

# Profile of the $L_\alpha$ line of hydrogen-like ions in a dense plasma with allowance for the fine structure and the Lamb shift

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(Submitted 11 December 1984; resubmitted 7 March 1985)

Zh. Eksp. Teor. Fiz. **89**, 470–481 (August 1985)

A theory of the profile of the  $L_\alpha$  line of hydrogen-like ions in a dense plasma is calculated allowing for the fine structure, as well as for the Lamb and density shifts of the levels. The influence of the ionic microfield on the collisional electron widths and probabilities of radiative transitions is taken into account. The distribution function of the ionic microfields is found allowing for ion correlations. The results are given of numerical calculations of the profiles of the lines of Ne x, Al XIII, and Ar XVIII in a wide range of electron densities.

## I. INTRODUCTION

Broadening of the spectral lines in a plasma has been attracting investigators for a long time. The interest in this effect is mainly due to the possibility of developing plasma diagnostics on the basis of the profiles of spectral lines without introduction of any probes into a plasma because these might distort its properties. Another important application of the theory of broadening is in studies of the processes of radiative transfer in the cores of stars.

The main mechanisms of broadening of the spectral lines in a plasma are the Stark splitting of levels due to plasma microfields, and the collisional, radiative, and Doppler broadening effects. Consequently, the theory of broadening has to deal with a large number of problems from atomic physics and from the theory of a fluctuating plasma microfield. The problem is therefore very difficult and a number of simplifying assumptions is made in its solution. The traditional object of theoretical investigations is the broadening of the spectral lines of the hydrogen ions because of the importance of the applications (such as a deuterium-tritium plasma in experiments on controlled thermonuclear fusion) and because of the simplicity of the radiation source. Recently there has been a tendency to extend the investigations of the broadening of the spectral lines of hydrogen-like ions to the range with moderately large nuclear charges ( $Z_0 \lesssim 30$ ). By way of example, we can mention here the experiments on inertial-confinement fusion in which small amounts of rare gases are added to a deuterium-tritium target. An increase in the charge of the radiation source enhances the role of the relativistic effects such as the fine structure and the Lamb shift. In the majority of the calculations reported so far it is assumed that the Stark splitting of the levels is much greater than the fine structure scale. This makes it possible to ignore the relativistic corrections and to consider the Stark effect in the hydrogen atom and in hydrogen-like ions, using the parabolic quantization approximation (see, for example, Ref. 1). In those cases when the Stark splitting becomes comparable with the fine structure intervals, an allowance has to be made for the dependences of the wave functions of the Stark states on the intensity  $F$  of the electric microfield.

Calculations of the broadening of the lines of hydrogen-like ions in a hot plasma have been published recently.<sup>2,3</sup> Apruzese *et al.*<sup>2</sup> allowed for the influence of the fine structure on the profile of the  $L_\alpha$  line of Ar XVIII ions, but ignored the Stark shifts of the level, which limits the validity of the results of Ref. 2 to low densities of charged particles. The relativistic effects and the radiative line widths were ignored by Held *et al.*<sup>3</sup>

We shall report a self-consistent calculation of the profiles of the  $L_\alpha$  lines of hydrogen-like ions with  $Z_0 \lesssim 30$  allowing for the fine structure, as well as for the Lamb and density shifts of the levels. The upper limit on the charge of the light-emitting ion is set by the use of the Pauli approximation to allow for the relativistic effects. Calculations of the probabilities of spontaneous emission of the components of the  $L_\alpha$  lines carried out using the Dirac wave functions indicate that a deviation from the Schrödinger-Pauli approximation, amounting to a few percent, appears beginning from  $Z_0 \gtrsim 50$ .

## 2. INITIAL ASSUMPTIONS

The fundamentals of the modern theory of the broadening of spectral lines can be found in several monographs (see, for example, Refs. 4 and 5). The following broadening pattern is generally accepted. Ionic microfields give rise to the Stark splitting of the levels and establish states of the radiation source which are subject to the collisional electron broadening; averaging of the distribution of microfields  $W(F)$  in a plasma gives the line profile  $I(\omega)$ . The relevant analytic expressions for an  $n \rightarrow n'$  transition, derived allowing for the Doppler broadening and for the natural width of the lines, are as follows:

$$I_{nn'}(\omega) = \int_0^\infty dFW(F) I_{nn'}(\omega, F),$$

$$I_{nn'}(\omega, F) = \frac{1}{\pi} \operatorname{Re} \left( \frac{1}{\pi^{1/2}} \int_{-\infty}^\infty \frac{dv}{v_0} e^{-v^2/v_0^2} \sum_{\alpha, \alpha', \beta, \beta'} |d_{\alpha\beta}|^2 \right. \quad (1)$$

$$\left. \times \left\{ i \left[ \omega - \omega_{\alpha\beta}^{(0)} - \delta\omega_{\alpha\beta}(F) - \omega \frac{v}{c} + \operatorname{Im}(-\Phi_{nn'})_{\alpha\beta, \alpha'\beta'} \right] \right\} \right)$$

$$+\operatorname{Re}(-\Phi_{nn'})_{\alpha\beta,\alpha'\beta'} + \frac{1}{2} A_{\alpha\beta} \left. \right\}^{-1}).$$

Here, the indices  $\alpha, \alpha'$  and  $\beta, \beta'$  label the Stark states of the upper and lower levels, respectively, with the principal quantum numbers  $n$  and  $n'$ ;  $v_0 = (2T/M)^{1/2}$ ;  $\mathbf{d}_{\alpha\beta}$  are the dipole matrix elements of  $\alpha \rightarrow \beta$  transitions normalized by the condition  $\sum_{\alpha\beta} |\mathbf{d}_{\alpha\beta}|^2 = 1$ ;  $(-\Phi_{nn'})_{\alpha\beta,\alpha'\beta'}$  are the matrix elements of the electron broadening operator;  $\omega_{\alpha\beta}^{(0)}$  is the unperturbed frequency of  $\alpha \rightarrow \beta$  transitions;  $\delta\omega_{\alpha\beta}(F)$  is the Stark shift of the transition frequency in a field  $F$ ;  $A_{\alpha\beta} = A_\alpha + A_\beta$ , where  $A_\alpha$  and  $A_\beta$  are the radiative widths of the Stark levels  $\alpha$  and  $\beta$ . The expression (1) is derived assuming equal populations of the Stark states  $\alpha$  of a level with the principal quantum number  $n$ .

The collisional approximation is applicable in the case when  $g \equiv \rho_0^3 N_e \ll 1$ , where  $\rho_0$  is the Weisskopf radius and  $N$  is the density of the particles.<sup>1,4,5</sup> In the case of electrons, we have

$$g_e = \rho_0^3 N_e \approx 10^{-4} Z^{-3} (T/1 \text{ keV})^{-3/2} (N_e/10^{24} \text{ cm}^{-3}),$$

from which it follows that in the range of interest to use, corresponding to  $T \sim 1$  keV and  $N_e = 10^{20} - 10^{24} \text{ cm}^{-3}$ , the electron broadening is of the collisional nature. However, in the case of ions, we find that

$$g_i = \rho_0^3 N_i \approx 25 Z^{3/2} (T/1 \text{ keV})^{-3/2} (N_e/10^{21} \text{ cm}^{-3}) \gg 1,$$

which justifies the use of the quasistatic approximation for the ion broadening.

We shall now estimate the contributions of the various broadening mechanisms to the profile of the  $L_\alpha$  line. A characteristic value of the intensity of ionic microfields is

$$F_0 = (4\pi/3)^{3/2} Z^{3/2} e N_e^{3/2},$$

which gives

$$\Delta\omega_i \sim 10^{-2} Z^{-2/3} (N_e/10^{21} \text{ cm}^{-3})^{2/3} (\text{Ry}/\hbar).$$

The collisional electron broadening is of the order of<sup>1</sup>

$$\Delta\omega_e \sim 10^{-2} (T/1 \text{ keV})^{-1/2} Z^{-2} (N_e/10^{21} \text{ cm}^{-3}) (\text{Ry}/\hbar),$$

i.e., if  $Z \gtrsim 10$ , then  $(\Delta\omega_e/\Delta\omega_i) \lesssim 0.1$ . Although, on the average, the contribution of the electron impact broadening is relatively small, it becomes significant near the line center. For this reason we shall allow for the electron broadening mechanism. The smallness of the ratio  $\Delta\omega_e/\Delta\omega_i$  allows us to calculate the electron impact broadening operator ignoring the off-diagonal matrix elements between various Stark sublevels; their contribution to the line profile is of the second order of smallness in respect of the parameter  $\Delta\omega_e/\Delta\omega_i$ .

The Lamb shift is small compared with the fine splitting. Nevertheless, it can influence greatly the electron collisional width of the line, since for  $\Delta E_{\text{Lamb}}/\hbar\Delta\omega_i \gtrsim 1$  the wave functions of the Stark sublevels depend strongly on its magnitude. Simple estimates indicate that the Lamb shift should be allowed for if  $Z \gtrsim 15$ . The formation of the Stark sublevels may be influenced, in a manner similar to the Lamb shift, also by a small density shift of the levels due to the static screening of the Coulomb potential of the emitting ion by the

surrounding electrons. It follows from estimates given below (Sec. 4) that

$$\Delta E_{\text{dens}}/\hbar\Delta\omega_i \approx 10^{-2} Z^{3/2} (N_e/10^{24} \text{ cm}^{-3})^{1/2} (T/1 \text{ keV})^{-1},$$

i.e., the density shift must be allowed for at the maximum densities  $N_e \sim 10^{24} \text{ cm}^{-3}$  considered by us in the range  $Z \gtrsim 20$ .

Simple estimates indicate that in the range of densities and temperatures under consideration the Doppler broadening and the radiative widths of the levels must also be taken into account when the calculations are made of the profile of a line emitted by a source of charge  $Z \gtrsim 10$ .

### 3. DISTRIBUTION OF MICROFIELDS IN A PLASMA

The simplest model of the distribution of plasma microfields was proposed by Holtsmark (see Refs. 1, 4, and 5). In this model an electric field in a plasma is created by the Coulomb field of immobile noninteracting ions distributed in a random manner. In several investigations an allowance has been made for ion-ion correlations and for the screening of ionic fields in a plasma (see Refs. 4–7). We shall use the distribution of microfields, which is a modification of the results of Hooper *et al.*<sup>6,7</sup> In the case of perturbing ions of several kinds (with charges  $Z_k$  and densities  $N_k$ ) and of a radiator with a charge  $Z_0$  the distribution of microfields is as follows:

$$W(F) dF = \frac{2}{\pi} \varepsilon \int_0^\infty dl l T(l) \sin(\varepsilon l) \frac{dF}{F_0}, \quad (2)$$

$$T(l) = \exp \left\{ \sum_k I_k(l) \right\}, \quad (3)$$

$$I_k(l) = 3 \frac{N_k}{N_e} \int_0^\infty dx x^2 \exp[-Z_k F(x)] \left\{ \frac{\sin[Z_k l G(x)]}{Z_k l G(x)} - 1 \right\}. \quad (4)$$

Here,

$$F(x) = \frac{Z_0 a^2}{3x} e^{-ax}, \quad G(x) = \frac{e^{-ax}}{x^2} (1+ax), \quad (5)$$

$$a = \frac{r_0}{r_D}, \quad r_D = \left( \frac{T_e}{4\pi e^2 N_e} \right)^{1/2}, \quad \varepsilon = \frac{F}{F_0}, \quad F_0 = \frac{e}{r_0^2},$$

$$\frac{4\pi}{3} N_e r_0^3 = 1,$$

$N_e$  and  $T_e$  are the electron density and temperature.

In the original work of Hooper *et al.*<sup>6,7</sup> the method of collective coordinates is used to obtain for  $W(F)$  an expression which contains terms of the second order in respect of the ion density in the argument of the exponential function occurring in the expression for  $T(l)$ . Moreover, we can reduce the errors associated with the dropping of the higher terms of this expansion by introducing an auxiliary parameter  $\alpha \sim 1$ , which should be selected in the range where the response is relatively insensitive to its variations. It should be pointed out that introduction into the original interaction Hamiltonian of a screened Coulomb potential with electron Debye radius  $r_D$  is justified for  $r_{0i}/r_D \ll 1$ , where  $r_{0i}$  is the average distance between ions. Under these conditions the retention of the terms of the second order in the ion density is

a pointless refinement. Therefore, we shall retain only the first-order terms and assume that  $\alpha = 1$ , which follows from the initial representation of the ion-ion interaction potential. A comparison of the results of calculations carried out using such a simplified distribution with the results of Hooper *et al.* shows that the agreement between them is good. Moreover, the expression obtained is much more convenient for numerical modeling. An asymptotic expression obtained in Refs. 8 and 9 in the limit of high fields contains a pair correlation function of ions and the total (and not just the electron) Debye radius appears in this function. This is in conflict with the initial formulation of the problem, in which an allowance for the ion-ion interaction is made by a potential averaged over the electron variables. In reality, the asymptote obtained from Eqs. (2)–(5) for the distribution function  $W(F)$  in the limit of high values of the fields  $F \rightarrow \infty$  is

$W(F) \approx$

$$\frac{3}{N_e} \sum_k \frac{N_k}{Z_k} \frac{x_k^4 \exp[-Z_0 Z_k (\alpha^2/3x_k) \exp(-\alpha x_k)] \exp(\alpha x_k)}{a[2+2/\alpha x_k + \alpha x_k]}, \quad (6)$$

where  $x_k$  is found from the condition

$$Z_k G(x_k) = \varepsilon. \quad (7)$$

The formulas (6) and (7) give the asymptote of  $W(F)$  in an implicit form. It follows from Eq. (6) that this asymptote is governed by the pair correlation function with the electron Debye radius.

#### 4. STARK STATES CALCULATED ALLOWING FOR THE RELATIVISTIC EFFECT AND FOR THE DENSITY SHIFT OF LEVELS

In the case of strong fields  $F$  or relatively small charges of the light-emitting ion the Stark shift is much greater than the fine splitting of the levels. The wave functions of the levels of hydrogen-like ions are then characterized by parabolic quantum numbers. Consequently, the matrix elements of the operator of the electron broadening  $\Phi_{\alpha\beta}$ , the dipole matrix elements  $\mathbf{d}_{\alpha\beta}$ , and the radiative widths of the levels  $A_{\alpha\beta}$  occurring in Eq. (1) should be all calculated in the parabolic quantization approximation.<sup>1</sup> In those cases when the Stark shift is comparable with the fine splitting, the wave functions of the Stark states depend on the field intensity  $F$ . A calculation of the line profile should then be carried out on the basis of these wave functions.

In the case of a level with the principal quantum number  $n = 2$  the wave functions of the Stark sublevels can be represented in the form

$$\psi_i = \sum_{k=1}^3 c_k(\xi_i) \varphi_k, \quad \psi_i = \varphi_i, \quad i=1, 2, 3,$$

where  $\varphi_k$  ( $k = 1, \dots, 4$ ) are the wave functions in the spherical quantization  $|nljm\rangle$ :

$$\begin{aligned} \varphi_1 &= |2p_{1/2}, \pm^1/2\rangle, & \varphi_2 &= |2p_{1/2}, \pm^1/2\rangle, \\ \varphi_3 &= |2s_{1/2}, \pm^1/2\rangle, & \varphi_4 &= |2p_{3/2}, \pm^3/2\rangle. \end{aligned} \quad (8)$$

The dimensionless quantities  $\xi_i$  are the Stark energy shifts of hydrogen-like levels expressed in units of  $\alpha^2 \text{Ry} Z_0^4$ :  $\xi_i = \delta E_i / (\alpha^2 \text{Ry} Z_0^4)$ , where  $\text{Ry} = mc^4 / (2\hbar^2)$  is the Rydberg unit of energy and  $\alpha$  is the fine-structure constant.

The radiative corrections shift the fine-structure levels and, in particular, they lift the degeneracy of the  $2s_{1/2}$  and  $2p_{1/2}$  levels (Lamb shift). The shifts of the  $p$  states are small compared with the shift of the  $s$  states and we shall ignore the former. The radiative shifts of the  $s$  states are calculated using the formulas in Ref. 10.

In the case of a sufficiently dense plasma there is shift of the energy levels of an atom because of the distortion of the potential of the interaction between the bound electrons and the nucleus. The magnitude of this shift (known as the density shift) is governed by the spatial distribution of free electrons and of the neighboring ions. We shall use the static screening approximation to obtain an estimate of the density shift of the levels of the ion with the Coulomb potential screened by electrons:

$$\begin{aligned} (\Delta E_{nl})_{\text{dens.}} &\approx -\frac{1}{2} \left\{ (\kappa a_0)^2 [3n^2 - l(l+1)] \right. \\ &\left. + \left( \frac{a_0}{R} \right)^3 \frac{n^2}{Z_0} \left[ 1 - \frac{1}{2} (\kappa R)^2 \right] (5n^2 + 1 - 3l(l+1)) \right\} \text{Ry}. \end{aligned} \quad (9)$$

Here,  $\kappa = r_D^{-1}$  and  $R = (3Z_0/4\pi N_e)^{1/3}$  is the radius of a quasineutral cell.

The positions of the Stark levels ( $\xi_i$ , where  $i = 1, 2, 3$ ) can be found allowing for the Lamb and density shifts using the following secular equation:

$$\begin{vmatrix} -\xi & 0 & \sqrt{6} A \\ 0 & -\frac{1}{16} + \delta_2 - \xi & \mp \sqrt{3} A \\ \sqrt{6} A & \mp \sqrt{3} A & -\frac{1}{16} + \delta_3 - \xi \end{vmatrix} = 0. \quad (10)$$

Here  $\delta_2$  and  $\delta_3$  are, respectively, the density shift of the level  $2p_{1/2}$  and the sum of the density and Lamb shifts of the level  $2s_{1/2}$  expressed in units of  $\alpha^2 \text{Ry} Z_0^4$ ;  $A = ea_0 F / (\alpha^2 \text{Ry} Z_0^5)$ . The energy shifts are measured from the position of the level  $2p_{3/2}$  in the absence of an ionic microfield ( $F = 0$ ), but allowing for its density shift  $\delta_1$ . The matrix elements  $\mp \sqrt{3} A$  correspond to projections of the total momentum amounting to  $m = \pm 1/2$ . The corresponding secular equation is derived in Ref. 11 ignoring the Lamb and density shifts. The coefficients in the expansion of Stark wave functions  $\psi_i$  in terms of the basis constants  $\varphi_k$  can be represented as follows

$$\begin{aligned} c_1(\xi_i) &= \left[ 1 + \frac{\xi_i^2}{2 \left( \xi_i + \frac{1}{16} - \delta_2 \right)^2} + \frac{\xi_i^2}{6A^2} \right]^{-1/2}, \\ c_2(\xi_i, m) &= \left[ -\frac{c_1 \xi_i}{\sqrt{2} \left( \xi_i + \frac{1}{16} - \delta_2 \right)} \right] \text{sign}(m) = c_2(\xi_i) \text{sign}(m), \\ c_3(\xi_i) &= \frac{c_1 \xi_i}{A\sqrt{6}}. \end{aligned} \quad (11)$$

The secular equation (10) has the same solutions for the states with  $m = \pm 1/2$ . The coefficients  $c_1$  and  $c_3$  are also independent of the sign of  $m$ , where  $c_2$  has different signs depending on the projection of the total momentum.

The wave function and the energy of the ground state of a hydrogen-like atom are assumed to be an unperturbed wave function and an energy  $E_0$  including the Lamb and density shifts of the  $1s_{1/2}$  line level.

## 5. MATRIX ELEMENTS OF THE ELECTRON BROADENING OPERATOR

The real and imaginary parts of the electron collisional broadening operator ( $-\Phi_{nn'}$ ) can determine the contribution of electrons to the broadening and shift of levels. The relevant matrix elements can be written in the form<sup>1,4,5</sup>

$$\text{Re}(-\Phi_{nn'})_{\alpha\alpha',\beta\beta'} = \frac{4\pi}{3} \left(\frac{\hbar}{m}\right)^2 N_e \langle v_e^{-1} \rangle M_{\alpha\beta}^R, \quad (12)$$

$$\text{Im}(-\Phi_{nn'})_{\alpha\alpha',\beta\beta'} = \left(-\frac{2\pi^2}{3}\right) \left(\frac{\hbar}{m}\right)^2 N_e \langle v_e^{-1} \rangle M_{\alpha\beta}^I, \quad (13)$$

where

$$M_{\alpha\beta}^R = \delta_{\beta\beta'} \sum_{\alpha_1} \langle \alpha | \mathbf{r} | \alpha_1 \rangle \langle \alpha_1 | \mathbf{r} | \alpha' \rangle \Lambda_{\alpha,\alpha_1,\alpha'} + \delta_{\alpha\alpha'} \sum_{\beta_1} \langle \beta | \mathbf{r} | \beta_1 \rangle \langle \beta_1 | \mathbf{r} | \beta' \rangle \Lambda_{\beta,\beta_1,\beta'} - 2\delta_{\alpha\alpha'} \delta_{\beta\beta'} \langle \alpha | \mathbf{r} | \alpha \rangle \langle \beta | \mathbf{r} | \beta \rangle \Lambda_{\alpha,\alpha,\alpha}, \quad (14)$$

$$M_{\alpha\beta}^I = \frac{2}{\pi} \left\{ \delta_{\beta\beta'} \sum_{\alpha_1} \langle \alpha | \mathbf{r} | \alpha_1 \rangle \langle \alpha_1 | \mathbf{r} | \alpha' \rangle b_{\alpha,\alpha_1,\alpha'} - \delta_{\alpha\alpha'} \sum_{\beta_1} \langle \beta | \mathbf{r} | \beta_1 \rangle \langle \beta_1 | \mathbf{r} | \beta' \rangle b_{\beta,\beta_1,\beta'} \right\}. \quad (15)$$

It is shown in Sec. 2 that in the range of densities and temperatures under consideration there is no overlap of the individual Stark components, i.e.,  $\Delta\omega_e \ll \Delta\omega_i$ . For this reason the off-diagonal matrix elements of the electron collisional broadening operator are small compared with the diagonal elements<sup>1,4,5</sup> and we can replace the quantities  $\Lambda_{\alpha,\alpha_1,\alpha'}$  with  $\delta_{\alpha\alpha'} \Lambda_{\alpha,\alpha_1,\alpha}$  and  $\delta_{\alpha\alpha'} b_{\alpha,\alpha_1,\alpha}$ . The parameters  $\Lambda_{\alpha,\alpha_1,\alpha}$  and  $b_{\alpha,\alpha_1,\alpha}$  are found by integration using the impact parameters  $\rho$ . An analysis of the integrands<sup>1,4,5</sup> shows that in the selected range of plasma parameters, we have

$$\Lambda_{\alpha,\alpha_1,\alpha} \approx \Lambda_{\alpha,\alpha,\alpha} \approx \Lambda_0 \approx \ln(\rho_{\max}/\rho_{\min}) + \lambda_0, \\ b_{\alpha,\alpha_1,\alpha}(\omega_{\alpha,\alpha_1}) \approx (\pi/2) \text{sgn } \omega_{\alpha,\alpha_1}, \quad \omega_{\alpha,\alpha_1} = (E_\alpha - E_{\alpha_1}) \hbar.$$

The quantities  $\rho_{\max}$  and  $\rho_{\min}$  cut off the diverging Coulomb logarithm on the side of high and low values of the impact parameters; the parameter  $\lambda_0$  allows for the contribution of "strong" collisions. The upper cutoff parameter is usually selected to be the electron Debye radius  $r_D$ . When the collisional broadening of the hydrogen lines is considered, the lower cutoff parameter is the Weisskopf radius  $\rho_{0e}$  (Refs. 1, 4, and 5); the lower values of the impact parameter (distance) correspond to strong collisions to which perturbation theory cannot be applied. An approximate analysis shows that the contribution of strong collisions is  $\lambda_0 \approx 0.215$ .

In the case of hydrogen-like ions with sufficiently large charges the process of selection of  $\rho_{\min}$  becomes more difficult. Firstly, the Weisskopf radius  $\rho_{0e}$  is now less than the de Broglie electron wavelength  $\lambda_D = h/mv$ , so that the approximation of classical trajectories becomes invalid; secondly, the effects of the hyperbolicity of the classical trajectories of electrons may become important (in the case of hydrogen these trajectories are usually assumed to be rectilinear); thirdly, if  $\rho \lesssim n_2 a_0 / (Z_0 + 1)$ , the restriction to the dipole interaction of the perturbing electrons with a bound electron of a light-emitting ion becomes invalid and it is necessary to include the contributions of higher multipoles. It follows from the above discussion that the parameter  $\rho_{\min}$  should be selected to satisfy the condition

$$\rho_{\min} = \max \left\{ \rho_{0e}, \frac{\hbar}{mv}, \frac{Z_0 e^2}{mv^2}, n^2 \frac{a_0}{Z_0 + 1} \right\}. \quad (16)$$

In the range of plasma parameters under discussion, for charges in the range  $Z_0 \lesssim 30$ , we find that  $\rho_{\min} = h/mv$ .

The deviation of the trajectories of the perturbing electrons from hyperbolic paths can be allowed for approximately if we replace  $\ln(\rho_{\max}/\rho_{\min})$  with  $\ln(\varepsilon_{\max}/\varepsilon_{\min})$ , where  $\varepsilon$  is the eccentricity of a Coulomb orbit.<sup>4</sup> However, in the range where  $T \sim 1$  keV and  $Z_0 \lesssim 30$  the difference between  $\ln(\varepsilon_{\max}/\varepsilon_{\min})$  and  $\ln(\rho_{\max}/\rho_{\min})$  is negligible.

A change in the lower cutoff parameter  $\rho_{\min}$  should be accompanied by a corresponding change in the contribution of strong collision  $\lambda_0$  corresponding to  $\rho < \rho_{\min}$ . A consistent calculation of  $\lambda_0$  can be carried out only within the framework of a quantum-mechanical theory. However, since the contribution of "weak" collisions is logarithmically large compared with  $\lambda_0$ , it follows that in the case when  $\ln(\rho_{\max}/\rho_{\min}) \gg 1$ , we can ignore the quantity  $\lambda_0 \lesssim 1$ . This approximation is admissible for  $N_e \lesssim 10^{22} \text{ cm}^{-3}$ , but it is too rough when the density is  $N_e \sim 10^{23} - 10^{24} \text{ cm}^{-3}$ , because we then have  $\ln(\rho_{\max}/\rho_{\min}) \approx 2-3$ . Since the electron collisional widths are small compared with the characteristic ion broadening, we shall ignore  $\lambda_0$  also in this range of densities.

The expressions (12)–(15) for  $\text{Re}(-\Phi)_{\alpha\alpha}$  and  $\text{Im}(-\Phi)_{\alpha\alpha}$  can be simplified greatly using the equality  $\Lambda_{\alpha,\alpha_1,\alpha} \approx \Lambda_0$ . Employing the unitarity of the matrix  $c_{ik} = c_i(\xi_k)$ , we obtain

$$\text{Re}(-\Phi)_{\alpha\alpha} = 2M\Lambda_0\gamma_\alpha, \quad M = 18\pi \left(\frac{\hbar}{m}\right)^2 \frac{N_e}{Z_0^2} \langle v_e^{-1} \rangle, \\ \gamma_\alpha = 1 - {}^2/3 p_\alpha^2, \quad p_\alpha^2 = 1 - c_3^2(\xi_\alpha), \quad c_3^2(\xi_\alpha) = 0. \quad (17)$$

The roots of the secular equation (10) will be numbered as follows:

$$\xi_1 = \max\{\xi_i\}, \quad \xi_2 = \min\{\xi_i\},$$

and, in accordance with the above discussion, we have  $\xi_4 = 0$  [see the comment in the vicinity of Eq. (10)]. Using these relationships we obtain

$$\text{Im}(-\Phi)_{\alpha\alpha} = -\pi M \beta_\alpha, \\ \beta_1 = \gamma_1 - D(\xi_1), \quad \beta_2 = -\gamma_2 + D(\xi_2), \quad \beta_3 = {}^2/3 - \gamma_1, \\ \beta_3 = -(\beta_1 + \beta_2 + \beta_1), \quad D(\xi_i) = {}^4/9 c_3^2(\xi_i) [c_2(\xi_i) - \sqrt{2} c_1(\xi_i)]^2. \quad (18)$$

## 6. DIPOLE MATRIX ELEMENTS

The dipole matrix elements of the 2→1 transition occur in the theory in two ways: firstly, the correlation function of these matrix elements is governed by the Stark line profiles; secondly, the radiative widths of the Stark states are expressed in terms of them. In the case of normalized squares of the dipole matrix elements of the 2→1 transitions, we obtain  $d_{\alpha}^2 = (1/3)p_{\alpha}^2$ , where the quantities  $p_{\alpha}^2$  are defined above [see Eq. (17)]. The radiative widths of the Stark states  $A_{\alpha}$  are

$$A_{\alpha} = 6.268 \cdot 10^8 Z_0^4 p_{\alpha}^2. \quad (19)$$

## 7. CALCULATION OF THE LINE PROFILES

When the above relationships are employed, the system (1) describing the profile of the  $L_{\alpha}$  line of a hydrogen-like ion can be represented as follows

$$I_{21}(\omega) = \int_0^{\infty} dF W(F) I_{21}(\omega, F), \quad (20)$$

$$I_{21}(\omega, F) = \frac{1}{\pi^{1/2}} \int_{-\infty}^{\infty} \frac{dv}{v_0} \exp\left(-\left[\frac{v}{v_0}\right]^2\right) \times \frac{1}{3} \operatorname{Re} \left\{ \sum_{\alpha=1}^4 p_{\alpha}^2 \left[ i \left\{ \omega - \frac{1}{\hbar} \operatorname{Ry} \left[ \frac{3}{4} Z_0^2 + \alpha^2 Z_0^4 \left( \xi_{\alpha} + \delta_1 - \delta_0 - \frac{1}{64} \right) - \omega \frac{v}{c} + \operatorname{Im}(-\Phi)_{\alpha\alpha} \right\} + \operatorname{Re}(-\Phi)_{\alpha\alpha} + \frac{A_{\alpha}}{2} \right]^{-1} \right\} \right\}.$$

Here,  $\delta_1$  and  $\delta_0$  are the density shift of the  $2p_{3/3}$  level and the sum of the density and Lamb shifts of the  $1s_{1/2}$  level expressed in units of  $\alpha^2 \operatorname{Ry} Z_0^4$ .

In the limit of strong fields when the Stark splitting is considerably greater than the fine structure intervals for the Lamb and density shifts, the solutions of the secular equation (10) are of the form  $\xi = \pm 3A, -1/24$ ; substitution of these values into Eqs. (11) and (17)-(20) gives the  $L_{\alpha}$  line profile in agreement with that obtained in Ref. 1 using the

parabolic quantization approximation and ignoring the relativistic effects. The profile of the  $L_{\alpha}$  line given by Eq. (20) was calculated by us ignoring the effects associated with the homogeneity of the ionic electric field over distances of the order of  $\sim a_0/Z$  (Ref. 12). This imposes an upper limit on the density of ions  $(a_0 N_i^{1/3})/Z \ll 1$ . However, this limit can be relaxed if we know the compatible distribution function of the ionic microfield and of its spatial derivative obtained allowing for the ion-ion interaction. At present the problem has not yet been solved and it requires numerical calculations which are much more cumbersome than those reported above. A similar comment applied also to an allowance for the thermal motion of ions, the correct description of which requires knowledge of a compatible distribution function of ionic microfields at different moments in time.<sup>13</sup>

Investigations have recently appeared<sup>14,15</sup> in which an analysis is made of the influence of the dynamics of the broadening ions on the profile of the lines in the Lyman series of hydrogen-like ions. In particular, a theory of collisional ion broadening is developed in Ref. 14 and it is valid in the case of a dense hot plasma when the broadening of the lines due to ions with high values of  $Z_0$  is governed by light ions. A similar problem is solved in Ref. 15, but the results are not reliable because the Doppler effect was not taken into account and the model was based on some unjustified approximations.

In calculations of the profile of the  $L_{\alpha}$  spectral line with the aid of the system of equations (20), we carried out numerical integration both with respect of the intensity of the ionic field  $F$  and with respect of the intensity of the velocities of the light-emitting ions. The procedure of integration with respect to the variable  $F$  is based on the use of eighth-order Newton-Cotes quadrature formulas.<sup>16</sup> For each value of the field intensity we solved numerically the secular equation (10) in order to determine the parameters  $\xi_{\alpha}$  dependent on  $F$ . Optimization of internal integration with respect to the velocities of the light-scattering ions was ensured by the integral transformation proposed in a monograph of Nikiforov and Uvarov,<sup>17</sup> followed by the subsequent application of Hermite quadrature formulas.<sup>18</sup>

In the calculation of  $I_k(I)$  we employed adaptive algorithms for the calculations of integrals using eighth-order

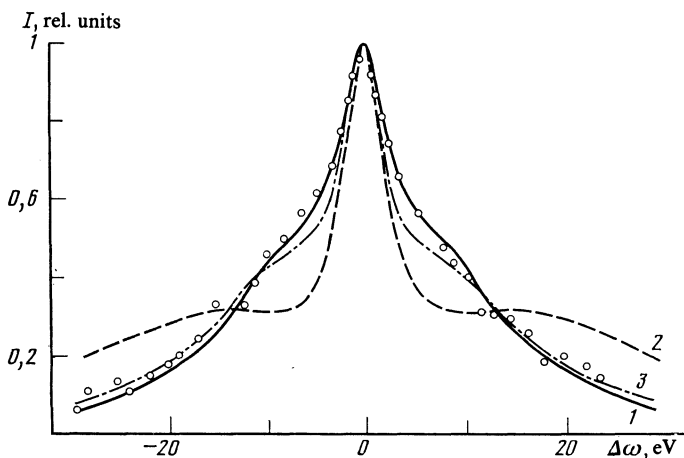


FIG. 1. Profile of the  $L_{\gamma}$  spectral line of the Ne x ion in units of  $I(\Delta\omega)/I(\Delta\omega = 0)$ . The plasma temperature is 0.3 keV and the electron density is  $7 \times 10^{22} \text{ cm}^{-3}$ . The fields created by ions are described by the Hooper distribution (curve 1) and by the Holtsmark distribution (curve 2). The experimental points and the theoretical calculations (curve 3) are taken from Ref. 20.

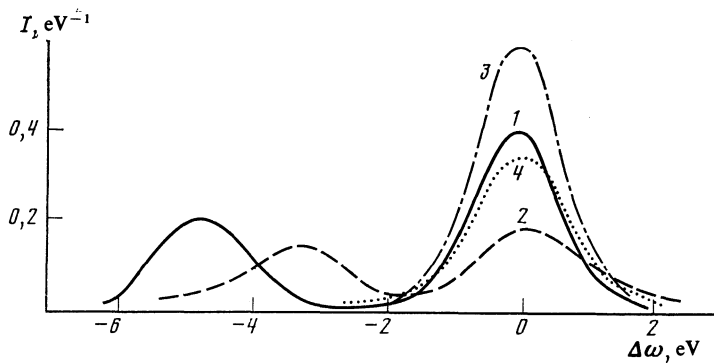


FIG. 2. Profile of the  $L_{\alpha}$  spectral line of the Ar XVIII ion. The plasma temperature is 1.4 keV and the electron densities are  $6.6 \times 10^{20} \text{ cm}^{-3}$  (curves 1 and 3) and  $10^{24} \text{ cm}^{-3}$  (curves 2 and 4). Curves 1 and 2 represent calculations in accordance with Eq. (20), whereas curves 3 and 4 are calculations carried out ignoring the relativistic effect and the density shift.

quadrature formulas in Eq. (4) (Ref. 16). A determination of  $W(F)$  was made by the fast Fourier transformation.<sup>19</sup>

## 8. RESULTS OF CALCULATIONS AND DISCUSSION

The proposed description was used to calculate the profiles of the  $L_{\alpha}$  spectral lines of hydrogen-like ions in a dense plasma for a series of values of charges of the light-emitting ions. The parameters of the plasma were varied in a wide range of temperatures and densities, typical of laser and thermonuclear plasmas. By way of illustration of the importance of an allowance for the relativistic effects we also carried out calculations ignoring the fine structure, and the Lamb and density shifts.

As pointed out in Sec. 3, in quantitative investigations of the profile of a line in a dense plasma it is necessary to use a realistic description of the distribution of plasma microfields created by ions. Figure 1 shows the profile of the  $L_{\gamma}$  line of the Ne X ion obtained ignoring the relativistic effects (small value of  $Z_0$ ). The calculations were carried out in two variants: using a distribution that allows for the ion-ion correlations and for the screening of the ionic fields (Hooper distribution), and neglecting these fields (Holtmark distribution). A comparison with the experimental results taken from Ref. 20 demonstrated a considerable improvement in respect of the agreement with the experiment when a more realistic distribution of plasma microfields was used in the calculations. Figure 1 also gives the results of theoretical calculations carried out using similar approximations and reported in Ref. 20. The slight discrepancies between the results may be attributed to differences in the calculation of the distribution of plasma microfields, shown in Sec. 3.

Figure 2 shows the results of calculations of the profile of the  $L_{\alpha}$  spectral line of the hydrogen-like ion Ar XVIII at a plasma temperature 1.4 keV for electron densities  $N_e$  amounting to  $6.6 \times 10^{20}$  and  $10^{24} \text{ cm}^{-3}$ . Our results for  $N_e = 6.6 \times 10^{20} \text{ cm}^{-3}$  agreed fully with the results of Ref. 2, the authors of which ignored the Stark shift of the levels. This approximation is justified for the selected density.

In the investigation of the influence of the relativistic effects on the spectral line profile, the center of a line calculated ignoring the fine structure was made to coincide, for the sake of convenience, with the center of the right-hand (short-wavelength) component of the line obtained allowing for the fine structure. In reality, the line calculated allowing for the relativistic effects is shifted toward higher frequen-

cies; in the case of the Ar XVIII ion this shift is about one rydberg.

An increase in the plasma density at a fixed temperature causes smearing of the left- and right-hand components of the line, accompanied by a simultaneous change in their relative intensities. When the electron density is  $N_e \sim 10^{24} \text{ cm}^{-3}$ , the relative intensity of the components is close to unity.

Figure 3 shows the profile of the  $L_{\alpha}$  spectral line of the Al XIII ion at a plasma temperature of 0.5 keV for electron densities  $10^{21}$  and  $10^{23} \text{ cm}^{-3}$ . In contrast to the preceding case (Fig. 2), the fine structure components are well-resolved only when the electron density is  $N_e \lesssim 10^{22} \text{ cm}^{-3}$ . An increase in the particle density merges the components into one line. When the electron density is  $N_e \approx 10^{24} \text{ cm}^{-3}$ , the profile of the line obtained allowing for the relativistic effects differs little from the profile of the line obtained ignoring them.

Figure 4 presents the results of calculations of the profile of the  $L_{\alpha}$  spectral line of the hydrogen-like ions Ar XVIII and Ne X carried out assuming the same plasma parameters as in Ref. 3 ( $T = 1.014 \text{ keV}$ ,  $N_e = 2 \times 10^{23} \text{ cm}^{-3}$ ). In this investigation the calculations were carried out ignoring the fine structure and the radiative line widths. It is clear from the figure that in the case of the Ne X ions ( $Z_0 = 10$ ) the relativistic effects give rise to a weak asymmetry of the spectral line. However, in the case of the Ar XVIII ions ( $Z_0 = 18$ ) the relativistic effects play a more important role and the

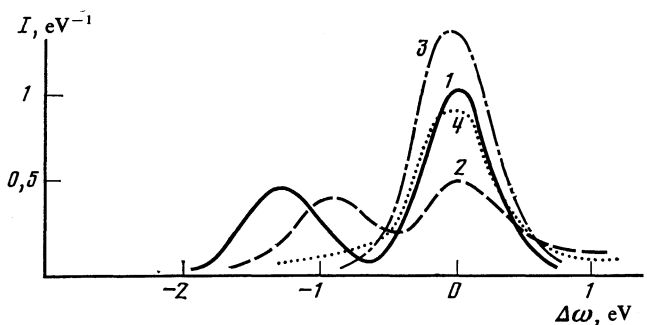


FIG. 3. Profile of the  $L_{\alpha}$  spectral line of the Al XIII ion. The plasma temperature is 0.5 keV and the electron densities are  $10^{21} \text{ cm}^{-3}$  (curves 1 and 3) and  $10^{23} \text{ cm}^{-3}$  (curves 2 and 4). Curves 1 and 2 represent calculations in accordance with Eq. (20), whereas curves 3 and 4 are calculations carried out ignoring the relativistic effects and the density shift.

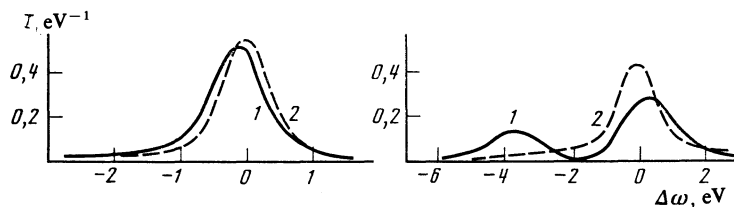


FIG. 4. Profile of the  $L_{\alpha}$  spectral line of the Ne x ion (left-hand side) and of the Ar xviii ion (right-hand side). The plasma temperature is 1.017 keV and the electron temperature is  $2 \times 10^{23} \text{ cm}^{-3}$ . Curves 1 and 2 correspond respectively to calculations carried out allowing and ignoring the relativistic effect and the density shift.

approximation employed in Ref. 3 does not provide a satisfactory description of the line profile.

It is clear from our calculations that allowance for the Lamb and density shifts results mainly in a shift of the spectral line and has a smaller effect on its profile.

An analysis of the results of the above calculations shows that the role of the relativistic effects in the formation of the profiles of the  $L_{\alpha}$  spectral lines of hydrogen-like ions increases on increase in the charge of the light-emitting ion and on reduction in plasma density. In the case of the Al XIII ions when the electron density is  $N_e \sim 10^{23} \text{ cm}^{-3}$  and the temperature is  $T = 0.5 \text{ keV}$ , the Stark splitting is comparable with the fine structure intervals and in this case the ionic microfield affects strongly not only the energies of the Stark states, but also their collisional and radiative widths, and this has a considerable influence on the whole line profile. In the case of the Ar xviii ions at  $T = 1.4 \text{ keV}$  the relativistic effects are important throughout the investigated range of the densities ( $N_e \sim 7 \times 10^{20} - 10^{24} \text{ cm}^{-3}$ ) and neglect of these effects results in a considerable deviation of the line profiles from the results of more rigorous calculations.

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Translated by A. Tybulewicz