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Effect of reduced mass in Stark broadening of hydrogen lines

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A theory is developed which describes the deformation of the Stark contour of hydrogen lines near the center, brought about by the thermal motion of the perturbing ions. The method of calculation is based on systematic perturbation theory with respect to the parameter $\dot{\Psi}_\tau < 1$, where $\dot{\Psi}$ is the characteristic rotation frequency of the ion field, while τ is the atom lifetime on the Stark sublevel and depends on the impact electron broadening $w \sim \tau^{-1}$. The main regularities of the "reduced mass effect" are explained, viz., the experimentally observed dependence of the spectral variation of the contour $I(\Delta\lambda)$ near the center of the hydrogen line on the concentration of the plasma N and the reduced mass of the perturbing ions μ. The effect is of interest as a means of determining the ion temperature T_i and of investigating the ion microfield fluctuations in the plasma.

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1. In the problem of the Stark broadening of spectral lines of the hydrogen atom, the reason for the systematic divergence of the calculated and observed shapes near the center has long remained unclear. These divergences have quite definite regularities: 1) the observed dip at the center of the lines without unshifted components (H_β, H_δ) is always less than theoretical; 2) for lines with unshifted components (H_α, H_γ) the observed intensity at the center is less and the halfwidth of the line is greater than calculated. Recently,[6,7] the supposition was advanced that the foregoing deviations are connected with the thermal motion of the ions. Experimental proof of such a connection was obtained by Wiese and coworkers,[8,9] who discovered the so-called reduced mass effect: the deformation of the central part of the line shape depends not only on the concentration of the charged particles N but also on the reduced mass of the exciting ion + radiating atom pair.

The largest amount of experimental data has been obtained for the H_β line, while the line contour was determined in Refs. 8, 9 principally by the static multiple mechanism of broadening

$$h_i = N\left(\frac{eC}{v_i}\right)^3 \gg 1,$$

where C is the Stark constant, e is the charge of the electron, and v_i is the thermal velocity of the ions.

The method of taking into account the effects of thermal motion in the many-particle case $h_i \gg 1$, based on the calculation of corrections to the static contours in terms of the parameter $h_i^{-1/2}$, was first developed within the framework of adiabatic theory by Kogan.[10] However, calculations [5] based on the adiabatic theory[10] led to corrections which did not agree with experiment not only in magnitude but even in sign. The negative result of the analysis of Ref. 5 is not surprising since, as was shown in Ref. 11, the principal role near the center of the line is played by effects connected with rotation of the electric field intensity vector of the ions $\mathbf{F}$, which were not taken into account in the adiabatic theory.[10] In the present work, thermal corrections to the contour for the case $h_i \gg 1$ are considered with account of the electron impact broadening and rotation of the ion field.

2. In calculation of the line shape $I_{ab}(\omega)$, taking into account both the electron impact broadening and also the dynamics of the ion field, the starting point is the following expression for the correction function $K_{ab}(\tau)$ (see Refs. 11 and 12):

$$K_{ab}(\tau) = \sum_{\alpha,\beta,\alpha',\beta'} \{ \langle\alpha|\hat{\mathbf{d}}(0)|\beta\rangle\langle\beta'|\hat{\mathbf{d}}(\tau)|\alpha'\rangle$$

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$$\ll\alpha'\beta'^{+}\left|\hat{P}\exp\left\{-\frac{i}{\hbar}\int_0^{\tau}dt'[\hat{H}^{(a)}(t')-\hat{H}^{(b)}(t')]+\hat{\Phi}_{ab}\tau\right\}\right|\alpha\beta^{+}\gg\Big\}_{Av} \quad (1)$$

$$\hat{H}^{(a),(b)}(t)=\hat{H}_0^{(a),(b)}-\hat{d}_z^{(a),(b)}F(t)+\hbar\hat{J}^{(a),(b)}\dot{\Psi}(t),$$

$$\hat{d}(\tau)=\hat{R}^{-1}(\tau)\hat{d}'\hat{R}(\tau),$$

$$\hat{R}(\tau)=\exp(iJ_z\theta_0)\exp(iJ_x\varphi_0)\exp\left(i\hat{J}\int_0^{\tau}\dot{\Psi}(t')\,dt'\right),$$

$$\dot{\Psi}(t)=[\mathbf{F}(t),\dot{\mathbf{F}}(t)]/F^2(t).$$

Here $\mathbf{d}'$ is the dipole moment operator in the laboratory system of coordinates, $\Psi(t)$ is the vector of the instantaneous angular velocity of the ion field $\mathbf{F}(t)$; φ_0, θ_0, $\psi_0=0$ are the Euler angles that determine the orientation of the vector $\mathbf{F}(0)$ relative to the laboratory system of coordinates. The operators $\hat{H}_0^{(a),(b)}$ of the Hamiltonian of the unperturbed hydrogen atom, $\hat{\mathbf{d}}^{(a),(b)}$ of the dipole moment, $\hat{\mathbf{J}}^{(a),(b)}$ of the angular momentum and, $\hat{\Phi}_{ab}$ of the impact electron broadening[12] are defined in the set of coordinates XYZ rotating with the vector $\mathbf{F}(t)$, so that $\mathbf{F}(t)\parallel OZ$. The indices α, α' and β, β' enumerate the Stark states of the upper (a) and lower (b) levels, respectively, $\hat{P}$ is the chronological operator, the symbol $[\ldots]_{Av}$ denotes averaging over the ensemble of plasma ions.

Assuming that the deformation of the contour $I_{ab}(\omega)$ due to the thermal motion of the ions is small, we expand $K_{ab}(\tau)$ in a series in powers of τ (cf. Rev. 11).

The evolution operator

$$\hat{T}_{ab}(\tau)=\hat{P}\exp\left\{-\frac{i}{\hbar}\int_0^{\tau}[\hat{H}^{(a)}(t')-\hat{H}^{(b)}(t')]dt'+\hat{\Phi}_{ab}\tau\right\}$$

can be represented at small τ in the form[1)]

$$\hat{T}_{ab}(\tau)\approx\exp\{-i\tau\hat{H}_{ab}\}, \quad (2)$$

$$\hat{H}_{ab}=\hat{H}_{ab}^{(0)}+\hat{V}^{(1)}(\tau)+\hat{V}^{(2)}(\tau), \quad (3)$$

$$\hat{H}_{ab}^{(0)}=(1/\hbar)[(\hat{H}_0^{(a)}-\hat{H}_0^{(b)})-(\hat{d}_z^{(a)}-\hat{d}_z^{(b)})F(0)]+i\hat{\Phi}_{ab}, \quad (4)$$

$$\hat{V}^{(1)}(\tau)=(J_x^{(a)}-J_x^{(b)})\dot{\Psi}_x(0)+(J_y^{(a)}-J_y^{(b)})\dot{\Psi}_y(0)$$
$$-(\hat{d}_z^{(a)}-\hat{d}_z^{(b)})\dot{F}(0)\tau/2\hbar, \quad (5)$$

$$\hat{V}^{(2)}(\tau)=[(J_x^{(a)}-J_x^{(b)})\ddot{\Psi}_x(0)+(J_y^{(a)}-J_y^{(b)})\ddot{\Psi}_y(0)]\tau/2$$
$$-(\hat{d}_z^{(a)}-\hat{d}_z^{(b)})\ddot{F}(0)\tau^2/6\hbar^2. \quad (6)$$

The expressions (2)–(6) were obtained by expansion of $F(\tau)$ and $\dot{\Psi}(\tau)$ in powers of τ with accuracy to terms of second order of smallness in the thermal velocity of the ions (atoms) inclusive, while the degree of v_i, corresponds to the number of differentiations with respect to time, namely, $\dot{\Psi}(0)\propto v_{i,a}$, $\ddot{F}(0)\propto v_{i,a}^2$ and so on. The possibility of such an expansion is due to the presence of the small parameter

$$\varepsilon\sim\dot{\Psi}(0)/|iC_{\alpha\beta}F(0)+w_{\alpha\beta}|\ll 1,$$

which determines the slowness of the ion motion in comparison with the damping due to the electron impact broadening. (Here, $w_{\alpha\beta}\equiv-\mathrm{Re}(\hat{\Phi}_{ab})_{\alpha\alpha,\beta\beta}$ is the impact electronic halfwidth, $C_{\alpha\beta}$ is the Stark constant of the component $\alpha-\beta$.) The effect of thermal motion can be taken into account, therefore, within the framework of perturbation theory (in the parameter ε), while, in contrast with Ref. 11, the calculation of the contour can be carried out up to the center of the line $\Delta\omega=0$, $\Delta\omega\equiv\omega-\omega_0$ (ω_0 is the unperturbed radiation frequency).

In the following, we assume that the matrix of the operator Φ_{ab} is diagonal in the basis of parabolic states.[2)]

3. Using the wave functions that diagonalize the operator (3) in the framework of perturbation theory in the parameter ε (cf. Ref. 11), and expanding $\{\hat{\mathbf{d}}(\tau)\otimes\hat{T}_{ab}(\tau)\}$ in a series in τ with accuracy to terms of second order in $v_{i,a}$ inclusive, we average $K_{ab}(\tau)$ over $\ddot{\mathbf{F}}(0)$ and $\dot{\mathbf{F}}(0)$ with the help of the set of distribution functions $W(\mathbf{F},\dot{\mathbf{F}},\ddot{\mathbf{F}})$.[13] We then average over the Euler angles φ_0 and θ_0 and, substituting the expression for $K_{ab}(\tau)$ in $I_{ab}(\omega)$, we integrate over τ. As a result, we obtain the following expression for the profile of the hydrogen line:

$$I_{ab}(\Delta\omega)=I_{ab}^{(0)}(\Delta\omega)+I_{ab}^{(n)}(\Delta\omega)+I_{ab}^{(f)}(\Delta\omega)+I_{ab}^{(am)}(\Delta\omega), \quad (7)$$

$$I_{ab}^{(0)}(\Delta\omega)=-\frac{\mathrm{Re}}{\pi}\int_0^{\infty}dF\,W(F)\sum_{\alpha\beta}|\mathbf{d}_{\alpha\beta}|^2[i(\Delta\omega-C_{\alpha\beta}F)-w_{\alpha\beta}]^{-1}, \quad (8)$$

$$I_{ab}^{(n)}(\Delta\omega)=-\frac{\mathrm{Re}}{\pi}\int_0^{\infty}dF\frac{W(F)\langle\dot{\mathbf{F}}_\perp^2\rangle_F}{F^2}\sum_{\alpha\beta}A_{\alpha\beta}^{(n)}(\Delta\omega;F), \quad (9)$$

$$I_{ab}^{(f)}(\Delta\omega)=-\frac{\mathrm{Re}}{\pi}\int_0^{\infty}dF\Big(\frac{W(F)\langle\dot{\mathbf{F}}_\perp^2\rangle_F}{F}\sum_{\alpha\beta}A_{\alpha\beta}^{(f_1)}(\Delta\omega;F)$$
$$+W(F)\langle\dot{\mathbf{F}}_\parallel^2\rangle_F\sum_{\alpha\beta}A_{\alpha\beta}^{(f_2)}(\Delta\omega;F)\Big), \quad (10)$$

$$I_{ab}^{(am)}(\Delta\omega)=-\frac{\mathrm{Re}}{\pi}\int_0^{\infty}dF\,W(F)\frac{\langle\dot{\mathbf{F}}_\perp^2\rangle_F}{F^2}\sum_{\alpha\beta}A_{\alpha\beta}^{(am)}(\Delta\omega;F). \quad (11)$$

The expression (8) describes the Stark profile in the absence of thermal motion, (9)—the thermal correction, associated with nonadiabatic effects, (10)—with phase modulation, (11)—with amplitude modulation (expansion of the rotation operator $\hat{R}(\tau)$). The expressions for $A_{\alpha\beta}^{(n)}(\Delta\omega;F)$, $A_{\alpha\beta}^{(f_1,2)}(\Delta\omega;F)$, $A_{\alpha\beta}^{(am)}(\Delta\omega;F)$ are determined by the perturbation-theory series and are given in the Appendix. It is easy to see that (9)–(11) is proportional to the small parameter $h_i^{-2/3}\ll 1$.

The formulas for the nonvanishing second moments of the distribution function $W(\mathbf{F},\dot{\mathbf{F}})$ with account of the results of Ref. 13 have the form[3)]

$$W(F)\langle\dot{\mathbf{F}}_\parallel^2\rangle_F=\frac{45}{8}\lambda F_0\Big\{N^{7/3}\langle v_i^2\rangle\beta^{1/2}\mathcal{I}(\beta)$$
$$+N^{7/3}\langle v_a^2\rangle\Big[\beta^{1/2}\mathcal{I}(\beta)+\Big(\frac{5}{12\pi}\Big)\Big(\frac{2}{3}\mathcal{H}(\beta)-\frac{\mathcal{H}(\beta)}{\beta}\Big)\Big]\Big\}, \quad (12)$$

$$W(F)\langle\dot{\mathbf{F}}_\perp^2\rangle_F=\frac{45}{8}\lambda F_0\Big\{N^{7/3}\langle v_i^2\rangle[\beta^{1/2}(G(\beta)-\mathcal{I}(\beta))]$$
$$+N^{7/3}\langle v_a^2\rangle\Big[\beta^{1/2}(G(\beta)-\mathcal{I}(\beta))+\Big(\frac{5}{12\pi}\Big)\Big(\frac{1}{3}\mathcal{H}(\beta)+\frac{\mathcal{H}(\beta)}{\beta}\Big)\Big]\Big\}, \quad (13)$$

where

$$W(F)=\frac{1}{F_0}\mathcal{H}(\beta)=\frac{2\beta}{\pi F}\int_0^\infty dx\exp(-x^{3/2})x\sin\beta x.$$

Here $\beta\equiv F/F_0$, $F_0=\lambda eN^{2/3}$ is the normal Holtsmark field; N is the concentration of ions in the plasma; $\lambda\equiv 2\pi(4/15)^{2/3}$ is the scale of the Holtsmark field; $\langle v_a^2\rangle\equiv 2T_a/m_a$; $\langle v_i^2\rangle\equiv 2T_i/m_i$; T_a and T_i are the temperatures of the radiating atoms and the exciting (single-charge) ions, and m_a and m_i are their masses. According to Ref. 13, the functions $G(\beta)$, $\tilde{I}(\beta)$ and $\mathcal{H}(\beta)$ have the form

$$\mathcal{H}(\beta)=\int_0^\beta d\beta'\mathcal{H}(\beta'),$$

$$G(\beta)=\left(\frac{2}{\pi}\right)\int_0^\infty dx\exp\left\{-\left(\frac{x}{\beta}\right)^{3/2}\right\}x^{-1/2}\sin x,$$

$$\tilde{I}(\beta)=\left(\frac{2}{\pi}\right)\int_0^\infty dx\exp\left\{-\left(\frac{x}{\beta}\right)^{3/2}\right\}x^{-3/2}(\sin x-x\cos x). \qquad (14)$$

The first terms in the curly brackets of (12) and (13) are connected with the ion field fluctuations due to thermal motion of the ions, and the second, with the ion field fluctuations due to the thermal motion of the atoms relative to the fixed background of the plasma ions. Since the second term in the square brackets at $N^{2/3}\langle v_a^2\rangle$ in (12), (13) is small in comparison with the first in the entire region of change of the parameter β,[4)] it follows that (12) and (13) are proportional to $\langle v_a^2\rangle+\langle v_i^2\rangle$. At $T_a\approx T_i$, (12) and (13) are proportional to the ion temperature and inversely proportional to the reduced mass $\mu\equiv m_am_i/(m_i+m_a)$ of the ion + atom pair.

The expressions (8)–(11) preserve the normalization of the spectrum by virtue of the normalization of the perturbation theory series. Since the zero profile (8) is normalized to unity, the normalization integral of the thermal corrections (9)–(11) is equal to zero. Whereas this condition is satisfied for (10) and (11) in the case of the individual terms of the sums, it is satisfied only for the entire sum in (13).

In the limit of large $\Delta\omega\gg w$, the formulas (9)–(11) go over into the corresponding expressions of Ref. 11. As to the amplitude modulation of the central component, its value is identical with the estimates of this effect given earlier.[14]

The results are applicable under the condition

$$I^{(0)}(\Delta\omega)\gg I^{(1)}(\Delta\omega), \qquad (15)$$

where $I^{(1)}(\Delta\omega)\equiv I^{(n)}(\Delta\omega)+I^{(f)}(\Delta\omega)+I^{(am)}(\Delta\omega)$. This criterion, on the one hand, is necessary for the applicability of perturbation theory and on the other, it corresponds to the condition of the quasistatic nature of the broadening ions, based on the smallness of the thermal corrections.

4. Integration over F for the contribution of the effect of amplitude modulation of the central component $I_c^{(am)}(\Delta\omega)$ in (11) is carried out directly and leads to the following result:

$$I_c^{(am)}(\Delta\omega)=\frac{3}{16}\Gamma\left(\frac{1}{3}\right)\frac{g_0}{\gamma_0}\mathrm{Re}\sum_{\alpha\beta}|d_{\bar\alpha\bar\beta}|^2(ix-\gamma_{\bar\alpha\bar\beta})^{-3}, \qquad (16)$$

where $g_0\equiv(10\lambda/\pi)((T_i/\mu)N^{2/3})/\gamma_0^2$, $x\equiv\Delta\omega/\gamma_0$, $\gamma_{\bar\alpha\bar\beta}\equiv w_{\bar\alpha\bar\beta}/\gamma_0$; $\Gamma(z)$ is the gamma function; the indices $\bar\alpha$ and $\bar\beta$ denote summation over the unshifted components of the line $a\to b$. The effective impact electron width γ_0 of the Stark components of the line is determined by the expression[15]

$$\gamma_0=\frac{3}{2}\pi\left(\frac{2m}{\pi T}\right)^{1/2}N_e(n_a^4+n_b^4)\ln(\rho_D/\rho_W), \qquad (17)$$

where m is the mass of the electron, ρ_D and ρ_W are the Debye and Weisskopf radii, respectively, n_a and n_b are the principal quantum numbers of the upper (a) and lower (b) levels. As follows from (16), the correction is proportional to $h_i^{-2/3}h_e^{-1}$ ($h_e\equiv N(eC/v_e)^3$ is the characteristic parameter of the theory of the broadening by electrons, v_e is the thermal velocity of the electrons), while under the conditions of applicability of the impact approximation $h_e\ll 1$.[12]

For the calculation of corrections for the effects of nonadiabaticity (9), phase (10) and amplitude (11), it is convenient to transform the modulation $I_i^{(am)}(\Delta\omega)$ of the sideband components to the complex plane F. The integrands in (9)–(11) can be continued analytically into the complex F plane. They have singularities only of the type of poles of first order of the "dispersion" denominators $R_{\alpha\beta}=[i(\Delta\omega-C_{\alpha\beta}F)-w_{\alpha\beta}]^{-1}$ (see the Appendix). Using the fact that the integrands in (9)–(11) are even, we extend the lower limit of the integration in F to $-\infty$.[5)] Closing the contour of integration in the upper half of the complex F plane, we obtain expressions for the integrals (9)–(11) by summing the residues of the integrands in the bands $F_{(\alpha\beta)}=(\Delta\omega+iw_{\alpha\beta})/C_{\alpha\beta}$, $C_{\alpha\beta}>0$. In two limiting cases, $\Delta\omega\gg w$ and $\Delta\omega\lesssim w$, it is possible to obtain with the help of expansions of the functions (12)–(14) and their derivatives at small and large values of the argument ($\beta\gg 1$, $\beta\ll 1$), simple analytic formulas for the thermal corrections. At $\Delta\omega\gg w$, the results of the previous paper are reproduced.[11] At $\Delta\omega\lesssim w$, the expression for the thermal corrections can be represented in the form of a series in powers of the parameter $h_e^{2/3}$:

$$I^{(n)}(\Delta\omega)+I^{(f)}(\Delta\omega)+I_i^{(am)}(\Delta\omega)=\sum_{n=1}^{\infty}a_n(\Delta\omega);$$

$$a_1\propto h_e^{-2/3},\quad a_2\propto\mathrm{const},\quad a_3\propto h_e^{2/3}$$

and so on. The principal term of the series is determined by the effects of nonadiabaticity from the lateral components and has the form

$$I_{ab}^{(n)}(\Delta\omega)=g_0\,\mathrm{Re}\sum_{\substack{\alpha\beta\\(C_{\alpha\beta}>0)}}\frac{1}{C_{\alpha\beta}F_0}B_{\alpha\beta}\left(\frac{\Delta\omega}{\gamma_0}\right); \qquad (18)$$

$$B_{\alpha\beta}(x)=\sum_{\alpha'\beta',\alpha''\beta''}{}'\{(U_{\alpha\alpha'}-U_{\beta'\beta})(U_{\alpha''\alpha}-U_{\beta\beta''})d_{\alpha'\beta'}d_{\beta''\alpha''}$$

$$+[(U_{\alpha'\alpha''}-U_{\beta''\beta'})(U_{\alpha''\alpha}-U_{\beta\beta''})+(U_{\alpha\alpha'}-U_{\beta''\beta})(U_{\alpha''\alpha'}-U_{\beta'\beta''})]d_{\alpha\beta}d_{\beta'\alpha'}\}$$

$$\times\frac{1}{Z_{\alpha''\beta''}(x)Z_{\alpha'\beta'}(x)}-|d_{\alpha\beta}|^2\sum_{\alpha'\beta'}{}'\frac{(U_{\alpha\alpha'}-U_{\beta'\beta})(U_{\alpha'\alpha}-U_{\beta\beta'})}{Z^2_{\alpha'\beta'}(x)}$$

$$\times\left(1-\frac{dZ_{\alpha'\beta'}(x)}{dx}\right), \qquad (19)$$

where

$\gamma_{\alpha\beta}\equiv w_{\alpha\beta}/\gamma_0$; $Z_{\alpha'\beta'}(x)\equiv x-i\gamma_{\alpha'\beta'}$
$-(C_{\alpha'\beta'}/C_{\alpha\beta})(x-i\gamma_{\alpha\beta})$; $U_{ik}\equiv(J_x)_{ik}$.

Formulas (18) and (19) give analytic expressions for the thermal correction near the center of any hydrogen line without central components. For lines with a central component, (18) is the second term of the expansion in h_e, since (16) is proportional to h_e^{-1}. As analysis shows, a description of the thermal corrections by the first terms of the obtained expansion in h_e, (16) and (18), is valid to $\Delta\omega\sim CF_0(x\sim h_2^{-1/3})$.

According to (16) and (18), in the case of lines of the type n_α (Ly-α, H_α, P_α, and so on), for which the principal fraction of the intensity goes to the unshifted component, the change in the intensity at the center is always negative, i.e., an effective increase of the "linewidth" takes place. Conversely, in the case of lines without a central component (Ly-β, H_β, H_δ and so on) the intensity at the center increases.

In the case of the Ly-α line, the thermal correction $I^{(1)}(\Delta\omega)$ near the center, calculated according to (16) and (18), is determined by the expression

$$I^{(1)}_{Ly\alpha}(\Delta\omega)=\frac{10\lambda}{\pi}\frac{(T_i/\mu)N^{2/3}}{w^2}\frac{1}{CF_0}\left[\frac{CF_0}{w}F_{1-\alpha}(x)+F_{2-\alpha}(x)\right], \qquad (20)$$

where w is the impact electron width of the central component (001) – (000)[15,16]; $C\equiv ea_0/\hbar$, $x\equiv\Delta\omega/w$.

$$F_{1-\alpha}(x)\equiv\frac{\Gamma(1/3)}{8}\frac{3x^2-1}{(x^2+1)^3};\quad F_{2-\alpha}(x)\equiv\frac{1}{12}\left[2\frac{x^2-1}{(x^2+1)^2}+\frac{x^2-2}{(x^2+1)(x^2+4)}\right] \qquad (21)$$

For the Ly-β line, we obtain in similar fashion,

$$I^{(1)}_{Ly\beta}(\Delta\omega)=\frac{10\lambda}{\pi}\frac{(T_i/\mu)N^{2/3}}{w_{01}^2}\frac{1}{C_1F_0}F_{2-\beta}(x), \qquad (22)$$

where w_{01} is the impact electron width of the Stark sublevel—(002) $C_1\equiv 9ea_0/\hbar$, $x=\Delta\omega/w_{01}$.

$$F_{2-\beta}(x)=\frac{1}{6}\left[\frac{4-x^2}{(x^2+4)^2}+\frac{2-x^2}{(x^2+4)(x^2+1)}\right]. \qquad (23)$$

The value of $I^{(1)}(\Delta\omega)$ is negative (20) at the center of the Ly-α line, positive (22) for Ly-β. The functions $F_{1,2-\alpha}(x)$ and $F_{2-\beta}(x)$ satisfy the normalization condition at zero.

5. The expressions found above for the thermal correction allow us to make more precise the criterion of applicability of the static approximation to the broadening by the ions (15). For lines without central components, at $\Delta\omega\lesssim w$, we obtain the following condition:

$$h_i^{-2/3}h_e^{-1}\Lambda^{-3}F\left(\frac{\Delta\omega}{w}\right)\ll 1. \qquad (24)$$

Here $\Lambda\equiv\ln(\rho_D/\rho_W)$ and the function $F(x)$, as well as the function (23), has the characteristic limiting values $F(x)\approx$ const~ 1 at $x\ll 1$ and $F(x)\sim -x^{-2}$ at $x\gg 1$. At $\Delta\omega\gg w$, it follows from (15) that

$$\Delta\omega\gg(eCNv_i)^{1/2}, \qquad (25)$$

which coincides with the corresponding criterion for $\Delta\omega\ll CF_0$, obtained previously.[11] At $\Delta\omega\ll\omega$, the expression (24) gives

$$h_i^{2/3}h_e\Lambda^3\gg 1,\quad\text{or}\quad\frac{\rho_{eff}}{v_i}w\gg 1,\quad \rho_{eff}\sim h_i^{-1/3}N^{-1/3}. \qquad (26)$$

The criterion (26) does not contain the frequency shift $\Delta\omega$ and has the illustrative meaning of the smallness of the lifetime w^{-1} of the atom on the Stark sublevel in comparison with the characteristic time ρ_{eff}/v_i. The value of ρ_{eff} is practically always indentical with the mean interparticle distance $N^{-1/3}$.

For lines with central components, at $\Delta\omega\lesssim w$, it follows from (15) that

$$h_i^{-2/3}h_e^{-1/3}\Lambda^{-2}\left[F_1\left(\frac{\Delta\omega}{w}\right)+h_e^{1/3}\Lambda F_2\left(\frac{\Delta\omega}{w}\right)\right]\left[\left(\frac{\Delta\omega}{w}\right)^2+1\right]\ll 1. \qquad (27)$$

Here the function $F_1(x)$, connected with the effect of amplitude modulation, has the limiting values (cf. (21)) $F_1(x)\propto$ const <0 at $x\ll 1$ and $F_1(x)\sim x^{-4}$ at $x\gg 1$. The function $F_2(x)$ is connected with the effects of nonadiabaticity and in the limiting cases has the form (cf. (21)) $F_2(x)\sim$ const <0 at $x\ll 1$ and $F_2(x)\sim x^{-2}$ at $x\gg 1$. At $\Delta\omega\ll w$, the main contribution to (27) is made by the first term

$$h_i^{2/3}h_e^{2/3}\Lambda^2\gg 1. \qquad (28)$$

At $\Delta\omega/w\gg h_e^{-1/6}$ the main contribution to (27) is made by the second term and the criterion has the form

$$h_i^{2/3}h_e^{1/3}\Lambda\gg 1. \qquad (29)$$

The criteria (27)–(29) take into account the contribution made to the zero contour $I^{(0)}(\Delta\omega)$ only by the central components. However, even at $\Delta\omega/w\gtrsim h_e^{-1/4}$, the main contribution to $I^{(0)}(\Delta\omega)$ is made by the sideband components and the criterion again takes the form (25).

6. The most detailed experimental investigations have been carried out for H_β. The estimate of the value of the thermal corrections is given on the basis of a very simple model of the line[12]: the set of Stark sideband components of the line are replaced by a single component with effective constant C, impact width w_0 and intensity of the sideband components of the line I_0. Use of such a model in general formula (18) gives for the thermal correction $I^{(1)}(\Delta\omega)$ an expression similar in structure to the formula (23):

$$I^{(1)}(\Delta\omega)\approx\frac{5\lambda}{\pi}\frac{(T_i/\mu)N^{2/3}}{w_0^2}\frac{U^2}{CF_0}\frac{1-x^2}{(1+x^2)^2}, \qquad (30)$$

where $x\equiv\Delta\omega/w_0$ and U^2 is the effective value of the square of the matrix element of the operator J_x. Formula (30) can be used for the determination of the rela-

tive value of the correction $I^{(1)}(\Delta\omega)$ and its dependence on the parameters N, T, μ and $\Delta\omega$ (or $\Delta\lambda$).

We estimate the relative value of the correction $I^{(1)}(0)$ at the center of the H_β line in comparison with I_{max}—the intensity of the line in the region of the maxima. In the framework of the given simplified treatment, the value of I_{max}, estimated with the help of the Holtsmark distribution, is $I_{max} \sim 0.37/CF_0$. The quantity U for transitions between components of the H_β line has two values: 1 and $3^{1/2}/2$, and we can set $U^2 \sim 1$ with good accuracy. Estimating w_0 from (17), we obtain $I^{(1)}(0)/I_{max} \approx 30\%$ for the experimental conditions of[8,9] ($T_{e,i} = 13,400$ K, $N_{e,i} \approx 8 \times 10^{16}$ cm^{-3}, $\mu = \frac{1}{2}$—the $H^+ + H$ pair). The value of this ratio, determined from the difference in the experimental contour[9] and the theoretical contour,[16] calculated without account of thermal motion, amounts to 20%. Figure 1 shows in relative units the shape of the contour of the thermal corrections $I^{(1)}(\Delta\lambda)$, calculated from Eq. (30) (solid curve) and deduced from the difference of the two contours: measured in Refs. 8 and 9, and found theoretically without account of the thermal motion, in Ref. 16 (the circles denote the $H^+ + H$ pair $\mu_1 = \frac{1}{2}$, and the crosses the $Ar^+ + H$ pair with $\mu_2 = 1$). The scale of the change $\Delta\lambda_0$ of the quantity $I^{(1)}(\Delta\lambda)$ in the scale of wavelengths is determined by the quantity w_0, calculated from Eq. (17) and is equal to $\Delta\lambda_0 \approx 5.2$ Å.

Greatest interest in the comparison of theory with experiment attaches to the difference characteristic $\delta_R(\Delta\lambda)$, determined from the ratio of the difference of the line shapes for two values of the reduced mass μ to the value of the intensity at the maximum, I_{max}:

$$\delta_R(\Delta\lambda) = [I_{\mu_1}(\Delta\lambda) - I_{\mu_2}(\Delta\lambda)]/I_{max}.$$

The characteristic $\delta_R(\Delta\lambda)$, determined from the experimental results for two values of μ, does not depend on the theoretically calculated line shape and describes the effect of the reduced mass in "pure form." The relative course of the quantity $\delta_R(\Delta\lambda)$, obtained from the experimental results of Refs. 8 and 9 for the values $\mu_1 = \frac{1}{2}$ and $\mu_2 = 1$ is also shown in Fig. 1 (∇). At the center of the line, the quantity $\delta_R(\Delta\lambda)$ can be expressed in terms of $I^{(1)}(\Delta\lambda)$ from (30):

$$\delta_R(\Delta\lambda) = \frac{I^{(1)}_{\mu_1}(\Delta\lambda) - I^{(1)}_{\mu_2}(\Delta\lambda)}{I_{max}} \propto \frac{T_i T_e}{N^{4/3}} \frac{|\mu_2 - \mu_1|}{\mu_1 \mu_2} F\left(\frac{\Delta\lambda}{\Delta\lambda_0}\right), \qquad (31)$$

where $F(x) = (1 - x^2)/(1 + x^2)^2$. It has been taken into account here that the thermal corrections fall off with

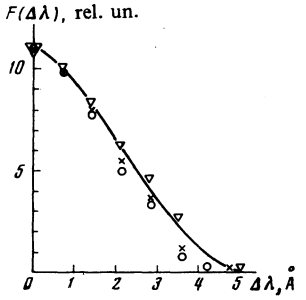

FIG. 1. Relative course of the thermal correction $F(\Delta\lambda)$ to the shape of the H_β line.

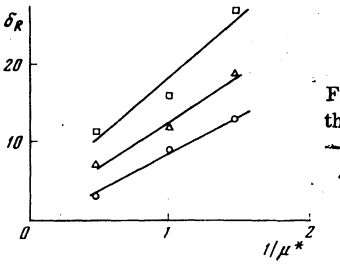

FIG. 2. Dependence of $\delta_R(0)$ on the reduced mass $\mu^* = \mu_i\mu_k/|\mu_k - \mu_i|$ of the ions; □—$N = 2 \times 10^{16}$, △—6×10^{16}, ○—1.1×10^{17} cm^{-3}.

increase in $\Delta\lambda$ and are insignificant in the region of maximal intensities. It is seen from Fig. 1 that both the scale of change of the corrections and the detailed course of the contour $F(x)$ are in good agreement with the experimental results. In the region $\Delta\lambda \gtrsim \Delta\lambda_0$ the corrections are extremely small and the observation of the course of the contour $\delta_R(\Delta\lambda)$ becomes difficult. The calculated and experimental dependences of the thermal corrections on the reduced mass μ of the exciting particles at a fixed value of the plasma concentration, are in good qualitative agreement as is seen from Fig. 2. However, the degree of quantitative agreement still remains insufficiently certain. The achieved measurement accuracy does not permit us to make an unambiguous choice between the dependence $1/\mu$ and the empirically determined dependence $1/\mu^{1/2}$, which, according to Refs. 8 and 9, also describes the results of the measurements. It appears that the principal reason for this is the insufficient accuracy in the determination of the plasma temperature, on which the thermal correction has a quadratic dependence, in correspondence with Eq. (31). At the same time, the range of measurement of μ is comparatively narrow.

As to the dependence of $\delta_R(0)$ on the plasma concentration, analysis of the experimental data leads to the conclusion that this dependence is weaker than $N^{-4/3}$. However, a significant indeterminacy is also possible here, connected with the insufficiently accurate knowledge of the temperature. Actually, an increase of the concentration in an arc discharge should be accompanied by an increase of the temperature and if the dependence of $\delta_R(0)$ on T is quadratic this can be the reason for the appreciable distortion of the true dependence. For a more complete test of the developed theory, further experiments with precision measurements of the temperature of the charged particles are desirable.

7. Thus, the main regularities of the effect of the reduced mass are explained by the nonadiabatic character of the rotation of the ion field. Recently, however, attempts have been made to attribute the smearing of the central dip of the H_β and H_δ lines to the presence in the plasma of intense one-dimensional noise due to ion-sound turbulence.[18] But this cannot explain all the main regularities of the effect. Actually, for lines with central components (H_α, H_β), the one-dimensional low-frequency turbulence should, according to Ref. 5, lead to an increase of the intensity near the center of the line, since the shape and intensity of the unshifted Stark component does not change, and a fraction of the intensity of the sideband components is transferred to

the center. This patently contradicts the experiment. For lines without central components, such as Ly-β, H_β, H_δ, the electric field of the one-dimensional noise should first of all be taken into account in the convolution that determines the distribution function of the total field. In this case, the spatial distribution of the noise turns out to be anisotropic with one preferred axis, along which the average value of the field amplitude has a somewhat larger value than along the other two. However, the probability of appearance of weak fields tends to zero as before in power-law fashion. It is not difficult to establish this by considering, for simplicity, the convolution of the one-dimensional Rayleigh distribution with the three-dimensional distribution, the behavior of which as $E \to 0$ does not differ from the Holtsmark distribution.[7)] A consistent approach to the calculation of profiles of lines of the type H_β in a plasma with one-dimensional electrostatic, low frequency noise, the average field intensity E_n of which does not exceed F_0 by a significant amount, leads only to a certain polarization effect,[19] without affecting the depth of the dip at the center. Only when the one-dimensional electrostatic noise is excited in the region of rarefied plasma, where $E_n \gg F_0$, and this region is spatially separated from the region where $E_n \ll F_0$, can one resort to the procedure of the convolution of the distribution functions of the low-frequency fields and use the corresponding superposition of the Gaussian and Holtsmark contours. However, in the experiments of Refs. 8 and 9, there scarecely exists a significant contribution to the total intensity from regions with a low concentration of electrons, especially in observation from the end.

So far as the possibile nonadiabatic effect of the ion-sound noise, it will be determined by the parameter ω_{pi}/w, where ω_{pi} is the ion plasma frequency. Since $v_i N^{1/3} \gg \omega_{pi}$, the smearing out of the dip that is associated with the individual thermal motion of the particles will predominate so long as $F_0 \gtrsim E_n$.

In conclusion, the authors consider it their pleasant duty to thank L. I. Rudakov for support in fulfilment of the present research. The authors are also grateful to W. Wiese, J. Chapelle, and V. I. Kogan for useful discussions.

APPENDIX

The functions $A_{\alpha\beta}^{(n)}(\Delta\omega; F)$ and so on, which determine the thermal corrections (8)–(10) to the line shape at fixed ion field F, are given by

$$A_{\alpha\beta}^{(n)}(\Delta\omega; F) = R_{\alpha\beta}\Bigg(\sum_{\alpha'\beta',\alpha''\beta''}{}' \{(U_{\alpha\alpha'}-U_{\beta'\beta})(U_{\alpha''\alpha}-U_{\beta\beta''})\mathbf{d}_{\alpha'\beta}\mathbf{d}_{\beta''\alpha''} + \tfrac{1}{2}[(U_{\alpha'\alpha''}-U_{\beta''\beta'})(U_{\alpha''\alpha}-U_{\beta\beta''})+(U_{\alpha\alpha''}-U_{\beta''\beta})(U_{\alpha''\alpha'}-U_{\beta'\beta''})]\mathbf{d}_{\alpha\beta}\mathbf{d}_{\beta'\alpha'}\} \frac{1}{[(C_{\alpha\beta}-C_{\alpha'\beta'})F-i(w_{\alpha\beta}-w_{\alpha'\beta'})][(C_{\alpha\beta}-C_{\alpha''\beta''})F-i(w_{\alpha\beta}-w_{\alpha''\beta''})]} - \frac{|\mathbf{d}_{\alpha\beta}|^2(U_{\alpha\alpha'}-U_{\beta'\beta})(U_{\alpha'\alpha}-U_{\beta\beta'})}{[(C_{\alpha\beta}-C_{\alpha'\beta'})F-i(w_{\alpha\beta}-w_{\alpha'\beta'})]^2}\Bigg) - i|\mathbf{d}_{\alpha\beta}|^2\sum_{\alpha'\beta'}{}'\frac{(U_{\alpha\alpha'}-U_{\beta'\beta})(U_{\alpha'\alpha}-U_{\beta\beta'})}{(C_{\alpha\beta}-C_{\alpha'\beta'})F-i(w_{\alpha\beta}-w_{\alpha'\beta'})}\frac{\partial}{\partial i\omega}R_{\alpha\beta}, \qquad (\text{II}.1)$$

$$A_{\alpha\beta}^{(fs)}(\Delta\omega; F) = |\mathbf{d}_{\alpha\beta}|^2 C_{\alpha\beta}\left(-\frac{i}{6}\frac{\partial^3}{\partial(i\omega)^3}R_{\alpha\beta}\right), \qquad (\text{II}.2)$$

$$A_{\alpha\beta}^{(fs)}(\Delta\omega; F) = |\mathbf{d}_{\alpha\beta}|^2 (C_{\alpha\beta})^2\left(-\frac{1}{8}\frac{\partial^4}{\partial(i\omega)^4}R_{\alpha\beta}\right),$$

$$A_{\alpha\beta}^{(sm)}(\Delta\omega; F) = -[(\mathbf{d}_z)_{\alpha\beta}^2+(\mathbf{d}_z)_{\alpha\beta}^2]\cdot\frac{1}{2}\frac{\partial^2}{\partial(i\omega)^2}R_{\alpha\beta}. \qquad (\text{II}.3)$$

Here $U \equiv J_x$, $R_{\alpha\beta} \equiv [i(\Delta\omega - C_{\alpha\beta}F) - w_{\alpha\beta}]^{-1}$ is the impact electron halfwidth of the Stark component $\alpha \to \beta$,[15] $C_{\alpha\beta}$ is the Stark constant of the component $\alpha \to \beta$.[15] In the derivation of (A.1), it was taken into account that in the Stark basis, only the nondiagonal matrix elements of the operator J_x differ from zero, and the operator equality $\hat{J}_x\hat{J}_x = \hat{J}_y\hat{J}_y$ is used.

1)The use of an expansion in τ allows us to remove the effect of the operator of chronological ordering $\hat{P}$.

2)This approximation is called the approximation of isolated components. Account of the nondiagonal elements Φ_{ab} does not alter, as a detailed calculation shows, the qualitative dependence of the thermal corrections on the parameters and leads in the region $\Delta\omega \lesssim w$ only to the appearance of an unimportant numerical factor close to unity.

3)The results (12) and (13) are easily generalized to the case of the presence of several types of exciting atoms.

4)It is easy to verify the noted smallness by considering the limiting cases $\beta \ll 1$ and $\beta \gg 1$. At $\beta \ll 1$, the second term in the square brackets is approximately 7 times smaller than the first. At $\beta \gg 1$ the first term increases as $\beta^{1/2}$ while the second falls off like β^{-1}. The difference in the contributions from the given terms disappears only in the thermal corrections from phase modulation,[5] which is unimportant for the considered effect.

5)It is first necessary to transform the expressions describing the effects of phase and amplitude modulation of the sideband components by using integration by parts.

6)Here and in the following, we designate the Stark sublevels by the parabolic quantum numbers $(n_1 n_2 m)$.

7)The difference in the asymptotic values of these functions as $E \to \infty$ is insignificant in the given case.

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Electron spectra from the autoionization of quasimolecules

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The energy spectra of the electrons emitted in collisions between heavy atomic particles, in which the molecule undergoes a transition to an autoionization state, are considered. The theory employed is a generalization of Fano's method to the case of the adiabatically time-dependent Hamiltonian. Spectrum features due to an extremum of the autoionization term are investigated. The spectra exhibit interference oscillations whose phase is numerically equal to the area of the figure bounded by the term and the horizontal line corresponding to the energy of the emitted electron. The shape of the atomic autoionization lines excited during the collisions and broadened as the atomic particles fly apart is determined. It is shown that the expressions usually employed in such cases are valid only for the line wing. The feasibility of an experimental observation of the spectral features is discussed.

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§1. INTRODUCTION

An effective autoionization mechanism in slow collisions between heavy atomic particles is the transition of the quasimolecule to an unstable autoionization state. Experimental and theoretical studies of the energy distributions (spectra) of electrons produced in such reactions can be used to obtain important information on the behavior of the states and on the physics of the process.

Transitions to the continuum of free states of the electron lead to autoionization, and it is important from the standpoint of a theoretical description of the spectra to determine the extent to which the continuum can be regarded as uniform. In fact, the uniformity of the continuum is violated by the presence of the autoionization state. However, we shall be concerned with the continuum states that are the initial states (for example, in the paper by Fano[1]) and correspond to the turning off of the interaction responsible for the decay of the autoionization state. For simplicity, such states will be referred to as diabatic. The uniformity of this type of continuum may be further violated by the presence of the limit of the continuous spectrum and a rapid variation in the wave functions with energy. The latter leads to a rapid change in the matrix elements, of which we shall be mainly concerned with that corresponding to the interaction with a discrete diabatic state lying against the background of the continuum. This matrix element will, in fact, determine the width of the adiabatic autoionization state.

The limit of the continuous spectrum of the quasimolecule will, in principle, always be present, and its correct inclusion in the theory presents an additional difficulty which has been considered in a number of papers (see Demkov[2] and Solov'ev,[3] and the references therein). However, if we are interested in the spectra of electrons at relatively low energies, the continuum can be assumed to be approximately uniform.[4–6] This results in a considerable simplification of the theoretical analysis of the spectra (§2) as compared with the case of the inhomogeneous continuum and, at the same time, yields an adequate description of a number of important physical effects responsible for the various spectrum features.

Although it is basically simple, a systematic analysis of the foregoing problems has not so far been made, and the theory formulated for the interpretation of particular experimental data has frequently been found to be subject to important inaccuracies and errors which will be noted below. In §§3 and 4 we consider the spectrum features that appear when the real part of the energy of the autoionization state has extrema for finite or infinite internuclear distances. The latter case corresponds to the inclusion of the broadening of atomic autoionization lines by the interaction between the atomic particles. In the important case of Coulomb interaction (the so-called Stark broadening of lines), it is possible to achieve an important improvement in the well-known formula of Berry[7] for the line shape, which is commonly used in the interpretation of experimental data.[8–11]

The main initial propositions of the theory of spectra

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