ionization process upon excitation of the L electrons is not taken into account.

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Quantum theory of Stark broadening of the lines of hydrogenlike ions

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An exact analytic solution of the problem of hydrogenlike-ion line broadening by electrons is obtained within the framework of the dipole approximation. The character of the solution is investigated at various values of the Coulomb paramter $Ze^2/\hbar v$. The transition to solutions for a neutral atom is tracked, as well as that to the impact theory of broadening, including its classical limit.

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§1. INTRODUCTION

The recent development of the theory of the hydrogen-atom (H) and of H-like-ion line broadening[1-4] was based on the use of the specific properties of the Coulomb symmetry of H-like systems, wherein the line contour could be described not only at high and low frequencies $\Delta\omega$, but also in the intermediate $\Delta\omega$ region. For neutral hydrogen, the line contours were calculated both in the classical[1] and in the quantum[3,4] cases. The situation here is analogous in many respects to nonrelativistic theory of bremsstrahlung in a Coulomb field, where classical and quantum solutions and the relations between them are also known.[5] Calculations of the line contours of H-like ions are known in the impact limit,[6] as well as in the intermediate frequency region,[2] but only in the classical-trajectory approximation.

We obtain in this paper general quantum solutions for the line contours of H-like ions, and investigate their connection with the known limiting cases. A new parameter of the problem compared with the case of neutral hydrogen is the parameter $Ze^2/\hbar v$, where Z is the ion charge and v is the velocity of the particle that causes the broadening. We note that allowance for the quantum effects is more important for H-like ions than for neutral hydrogen (see Ref. 7, Chap. 4). The reason is the decrease of the effective collision radius (the so-called Weisskopf radius[8]) with increasing Z. It is interesting that the theory developed is similar in many respects to the relativistic bremsstrahlung theory.[9]

§2. WAVE FUNCTION OF BROADENING PARTICLE AND FORMAL EXPRESSION FOR THE LINE CONTOUR

The line contour of a radiating atom or ion can be expressed in terms of the overlap integrals of the broadening particles, assumed for the sake of argument to be electrons.[4] Of interest for the broadening particles are

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small frequency shifts $\Delta\omega \ll \omega_{nn'}$ ($\omega_{nn'}$ is the frequency of the optical transition) and it suffices therefore to retain in the Hamiltonian of the interaction between the ion and the broadening electron the dipole term (on top of the Coulomb term):

$$\hat{H}=\hat{H}_0-\frac{Ze^2}{r}+\frac{\hat{\Lambda}}{2Mr^2}; \quad \hat{\Lambda}=\hat{l}^2-2M\frac{\mathbf{r}_A\mathbf{r}_e}{r_e}e^2, \tag{2.1}$$

where $\hat{H}_0$ is the Hamiltonian of the unperturbed ion, the operator $\hat{\Lambda}$ takes into account the sum of the centrifugal and the dipole potentials ($\hat{l}, M$, and $\mathbf{r}_e$ are respectively the orbital momentum, the mass, and the coordinate of the broadening electron, and $\mathbf{r}_A$ is the coordinate of the atomic electron).

It is seen from (2.1) that since the centrifugal and the dipole potentials decrease in identical fashion with distance, it is possible to separate the radial and the angular motions. Indeed, using the wave functions corresponding to definite values λ of the operator $\hat{\Lambda}$ and of the total angular momentum of the system L, we easily see that the radial Schrödinger equation that follows from (2.1) differs from the equation for the free motion in the Coulomb field only in that the eigenvalues of the orbital momentum l are replaced by the eigenvalues λ of the operator $\hat{\Lambda}$. As a result we can immediately write down the expression for the radial function $R_q(r)$ of the broadening electron:

$$R_q(r)=\left(\frac{2}{\pi}\right)^{1/2}qe^{\pi\eta/2}\frac{|\Gamma(a)|}{\Gamma(b)}(2qr)^{\nu-1/2}e^{-iqr}F(a,b,2iqr), \tag{2.2}$$
$$\nu=(\lambda+1/4)^{1/2},\ a=\nu+1/2+i\eta,\ \eta=Ze^2/\hbar v,\ b=2\nu+1,$$

where $F(a,b,x)$ is a confluent hypergeometric function that is regular at zero; $\Gamma(z)$ is the gamma function. The radial function $R_q(r)$ is normalized to $\delta(q-q')$.

The angular part of the problem, which reduces to finding the eigenvalues λ and the eigenvectors $a_L^{\lambda L}$ of the operator $\hat{\Lambda}$, turns out to be the same for an ion as for a neutral atom. In analogy with the known result for neutral hydrogen[4] the contour of the Lyman series of the ion lines $I(\omega)$ is represented in the form

$$I(\omega)=\frac{\pi^2\hbar}{3Eq'}\sum_{\lambda L}\{|a_{L+1}^{\lambda L}A_{L+1}^{\lambda L}|^2+|a_{L-1}^{\lambda L}A_{L-1}^{\lambda L}|^2\}. \tag{2.3}$$

The explicit forms of λ and $a_{L\pm1}^{\lambda L}$ for the $n=2$ level (the L_α line) is given in Ref. 4.

The basic problem is to calculate the overlap integrals of the radial wave functions A, expressed in the form

$$\int_0^\infty r^2R_{q_1}(r)R_{q_2}(r)\,dr=\frac{\nu_1^2-\nu_2^2}{q_1^2-q_2^2}\int_0R_{q_1}(r)$$
$$\times R_{q_2}(r)\,dr=\frac{\nu_1^2-\nu_2^2}{q_1^2-q_2^2}A. \tag{2.4}$$

Using the explicit form (2.2) of the functions $R_q(r)$ we obtain the formal solution of the problem:

$$A=\frac{(q_1q_2)^{1/2}}{\pi}x^{\nu_1}(-y)^{\nu_2}\exp\left[-i\frac{\pi}{2}\alpha+\frac{\pi}{2}(\eta_1+\eta_2)\right]$$
$$\times\Gamma(\alpha)\frac{|\Gamma(a_1)\Gamma(a_2)|}{\Gamma(b_1)\Gamma(b_2)}F_2\left(\alpha\left|\begin{matrix}a_1 & a_2\\ b_1 & b_2\end{matrix}\right|x,y\right), \tag{2.5}$$
$$\alpha=(b_1+b_2-2)/2,\ a_{1,2}=\nu_{1,2}+1/2\pm i\eta_{1,2},\quad \eta_{1,2}=Z/q_{1,2},$$
$$x=\frac{2q_1}{q_1-q_2},\quad y=-\frac{2q_2}{q_1-q_2},\quad q_1^2-q_2^2=2M\hbar\Delta\omega,$$

where F_2 is a hypergeometric function of two variables, the Appel function,[10] defined by the series

$$F_2\left(\alpha\left|\begin{matrix}a_1 & a_2\\ b_1 & b_2\end{matrix}\right|x,y\right)=\sum\frac{(\alpha)_{m+n}(a_1)_m(a_2)_n}{(b_1)_m(b_2)_n}\frac{x^my^n}{m!n!};$$
$$(\alpha)_m=\frac{\Gamma(\alpha+m)}{\Gamma(\alpha)},$$

which converges if $|x+1|<1$.

In our case $x+y\equiv2$ in (2.5), so that the solution obtained remains formal until we obtain its analytic continuation in the variable range of interest to us. The indicated analytic continuation can be obtained in analogy with the theory of relativistic bremsstrahlung.[9] The analytic-continuation formulas are given in the Appendix, where the method used to obtain them is briefly described and some inaccuracies of Ref. 9 have been corrected. The results are expressed in the form of rapidly converging double hypergeometric series and can be used for numerical calculations.

§3. TRANSITION TO THE LIMIT OF STRAIGHT TRAJECTORIES ($Ze^2/\hbar v\to0$)

We now trace in general formula (2.5) the transition to straight trajectories, $Z/q\to0$, including to the known results[4] for neutral hydrogen ($Z\equiv0$). The radial integral (2.5) is expressed in terms of an analytic function and can therefore be in principle investigated also without an analytic continuation. Under the condition $Z/q\to0$ we have in formula (2.5) $a_{1,2}=\nu_{1,2}+\frac{1}{2}$ and $b_{1,2}=2a_{1,2}$. Using the quadratic transformations of the hypergeometric function [Ref. 10, §2.11], we obtain

$$F_2\left(\alpha\left|\begin{matrix}a_1 & a_2\\ 2a_1 & 2a_2\end{matrix}\right|x,y\right)=\left(1-\frac{x}{2}\right)^{-\alpha}H_4\left(\alpha,a_2,a_1+\frac{1}{2},\ 2a_2|x',y''\right), \tag{3.1}$$
$$H_4\left(\alpha,a_2,a_1+\frac{1}{2},2a_2|x',y'\right)$$
$$=\left(1-\frac{y'}{2}\right)^{-\alpha}F_4\left(\frac{\alpha}{2},\frac{\alpha+1}{2},a_2+\frac{1}{2},a_1+\frac{1}{2}\middle|\,x'',y''\right).$$

Here H_4 and F_4 are the standard symbols for double hypergeometric series (see Ref. 10, §5.7);

$$x'=\frac{y^2}{4(2-y)^2},\quad y'=\frac{2x}{2-y},$$
$$x''=\frac{16x'}{(2-y')^2},\quad y''=\frac{y'^2}{(2-y')^2}. \tag{3.2}$$

If $z+y\to2$, then,

$$x''=y^2(2-x-y)^{-2}\to\infty,\quad y''=x^2(2-x-y)^{-2}\to\infty.$$

Using Ref. 10 (p. 225), we continue $F_4(x'',y'')$ analytically into the region of larger arguments. For the condition $x+y\to2$ of interest to us we can verify that in this analytic continuation there remains one term that degenerates into a hypergeometric function of a single variable,[1)] as a result of which we get

$$F_2\left(\alpha\left|\begin{matrix}a_1 & a_2\\ 2a_1 & 2a_2\end{matrix}\right|x,y\right)=\left(\frac{y}{2}\right)^{-\alpha}\frac{\Gamma(a_2+1/2)\Gamma(1/2)e^{-i\pi\alpha/2}}{\Gamma(a_2+1/2-\alpha)\Gamma(\alpha/2+1/2)}$$
$$\times{}_2F_1(\alpha/2,(\alpha+1-2a_2)/2,a_1+1/2,(x/y)^2). \tag{3.3}$$

Substitution of (3.3) in (2.3) yields directly for the contour the expression previously[4] obtained for the neutral hydrogen atom.

§4. IMPACT LIMIT. TRANSITION TO CLASSICAL THEORY

In the impact limit, corresponding to small frequency deviations ($\Delta\omega \to 0$), the line contour $I(\omega)$ is known[8] to be Lorentzian with a width γ expressed in terms of the difference between the phase shifts for the scattering of the broadening electron by the levels of the radiating atom. In the considered case of ion lines, a peculiar relation appears between the scattering phase shifts in the Coulomb and in the dipole potentials.

We obtain now the corresponding expressions, by starting from the analytic-continuation formulas (A.2) of the Appendix. Putting $\Delta\omega \to 0$ we verify that the arguments of the double series $1/x$, $1/y \to 0$ and their ratio $y/x \to 1$. The third term of (A.2) has a singularity in the Γ function, which is cancelled out by an analogous singularity in the second term. As a result, the first and second terms of (A.2) yield single hypergeometric series, ${}_2F_1$ and ${}_3F_2$ respectively, with unity argument. The ratio of the indices in ${}_3F_2(1)$, is such that ${}_3F_2(1)$ can be summed, just as ${}_2F_1(1)$, with the aid of Γ functions (see Ref. 10, $\S$ 4.4).

After straightforward but rather laborious transformations we obtain, taking (2.5) into account,

$$A = \frac{2q}{\nu_1^2-\nu_2^2}\sin\left[\frac{\pi}{2}(\nu_2-\nu_1)+\Delta_1-\Delta_2\right], \qquad \Delta_{1,2}=\arg\Gamma(\nu_{1,2}+{}^1/_2+i\eta). \tag{4.1}$$

In the limit as $Z/v \to 0$ (the phase shifts $\Delta_{1,2} \to 0$) we get from (4.1) and (2.3) the known result for the impact width of a neutral hydrogen atom (see. e.g., Ref. 4). At $Z \neq 0$ the Coulomb scattering leads, as is seen from (4.1), to the appearance of an additional phase difference $\Delta_1 - \Delta_2$. We note that the Coulomb phase shifts $\Delta_{1,2}$ depend also on the dipole-interaction constant that enters in $\nu_{1,2}$ (this is precisely why their difference in the upper and lower states does not vanish).

It is convenient to continue the analysis within the framework of the so-called adiabatic model, corresponding to a spherically symmetrical potential $U = -Ze^2/r + \alpha r^2$, inasmuch as allowance for the complicating angular part (i.e. for the concrete form of the parameters λ and $a_{L\pm1}^{\lambda L}$) does not introduce any new parameters into the problem and influences only the numerical coefficients. The order of magnitude of the dipole-interaction constant α for an ion level with a given n is the following[8]: $\alpha \sim n^2\hbar/Zm$. The scattering phase shifts $\delta_{1,2}$ take in the adiabatic model the form

$$\delta = \frac{\pi}{2}(l+{}^1/_2-[(l+{}^1/_2)^2+2M\alpha]^{1/2}).$$

The line width γ determined from the general formulas (2.3) for the contour and (2.5) for the overlap-integral structure take in the adiabatic model the form

$$\gamma = N_e v\frac{4\pi}{q^2}\sum(2L+1)\sin^2\left[\frac{\pi}{2}(\nu_2-\nu_1)+\Delta_1-\Delta_2\right]. \tag{4.2}$$

We consider now different limiting cases of (4.2). We go first to the classical limit. In this limit the effective values of the angular momenta l are large, so that the following expansion is valid for the Coulomb phase difference

$$\Delta_1-\Delta_2 \approx \frac{d\Delta}{d\nu}(\nu_1-\nu_2) \approx (\nu_1-\nu_2)\operatorname{arctg}\frac{\varkappa}{\nu}. \tag{4.3}$$

Putting next $\nu_1 \approx \nu_2 = Mv\rho$, we obtain

$$\gamma = 2N_e v\int_0^{\rho_{max}} 2\pi\rho\, d\rho\left\{1-\cos\left[\frac{\pi\alpha}{\rho v}\left(1\pm\frac{2}{\pi}\operatorname{arctg}\frac{Ze^2}{Mv^2\rho}\right)\right]\right\}. \tag{4.4}$$

The plus and minus signs correspond respectively to attraction and repulsion. The parameter ρ_{max} was introduce to cut off the logarithmic divergence that characterizes the broadening by charged particles, and is assumed below to be equal to the Debye radius ρ_D (for more details see Refs. 7 and 8).

At $Ze^2/\hbar v \ll 1$ we obtain from (4.4) the impact line width of a neutral atom. At $Ze^2/\hbar v \gg 1$ the answer depends on the relation between ρ_{max} and Ze^2/Mv^2. Under ideal-plasma conditions the values of these parameters are usually such that the line width changes insignificantly. It is nonetheless seen from (4) that line narrowing (in the case of repulsion) and additional broadening (in the case of attraction) are both possible.

The classical formula (4.4) contains automatically a cutoff at small impact parameters $\sim \alpha/v$ as a result of the rapid oscillations at values of ρ smaller than the Weisskopf radius $\rho_b \sim \alpha/v$. At large values of the ion charges Z the value of ρ_b may turn out to be smaller than the de Broglie wavelength λ of the electron. This is important for levels n that are not too high, and particularly for the L_α ($n = 2$) line. In this case the classical treatment becomes unsuitable.

To analyze the situation at $\rho_b \lesssim \lambda$ we consider in the general quantum formula the limiting case $Z \gg 1$, which ensures satisfaction of the condition $\rho_b/\sim n^2/Z \sim \alpha$ [at. un.] $\ll 1$. It is easily seen that in this case it is also possible to use the expansion (4.3), which is valid down to $l = 0$. At the same time, in view of the small phase difference $\nu_1 - \nu_2$ we can replace the sine function in (4.2) by its argument, and obtain

$$\gamma \approx 8\pi^3\frac{N_e\alpha^2}{v}\sum_{l=0}^{l_{max}}\frac{1}{l+{}^1/_2}\left\{1\pm\frac{2}{\pi}\operatorname{arctg}\frac{Ze^2}{\hbar v(l+{}^1/_2)}\right\}^2, \qquad l_{max} \approx Mv\rho_D. \tag{4.5}$$

We consider for the sake of argument the case of attraction [the plus sign in (4.5)]. Putting $\varkappa = Ze^2/\hbar v \gg 1$ and $l_{max} \gg 1$, we obtain with logarithmic accuracy

$$\sum_{l=0}^{l_{max}}(\ldots) \approx \begin{cases} 4\ln 2\varkappa + \ln(l_{max}/\varkappa), & l_{max} > \varkappa, \\ 4\ln 2l_{max}, & l_{max} < \varkappa. \end{cases} \tag{4.6}$$

It is seen that (4.5) and (4.6) do not contain the Weisskopf radius at all, whereas the cutoff at the de Broglie length plays an essential role. We note that in contrast to the classical theory[6] the cutoff at the de Broglie length appears automatically in the quantum approach.

In the case of the most practical interest $l_{max} > \varkappa$, the bending of the Coulomb trajectories, as follows from (4.6), affects noticeably the line width. The case $l_{max} < \varkappa$ is more of academic interest, since it can be realized only if the plasma is significantly nonideal. In the case of repulsion the lower cutoff parameter is the Landau radius $\rho_L = Ze^2/Mv^2$. We note that at $\varkappa > l_{max}$ there is no

logarithmic dependence of the impact width at all.

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APPENDIX

We represent the Appel function in the form of a series of hypergeometric Gauss functions:

$$F_2\left(\alpha\left|\begin{matrix}a_1 & a_2\\ b_1 & b_2\end{matrix}\right| x,y\right)=\sum_{l=0}^{\infty}\frac{(\alpha)_l(a_2)_l}{(b_2)_l}\frac{y^l}{l!}\,{}_2F_1(\alpha+l,a_1,b_1x). \qquad \text{(A.1)}$$

We continue ${}_2F_1$ analytically to the outside of the unit circle $|x|>1$.[10] One of the obtained terms converges under the condition $|x+y|>1$, and the other turns into a series of hypergeometric Gauss functions with argument y. By analytic continuation beyond the unit circle $|y|>1$ we obtain the final expression

$$\begin{aligned}
&F_2\left(\alpha\left|\begin{matrix}a_1 & a_2\\ b_1 & b_2\end{matrix}\right| x,y\right)=(-x)^{-\alpha}\Gamma\left(\begin{matrix}b_1, a_1-\alpha\\ a_1, b_1-\alpha\end{matrix}\right)\\
&\times Q_1\left(\begin{matrix}\alpha, & 1+\alpha-b_1, & a_2\\ & 1+\alpha-a_1, & b_2\end{matrix}\;\middle|\; -\frac{y}{x},\frac{1}{x}\right)+(-x)^{-\alpha_1}(-y)^{-\alpha+\alpha_1}\\
&\times\Gamma\left(\begin{matrix}b_1, & b_2, & \alpha-a_1, & a_1+a_2-\alpha\\ b_1-a_1, & \alpha, & b_2-\alpha+a_1, & a_2\end{matrix}\right)\\
&\times Q_2\left(\begin{matrix}a_1, & a_1+1-b_1, & a_1+a_2-\alpha\\ a_1+b_2-\alpha, & 1-\alpha+a_1\end{matrix}\;\middle|\; -\frac{y}{x},-\frac{1}{y}\right)+(-x)^{-\alpha_1}(-y)^{-\alpha_2}\\
&\times\Gamma\left(\begin{matrix}b_1, b_2, & \alpha-a_1-a_2\\ \alpha, & b_1-a_1, & b_2-a_2\end{matrix}\right)F_3\left(\begin{matrix}a_1, & a_2, & a_1+1-b_1, & a_2+1-b_2\\ & & a_1+a_2+1-\alpha\end{matrix}\;\middle|\; \frac{1}{y},\frac{1}{x}\right);
\end{aligned} \qquad \text{(A.2)}$$

$$\Gamma\left(\begin{matrix}a, & b\\ c, & d\end{matrix}\right)=\frac{\Gamma(a)\Gamma(b)}{\Gamma(c)\Gamma(d)},\quad \arg(-x)=-\pi,$$

$$Q_1\left(\begin{matrix}a, & b, & c\\ d, & e\end{matrix}\;\middle|\; x,y\right)=\sum_{l,m=0}^{\infty}\frac{(a)_{l+m}(b)_{l+m}(c)_l}{(d)_{l+m}(e)_l}\frac{x^ly^m}{l!m!}.$$

$$Q_2\left(\begin{matrix}a, & b, & c\\ d, & e\end{matrix}\;\middle|\; x,y\right)=\sum_{l,m=0}^{\infty}\frac{(a)_l(b)_l(c)_{l-m}}{(d)_{l-m}(e)_{l-m}}\frac{x^ly^m}{l!m!},$$

$$F_3\left(\begin{matrix}a, & b, & c, & d\\ & e\end{matrix}\;\middle|\; x,y\right)=\sum_{l,m=0}^{\infty}\frac{(a)_l(b)_m(c)_l(d)_m}{(e)_{l+m}}\frac{x^ly^m}{l!m!}$$

Equation (A.2) coincides with the analogous formula of Ref. 9 if some of its inaccuracies are corrected.

[1)]Equation (3.3) is, along with those given in Ref. 9, one more particular case of an analytic continuation of the Appel function, which can be of interest also for relativistic bremsstrahlung theory.

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