Classical and quantum treatment of the Stark broadening of hydrogen lines

F. F. Baryshnikov and V. S. Lisitsa

I. V. Kurchatov Institute of Atomic Energy
(Submitted September 17, 1976)
Zh. Eksp. Teor. Fiz. **72**, 1797–1808 (May 1977)

The dipole approximation is used to obtain an exact quantum-mechanical solution for the Stark broadening of a hydrogen line. This solution provides an analytic description of the entire line contour. The quantum-mechanical solution is compared with the exact classical solution, and the range of validity of the latter is elucidated.

PACS numbers: 32.60.+i, 32.70.Jz

§ 1. INTRODUCTION

There are two main approaches to the problem of Stark broadening of atomic lines, and it is convenient to describe them as the classical and the quantum-mechanical. Their essence can be easily understood if we regard the radiating and perturbing particles (respectively, the atom and, say, the ion) as the components of a single system emitting a quantum of radiation. The system is represented by the wave function $\Psi(r_A, r_i)$ which can be written as the product of the atomic wave function $\psi(r_A)$ and the wave function $\psi(r_i)$ of the ion. This way of writing the wave function is justified by the fact that the broadening process involves only a small spectral range $\Delta\omega$ near the atomic transition and corresponds to a small energy transfer (i. e., large distances) between the atom and the ion. In the classical treatment of the problem of broadening, one examines the evolution of the atomic wave function $\psi(r_A)$ in the field of the ion, the motion of which is assumed unperturbed and classical [$\psi(r_i)$ is the classical wave packet]. In the quantum-mechanical formulation, on the other hand, one is interested in the motion of the perturbing particle (ion) in the potential produced by the radiating atom. The change ΔE in the energy of the scattered ion determines the change $\Delta\omega = \Delta E/\hbar$ in the frequency of the light emitted by the atom.

The great majority of papers on the theory of broadening has been concerned with the classical treatment.[1] The quantum-mechanical formulation was first used by Jablonski.[3] Specific calculations were, however, performed by Jablonski[3] only in the quasiclassical approximation, in the case of broadening by heavy particles. The corresponding results were, therefore, valid only for the distant, static wing of the line. Sobel'man[4] (see also Sobel'man[11]) and Baranger[5] used the quantum-mechanical formulation to calculate broadening by fast light particles (electrons). The quantum-mechanical description of the motion of the electrons enabled them to relate the broadening parameters (linewidth and shift) to the electron-atom scattering cross sections. These calculations were concerned with the central (collisional) part of the line contour and did not, therefore, incorporate the results of Jablonski[3] for the distant wing of the line. Further development of Jablonski's theory,[3] undertaken by Szudy,[6] resulted in a description of the transition between the central (collisional) part of the contour and the static wing of the line. We note that this transition was achieved in[6] with the aid of quasiclassical wave functions for the perturbing particle.

More recently, Tran Minh *et al.*[7,8] and Szudy and Baylis[9] gave a sufficiently general quantum-mechanical treatment of line broadening. Their results apply to the case of two isolated atomic levels between which a radiative transition takes place. The method used by Tran Minh *et al.*[7,8] is more general and can, in principle, take into account the degeneracy of levels that is important for hydrogen-like systems. It is important to note, however, that all these workers were forced to use the quasiclassical approximation for specific calculations. This is so because the quantum-mechanical treatment of the problem requires a knowledge of the exact wave function $\psi(r_i)$ of the perturbing particle in the field of the radiating atom. This function can, as a rule, be found only numerically. We emphasize that the scattering phase alone is insufficient for the determination of the entire line contour. Thus, the generality of the quantum-mechanical treatment of the broadening problem is, therefore, to some extent determined by the associated computational difficulties.

The hydrogen atom is an exception to all this and, as will be shown below, it admits of an analytic solution in both the classical and the quantum-mechanical formulations. This is connected with the particular properties of the Coulomb field which gives rise to a "fortuitous" degeneracy of the hydrogen lines. The symmetry properties of the hydrogen atom can, in fact, be used (in the dipole approximation) to obtain an exact solution for the broadening problem in the classical formulation.[10][1)] In this paper, we shall derive (again in the dipole approximation) the exact solution of the quantum-mechanical problem and consider its relation to the solution[10] obtained in the classical formulation.

The fact that an exact solution for hydrogen-line broadening during collisions with ions *can* be obtained is quite clear *a priori*. Thus, the potential due to the (dipole) interaction between the ion and the excited hydrogen atom falls off as r_i^{-2}, i.e., like a centrifugal potential. The wave functions of the ion moving in the dipole potential must, therefore, be Bessel functions.

 0038-5646/77/4505-0943$02.40

The calculations are complicated because a large number (n^2) of states associated with the degenerate hydrogen level with principal quantum number n participate in the interaction. In this respect, the problem is completely analogous to the strong-coupling approximation in the multichannel problem of inelastic atomic collisions, discussed by Seaton.[13] We note in this connection that, as observed by Demkov, Ostrovskiĭ, and Solov'ev,[14,15] the four-dimensional symmetry properties of the hydrogen atom can be used in the quasiclassical approximation to solve the scattering problem, just as in the classical case. It is important to note, however, that, in contrast to the theory of scattering, the final result for the line profile in the theory of broadening is not expressed in terms of the scattering phases, but contains information about the total structure of the wave function.

§ 2. SET OF WAVE FUNCTIONS FOR THE EXCITED HYDROGEN ATOM AND THE BROADENING PARTICLE

In this section, we shall construct the set of functions $|\pm q l_A m_A\rangle$ that transform, at large distances between the atom and the perturbing particle, into a plane wave, a convergent or divergent spherical wave associated with the perturbing particle, and the hydrogen function of the atom in the state $l_A m_A$. These functions will then be used to determine the spectrum of the hydrogen atom. Let us begin by considering the Hamiltonian of the system consisting of an excited hydrogen atom and the broadening particle (ion):

$$\hat{H}=\hat{H}_A+\hat{H}_i+\hat{V}_{Ai}. \tag{2.1}$$

In this expression, $\hat{H}_A$ and $\hat{H}_i$ are the Hamiltonians of the free atom and ion, respectively, and $\hat{V}_{Ai}$ is the operator corresponding to their dipole interaction:

$$\hat{V}_{Ai}=\frac{1}{r_i}-\frac{1}{|\mathbf{r}_A-\mathbf{r}_i|}\approx-\frac{\mathbf{r}_i\mathbf{r}_A}{r_i^3}, \tag{2.2}$$

where $\mathbf{r}_A$ and $\mathbf{r}_i$ are the position vectors of the atomic electron and ion, respectively.

The main contribution to broadening is provided[1,2] by the states of the atom that correspond to the given degenerate level with fixed principal quantum number n (and lie on the "equal energy" surface). The wave function of the system under investigation can, therefore, be written in the form of the product

$$\Psi(r_A, r_i)=\psi_n(r_A)\psi(r_i), \tag{2.3}$$

where $\psi_n(r_A)$ is the unperturbed wave function for the hydrogen level n.

If we substitute (2.3) into the Schrödinger equation with the Hamiltonian given by (2.1), (2.2), we obtain a set of equations for the wave function of the ion interacting with the n^2 degenerate states of hydrogen. The potential for this multichannel interaction, given by (2.2), is noncentral and, therefore, the orbital angular momentum l_i of the scattered ion is not conserved. To simplify the resulting multichannel problem, we can use the symmetry properties of the dipole potential. Thus, it is known[15,16] that, in addition to the resultant angular momentum of the system $\mathbf{L}=\mathbf{l}_i+\mathbf{l}_A$ ($\mathbf{l}_A$ is the orbital angular momentum of the atom) and its component M, there is the additional constant of motion

$$\hat{\Lambda}=\hat{\mathbf{l}}_i^2-2Mr_A(\mathbf{n}_i\mathbf{n}_A), \quad \hat{\Lambda}\Psi=\lambda\Psi. \tag{2.4}$$

In this expression, M is the mass of the ion, $\mathbf{n}_i$, $\mathbf{n}_\lambda$ are unit position vectors $\mathbf{n}=\mathbf{r}/r$, and we are using atomic units in which $e=\hbar=m=1$.

Since $\hat{\Lambda}$ is conserved, we can immediately write down the radial Schrödinger equation for the motion of the ion in the potential given by (2.2) (cf. Ostrovskiĭ and Solov'ev[15]):

$$\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}+\left(q^2-\frac{\lambda}{r^2}\right)R=0. \tag{2.5}$$

The solution of this equation can be expressed in terms of Bessel functions:

$$R^{\lambda L}=\left(\frac{q}{r}\right)^{1/2}J_{(\lambda+1/4)^{1/2}}(qr). \tag{2.6}$$

where $q^2/2M=E$ is the energy of the free motion of the ion and r is the modulus of its position vector (the subscript i will be omitted henceforth).

We must recall that (2.6) was obtained in the dipole approximation which is valid only for sufficiently distant encounters. Encounters involving small angular momenta may result in the "fall" of the particle on the atom[17] (Sec. 35). It is clear, however, that, as the distance decreases, the dipole approximation eventually ceases to be valid and the "fall" will not, in fact, occur. For the $n=2$ level, the fall of the particle is already absent for $l_i>2$. We shall, therefore, suppose that such encounters provide a small contribution to the resultant contour. They may have an effect on the distant wings of the line contour, where the dipole approximation is not valid. We note that, from the mathematical point of view, the fall effect is connected with the appearance of an imaginary index of the functions given by (2.6), so that the condition for an encounter without the "fall" is $\lambda>-1/4$.

Despite the simple form of the solution (2.6), it is important to recall that, before it can be used, we must find the values of λ, i.e., solve the secular equation (2.4). The wave function $\Psi_{\lambda LM}$, which diagonalizes (2.4), is conveniently sought in the form of a combination of functions with definite total angular momentum L and projection M:

$$\Psi_{\lambda LM}=R^{\lambda L}(q)|\lambda LM\rangle, \quad |\lambda LM\rangle=\sum\langle l_A l_i|\lambda L\rangle|l_A l_i LM\rangle. \tag{2.7}$$

The coefficients $\langle l_A l_i|\lambda L\rangle$ are found in the course of the diagonalization of the constant of motion Λ. If we write

$$|l_A l_i LM\rangle=\sum_{m_A m_i}\langle m_A m_i|LM\rangle|n_A l_A m_A\rangle|l_i m_i\rangle \tag{2.8}$$

and substitute for $\Psi_{\lambda LM}$ in (2.4), we obtain the following set of equations for the coefficients $\langle l_A l_i | \lambda L\rangle$:

$$\sum_{l_A l_i} \langle l_A l_i|\lambda L\rangle\langle l_A' l_i' LM|\hat{\Lambda}-\lambda|l_A l_i LM\rangle=0. \tag{2.9}$$

The consistency condition for (2.9) is

$$\det \langle l_A' l_i' LM|\hat{\Lambda}-\lambda|l_A l_i LM\rangle=0 \tag{2.10}$$

and this can be used to find the values of λ and then, after substituting into (2.9), the coefficients $\langle l_A l_i | \lambda L\rangle$. These coefficients satisfy the orthogonality condition

$$\sum_{l_A l_i} \langle l_A l_i|\lambda L\rangle\langle l_A l_i|\lambda' L\rangle=\delta(\lambda'\lambda). \tag{2.11}$$

Using the well-known relationships for the matrix elements of tensor operators (see, for example, Landau and Lifshitz[17]), we obtain the following expression for the constant of motion (2.4):

$$\langle l_A' l_i' LM|\hat{\Lambda}-\lambda|l_A l_i LM\rangle=[l_i(l_i+1)-\lambda]\delta(l_A l_A')\delta(l_i l_i')$$

$$-\alpha\sqrt{3}(-1)^{l_{Amin}+l_{imax}+L}\begin{Bmatrix} L & l_i' & l_A' \\ 1 & l_A & l_i \end{Bmatrix}\langle l_A'\|n_A\|l_A\rangle\langle l_i'\|n_i\|l_i\rangle. \tag{2.12}$$

In this expression, $\alpha=Mn[3(n^2-l_{A\,max})]^{1/2}$ ($\alpha=6M$ for $n=2$), n is the principal quantum number, l_{min}, l_{max} are the minimum and maximum values of l, l'; the symbols $\{\ldots\}$ represent the $6J$-symbol of Wigner, and $\langle l' \| n \| l\rangle$ are the reduced matrix elements of the operator n, which can be expressed in terms of the $3J$-symbol.[17]

The solution of (2.9) and (2.10) in a general form is difficult because of the high degree of degeneracy of the hydrogen levels. The solution is simplified, however, if, for example, the main contribution to the contour is provided by encounters with high angular momenta. We can then use the asymptotic expressions for the $6J$ symbols. The aim of the present analysis is not, however, the solution of this problem for an arbitrary n. Henceforth, we shall suppose that the values of λ and of the coefficients $\langle l_A l_i | \lambda L\rangle$ are known and the specific calculation will be carried out for $n=2$ for which the degree of degeneracy is not high.

We must now construct the system of functions $|\pm q l_A m_A\rangle$. We shall expand it in terms of the complete set of functions $\Psi_{\lambda LM}$ (2.7):

$$|\pm q l_A m_A\rangle=\sum_{\lambda LM}\langle\lambda LM|\pm q l_A m_A\rangle\Psi_{\lambda LM}. \tag{2.13}$$

The asymptotic expression for the function given by (2.13) is

$$|\pm q l_A m_A\rangle \underset{r\to\infty}{\approx} |l_A m_A\rangle e^{iqr}+\frac{f^{(\pm)}}{r}e^{\pm iqr}, \tag{2.14}$$

where r is the distance between the ion and the atom. Equating the corresponding coefficients in (2.13) and (2.14), and using the orthogonality properties of $\langle l_A l_i | \lambda L\rangle$ and $\langle m_A m_i | LM\rangle$, we obtain

$$\langle\lambda LM|\pm q l_A m_A\rangle=\frac{(2\pi)^{1/2}}{q}\exp\left[\mp i\frac{\pi}{2}\left(\nu_{\lambda L}-\frac{1}{2}\right)\right]$$

$$\times\sum_{lm}(\mp 1)^l\langle m_A m|LM\rangle\langle l_A l|\lambda L\rangle Y_{lm}^*(\mathbf{q}), \tag{2.15}$$

where the corresponding signs on the left and right must be taken, i.e., either the upper or the lower, and $\nu_{\lambda L}=(\lambda+\frac{1}{4})^{1/2}$. The coefficients in (2.15) and the functions (2.7) jointly provide us with the solution of our problem. Let us consider in greater detail the states with $n=2$. In this case, there are no difficulties with the diagonalization of the matrix Λ. Since the $n=2$ wave functions are superpositions of only the S and P states, the corresponding results coincide, as expected, with the results obtained by Seaton[13] for problems involving strong coupling between the S and P channels during scattering. For the $n=2$ level, Eq. (2.10) together with the explicit expression for the $6J$ symbols in (2.11) assumes the form

$$\det\begin{Vmatrix} L(L+1)-\lambda & -\alpha[L/(2L+1)]^{1/2} & -\alpha[(L+1)/(2L+1)]^{1/2} \\ -\alpha[L/(2L+1)]^{1/2} & L(L-1)-\lambda & 0 \\ -\alpha[(L+1)/(2L+1)]^{1/2} & 0 & (L+1)(L+2)-\lambda \end{Vmatrix}=0, \tag{2.16}$$

where $\alpha=6M$. The numbers of rows and columns in this matrix correspond to the coefficients $\langle 0L|\lambda L\rangle$, $\langle 1L-1|\lambda L\rangle$, and $\langle 1L+1|\lambda L\rangle$, respectively. The eigenvalues λ and eigenvectors $\langle l_{Ai}|\lambda L\rangle$ have the form

$$\lambda=\lambda_0=L(L+1),$$

$$\begin{bmatrix}\langle 0L|\lambda L\rangle \\ \langle 1L-1|\lambda L\rangle \\ \langle 1L+1|\lambda L\rangle\end{bmatrix}=\frac{1}{N_0}\begin{bmatrix}1 \\ -\alpha/2[L(2L+1)]^{1/2} \\ -\alpha/2[(L+1)(2L+1)]^{1/2}\end{bmatrix},$$

$$N_0=[1+\alpha^2/4L(L+1)]^{1/2}; \tag{2.17}$$

$$\lambda=\lambda_\pm=L(L+1)+1\pm(2L+1)[1+[\alpha/(2L+1)]^2]^{1/2},$$

$$\begin{bmatrix}\langle 0L|\lambda L\rangle \\ \langle 1L-1|\lambda L\rangle \\ \langle 1L+1|\lambda L\rangle\end{bmatrix}=\frac{1}{N_\pm}\begin{bmatrix}1 \\ -\alpha L^{1/2}/(2L+1)^{3/2}(1\pm\xi) \\ -\alpha(L+1)^{1/2}/(2L+1)^{3/2}(-1\pm\xi)\end{bmatrix}, \tag{2.18}$$

$$N_\pm=\left\{2\left[1+\left(\frac{2L+1}{\alpha}\right)^2\pm\xi\frac{2L+1}{\alpha^2}\right]\right\}^{1/2},$$

$$\xi=\left[1+\left(\frac{\alpha}{2L+1}\right)^2\right]^{1/2}. \tag{2.19}$$

The expressions given by (2.17) and (2.18), taken together with (2.6), (2.7), (2.13), and (2.15), define the exact wave functions of the broadening particle, moving in the field of the excited hydrogen atom in the $n=2$ state. These functions will be used below in a specific calculation concerned with the spectrum of the Ly-α line.

§3. CONTOUR OF A HYDROGEN LINE AND THE OVERLAP INTEGRAL FOR THE WAVE FUNCTIONS OF BROADENING PARTICLES

To determine the contour $I(\omega)$, we shall use the well-known expression for the transition probability in the continuous spectrum

$$W=\frac{2\pi}{\hbar}|\hat{V}_{ab}|^2\delta(\mathscr{E}_b-\mathscr{E}_a)\frac{d\mathbf{q}_b}{(2\pi)^3}\frac{d\mathbf{k}}{(2\pi)^3}. \tag{3.1}$$

Here, $\hat{V}$ is the operator representing the interaction between the atom and the radiation field, $\mathcal{E}_b - \mathcal{E}_a = (\hbar^2/2M)(q_b^2 - q_a^2) - \hbar\Delta\omega$, $\Delta\omega = \omega_{ab} - \omega$ is the difference between the atomic and observed frequencies, and $\mathbf{k}$ is the wave vector of the emitted photon.

We begin by considering the case of a two-level atomic system with arbitrary spherically symmetric interaction potentials $U_a(r)$ and $U_b(r)$. The particular form of the potential is unimportant. We shall use this example to demonstrate the possibilities of the quantum-mechanical approach to the theory of broadening. This approach enables us to use the well-established formalism of scattering theory. However, whilst the asymptotic form of the wave functions is sufficient in the scattering theory, to calculate the complete contour we must know the wave functions throughout space.

Let the wave functions for the initial a and final b states of the system be of the form

$$|a\rangle = \varphi_a v_a^{-1/2}\psi(\mathbf{q}_a^+), \quad |b\rangle = \varphi_b\psi(\mathbf{q}_b^-), \tag{3.2}$$

where $\varphi_{a,b}$ are the atomic wave functions and $\psi(\mathbf{q}^\pm) \underset{r\to\infty}{\approx} e^{i\mathbf{qr}} + f^\pm r^{-1} e^{\pm iqr}$ (see Sobel'man[11]). The chosen normalization of the wave functions is analogous to the normalization used[1] to determine the bremsstrahlung cross section $d\sigma/d\omega$. The cross section $d\sigma$ is given directly by (3.1) after averaging over initial and summing over final states of the system. In our case, it is not the external particle that interacts with the radiation field but the atom itself and, therefore, the resulting cross section will characterize the broadening process. Following the treatment used for bremsstrahlung,[1] we obtain

$$\frac{d\sigma}{d\omega} = \frac{4\omega^3|\mathbf{d}_{ab}|^2}{3c^3}\frac{\pi^2}{v_a E_a q_b}\sum_l (2l+1)|A_l|^2,$$
$$E_a = \frac{\hbar^2 q_a^2}{2M}, \quad A_l = \int_0^\infty dr\, r^2 R_l(q_a r) R_l(q_b r), \tag{3.3}$$

where $R_l(q_i r)$ is the solution of the radial equation with angular momentum l in the potential $U_i(r)$ with momentum $\hbar q_i$ $(i = a, b)$:

$$R_l(q_i r) \underset{r\to\infty}{\approx} \left(\frac{2}{\pi}\right)^{1/2}\frac{1}{r}\sin\left(q_i r - l\frac{\pi}{2} + \eta_l^i\right).$$

The power radiated per unit volume, $Q(\omega)\,d\omega$, is related to $d\sigma/d\omega$ in a simple fashion, as in the bremsstrahlung case:

$$Q(\omega) = N_A N_i \hbar\omega \int_0^\infty v_a f(v_a)\frac{d\sigma}{d\omega}dv_a.$$

In this expression, $f(v_a)$ is the distribution over the initial relative velocities. We shall not carry out the averaging with respect to velocity. If necessary, this can be done at the end. We thus obtain

$$Q(\omega) = N_A N_i \frac{4\omega^4|\mathbf{d}_{ab}|^2}{3c^3}\frac{\pi^2\hbar}{E_a q_b}\sum_l (2l+1)|A_l|^2. \tag{3.4}$$

This yields the following expression for the line contour:

$$I(\omega) = N_i\frac{\pi^2\hbar}{E_a q_b}\sum_l (2l+1)|A_l|^2. \tag{3.5}$$

The expression given by (3.5) is identical with the corresponding expression given by Szudy,[6] but we have obtained it by the direct method that does not require an analysis of the motion of the broadening particles in a finite volume. It can be shown[6,9] that (3.5) contains all the results of the adiabatic theory of broadening.

Let us apply our formalism to the radiation emitted by a hydrogen atom. The overlap integral is difficult to evaluate in this case because, as noted above, the states a and b by which the broadening ion is scattered are degenerate. However, the existence of the additional constant of motion Λ enables us to isolate independent scattering channels characterized by different quantum numbers λ. The overlap integral then splits into a series of two-level integrals corresponding to different pairs of values λ_a, λ_b for the levels a, b. Using the wave functions given by (2.13), we find that, as in the case of the two-level system, the expression for the power $Q(\omega)$ radiated per unit volume per unit frequency is

$$Q(\omega) = \frac{4\omega^4}{3c^3}N_A\frac{1}{n^2}|d_{AA'}|^2 I(\omega),$$
$$|d_{AA'}|^2 = \sum_{l_A l_A'}|\langle n_A' l_A'\|d\|n_A l_A\rangle|^2, \quad I(\omega) = |d_{AA'}|^{-2}\sum_{\lambda\lambda'} I_{\lambda\lambda'}, \tag{3.6}$$
$$I_{\lambda\lambda'} = N_i\frac{\pi^2\hbar}{Eq'}\sum_{LL'}(2L+1)(2L'+1)(A_{\lambda'L'}^{\lambda L})^2|\langle\lambda L|\lambda' L'\rangle|^2, \tag{3.7}$$
$$\langle\lambda' L'|\lambda L\rangle = \sum_{l_A l_A' l_i}(-1)^{l_A+l_i}\langle l_A l_i|\lambda L\rangle\langle l_A' l_i|\lambda' L'\rangle\begin{Bmatrix} l_A' & L' & l_i \\ L & l_A & 1\end{Bmatrix}\langle n' l_A'\|d\|n l_A\rangle,$$
$$A_{\lambda L}^{\lambda' L'} = \int_0^\infty r^2 R^{\lambda L}(qr) R^{\lambda' L'}(q' r)\,dr. \tag{3.8}$$

The primed and unprimed variables refer to states b and a of the system, respectively. The general expression (3.6) for $Q(\omega)$ is rather unwieldy and we shall, therefore, consider the lines belonging to the Lyman series. The resulting conclusions on the structure of the overlap integrals $A_\lambda^{\lambda' L'}$ will, however, be of a general character. For the Lyman lines, we can neglect the interaction in the lower state as compared with the upper state.

Using (3.6) and substituting $\langle 0L'|\lambda' L'\rangle = 1$, we obtain

$$I(\omega) = \frac{\pi^2\hbar}{3Eq'}\sum_{\lambda L}(2L+1)\{[\langle 1L-1|\lambda L\rangle A_{\lambda L}^{L-1}]^2 + [\langle 1L+1|\lambda L\rangle A_{\lambda L}^{L+1}]^2\}. \tag{3.9}$$

The expressions given by (3.8) and (3.9) and the coefficients $\langle l_A l_i|\lambda L\rangle$ given by (2.17) and (2.18) for $n=2$ are the starting point for evaluating the Ly-α contour. In contrast to the two-level approximation[6] and (3.5), the expression for the contour now includes contributions due to the different angular momenta $L_a = L_b \pm 1$ of the upper state and, in addition, all three scattering

channels corresponding to λ_0 and $\lambda_\pm$ [see (2.17) and (2.18)]. In the general case of an arbitrary Lyman line, the expression in (3.9) should be summed over all the scattering channels, i.e., all λ obtained by solving (2.10).

For arbitrary (non-Lyman) lines, the contour $I_{ab}(\omega)$ has a relatively complicated structure, largely due to the complexity of the solution of the secular equation determined by the value of the constant of motion λ. The latter is clear from (3.6). This problem can be simplified in the quasiclassical limit by using the symmetry properties of the hydrogen atom.[10] However, we shall be interested in the possibility of obtaining the quantum-mechanical expression for the contour and in its relation to the classical expression.

It follows from (3.9) that the main problem in calculating the spectrum is the evaluation of the overlap integral (3.8). The radial wave functions (2.6) are normalized to the delta function of q so that we must investigate the integral

$$A_{\nu\nu'}=(q_aq_b)^{1/2}\int_0^\infty rJ_\nu(q_ar)J_{\nu'}(q_br)\,dr. \tag{3.10}$$

This integral contains singularities that impede its evaluation. It is, however, possible to isolate these terms explicitly. The integral can then be written as the sum of a regular part and delta-function type singularities. The singularities are unimportant for the main part of the line contour and can be ignored.

To isolate the regular part, we use the following property of the indefinite integral of Bessel functions[18]:

$$\int rJ_\nu(kr)J_{\nu'}(k'r)\,dr=\frac{\nu'^2-\nu^2}{k'^2-k^2}\int\frac{dr}{r}J_\nu(kr)J_{\nu'}(k'r)$$
$$+\frac{r}{k'^2-k^2}[k'J_\nu(kr)J_{\nu'+1}(k'r)-kJ_{\nu+1}(kr)J_{\nu'}(k'r)]-\frac{\nu'-\nu}{k'^2-k^2}J_\nu(kr)J_{\nu'}(k'r). \tag{3.11}$$

If we insert the limits $r=0$ and $r=\infty$, the last term will vanish for $\nu+\nu'>0$, which is satisfied in our case. The second term on the right-hand side of (3.10) is zero when $r=0$ and, as $r\to\infty$, we can substitute the asymptotic form of the Bessel functions. This leads to the above-mentioned singularities of the delta-function type:

$$-\sin\left[\frac{\pi}{2}(\nu+\nu')\right]\delta(q_a+q_b)+\cos\left[\frac{\pi}{2}(\nu-\nu')\right]\delta(q_a-q_b). \tag{3.12}$$

If we exclude the small neighborhood of the point $\Delta\omega=0$ ($q_a^2=q_b^2$) from our analysis, we can ignore this singularity.[2)]

The remaining term in (3.11) is regular. The corresponding integral can be expressed in terms of the complete hypergeometric function $F(a, b, c, z)$.[19] The final result is

$$A_{\lambda L}^{\nu'L'}=\frac{(q_aq_b)^{1/2}}{2}\frac{\nu_b^2-\nu_a^2}{q_b^2-q_a^2}\left(\frac{q_a}{q_b}\right)^{\nu}\frac{\Gamma((\nu_a+\nu_b)/2)}{\Gamma(1+(\nu_b-\nu_a)/2)\Gamma(1+\nu_a)}$$
$$\times F\left[\frac{\nu_a+\nu_b}{2},\frac{\nu_a-\nu_b}{2},\nu_a+1,\left(\frac{q_a}{q_b}\right)^2\right],\quad \nu+\nu'>0, \tag{3.13}$$
$$(q_a/q_b)^2=[1+2M\Delta\omega/q_a^2]^{-1},\quad q_b>q_a>0.$$

Substituting this expression in (3.9), we obtain the exact quantum-mechanical expression for the contour of an arbitrary Lyman line, including Ly-α, in the dipole approximation. Since the structure of the function $I_{ab}(\omega)$ is quite clear from (3.9) and (3.13), we shall not write out the somewhat unwieldy general expression.

We thus see that an exact expression for the line contour can be obtained from the quantum-mechanical treatment of the broadening of the hydrogen lines. As noted above, an exact solution can also be obtained[10] in the classical formulation corresponding to the classical motion of the perturbing ion. The problem is to determine the relation between the two solutions. One would expect the classical solution to be a special case of the quantum-mechanical solution as the latter is taken to the classical limit. This transition will be investigated below. All we need to say now is that we are concerned with the direct correspondence between the two analytic solutions for arbitrary values of $\Delta\omega$. When they are compared, we need not therefore use the quasiclassical wave functions of the form

$$\cos\int p(r)\,dr,$$

which was done by Szudy[6] and Tran Minh *et al.*[7-9]

§ 4. CLASSICAL LIMIT

The expression given by (3.9) for the line contour contains the sum over different angular momenta of the incident particle. Motion with large relative momenta should be close to the classical situation. For a heavy particle, the main contribution to broadening is, in fact, due to encounters with high angular momenta. Therefore, by passing to the limit of high angular momenta in (3.9), we obtain the expression for the line contour broadened by classical particles.

The overlap integral (3.7) in (3.6) and (3.9) is proportional to the hypergeometric function which, for high angular momenta, transforms into the confluent hypergeometric function of the second kind[20]

$${}_2F_1=F\left[\frac{\nu_a+\nu_b}{2},\frac{\nu_a-\nu_b}{2},\nu_a+1,\left(\frac{q_a}{q_b}\right)^2\right]$$
$$\approx\exp\left[\frac{\Delta\omega(\nu_a+1)}{Mv^2}\right](\nu+1)^{(\nu_a-\nu_b)/2}W_{(\nu_b-\nu_a)/2,\,1/2}\left(\frac{2\Delta\omega(\nu_a+1)}{Mv^2}\right). \tag{4.1}$$

When $\nu_a\gg|\nu_b-\nu_a|$, this is equivalent to

$$L\gg\bar{\gamma}\alpha, \tag{4.2}$$

and the factor in front of the hypergeometric function in (3.13) is then simplified, eventually yielding

$$A_{\lambda L}^{\lambda'L'}=\frac{(q_aq_b)^{1/2}}{2}\frac{\nu_b^2-\nu_a^2}{1+\nu_a}\frac{\exp(\Delta\omega/Mv^2)}{q_b^2-q_a^2}k_{\nu_b-\nu_a}\left[\frac{\Delta\omega(\nu_a+1)}{Mv^2}\right], \tag{4.3}$$

where $k_\nu(x)=W_{\nu/2,1/2}(2x)/\Gamma(1+\nu/2)$ is the Bateman function.[20]

The exponential in (4.3) can be ignored under our conditions. The coefficients in (2.17) and (2.18) are substantially simplified in the limit of high angular momenta. The final result for the Ly-α contour is

$$I(\omega)=\frac{1}{24}N_i\frac{\hbar^2\alpha\pi^2}{M^2v\Delta\omega^2}\sum_L\frac{1}{x(1+x^2)}\{[k^2_{\sqrt{1+x^2}+1}(x\beta)+k^2_{\sqrt{1+x^2}-1}(x\beta)+2x^2k_1^2(x\beta)]+[k_\nu\to k_{-\nu}]\},\qquad(4.4)$$

where $\beta=\alpha\Delta\omega/Mv^2$, $x=(2L+1)/\alpha$. The expression in the second brackets differs from the first by the signs of the indices of the k_ν-functions.

The expression given by (4.4) was obtained on the assumption that $\beta>0$. It is readily shown by examining the derivation of (4.4) that the same expression is valid for $\beta<0$. We can, therefore, use it for both signs of β by defining $k_\nu(\beta)$ for $\beta<0$ in the same way as for $\beta>0$[20]:

$$k_\nu(\beta)=\frac{2}{\pi}\int_0^{\pi/2}\cos[\beta\,\mathrm{tg}\,\vartheta-\nu\vartheta]\,d\vartheta.\qquad(4.5)$$

It follows from this expression that $k_\nu(\beta)=k_{-\nu}(-\beta)$. The expression in the second brackets in (4.4) is, therefore, identical with that in the first if we substitute $\beta\to-\beta$, which, of course, represents the symmetrization of the contour. If we replace the summation in (4.4) over the angular momenta by integration with respect to the impact parameter $\rho\sim x$, we obtain an expression that is exactly the same as the result of the classical calculation.[10]

We can use (4.2) to obtain the criterion for the validity of the classical expression for the line contour. In the collisional region ($\alpha\Delta\omega/Mv^2\ll1$), the effective impact parameter is determined by the Weisskopf length[1] $\rho_W\sim\alpha/Mv$. Condition (4.2) is, therefore, equivalent to

$$\sqrt{\alpha}\gg1,\qquad(4.6)$$

which is satisfied with a considerable margin. The validity of the classical expression given by (4.4) in the collisional region is quite clear *a priori* because the main contribution to the central part of the contour is due to distant encounters with high angular momenta. In the static region ($\alpha\Delta\omega/Mv^2\gg1$) the validity of (4.4) is not so obvious. In this case, the effective impact parameter is $\rho_{eff}\sim\rho_\omega\sim(\alpha/M\Delta\omega)^{1/2}$. Condition (4.2) is then satisfied provided

$$\Delta\omega\ll Mv^2.\qquad(4.7)$$

This condition is identical with the usual criterion for the validity of the approximation of classical trajectories which assumes that the change in the particle energy during the interaction process is small in comparison with its initial energy.

§ 5. CONCLUSIONS

We have investigated the quantum-mechanical treatment of the theory of broadening of spectral lines, based on an analysis of the overlap integrals for the wave functions of the broadening particle. This approach provides us with a simple means of formulating the broadening problem itself in complete analogy with the theory of inelastic scattering and the emission of bremsstrahlung. The quantum-mechanical treatment thus yields a clearer expression of the connection between the broadening of spectral lines and the latter two effects.

The broadening of hydrogen lines considered above is interesting in the first place because exact analytic expressions can be obtained for the entire line contour, both in the classical and quantum-mechanical treatments of the problem. This means that the two results can be compared. Comparisons of this kind usually encounter considerable computational difficulties. They are usually carried out either within a restricted part of the contour (collisional or static) or by substituting simplified quasiclassical wave functions into the quantum-mechanical expression. The hydrogen atom provides us with an interesting possibility of a direct comparison of quantum-mechanical and classical results for the entire line contour using the exact solutions without the quasiclassical approximations.

APPENDIX (DECEMBER 27, 1976)

Tran Minh *et al.* have recently published two new papers,[21,22] the second of which is devoted to the comparison between the quantum-mechanical results for the Ly-α line ($n=1$ level) and the classical result. The main difference as compared with the present work is that Tran Minh *et al.* considered the problem in a general form and did not, therefore, use the additional symmetry properties of the dipole potential associated with the constant of motion Λ [cf. (2.4)]. The contribution of the different Λ-channels to the broadening is, therefore, not isolated right from the outset by Tran Minh *et al.*[22] This leads to much more complicated expressions for the line contour than those given by (3.6) and (3.9). The separation of the Λ-channels can, in fact, be carried out at the initial stage by considering the wave functions (2.7) and (2.13). The use of the Λ-integral shows that the generalization of the results to other lines involves only an increase in the additive contribution of the Λ-channels [see (3.9)].

Comparison of (3.9) in the special case of the Ly-α ($n=2$) with the results reported by Tran Minh[22] [see their formulas (5.7) and (5.8)] enables us to establish that the two sets of results are completely equivalent once the intermediate summations are completed. This establishes the equivalence of the two treatments of the Ly-α line. We note that the approach used above reveals the possibility of obtaining simple quantum-mechanical solutions for higher-lying lines.

We note in conclusion that the wave functions given by (2.7) and (2.13) are of independent interest for the solution of other physical problems, for example, the quantum-mechanical determination of the cross sections for scattering accompanied by transitions between degenerate sublevels of an atom.

The authors are grateful to V. I. Kogan for valuable discussions.

[1)]We note that this solution was first obtained by Spitzer[11] for the special case of Ly-α. The method was subsequently

employed by Pfennig.[12]

[2)]The more rigorous criterion is $\Delta\omega \gg \gamma$, where γ is the collisional linewidth. For electron broadening, this region is commonly referred to as the single-electron region.[1,2]

[1]I. I. Sobel'man, Vvedenie v teoriyu atomnykh spektrov (Introduction to the Theory of Atomic Spectra), Fizmatgiz, M., 1963 (English transl. publ. by Pergamon Press, Oxford, 1972).
[2]R. G. J. Breene, The Shift and Shape of Spectral Lines, Pergamon Press, Oxford, 1961.
[3]A. Jablonski, Phys. Rev. **68**, 78 (1945).
[4]I. I. Sobel'man, Opt. Spektrosk. **1**, 617 (1956).
[5]M. Baranger, Phys. Rev. **111**, 481 (1958); **112**, 855 (1958).
[6]J. Szudy, Acta Phys. Pol. A **40**, 361 (1971).
[7]N. Tran Minh and H. Van Regemorter, J. Phys. B **5**, 903 (1972).
[8]N. Tran Minh, N. Feautrier, and H. Van Regemorter, J. Phys. B **8**, 1810 (1975).
[9]J. Szudy and W. E. Baylis, J. Quant. Spectrosc. Radiat. Transfer **15**, 641 (1974).
[10]V. S. Lisitsa and G. V. Sholin, Zh. Eksp. Teor. Fiz. **61**, 912 (1971) [Sov. Phys. JETP **34**, 484 (1972)].
[11]L. Spitzer, Phys. Rev. **58**, 348 (1940).
[12]H. Pfennig, J. Quant. Spectrosc. Radiat. Transfer **12**, 821 (1972).
[13]M. J. Seaton, Proc. Phys. Soc. London **77**, 174 (1961).
[14]Yu. N. Demkov, V. N. Ostrovskiĭ, and E. A. Solov'ev, Zh. Eksp. Teor. Fiz. **66**, 125 (1974) [Sov. Phys. JETP **39**, 57 (1974)].
[15]V. N. Ostrovskiĭ and E. A. Solov'ev, Zh. Eksp. Teor. Fiz. **66**, 1590 (1974) [Sov. Phys. JETP **39**, 779 (1974).
[16]A. Hautot, J. Math. Phys. (N.Y.) **14**, 1320 (1973).
[17]L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Nauka, M., 1974 (English transl. publ. by Pergamon Press, Oxford, 1975).
[18]G. N. Watson, Theory of Bessel Functions, Cambridge University Press, 1944 (Russ. Transl., IIL, 1949).
[19]I. S. Gradshteĭn and I. M. Ryzhik (Gradshteyn and Ryshik), Tablitsy integralov, summ, ryadov, i proizvedenii (Table of Integrals, Series, and Products) Nauka, M., 1971 (English trans. of an earlier ed. publ. by Academic Press, New York, 1966).
[20]H. Bateman and A. Erdelyi, Higher Transcendental Functions, McGraw-Hill, New York, 1953 (Russ. Transl., Nauka, 1966, Vol. 1).
[21]N. Feautrier, N. Tran Minh, and H. Van Regemorter, J. Phys. B **9**, 1871 (1976).
[22]N. Tran Minh, N. Feautrier, and H. Van Regemorter, J. Quant. Spectrosc. Radiat. Transfer **16**, 849 (1976).

Translated by S. Chomet

Finite amplitude Langmuir oscillations in the plasma resonance region

S. V. Bulanov, L. M. Kovrizhnykh, and A. S. Sakharov

P. N. Lebedev Physical Institute, USSR Academy of Sciences

(Submitted September 20, 1976)
Zh. Eksp. Teor. Fiz. **72**, 1809–1823 (May 1977)

We consider, in the multi-fluid hydrodynamical approximation, induced Langmuir oscillations of an inhomogeneous plane plasma layer in an external harmonic hf field. We study the limitation of the electric field amplitude near the plasma resonance point as the result of a linear transformation into plasma waves, the self-intersection of electron trajectories, the anharmonicity of the Langmuir oscillations, and the non-stationarity of the plasma for various density profiles. We study numerically the generation of non-linear plasma waves and the acceleration of particles when resonance break down takes place which leads to an effective dissipation of the energy of the oscillations in the resonance region. We analyze qualitatively the role of the ion motion which is the result of striction forces and we indicate conditions under which modulational, parametric, and other instabilities which are connected with ion motion turn out to be unimportant.

PACS numbers: 52.35.Mw

1. The amplification of an hf field near the plasma resonance point is of great interest in connection with the problem of the anomalous absorption of electromagnetic waves in a non-uniform plasma and the generation of accelerated particles.[1,2] The magnitude of the field at the resonance is determined by collisions, the linear transformation into plasma waves, and in strong fields by the electron non-linearity and the change in the plasma density under the influence of striction forces.[3–11]

In the present paper we consider the establishment of the field in the plasma resonance region under conditions where the modulational, parametric, and other instabilities, connected with ion motion in the self-consistent field, turn out to be unimportant (see inequalities (68), (70)).

We consider a plane layer of plasma with ion density n_i which is non-uniform in x. The plasma is in a uniform external electric field which depends on the time as $E = E_0 \sin\omega t$ and is parallel to the inhomogeneity gradient. We choose the origin $x = 0$ at the plasma resonance point, i.e., $\omega = \omega_p(x = 0)$. We denote by s the ratio of the amplitude of the acting field to the maximum

0038-5646/77/4505-0949$02.40