}\right)^{l}\left(\frac{\sinh u}{u}\right). \tag{8}$$

New variables used in Eqs (4)–(8) are defined as follows:

$$v=\rho x^{1/2},$$

$$\varepsilon_{p}=Z_{p}y^{-2}(1+vy)\exp(-vy),$$

$$u=R_{D}vy,$$

$$R_{D}=\left[1+\frac{Z_{p1}^{2}+C(Z_{p2}^{2}-Z_{p1}^{2})}{Z_{p1}+C(Z_{p2}-Z_{p1})}\right]^{1/2},$$

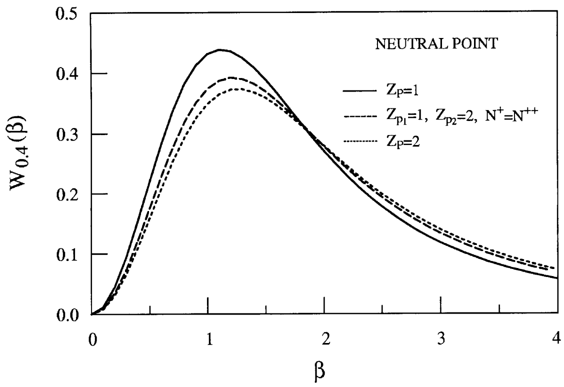

Fig. 1. The electric microfield distributions function $W_\rho(\beta)$ at a neutral point as a function of the reduced electric field β for a fixed screening parameter $\rho = 0.4$, but for different perturber ion charge numbers.

and

$$C = N_{p2}/(N_{p2} + N_{p1}).$$

The extensive tables of the numerical values of $W_\rho(\beta)$, calculated according to the presented procedure, are accessible under the address: (http://draco.uni.opole.pl/Halenka.html). In Fig. 1 the results of calculations for the function $W_{0.4}(\beta)$ are presented as an example. The correctness of our numerical code is demonstrated by the effect that for singly ionized plasmas ($C = 0$ in the code) our distribution functions $W_\rho(\beta)$ excellently agree with the Hooper's [21] distributions.

3. Line profile calculations

In order to describe the hydrogen line profile formed by emitter–plasma interactions, we have accepted the conventional assumptions similarly as in [6]. Thus, the relation between the spectral line profile and the average of the atomic dipole autocorrelation function $C(t)$, may be written

$$I(\omega) = \lim_{t_f \to \infty} \pi^{-1} \Re e \int_0^{t_f} C(t) e^{i\Delta\omega t} \, dt, \tag{9}$$

$$C(t) = Tr\{\mathbf{d}_{if} \cdot U^\dagger_{ff'}(t) \mathbf{d}_{f'i'} U_{i'i}(t)\}_{av} / Tr\{\mathbf{d}_{if} \cdot \mathbf{d}_{fi}\}, \tag{10}$$

where $\mathbf{d}$ is the dipole operator for the hydrogen atom, ii′ and ff′ indicate the sublevels of the initial (E_i) and final (E_f) states of the unperturbed atom, respectively. The relative frequency is given by $\Delta\omega = \omega - (E_i - E_f)/\hbar$, whereas $U(t)$ is the time development operator for the hydrogen atom in the presence of the electric field produced by electrons and ions. The averaging, $\{\}_{av}$, is taken over all the initial field strengths and possible time histories. The time-evolution operators $U_{i'i}(t)$ and $U_{f'f}(t)$ (corresponding to the initial and final states, respectively) satisfy the following Schrödinger equation:

$$i\hbar \dot{U}(t) = (H_0 + V(t))U(t), \tag{11}$$

where H_0—the Hamiltonian of the isolated radiator; $V(t) \approx -\mathbf{d} \cdot (\mathbf{F}_i(t) + \mathbf{F}_e(t))$—the radiator–plasma interaction, limited to the dipole approximation; $\mathbf{F}_i(t)$ and $\mathbf{F}_e(t)$—the uniform electric fields produced by ions and electrons, respectively, at the position of a given emitter. The electric field-strength variations with time were obtained by means of the computer simulation method. We used the so-called μ^*-ion model (introduced in [4]), which allowed us to take into account—at least approximately—the coupling between Stark and Doppler broadening (contrary to the usually used μ-ion model, which completely ignores this effect). The analysis of the accuracy of the calculated results was carried out according to [6]. Each simulated profile was obtained taking 1000 perturber configurations for averaging. We estimate that the statistical uncertainty of the simulated FWHMs is equal to about 3%. The matrix elements of the time-evolution operators $U_{ii'}$ and $U_{ff'}$ were taken by solving the Schrödinger Equation (11) using Fehleberg's numerical procedure.

4. Results

We calculated the Stark profiles for Ly_α, Ly_β, H_α, and H_β hydrogen lines (as an example see Fig. 2) formed in the helium plasmas of the electron concentrations ranging from 10^{18} cm^{-3} up to 10^{19} cm^{-3} at increasing temperature values from 7 to 10 eV (as in [1]). The calculations were made in the framework of two variants of the perturbing helium ions: (i) as the perturbers are the singly ionized helium ions ($Z_p = 1$) alone; (ii) as the perturbers are exclusively the doubly ionized helium ions ($Z = 2$). In Fig. 3, the values of the ratio of the proper full half-widths, $\Delta\lambda_{1/2}(Z_p = 2)/\Delta\lambda_{1/2}(Z_p = 1)$, are presented as a function of electron concentration N_e. The results are almost identical to those obtained in Ref. [16] by using approximate methods. The calculated values of the ratio are significantly smaller compared with the value $2^{1/3}$ (being the upper edge of Fig. 3), resulting from the relation

$$\alpha = \frac{\Delta\lambda_{1/2}(Z_p = 1)}{F_i(Z_p = 1)} = \frac{\Delta\lambda_{1/2}(Z_p = 2)}{F_i(Z_p = 2)}$$

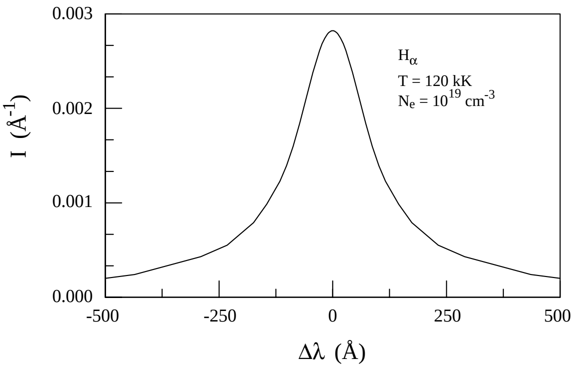

Fig. 2. The simulated line profile of the H_α line at the physical conditions of the helium plasmas: $N_e = 10^{19}$ cm^{-3}, $T = 120$ kK, the perturbing ion charge $Z_p = 2$, as an example.

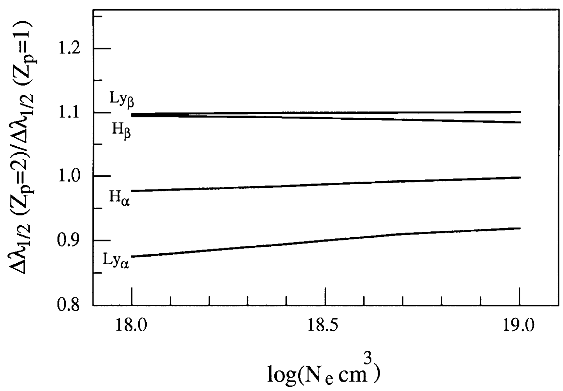

Fig. 3. The values of the ratio of the proper (full) half-widths, $\Delta\lambda_{1/2}(Z_p = 2)/\Delta\lambda_{1/2}(Z_p = 1)$, as a function of electron concentration N_e.

(where $F_i = Z_p^{1/3} F_0$ is mean ionic field), recommended e.g. in Refs. [24,25] as a tool approximately evaluating the influence of the multifold ionized perturbing ions on the half-widths of the hydrogen lines in plasma. In Fig. 3, we see that for the H_α line, mostly interesting from the point of view of the aim of the present paper, the value of the ratio equals approximately 1.0. This means that the effect examined in this paper does not contribute at all to the benefit of the improvement of the theory–experiment relations. It is proper to notice furthermore, that we obtained a surprising result for the Ly_α line: instead of the expected increasing values of the half-width of the line, we have received about 10 percent diminishing of them.

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