

state $X^1\Sigma_g^+$ into the state $C^3\Pi_u$, then the N_2 -system 2^+ spectrum connected with the transitions of the cold molecules would reveal a characteristic intensity alternation wherein triplets with even K' would be more intense than triplets with odd K' , owing to the influence of the nuclear spin. We, however, did not observe such an alternation. This question deserves a special investigation.

The authors thank L. P. Presnyakov for consultations on questions pertaining to collision theory, as well as P. L. Rubin, V. I. Man'ko, and L. A. Shelepin for a discussion of the results.

- ¹This phenomenon was pointed out in the report,^[6] and while the experimental conditions in that reference are not quite clear, it can be assumed that disequilibrium was observed there not only in the RF discharge in the N_2 -Ar mixture, but also in pure N_2 .
 - ²The radiating state $B^1\Sigma^+$ for the Angstrom band system is populated in the discharge by direct electron impact from the state $CO(X^1\Sigma^+)$.
 - ³The wave function is positive if it remains unchanged upon reflection in a plane passing through the axis joining the nuclei, and negative if its sign is reversed by this reflection.
 - ⁴We note that when one speaks of the symmetry of an electron wave function relative to reflection in a plane passing through an internuclear axis the reference is to symmetry of its coordinate part.^[9]
 - ⁵This was verified by experiment.
- ¹V. N. Ochkin, S. Yu. Savinov, and N. N. Sobolev, Preprint Fiz. Inst. Akad. Nauk No. 150, 1977.
²E. S. Fishburne, J. Chem. Phys. **47**, 58 (1967).
³D. W. Setser and D. H. Stedman, J. Chem. Phys. **53**, 1004 (1970).

- ⁴O. P. Bochkova and N. V. Chernyshova, Opt. Spektrosk. **31**, 677 (1971).
⁵J. Dechamps and A. Ricard, J. Phys. (Paris) **34**, C2, 123 (1973).
⁶G. H. Dieke and D. F. Heath, Johns Hopkins Spectroscopy Report, No. 17, Baltimore, Md., 1959.
⁷J. R. Howarth, J. Phys. B **5**, 402 (1972).
⁸O. V. Ravodina, Candidate's Dissertation, Sov. Phys. Tech. Inst. at Tomsk University, Tomsk, 1974.
⁹I. P. Zapesochnyi and V. V. Skubenich, Opt. Spektrosk. **21**, 140 (1966) [Opt. Spectrosc. (USSR)].
¹⁰V. M. Kaslin and G. G. Petrash, Tr. Fiz. Inst. Akad. Nauk **81**, 88 (1975).
¹¹S. É. Frish, in: Spektroskopiya gazorazryadnoy plazmy (Spectroscopy of Gas-Discharge Plasma), ed. S. É. Frish, Nauka, Leningrad, 1970, p. 7.
¹²G. N. Hays, C. J. Tracy, A. R. Demonchy, and H. J. Oskam, Chem. Phys. Lett. **14**, 352 (1972); G. N. Hays and H. J. Oskam, J. Chem. Phys. **59**, 6088 (1973).
¹³A. S. Sokolov, Candidate's Dissertation, Inst. of Inorganic Chemical Compounds, Akad. Nauk SSSR, Moscow, 1976.
¹⁴D. E. Golden, D. J. Burns, and V. C. Sutcliffe, Jr. Phys. Rev. A **40**, 2123 (1974).
¹⁵D. E. Golden, D. J. Burns, and D. W. Galliardt, J. Chem. Phys. **65**, 2616 (1976).
¹⁶P. Bleeckrode, Physica (Utrecht) **41**, 24 (1969).
¹⁷D. W. Setser and D. H. Stedman, J. Chem. Phys. **53**, 1004 (1970).
¹⁸M. A. El'yashevich, Atomnaya i molekulyarnaya spektroskopiya (Atomic and Molecular Spectroscopy), Fizmatgiz, 1962.
¹⁹L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika. Nerelyativistskaya teoriya (Quantum Mechanics. Nonrelativistic Part), Nauka, Moscow, 1974. [Pergamon, 1976].
²⁰G. Herzberg, Molecular spectra and molecular structure. I. Spectra of diatomic molecules, 2nd ed. D. van Nostrand, N. Y., 1951, p. 207.
²¹A. D. Sakharov, Izv. Akad. Nauk SSSR Ser. Fiz. **12**, 372 (1948).

Translated by J. G. Adashko

Highly excited states of the hydrogen atom in an electric field

G. F. Drukarev

A. A. Zhdanov Leningrad State University
 (Submitted 15 March 1978)
 Zh. Eksp. Teor. Fiz. **75**, 473-483 (August 1978)

We discuss the levels E and their widths Γ of hydrogen atom in the quasiclassical approximation in the presence of a uniform electric field E (all quantities are in atomic units). The effective quantum number $\nu = (-2E)^{-1/2}$ depends on E and on the parabolic quantum numbers n_1 , n_2 , and $|m|$. For $|m| \ll n_{1,2}$ the ratio ν/n (n is the principal quantum number) with accuracy to quantities of order $(m/n)^2$ is a universal function of two parameters: $S = (n_1 - n_2)/n$ and $T = 4n^{-1}E$. The value of ν/n is determined by Eqs. (3.4)-(3.6) and the value of Γ by Eq. (5.8). The values obtained with these relations are close to the results obtained by numerical integration of the Schrödinger equation.

PACS numbers: 32.60.+i, 32.70.Jz

1. INTRODUCTION

The hydrogen atom in the presence of a uniform electric field is described in parabolic coordinates by well known equations.^[1]

We shall designate the energy of the atom by E , \mathcal{E} is

the field strength, ξ and η are parabolic coordinates in the atomic system of units, and we introduce the effective quantum number

$$\nu = (-2E)^{-1/2}, \quad (1.1)$$

the reduced field strength

$$w = \mathcal{E}v^3 \quad (1.2)$$

and the coordinates

$$x = v^{-1}\xi, \quad y = v^{-1}\eta. \quad (1.3)$$

Using these designations, the equations mentioned take the form

$$\frac{d^2\varphi_1}{dx^2} + \frac{1}{4} \left(-1 + \frac{4\alpha_1}{x} - \frac{m^2-1}{x^2} - wx \right) \varphi_1 = 0, \quad (1.4)$$

$$\frac{d^2\varphi_2}{dy^2} + \frac{1}{4} \left(-1 + \frac{4\alpha_2}{y} - \frac{m^2-1}{y^2} + wy \right) \varphi_2 = 0, \quad (1.5)$$

$$\alpha_1 + \alpha_2 = v. \quad (1.6)$$

The boundary conditions are

$$\varphi_1(0) = 0, \quad \varphi_1(\infty) = 0, \quad \varphi_2(0) = 0, \quad \varphi_2(\infty) = 0.$$

The form of the functions

$$V_1 = -\frac{4\alpha_1}{x} + \frac{m^2-1}{x^2} + wx, \quad V_2 = -\frac{4\alpha_2}{y} + \frac{m^2-1}{y^2} - wy$$

at small distances is determined mainly by the Coulomb and centrifugal terms, and at large distances by the term containing the field w . Here $V_2 \rightarrow -\infty$ as $y \rightarrow \infty$, so that a potential barrier is formed along the y coordinate.

The energy spectrum is formally continuous. However, in practice we are dealing with a set of quasistationary states. The spectral density, defined as $|J|^{-2}$, where J is the Jost function (see Sec. 4), consists of a series of more or less sharp peaks in a background of a smooth variation, which correspond to the quasistationary states. In the energy region in which these peaks are sufficiently well separated from each other, the shape of a peak is given by the well known expression $[(E - E')^2 + \Gamma^2/4]^{-1}$ where E' and $\Gamma/2$ are the real and imaginary parts of the complex zero of the Jost function; E' defines the location of the quasistationary state on the energy scale; Γ is the width, which is related to the lifetime τ against ionization (i.e., passage through the barrier) by the expression $\Gamma = \tau^{-1}$ (Γ and τ are in atomic units).

In the quasiclassical approximation without taking into account the finite width of the level (i.e., without taking into account passage through the barrier) the dependence of α_1 and α_2 on w is determined by the quantization conditions^[1]

$$\frac{1}{2} \int_{x'}^{x''} \left(-1 + \frac{4\alpha_1}{x} - \frac{m^2}{x^2} - wx \right)^{1/2} dx = \left(n_1 + \frac{1}{2} \right) \pi, \quad (1.7)$$

$$\frac{1}{2} \int_{y'}^{y''} \left(-1 + \frac{4\alpha_2}{y} - \frac{m^2}{y^2} + wy \right)^{1/2} dy = \left(n_2 + \frac{1}{2} \right) \pi, \quad (1.8)$$

where $n_{1,2}$ are non-negative integers which are assumed to be large. The points x' , x'' , and y' , y'' are the zeros of the integrand functions. Equation (1.6) determines the dependence of v on w , and Eq. (1.2) the dependence of v on \mathcal{E} (of course, in implicit form).

For $\mathcal{E} \neq 0$, v depends on the three quantum numbers n_1 , n_2 , and $|m|$ independently. For $\mathcal{E} = 0$, degeneracy sets in:

$$v_{\mathcal{E}=0} = n_1 + n_2 + |m| + 1 = n.$$

The quantization condition (1.7) is satisfied for all values of w . However, the condition (1.8) is satisfied only for those w which do not exceed some critical value w_0 . In the case when $w > w_0$ there is no real upper limit y'' in (1.8), in which case the integrand vanishes. The physical meaning of w_0 is that the energy level reaches the peak of the potential barrier along the y axis.

In the absence of a field we have the equality

$$\int_{x'}^{x''} \left(-1 + \frac{4\alpha_1}{x} - \frac{m^2}{x^2} \right)^{1/2} dx = \int_0^{\pi} \left(-1 + \frac{4\alpha_1}{x} \right)^{1/2} dx + |m|\pi, \quad (1.9)$$

here x' , x'' , and x_1 are the zeros of the corresponding integrands.

In the presence of a field the exact equality of the form (1.9) does not exist. However, in the case when $|m|/\alpha_{1,2} \ll 1$ it is possible with accuracy to small corrections of order $(\alpha_{1,2}w)(m/\alpha_{1,2})^2$ to represent (1.7) and (1.8) in the form

$$\frac{1}{2} \int_{x'}^{x''} \left(-1 + \frac{4\alpha_1}{x} - wx \right)^{1/2} dx = \left(n_1 + \frac{|m|+1}{2} \right) \pi, \quad (1.10)$$

$$\frac{1}{2} \int_0^{y''} \left(-1 + \frac{4\alpha_2}{y} + wy \right)^{1/2} dy = \left(n_2 + \frac{|m|+1}{2} \right) \pi. \quad (1.11)$$

Analysis of Eqs. (1.10) and (1.11) (see Sec. 2) shows that in this approximation the ratio v/n depends only on the two parameters

$$S = (n_1 - n_2)/n, \quad T = 4n^4 \mathcal{E}, \quad (1.12)$$

i.e.,

$$v/n = f(S, T), \quad (1.13)$$

where f is a universal function. Quantities of order $(m/n)^2$ have not been taken into account, which does not introduce a substantial error if $|m| \ll n$.

We note that the same relation (1.13) is observed also in the well known formulas of perturbation theory if we apply them to the case of large quantum numbers n and neglect terms of order $(m/n)^2$.

The phase integrals which enter into Eqs. (1.10) and (1.11) were discussed in 1930 by Lanczos^[2] who expressed them in terms of elliptic integrals. His example was followed in 1961 by Rice and Good.^[3] However, expression of the phase integrals in terms of elliptic integrals introduces completely unnecessary complications into the calculation and unnecessarily makes the formulas extremely cumbersome. As a result the analytic investigation of the phase integrals in the studies cited remained to a certain degree incomplete. In particular, the authors of Refs. 2 and 3 did not note the existence of the universal dependence (1.13) for $|m| \ll n$. In addition, a number of errors exist in these studies.

In the present work the phase integrals are expressed in terms of the hypergeometric function $F(-1/2, 1/2, 2, z)$. Although it is possible with recurrence relations to

reduce this function to a combination of elliptic integrals, it is much more convenient to deal directly with $F(-1/2, 1/2, 2, z)$.

On the basis of a study of the relations (1.10) and (1.11), we establish in Sec. 3 a system of equations for determination of the function f (1.13). In Sec. 4 we take into account the finite width of the level. An expression is established for the Jost function, and its complex zeros with a small imaginary part are discussed. In Sec. 5 we calculate the level width and present approximate analytic expressions for weak and strong fields. In Sec. 6 we give a comparison with the calculations of other authors.

2. TRANSFORMATION AND STUDY OF THE PHASE INTEGRALS

We shall consider first the integral

$$L_1 = \frac{1}{2} \int_0^{z_1} \left(-1 + \frac{4\alpha_1}{x} - wx \right)^{1/2} dx. \quad (2.1)$$

By means of the well known integral representation of the hypergeometric function

$$F(\alpha, \beta, \gamma, x) = \frac{\Gamma(\gamma)}{\Gamma(\beta)\Gamma(\gamma-\beta)} \int_0^1 t^{\beta-1} (1-t)^{\gamma-\beta-1} (1-xt)^{-\alpha} dt$$

the integral L_1 is reduced to the form

$$L_1 = \pi \alpha_1 (1-z_1)^{1/2} F(-1/2, 1/2, 2, -z_1), \quad (2.2)$$

where

$$z_1 = \frac{(1+16\alpha_1 w)^{1/2} - 1}{(1+16\alpha_1 w)^{1/2} + 1}. \quad (2.3)$$

Taking into account (1.10), we obtain

$$\alpha_1 = \frac{n_1 + 1/2 (|m|+1)}{(1-z_1)^{1/2} F(-1/2, 1/2, 2, -z_1)}. \quad (2.4)$$

It is evident from this that

$$\alpha_1 \geq n_1 + 1/2 (|m|+1).$$

We then carry out the following transformation: We express $\alpha_1 w$ in terms of z_1 by means of Eq. (2.3):

$$\alpha_1 w = z_1 / 4(1-z_1)^2$$

and substitute into this Eq. (2.4) for α_1 . We obtain

$$[n_1 + 1/2 (|m|+1)] w = \frac{z_1}{4(1-z_1)^{3/2}} F(-1/2, 1/2, 2, -z_1). \quad (2.5)$$

Relations (2.4) and (2.5) express the dependence of α_1 on w in parametric form.

Let us turn now to the integral

$$L_2 = \frac{1}{2} \int_0^{z_2} \left(-1 + \frac{4\alpha_2}{y} + wy \right)^{1/2} dy. \quad (2.6)$$

like Eq. (2.1), it can be reduced to the form

$$L_2 = \pi \alpha_2 (1+z_2)^{1/2} F(-1/2, 1/2, 2, z_2), \quad (2.7)$$

where

$$z_2 = \frac{1 - (1-16\alpha_2 w)^{1/2}}{1 + (1-16\alpha_2 w)^{1/2}}. \quad (2.8)$$

Taking into account (2.7), we have

$$\alpha_2 = \frac{n_2 + 1/2 (|m|+1)}{(1+z_2)^{1/2} F(-1/2, 1/2, 2, z_2)}. \quad (2.9)$$

From this it follows that

$$\alpha_2 \leq n_2 + 1/2 (|m|+1).$$

The least value of α_2 is achieved for $z_2 = 1$ and is equal to

$$\alpha_{2 \min} = \frac{n_2 + 1/2 (|m|+1)}{2^{1/2} F(-1/2, 1/2, 2, 1)} = \frac{3\pi}{2^{1/2} \cdot 8} [n_2 + 1/2 (|m|+1)].$$

As can be seen, α_2 does not change greatly over the entire attainable interval of variation of z_2 .

Expressing $\alpha_2 w$ by means of (2.8) in terms of z_2 and combining it with (2.9), we obtain, similarly to (2.5),

$$\left[n_2 + \frac{1}{2} (|m|+1) \right] w = \frac{z_2 F(-1/2, 1/2, 2, z_2)}{4(1+z_2)^{3/2}}. \quad (2.10)$$

Relations (2.9) and (2.10) express the dependence of α_2 on w in parametric form.

It follows from Eq. (2.10) that the maximum value of w (for a given n_2) is reached at $z_2 = 1$ and is equal to

$$w_0 = \left[3\pi \cdot 2^{1/2} \left(n_2 + \frac{|m|+1}{2} \right) \right]^{-1}, \quad (2.11)$$

and from Eqs. (2.10) and (2.11) we obtain

$$\frac{w}{w_0} = \frac{3\pi \cdot 2^{1/2}}{4} \frac{z_2}{(1+z_2)^{3/2}} F(-1/2, 1/2, 2, z_2). \quad (2.12)$$

3. EQUATIONS FOR DETERMINATION OF THE EFFECTIVE QUANTUM NUMBER

Substituting into Eq. (1.6) expressions (2.4) and (2.9) for α_1 and α_2 and using the designation (1.12), we have

$$\frac{v}{n} = \frac{1+S}{2(1-z_1)^{1/2} F(-1/2, 1/2, 2, -z_1)} + \frac{1-S}{2(1+z_2)^{1/2} F(-1/2, 1/2, 2, z_2)} \quad (3.1)$$

Then, adding (2.5) and (2.10), taking into account (1.2), and using the designation (1.12), we obtain

$$\left(\frac{v}{n} \right)^3 T = \frac{z_1 F(-1/2, 1/2, 2, -z_1)}{(1-z_1)^{3/2}} + \frac{z_2 F(-1/2, 1/2, 2, z_2)}{(1+z_2)^{3/2}}. \quad (3.2)$$

Finally, subtracting (2.10) from (2.5), we have

$$\left(\frac{v}{n} \right)^3 TS = \frac{z_1 F(-1/2, 1/2, 2, -z_1)}{(1-z_1)^{3/2}} - \frac{z_2 F(-1/2, 1/2, 2, z_2)}{(1+z_2)^{3/2}}. \quad (3.3)$$

Equations (3.1)–(3.3) are inconvenient, since they involve combinations of all the quantities S , T , and v .

However, by means of simple transformations it is possible to break up these combinations and reduce Eqs. (3.1)–(3.3) to the form

$$\frac{v}{n} = \frac{z_1(1-z_1)^{-1/2} + z_2(1+z_2)^{-1/2}}{z_1(1-z_1)^{-1/2} F(-1/2, 1/2, 2, -z_1) + z_2(1+z_2)^{-1/2} F(-1/2, 1/2, 2, z_2)} \quad (3.4)$$

$$S = \frac{z_1(1-z_1)^{-1/2} F(-1/2, 1/2, 2, -z_1) - z_2(1+z_2)^{-1/2} F(-1/2, 1/2, 2, z_2)}{z_1(1-z_1)^{-1/2} F(-1/2, 1/2, 2, -z_1) + z_2(1+z_2)^{-1/2} F(-1/2, 1/2, 2, z_2)} \quad (3.5)$$

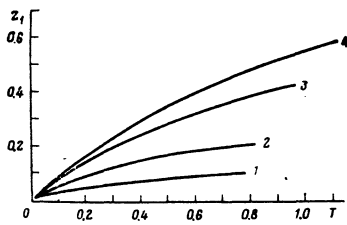


FIG. 1. Dependence of z_1 on T for $S = -0.5$ (1), 0 (2), 0.5 (3), and 0.5 (4).

$$T = \frac{[z_1(1-z_1)^{-1/2}F(-1/2, 1/2, 2, -z_1) + z_2(1+z_2)^{-1/2}F(-1/2, 1/2, 2, z_2)]^4}{[z_1(1-z_1)^{-2} + z_2(1+z_2)^{-2}]^2} \quad (3.6)$$

The relations (3.5) and (3.6) are the key system of equations to which the entire problem reduces. Finding the parameters z_1 and z_2 by means of Eqs. (3.5) and (3.6) for given S and T and substituting them into (3.4), we obtain the desired quantity ν/n .

Solution of (3.5) and (3.6) is possible only in numerical form. In Figs. 1 and 2 we have shown the dependence of z_1 and z_2 on T for several values of S .

4. THE JOST FUNCTION

For calculation of quasistationary states with inclusion of the width, the quasiclassical approximation in its simplest form is inadequate. It is necessary to use a more refined approach.

We shall use the method developed by N. Fröman and P. Fröman.^[4] According to this method, an approximate solution of (1.5) $\varphi(y)$ is represented in the form of a superposition of two linearly independent quasiclassical functions:

$$\varphi(y) = a_1(y)Q^{-1/2} \exp\left(i \int Q dy\right) + a_2(y)Q^{-1/2} \exp\left(-i \int Q dy\right). \quad (4.1)$$

The quantity Q in the simplest approximation is equal to

$$Q = 1/2(-1 + 4\alpha_2/y - m^2/y^2 + wy)^{1/2}. \quad (4.2)$$

(The Frömans developed a technique for calculation of higher-order corrections to (4.2), but we will not take these corrections into account here). In the Fröman method a major role is played by the matrix F which relates the values of $a_{1,2}$ with each other at two points:

$$a_i(y) = \sum_k F_{ik}(y, y') a_k(y'). \quad (4.3)$$

The properties of the matrix F and the technical details of its application have been set forth in detail in the Frömans' book.^[4] We present here only the results necessary to us on application of this method to the problem of interest here.

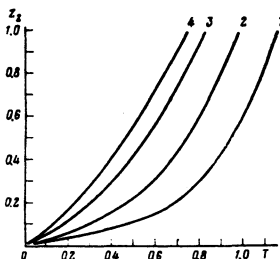


FIG. 2. Dependence of z_2 on T for $S = -0.5$ (1), 0 (2), 0.5 (3), and 0.75 (4).

The asymptotic behavior of φ as $y \rightarrow \infty$ we represent in the form

$$\varphi \sim (2iQ)^{-1/2} [J^* \exp(i \int Q dy) - J \exp(-i \int Q dy)]. \quad (4.4)$$

The coefficient J is a Jost function. We can construct for it an expression in terms of the elements of the matrix F :

$$J = N \{ |F_{12}(0, \infty)| e^{-i\phi} - |F_{22}(0, \infty)| e^{i\phi} \}. \quad (4.5)$$

where N is a normalization factor whose explicit form is not needed here;

$$\Phi = \int_{y''}^{y'''} Q dy + \delta, \quad (4.6)$$

$$\delta = 1/2(\arg F_{22} - \arg F_{12}). \quad (4.7)$$

The location of the quasistationary states E_n on the energy scale is determined by the condition

$$\Phi(E_n) = (n_2 + 1/2)\pi, \quad (4.8)$$

which represents a direct generalization of the condition (1.8) and differs from (1.8) in the presence of the additional term δ in the left-hand side.

For the quantities $|F_{12}|$ and $|F_{22}|$ in Ref. 4 we have obtained the approximate expressions

$$|F_{12}| \approx (1 + e^{-2K})^{1/2}, \quad |F_{22}| \approx 1, \quad (4.9)$$

where

$$K = \int_{y''}^{y'''} Q dy \quad (4.10)$$

(y''' is the turning point to the right of the barrier, and y'' is the turning point to the left of the barrier). The expressions (4.9) are exact for a parabolic barrier. In our problem the barrier near the top is very close to a parabolic shape. Therefore the expressions (4.9) are a good approximation for small K . On the other hand, for large K expressions (4.9) go over to well known formulas obtained in the elementary quasiclassical approximation. Therefore Eq. (4.9) can be considered a good approximation for all K .

The approximate expression for δ at small K has the form

$$\delta = \delta_0 + \left[\frac{1}{2\pi} K \left(1 - \ln \frac{K}{\pi} \right) + \frac{1}{2} \arg \Gamma \left(1 + i \frac{K}{\pi} \right) \right]. \quad (4.11)$$

The expression contained in the brackets in the right-hand side of (4.11) is exact for a parabolic barrier and is given in Ref. 5. Similar expressions have been considered also in a number of other studies (for example, Ref. 3). The value of δ_0 depends on the shape of the barrier at large distances from the top and in the general case cannot be represented in analytic form. For an approximate evaluation of δ_0 we shall proceed as follows.

We shall assume expression (4.11) valid for large K and require that as $K \rightarrow \infty$ the value of δ goes to zero (since on removal of the turning point y''' to infinity it should enter into the quantization condition (4.8)). Using

the known asymptotic expression for $\arg\Gamma(x)$ at large x , we find that $\delta_0 = \pi/8$. Finally we have

$$\delta = \frac{1}{2} \left[\frac{\pi}{4} + \arg \Gamma \left(\frac{1}{2} + i \frac{K}{\pi} \right) + \frac{K}{\pi} \left(1 - \ln \frac{K}{\pi} \right) \right]. \quad (4.12)$$

In any case—for small or large K —the contribution of δ to the quantization condition (4.8) is small, especially for large quantum numbers. Therefore in the first approximation we shall neglect the quantity δ and determine the position of the level from the condition (1.8). When necessary it is possible to take into account the correction introduced by δ . The condition (4.8), as shown by the Frömans, can be generalized in such a way that it will determine also the quasistationary states above the barrier.

In the case in which a quasistationary state has a sufficiently small width, it is possible to obtain an expression for Γ from (4.5), expanding Φ in series in powers $E - E_n$ and assuming all remaining quantities constant. We set

$$\Phi = \left(n_2 + \frac{1}{2} \right) \pi + \left(\frac{d\Phi}{dE} \right)_{E_n} (E - E_n) + \dots \quad (4.13)$$

Then to first order in the difference $E - E_n$ we have

$$J = J_0(E - E_n + i\Gamma/2), \quad (4.14)$$

where

$$\Gamma = \frac{2}{(d\Phi/dE)_{E_n}} \frac{|F_{12}| - |F_{22}|}{|F_{12}| + |F_{22}|}. \quad (4.15)$$

We note that in a quasiclassical situation the quantity $(d\Phi/dE_n)^{-1}$ has the meaning of the average distance between levels. Therefore expression (4.15) can be used only for the condition $\Gamma d\Phi/dE_n \ll 1$, i.e., for

$$|F_{12}| - |F_{22}| \ll 1/2 (|F_{12}| + |F_{22}|),$$

which in view of (4.9) reduces to the condition $2K \geq 1$. Here it is possible with sufficient accuracy to replace (4.15) by the simpler expression

$$\Gamma = \frac{1}{2(d\Phi/dE)_{E_n}} e^{-2K}. \quad (4.16)$$

In calculation of the quantity $d\Phi/dE$ which enters into (4.16), the term $d\delta/dE$ is particularly important for small K and must be taken into account. The point is that the quantity

$$\frac{d}{dE} \int_{y'}^{y''} Q dy, \quad (4.17)$$

which enters into $d\Phi/dE$, is proportional to the classical period of oscillations between the points y' and y'' . This period approaches $+\infty$ when the energy level approaches the top of the barrier. On the other hand, the quantity $d\delta/dE$ approaches $-\infty$ in such a way that a finite value is obtained in the sum.

5. LEVEL WIDTH

Let us consider the quantities which determine the numerical value of Γ . We begin with the quantity K .

Neglecting the centrifugal energy in the barrier region, we have

$$K = \frac{1}{2} \int_{y_1}^{y_2} \left(1 - \frac{4\alpha_2}{y} - wy \right)^{1/2} dy. \quad (5.1)$$

By means of transformations similar to those used in Sec. 2, we obtain the expression

$$K = \frac{1}{2w} g(z_2), \quad (5.2)$$

where

$$g(z_2) = \frac{\pi}{8} \frac{(1-z_2)^2}{(1+z_2)^{3/2}} F(1/2, 3/2, 3, 1-z_2). \quad (5.3)$$

The parameter z_2 can be expressed either in terms of S and T by means of Eqs. (3.5) and (3.6), or in terms of the ratio w/w_0 by means of (2.12). We shall now proceed with calculation of the quantity (4.17).

We shall use the approximation (1.11), in which the problem reduces to calculation of the quantity dL_2/dE . We represent it in the form

$$\frac{dL_2}{dE} = v^3 \frac{dL_2}{dv}.$$

According to (2.5) for fixed α_1 we have $dL_2/dv = dL_2/d\alpha_2$. From expressions (2.7) and (2.8) it follows that L_2 , before the quantization condition is imposed, is a function of two independent variables: w and α_2 . For the purposes of the present calculation we need the derivative for $w = \text{const}$. A calculation gives

$$\frac{dL_2}{dE} = \pi v^3 \frac{(1+z_2)^{3/2}}{1-z_2} \left\{ \left(1 - \frac{z_2}{2} \right) F(-1/2, 1/2, 2, z_2) - z_2(1+z_2) F(1/2, 3/2, 3, z_2) \right\}. \quad (5.4)$$

Finally, let us consider the quantity $d\delta/dE$. Using expression (4.11), we represent it in the form

$$\frac{d\delta}{dE} = \frac{v^3}{2\pi} \left\{ \text{Re} \psi \left(\frac{1}{2} + i \frac{K}{\pi} \right) - \ln \frac{K}{\pi} \right\} \left(\frac{dK}{dz_2} \right) \left(\frac{dz_2}{d\alpha_2} \right)_{w = \text{const}},$$

where ψ is the logarithmic derivative of the Γ function. Calculating

$$\left(\frac{dK}{dz_2} \right) \left(\frac{dz_2}{d\alpha_2} \right)_{w = \text{const}},$$

we obtain

$$\frac{d\delta}{dE} = \frac{v^3}{16} (1+z_2)^{3/2} \left\{ \ln \frac{K}{\pi} - \text{Re} \psi \left(\frac{1}{2} + i \frac{K}{\pi} \right) \right\} \times \left\{ \frac{7+z_2}{1+z_2} F(1/2, 3/2, 3, 1-z_2) + \frac{1-z_2}{2} F(3/2, 5/2, 4, 1-z_2) \right\}. \quad (5.5)$$

From (5.4) and (5.5) we find

$$2 \left(\frac{dL_2}{dE} + \frac{d\delta}{dE} \right) = v^3 h(z_2). \quad (5.6)$$

where

$$h(z_2) = 2\pi \frac{(1+z_2)^{3/2}}{1-z_2} \left\{ \left(1 - \frac{z_2}{2} \right) F(-1/2, 1/2, 2, z_2) - z_2(1+z_2) F(1/2, 3/2, 3, z_2) \right\} + \frac{(1+z_2)^{3/2}}{8} \left\{ \ln \frac{K}{\pi} - \text{Re} \psi \left(\frac{1}{2} + i \frac{K}{\pi} \right) \right\} \left\{ \frac{7+z_2}{1+z_2} F(1/2, 3/2, 3, 1-z_2) + \frac{1-z_2}{2} F(3/2, 5/2, 4, 1-z_2) \right\}. \quad (5.7)$$

Substituting (5.2) and (5.6) into (4.16), we obtain

$$\Gamma = \frac{1}{v^3 h(z_2)} \exp\left(-\frac{g(z_2)}{w}\right). \quad (5.8)$$

Let us consider the functions g and h in the limiting cases $z_2 \ll 1$ and $1 - z_2 \ll 1$.

1) $z_2 \ll 1$. In estimation of g it is necessary to take into account that the hypergeometric function $F(1/2, 3/2, 3, 1 - z_2)$ belongs to the form $F(\alpha, \beta, \alpha + \beta + n, x)$, where $n = 0, 1, 2, \dots$. For functions of this type the expansion of F as $x \rightarrow 1$ contains in addition to powers of $1 - x$ also $\ln(1 - x)$ (see for example Ref. 6). Using this expansion, we have

$$F(1/2, 3/2, 3, 1 - z_2) = \frac{16}{3\pi} - \frac{4}{\pi} \left(4 \ln 2 - \frac{11}{3} - \ln z_2 \right) z_2 + \dots$$

For g we obtain

$$g = \frac{2}{3} - \left(\frac{1}{2} + \ln 4 \right) z_2 + \frac{1}{2} z_2 \ln z_2 + \dots$$

Substituting the approximate expression for z_2 , which follows from (2.12) for $z_2 \ll 1$:

$$z_2 \approx \frac{4}{3\pi 2^n} \frac{w}{w_0},$$

and taking into account expression (2.11) for w_0 , we find

$$g \approx \frac{2}{3} - w \{ 2n_2 + |m| + 1 \} \left\{ 1 - \ln \left[\frac{w}{4} \left(n_2 + \frac{|m| + 1}{2} \right) \right] \right\}. \quad (5.9)$$

In regard to $h(z_2)$, we have for $z_2 \rightarrow 0$

$$h(0) = 2\pi. \quad (5.10)$$

In this approximation we obtain for Γ

$$\Gamma = \frac{1}{\pi v^3} \left(\frac{4}{\mathcal{E} v^3} \right)^{2n_2 + |m| + 1} \exp \left\{ -\frac{2}{3\mathcal{E} v^3} + [2n_2 + |m| + 1] \times \left[1 - \ln \left(n_2 + \frac{|m| + 1}{2} \right) \right] \right\}. \quad (5.11)$$

2) $1 - z_2 \ll 1$. In this case

$$g \approx \frac{\pi}{2^{3/2} \cdot 16} (1 - z_2)^2. \quad (5.12)$$

Considering $h(z_2)$ as $z_2 \rightarrow 1$, we can observe two terms proportional to $\ln(1 - z_2)$ and going to infinity at $z_2 = 1$. One of them originates from $\ln(K/\pi)$ on substitution of expressions (5.2) and (5.3). The other originates from the logarithmic terms in the expansion of the hypergeometric functions $F(-1/2, 1/2, 2, z_2)$ and $F(1/2, 3/2, 3, z_2)$ in the quantity $1 - z_2$ (see Ref. 6). These two terms mutually cancel, and a finite expression remains. The limiting value for $z_2 = 1$ is

$$h(1) = 2^{3/2} [6 - \ln(2^{3/2} \cdot 32 w_0) - \psi(1/2)]. \quad (5.13)$$

TABLE I.

	ν		$\Gamma \cdot 10^6$	
	From Ref. 7	Present calculation	From Ref. 7	Present calculation
$n=5, \mathcal{E}=1.8 \cdot 10^{-4}$	4.9240	4.929	2.282	2.55
$n=11, \mathcal{E}=10^{-5}$	10.6882	10.722	2.815	3.3
$n=15, \mathcal{E}=3 \cdot 10^{-6}$	14.5771	14.619	1.338	1.74

6. COMPARISON WITH RESULTS OF OTHER CALCULATIONS

An exact numerical calculation of the energy levels was carried out by Damburg and Kolosov.^[7]

We have compared values of ν obtained by means of relations (3.4)–(3.6) and values of Γ determined from Eq. (5.8) with the corresponding values calculated by the method of Ref. 7, for three states with $n_1 = n_2$, $m = 0$, and $n = 5, 11$, and 15. The results are given in the table.

For weak fields Damburg and Kolosov^[8] found by means of an asymptotic method an analytic expression for Γ . If the factorials of the quantum numbers in the formula for Γ from Ref. 8 are expressed approximately by means of Stirling's formula, we obtain an expression which coincides with our formula (5.11) with accuracy to small corrections.

In conclusion the author extends his thanks to N. Fröman and P. Fröman for discussion of the questions taken up in Sec. 4 and for valuable observations, to I. Yu. Yurova for carrying out the numerical solution of Eqs. (3.5) and (3.6), and to V. V. Kolosov for carrying out numerical calculations by the method of Ref. 7, the results of which are given in the Table.

¹L. D. Landau and E. M. Lifshits, *Kvantovaya mekhanika* (Quantum Mechanics), Third Edition, Moscow, 1974, Chapter 10, Sec. 77.

²C. Lanczos, *Z. Phys.* **62**, 518 (1930).

³M. H. Rice and R. H. Good, *JOSA* **52**, 239 (1962).

⁴N. Fröman and P. Fröman, *The JWKB Approximation*, North-Holland, 1965. Russ. transl., Mir, 1967.

⁵N. Fröman, P. O. Fröman, U. Myhrman, and R. Paulsson, *Ann. Phys. (N. Y.)* **74**, 314 (1972).

⁶N. N. Lebedev, *Spetsial'nye funktsii i ikh primeneniya* (Special Functions and Their Applications), Fizmatgiz, 1963, Chapter 10, Sections 9 and 7.

⁷R. Damburg and V. Kolosov, *J. Phys.* B9, 3149 (1976).

⁸R. Ya. Damburg and V. V. Kolosov, *Asimptoticheskiĭ podkhod k zadache Shtarka dlya atoma vodoroda* (Asymptotic Approach to the Stark Problem for the Hydrogen Atom), Riga, Zinatne, 1977.

Translated by Clark S. Robinson