Generalization of the Gamow formula to the multidimensional case

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A generalization of the Gamow formula for the width Γ of a quasistationary level (with energy $E = E_r - i\Gamma/2$) is given for the case of multidimensional systems with separable variables. The condition for applicability of this approximation is obtained, and some examples are considered.

1. In atomic and nuclear physics, quantum scattering theory, etc., one often needs to calculate the positions and widths of quasistationary states (resonances). Because of the exponential growth of the Gamow wave function at infinity, numerical solution of the Schrödinger equation for such problems encounters certain difficulties.[3)]

We shall consider this problem in the quasiclassical approximation. If the potential $U(r)$ is smooth and the width of the level is exponentially small, then in the one-dimensional case the width can be calculated using the well known formula of Gamow[6,7]

$$\Gamma = \frac{\hbar}{T}\exp\left\{-\frac{2}{\hbar}\int_{r_1}^{r_2}(-p^2)^{1/2}\,dr\right\}, \tag{1}$$

$$T=2m\int_{r_0}^{r_1}\frac{dr}{p(r)}, \qquad p=\{2m[E-U(r)]\}^{1/2}, \tag{1a}$$

where T is the period of radial oscillations of the particle inside the potential well ($r_0 < r < r_1$) and r_i are the turning points (see Fig. 1 in Ref. 8); below, we set $\hbar = m = 1$. In a D-dimensional problem with spherical symmetry the effective potential which includes the centrifugal energy is $U(r) = V(r) + [l + \frac{1}{2}(D-2)]^2/(2r^2)$.

There arises the problem of generalizing Eq. (1) to the multidimensional case. We shall consider the particular but important case in which the variables in the Schrödinger equation can be separated in a certain system of coordinates $q_1, q_2, \ldots, q_f$ (f is the number of degrees of freedom). The results of the present paper have been reported briefly in Ref. 9.

2. Using the modification of the Bohr–Sommerfeld quantization rules to take into account the finite penetrability of the barrier,[8,10] it can be shown that

$$\Gamma=cT_f^{-1}\exp(-2\pi a_f), \tag{2}$$

where

$$c=\left[\alpha\bar{v}_f\sum_{i=1}^{f}\frac{1}{\bar{v}_i}\right]^{-1}, \qquad T_f=2\int_{q_f^{(0)}}^{q_f^{(1)}}\frac{dq_f}{p_f}, \tag{2a}$$

$$a_i=\frac{1}{\pi}\,\mathrm{Im}\,S_i=\frac{1}{\pi}\int_{q_i^{(1)}}^{q_i^{(2)}}(-p_i^2)^{1/2}\,dq_i. \tag{3}$$

In Eq. (2) we have taken into account the fact that in a multidimensional potential the tunneling actually occurs along one of the coordinates, taken here as q_f, provided that

$$\exp(-2\pi a_f)\gg\exp(-2\pi a_i), \quad 1\leqslant i\leqslant f-1.$$

In the quasiclassical case this condition is always satisfied, with the possible exception of systems with special symmetry properties. The remaining notation is as follows: $q_i^{(0,1,2)}$ are the turning points, where $q_i^{(0)} < q_i < q_i^{(1)}$ is the classically admissible region of motion in the coordinate q_i, and $q_i^{(1)} < q_i < q_i^{(2)}$ is the sub-barrier region (where $p_i^2 < 0$); $\bar{v}_i$ is the mean value of $v_i(q)$ with respect to the quasiclassical wave function:

$$\bar{v}_i=\int v_i(q)\,\psi^2(q)\,dq\approx\int_{q_i^{(0)}}^{q_i^{(1)}}\frac{v_i(q)}{p_i(q)}\,dq\Big/\int_{q_i^{(0)}}^{q_i^{(1)}}\frac{dq}{p_i(q)}. \tag{4}$$

In the derivation of these expressions it is assumed that

$$S=\sum_{i=1}^{f}S_i=\sum_{i=1}^{f}\int p_i\,dq_i,$$
$$p_i=\{2[\alpha E-u_i(q_i)-\beta_i v_i(q_i)]\}^{1/2}, \tag{5}$$

where S is the action, β_i are the separation constants, satisfying the condition $\Sigma_{i=1}^{f}\beta_i = \mathrm{const}$, α is a constant that depends on the problem under consideration and whose value is determined in the process of separating the variables,[4)] and $u_i(q_i) + \beta_i v_i(q_i)$ is the potential for the coordinate q_i.

The explicit form of the functions u_i and v_i depends on the problem under consideration. For example, in the case of the Stark effect in the hydrogen atom the variables can be separated in the parabolic coordinates[11] $\xi = r + z$, $\eta = r - z$, and

$$\alpha=1/4, \quad \beta_1+\beta_2=1,$$
$$u_i(q)=1/8[m^2/q^2+(-1)^{i-1}\mathscr{E}q], \quad v_i(q)=-1/2q, \tag{6}$$

where $q = \xi, \eta$ for $i = 1, 2$; m is the magnetic quantum number, and $\mathscr{E}$ is the strength of the electric field ($\hbar = e = m_e = 1$).

Another example is the problem of two Coulomb centers, where

$$\alpha=1/4R^2, \quad \beta_1+\beta_2=0,$$
$$u_1=\frac{m^2-1}{2(\xi^2-1)^2}-\frac{(Z_1+Z_2)R\xi}{2(\xi^2-1)}, \qquad v_1=\frac{1}{2(\xi^2-1)},$$
$$u_2=\frac{m^2-1}{2(1-\eta^2)^2}+\frac{(Z_1-Z_2)R\eta}{2(1-\eta^2)}, \qquad v_2=\frac{1}{2(1-\eta^2)}, \tag{7}$$

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in which $\xi = (r_1 + r_2)/R$ and $\eta = (r_1 - r_2)/R$ are prolate spheroidal coordinates, R is the distance between the nuclei, and $Z_{1,2}$ are their charges.

3. Comparing Eqs. (1) and (2), it can be seen that the multidimensional problem differs from the one-dimensional one by the factor c in front of the exponential, which effectively takes into account the influence of the motion in the coordinates q_i $(i \neq f)$ on the frequency of the collisions of the particle in the classically allowed region with the barrier wall at $q_f = q_f^{(1)}$.

In the one-dimensional case we have $c = \alpha^{-1} = 1$, and Eq. (2) takes the form of the conventional Gamow formula (1).

In order to illustrate (2) in a nontrivial example, let us consider the Stark effect in the hydrogen atom. Performing a scale transformation[5)]

$$\xi = n^2 x, \quad \eta = n^2 y, \quad \mu = m/n, \quad F = n^4 \mathscr{E},$$
$$\varepsilon = 2n^2 E^{(n_1 n_2 m)}, \quad \mathrm{Im}\,\varepsilon = -n^2 \Gamma^{(n_1 n_2 m)} \tag{8}$$

we obtain

$$p_\xi = \frac{1}{2n} k_1(x), \qquad p_\eta = \frac{1}{2n} k_2(y),$$
$$k_i(q) = (\varepsilon + 4\beta_i/q - \mu^2/q^2 + (-1)^i F q)^{1/2}. \tag{9}$$

Substituting these expressions into (2), we easily find

$$c = \frac{4\sigma_1\tau_2}{\sigma_1\tau_2 + \sigma_2\tau_1}, \qquad T_\eta = 2\int_{\eta_0}^{\eta_1} \frac{d\eta}{p_\eta} = 4n^3\tau_2, \tag{10}$$

$$a_\eta = \frac{n(-\varepsilon)^{3/2}}{3\pi F} J(F), \tag{11}$$

$$\Gamma^{(n_1 n_2 m)} = \frac{\sigma_1}{n^3(\sigma_1\tau_2 + \sigma_2\tau_1)} \exp(-2\pi a_\eta), \tag{12}$$

where

$$\sigma_i = \int_{q_0}^{q_1} \frac{dq}{q k_i(q)}, \qquad \tau_i = \int_{q_0}^{q_1} \frac{dq}{k_i(q)},$$
$$J(F) = \frac{3}{2} \int_{u_1}^{u_2} \frac{du}{u} (A - Bu + u^2 - u^3)^{1/2}, \tag{13}$$

with

$$A = \mu^2 F^2/(-\varepsilon)^3, \; B = 4\beta_2 F/\varepsilon^2, \; y = -\varepsilon u/F.$$

When $F = 0$, we have $A = B = 0$ and $J(0) = 1$. Expansions in the region of the weak field are given in Appendix 1.

For the states with $m = 0$ the integrals in (13) can be calculated analytically (see Appendix 1):

$$\sigma_i = \pi(-\varepsilon)^{-1/2} F(1/4, 3/4; 1; z_i),$$
$$\tau_i = 2\pi\beta_i(-\varepsilon)^{-3/2} F(3/4, 5/4; 2; z_i),$$
$$a_\eta = \frac{n(-\varepsilon)^{3/2}}{2^{1/2} F}(1 - z_2) F(1/4, 3/4; 2; 1 - z_2), \tag{14}$$

where $z_i = (-1)^i 16\beta_i F \varepsilon^{-2}$ for $i = 1$ and 2.

Another case in which the quasiclassical width (12) can be calculated explicitly corresponds to the states $(0, 0, n-1)$, which in the limit $n \to \infty$ correspond to circular electron orbits orthogonal to the direction of the electric field $\mathscr{E}$. Referring the reader to Appendix 2 for details of the calculations, we present only the final expressions:

$$\Gamma_n = A_n c T_\eta^{-1} D, \tag{15}$$
$$A_n = 2^{1/2}\pi(n/e)^{n+1/2}/n!,$$
$$c = 2(1+\tau), \; T = 2\pi/\omega_\eta, \tag{16}$$

where

$$D = (2nez)^{1/2}\left(\frac{2z}{1+z}\right)^2 \exp\left\{-\frac{2n[-\varepsilon^{(0)}]^{3/2}}{3F} J(F) + \Delta(F)\right\}, \tag{17}$$

with

$$J(F) = 3^{-1/2}(1 - 2/3 z^2)^{-3/2}[z - 2/3 z^3 - (1 - z^2)\,\mathrm{arth}\,z], \tag{17a}$$
$$\Delta(F) = z(1-\tau)\tau^{-1}[(1+3\tau)^{1/2} + (1-3\tau)^{1/2} - 2], \tag{17b}$$

$z = 2\omega_2$ [here $\omega_\xi = n\omega_1/\xi_0^2$ and $\omega_\eta = n\omega_2/\eta_0^2$ are the frequencies of small oscillations around the equilibrium points ξ_0 and η_0 in the effective potentials $U_1(\xi)$ and $U_2(\eta)$], and the variable τ, which determines the dependence of all the quantities on the field strength F, is found from Eq. (A27).

4. The analytic expressions obtained above for the quantities σ_i, τ_i, etc., allow us to discuss the accuracy and the region of applicability of the generalized Gamow formula (2).

The results of the calculations for hydrogen states with $n = 10$ and 11 are presented in Fig. 1 (we use the atomic system of units with $\hbar = e = m_e = 1$; the strength of the electric field $\mathscr{E}$ is measured in the units $m_e^2 e^5 \hbar^{-4} = 5.142 \cdot 10^9$ V/cm). The solid curve, calculated by the method of Padé–Hermite approximants,[6)] is in good agreement with the results of Kolosov[17] obtained by a different numerical method. Note that Eq. (2) is highly accurate if $a \geqslant 1$ and is qualitatively correct up to $a \simeq 0.05$.

We have obtained analogous results for other states (n_1, n_2, m) as well [see Fig. 2, which shows the values of $\log \Gamma_n$ for the states $(0, 0, n-1)$ corresponding to circular electron orbits]. Here the principal quantum number n varies from 1 (the ground state) to 100. With growth of n, the region in which the quasiclassical formula (12) gives results close to the exact values of $\Gamma^{(n_1, n_2, m)}$ (calculated using Padé–Hermite approximants[14,15]) becomes somewhat larger. This follows from Eq. (20) below and can be seen from Fig. 3, showing the ratios

$$\rho_n = \tilde{\Gamma}_n(F)/\Gamma_n(F). \tag{18}$$

Here $\tilde{\Gamma}_n$ correspond to the quasiclassical formula (15), and Γ_n are the exact values of the widths, which for $F \geqslant 0.05$ were calculated using Padé–Hermite approximants, and for $F \lesssim 0.02$ by means of the asymptotic formula

$$\Gamma_n = \Gamma^{(0,0,n-1)}$$
$$\approx \frac{1}{n^2 n!} \exp\left\{-n\left[\frac{2}{3F} + \ln\frac{F}{4n} + \frac{33n^2 + 54n + 20}{12n^2} F\right]\right\}, \tag{19}$$

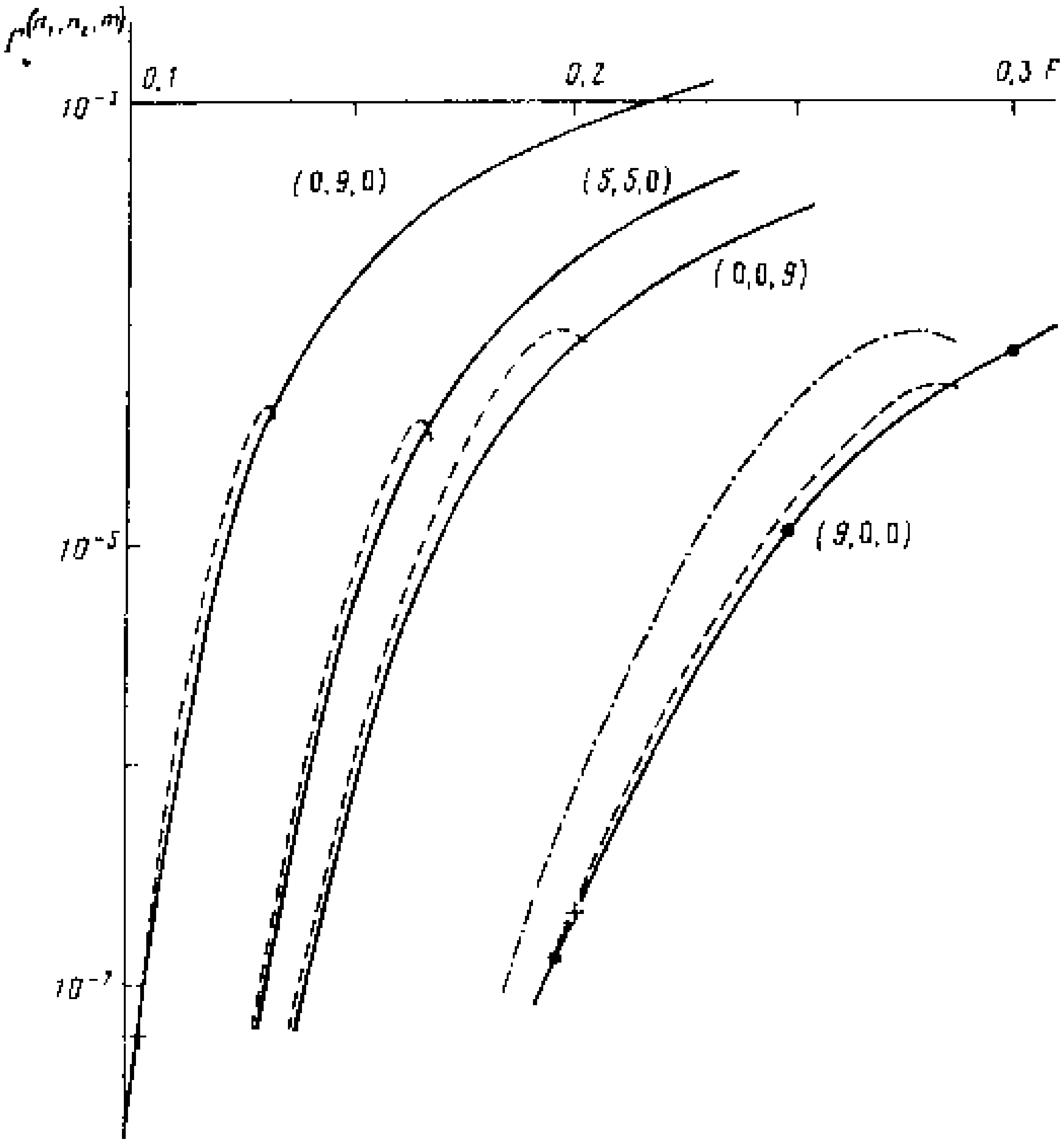

FIG. 1. Dependence of the widths of the atomic levels (n_1, n_2, m) on the electric field. Here and in Fig. 2 the solid curves correspond to the Padé–Hermite approximants, the dashed curves correspond to Eq. (12), and the dot–dashed curves correspond to the one-dimensional Gamow formula ($c = 1$); the points ● are the values taken from Ref. 17, and + are the points for which $a = 1$.

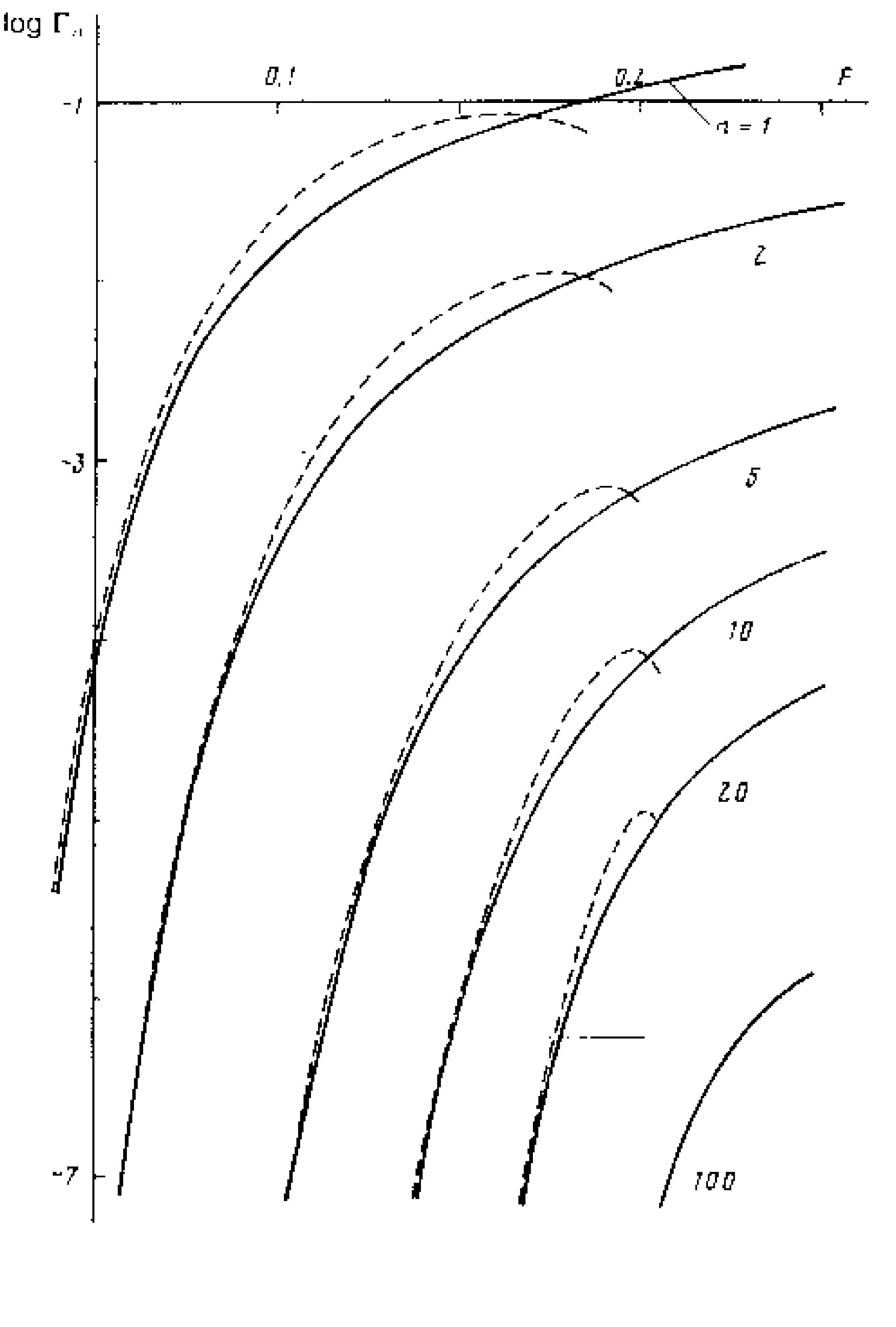

FIG. 2. Widths Γ_n for the states $(0, 0, n - 1)$ of the hydrogen atom.

which is very accurate for $F < 0.01$. From Fig. 3 it follows that in the sub-barrier region $F < F_*$ Eq. (15) is better, the larger the value of n, as we should expect in the quasiclassical approximation. However, when $F \geqslant F_*$ this formula ceases to work [here F_* is the classical ionization threshold, which for the states $(0, 0, n - 1)$ under consideration has the value[14] $F_* = 0.2081$).

We note that in this case the factor c multiplying the exponential, which is associated with the multidimensional character of the problem, is quite different from unity [see Ref. 9 and also (A13)]. Therefore the difference of (2) from the one-dimensional Gamow formula is considerable, as is also clear from comparison of the curves in Fig. 1 pertaining to the state (9, 0, 0) with $n = 10$.

5. Let us formulate the condition for applicability of the Gamow formula and its generalization (2).

When the energy E of the level approaches the top of the barrier, we have the parameter $a = (U_m - E)/\omega \to 0$, and the oscillation period T diverges logarithmically (see Appendix 3), as a result of which the approximate formulas (1) and (2) become meaningless. As can be seen from Fig. 1, it is natural to take the point of the maximum of the dashed curve ($a = a_m$) as the limit of applicability of these expressions. This leads to the required condition of applicability:

$$a \gg a_m = \{2\pi[\ln(n_0 + 1/2) + b]\}^{-1}. \tag{20}$$

Here n_0 is the number of levels with energy $E < U_m$, and b is a calculable constant which depends on the specific problem (see the examples in Appendix 3). For example, in the case of the Stark effect $b = 2.16$, and n_0 must be replaced by n_2 (since tunneling is possible only along the variable η associated with the parabolic quantum number n_2).

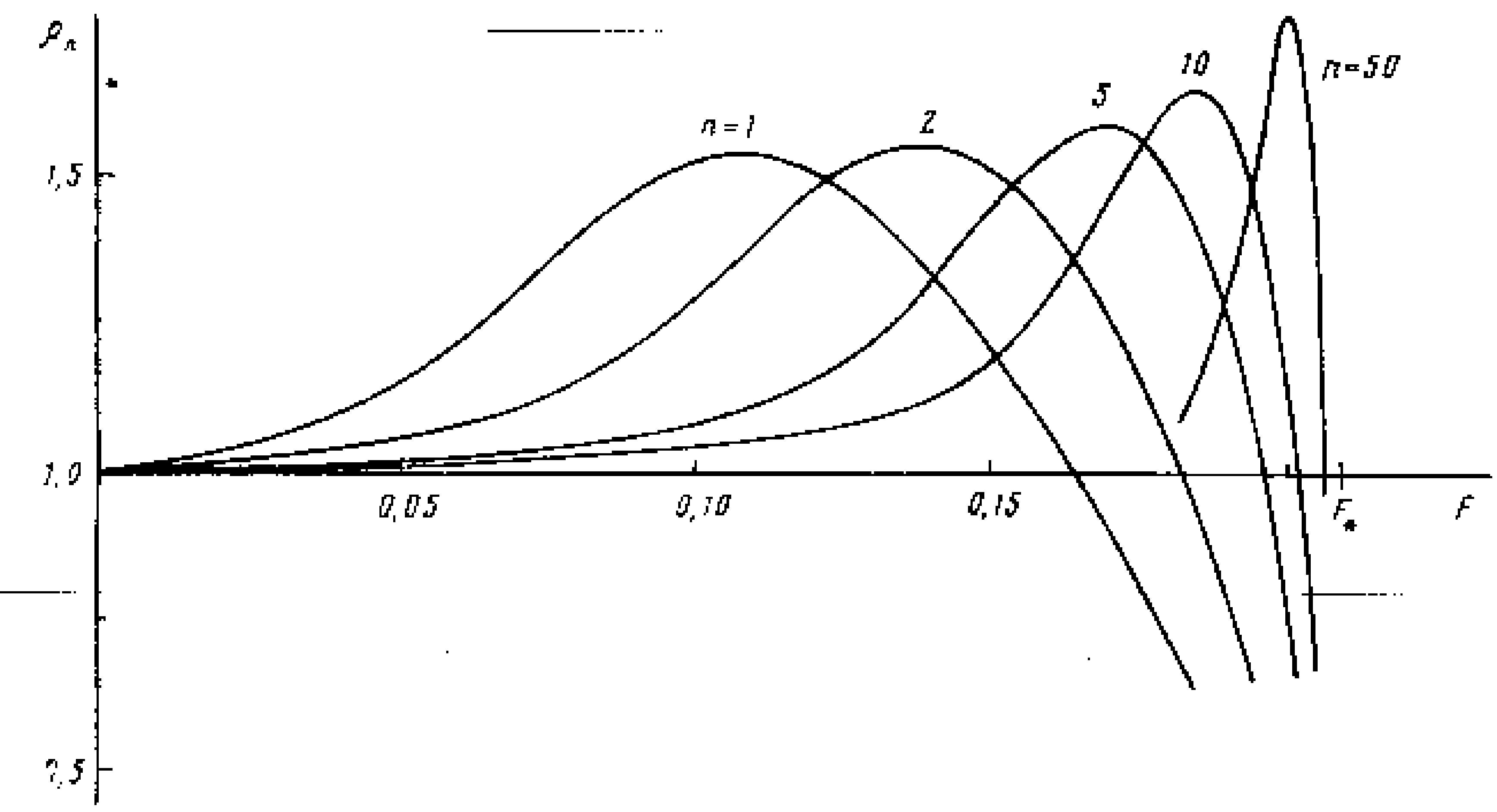

FIG. 3. The ratios ρ_n defined by Eq. (18) for the states $(0, 0, n-1)$ of the hydrogen atom as functions of the reduced field F.

The parameter a_m is numerically small even when $n_0 \sim 1$, and with growth of n_0 it decreases (logarithmically). Therefore, the Gamow formula, as well as its generalization (2), ceases to be valid only in a narrow region of energies $E \approx U_m$ where the level width Γ is no longer exponentially small.

When $E \approx U_m$, and all the more so for above-barrier resonances ($E > U_m$) the values of E_r and Γ can be found by solving (in the complex plane) the equations that follow from the quasiclassical quantization conditions with allowance for the finite penetrability of the barrier. Such a calculation[15] is, however, considerably more complicated than the explicit quasiclassical formulas (1) and (2).

6. Calculation of the penetrability of three-dimensional barriers that do not possess spherical symmetry is of interest for many problems of physics and chemistry. Usually, separation of variables is not assumed, and the barrier penetrability is regarded as exponentially small. In this case the calculation of the probability of tunneling reduces to determination of the most probable sub-barrier trajectory and of the bundle of trajectories close to it, which is required for the calculation of the pre-exponential factor. Such an approach has been long in use in the theory of multiphoton ionization of atoms and ions (the imaginary-time method[18,19]) and in the calculation of the probability of creation of e^+e^- pairs in a variable electric field,[20,21] and it has also been developed in detail (for the example of the two-dimensional anisotropic anharmonic oscillator) for the calculation of the asymptotic behavior of the higher orders of perturbation theory.[22] Further development of this method can be found in Refs. 23–25.

The success of this method is wholly dependent on the possibility of finding the most probable sub-barrier trajectory in an explicit form. It seems that in this way one can also obtain the formula (2) for a system of f degrees of freedom and separable variables. However, this result is not contained in the quoted literature. For a particular case such a formula was obtained[26] by a direct but more involved calculation of the flux of the particles emitted to infinity.

APPENDIX 1

The integral $J(F)$ in (13), which determines the barrier penetrability, is in general (for arbitrary quantum numbers n_1, n_2, and m) a rather complicated elliptic integral. We consider several cases in which the calculations can be simplified.

1) If $m = 0$, then in the effective potential $U_2(\eta)$ the centrifugal term is absent. $A = 0$, and

$$J(F)=3\pi\cdot 2^{-1/2}(1-z_2)F(1/4, 3/4; 2; 1-z_2) = \begin{cases} 1+3/16\, z_2[\ln z_2-(1+6\ln 2)]+\ldots, & z_2\to 0, \\ 3\pi\cdot 2^{-1/2}(1-z_2)+O((1-z_2)^2), & z_2\to 1, \end{cases} \tag{A1}$$

where $z_2 = 4B = 16\beta_2 F\varepsilon^{-2}$. The value $z_2 = 1$ corresponds to the classical ionization threshold[14,16] F_*, at which the barrier in the potential $U_2(\eta)$ vanishes. The expressions (14) for σ_i and τ_i follow[7)] from the identity

$$\int_0^{x_1}\left(-1\mp x+\frac{\lambda}{4x}\right)^{1/2} x^\nu\, dx$$

$$=\frac{\pi^{1/2}\Gamma(\nu+3/2)}{\Gamma(\nu+2)}\left(\frac{\lambda}{4}\right)^\nu F\left(\frac{2\nu+3}{4},\frac{2\nu+5}{4};\nu+2;\mp\lambda\right),$$

where $x_1 = \frac{1}{2}[(1+\lambda)^{1/2}-1]$ and $x_1 = \frac{1}{2}[1-(1-\lambda)^{1/2}]$ for the upper and lower sign, respectively. In the derivation of Eqs. (A1) and (A2) use has been made of the integral representation of the hypergeometric function and the Kummer transformation.[27]

2) For the states $|0, 0, n-1\rangle$ with $n\to\infty$ the polynomial $A - Bu + u^2 - u^3$ in (13) has a multiple root:

$$u_0=u_1=1/3[1-(1-\sigma)^{1/2}],\quad u_2=1/3[1+2(1-\sigma)^{1/2}], \tag{A3}$$

where $\sigma = \frac{3}{4}z_2$. This can be seen by using the expressions for the minimum of $U_2(\eta)$ and other quantities given in the parametric form [see (A26) and (A27)]. Here

$$u_0=u_1=\frac{\tau(1+\tau)}{1+3\tau^2},\quad u_2=\frac{(1-\tau)^2}{1+3\tau^2},\quad u_0+u_1+u_2=1, \tag{A4}$$

$$A=\tau^2(1-\tau^2)^2/(1+3\tau^2)^3=u_0u_1u_2, \tag{A5}$$

which indicates the existence of a multiple root. The integral (13) can therefore be calculated in terms of elementary functions [see (17a)].

3) In the weak-field region it is possible to calculate $J(F)$ for any values of n_1, n_2, and m. In this case we have $u_1 = c_1F + \ldots$ and $u_2 = 1 - c_2F + \ldots$, where

$$c_1 = {}^1/_2[(\rho+\mu)^{1/2}+(\rho-\mu)^{1/2}]^2, \quad c_2=2\rho, \tag{A6}$$

$$\rho=(2n_2+m+1)/n, \quad \mu=m/n. \tag{A7}$$

Introducing a matching point $\bar{u}$ such that $u_1 \ll \bar{u} \ll 1$, we split the integral into two parts: $J(F) = \frac{1}{2}(J_1 + J_2)$, with

$$J_1 = \int_{u_1}^{\bar{u}} \frac{du}{u}(A-Bu+u^2)^{1/2} = \bar{u} - \frac{1}{4}\bar{u}^2 - \frac{1}{4}B\bar{u} + A^{1/2}\,\mathrm{arth}\,\xi - \frac{1}{2}B\left[\ln(4\bar{u}/B)+1-\frac{1}{2}\ln(1-\xi^2)\right],$$

$$J_2 = \int_{\bar{u}}^{1} \frac{du}{u}\left\{(u^2-u^3)^{1/2} + \frac{A-Bu}{2u(1-u)^{1/2}} + \ldots\right\} = \frac{2}{3} - \bar{u} + \frac{1}{4}\bar{u}^2 + \frac{1}{2}B(\ln\bar{u} - 2\ln 2) + \frac{1}{4}B\bar{u} + \ldots,$$

whence[8)]

$$J(F) = 1 + {}^3/_4 B[\ln B - (1+4\ln 2) + \varphi(\xi)] + \ldots, \tag{A8}$$

where

$$\varphi(\xi) = {}^1/_2[(1+\xi)\ln(1+\xi) + (1-\xi)\ln(1-\xi)], \quad \xi = 2A^{1/2}B^{-1} = \mu/\rho + O(F). \tag{A9}$$

Inserting here the expansion $B = 2\rho F + \ldots$ when $F \to 0$, we find

$$J(F) = 1 + {}^3/_2\rho F\ln F - kF + \ldots, \quad k = {}^3/_2\rho[1+3\ln 2 - \ln\rho - \varphi(\mu/\rho)], \tag{A10}$$

and we finally obtain

$$2\pi a_\eta = 2n/3F + (2n_2+m+1)\ln F - n\{3 + (3\ln 2 - 2)\rho - {}^1/_2[(\rho+\mu)\ln(\rho+\mu) + (\rho-\mu)\ln(\rho-\mu)]\} + \ldots \tag{A11}$$

We note also that

$$\sigma_2 = \pi(1 - {}^3/_2F + \ldots), \quad \tau_2 = \pi\left[1 - \varkappa + 3\left(1 - \varkappa + \frac{m^2-1}{12n^2}\right)F + \ldots\right], \tag{A12}$$

$$c = 2(1-\varkappa) + 3(1 - \varkappa^2 + (m^2-1)/6n^2)F + \ldots, \quad c/T_\eta = (1/2\pi n^3)[1 - {}^3/_2\rho F + O(F^2)] \tag{A13}$$

(the expansions for σ_1 and τ_1 are obtained by replacing $\varkappa$ by $-\varkappa$ and F by $-F$). Here $\varkappa = (n_1 - n_2)/n$, $\rho = 1 - \varkappa$, where $2 - n^{-1} \geqslant \rho \geqslant n^{-1}$, $1 - n^{-1} \geqslant \mu \geqslant 0$, and $\rho > \mu$ for all the states (n_1, n_2, m) with a given value of n.

APPENDIX 2

Let

$$V(r) = -g(\hbar^2/mR^2)v(r/R), \tag{A14}$$

where g is a dimensionless coupling constant and R is a characteristic range of the forces (below, we set $\hbar = m = R = 1$). If $l \gg 1, n_r$, then the particle is localized in the vicinity of the classical equilibrium point $r = r_0$ in the potential $U(r) = V(r) + l(l+1)/(2r^2)$, which can be found from the equation $r^3v'(r) = -\nu$. This explains the validity of the $1/n$ expansion.[28] We apply a variation of this method, developed in Refs. 29 and 30, and restrict ourselves to nodeless states. Setting

$$\nu = n^2/g, \quad E_{nl} = g^2\varepsilon_{nl}/2n^2, \quad n = l+1, \quad r = r_0(1 + n^{-1/2}\rho), \tag{A15}$$

in the region $|\rho| \ll n^{1/2}$ we have

$$\chi_n(r) \equiv rR_{n,n-1}(r) = (n\omega/\pi r_0^2)^{1/4}e^{-1/2\omega\rho^2}[1 + O(n^{-1/2})], \quad \omega = [3 + r_0v''(r_0)/v'(r_0)]^{1/2}, \tag{A16}$$

and $\int_0^\infty \chi_n^2(r)dr = 1 + O(1/n)$. The last expression is valid in the classically allowed region including the turning points $r_\pm$ (or $\rho_\pm = \pm\omega^{-1/2}$). By means of the WKB method it can be continued into the sub-barrier region ($\rho < \rho_-$ and $\rho > \rho_+$). In particular, for $r_+ < r < r_2$ we have

$$\chi_n(r) = (\pi e)^{-1/4}\left[\frac{\omega}{2r_0^2Q(r)}\right]^{1/2}\exp\left\{-n\int_{r_+}^{r} Q(r)dr\right\}, \tag{A17}$$

where

$$Q^2 = \frac{(l+{}^1/_2)^2}{n^2r^2} - \frac{2}{\nu}v(r) + q^2 = Q_0^2 - \frac{1}{n}S_0 + O\left(\frac{1}{n^2}\right), \quad Q_0^2 = r^{-2} - (2/\nu)v(r) + q_0^2, \quad S_0 = r^{-2} + s_0, \; s_0 = (\omega-1)r_0^{-2}, \quad q^2 = -\varepsilon/\nu^2, \; q_0^2 = (2/\nu)v(r_0) - r_0^{-2}. \tag{A18}$$

We note the following expansion, which will be useful later:

$$\int_{r_+}^{r} Q\,dr = \int_{r_0}^{r} Q_0\,dr + \frac{1}{n}\int_{r_0}^{r} dr\left[\frac{1}{r-r_0} - \frac{S_0(r)}{Q_0(r)}\right] - \frac{1}{4n}\ln\left[4ne\omega\left(\frac{r}{r_0} - 1\right)^2\right] + \ldots \tag{A19}$$

Using the usual matching rules, from (A17) we obtain the divergent wave corresponding to the quasistationary state:

$$\chi_n^{(+)}(r) = (\pi e)^{-1/4}\left[\frac{\omega D}{2r_0^2P(r)}\right]^{1/2} \times \exp\left\{i\left[n\int_{r_2}^{r} P(r)dr + \frac{\pi}{4}\right]\right\}, \quad r > r_2, \tag{A20}$$

where $p(r) = nP(r)$ is the quasiclassical momentum [under the barrier we have $P(r) = iQ(r)$] and $D = \exp\{-2n\int_{r_+}^{r_2} Q\,dr\}$ is the penetrability of the barrier.

Let us apply these formulas to the Stark effect in the hydrogen atom. Consider the states $|0, 0, n-1\rangle$ in which "radial" (in the variables ξ and η) excitations are absent and where in the limit $n\to\infty$ the particle is at rest at the classical equilibrium point ξ_0, η_0. Going over to the scaled variables (8), we have

$$U_1(x)=\frac{1-2n^{-1}}{x^2}-\frac{4\beta_1}{x}+Fx,\quad U_2(y)=\frac{1-2n^{-1}}{y^2}-\frac{4\beta_2}{y}-Fy,$$

$$\psi(\mathbf{r})=Ne^{im\varphi}(\xi\eta)^{-1/2}\chi_n(x)\begin{cases}\chi_n(y), & y_-<y<y_+,\\ \chi_n^{(+)}(y), & y>y_2.\end{cases}\qquad \text{(A21)}$$

The condition of normalization to one particle in the well,[11]

$$\frac{\pi}{2}\int|\psi|^2(\xi+\eta)d\xi\,d\eta=1,$$

defines the constant N:

$$N=\frac{1}{n}\left[\frac{2x_0y_0}{\pi(x_0+y_0)}\right]^{1/2}.\qquad \text{(A22)}$$

Calculating the flux of particles moving to infinity by means of (A21), we find the width of a Stark resonance:

$$\Gamma_n=A_ncT_\eta^{-1}D,\qquad \text{(A23)}$$

where[9]

$$c=\frac{4y_0}{x_0+y_0},\qquad T_\eta=\frac{2\pi}{\omega_\eta}=2\pi n^3\frac{y_0^2}{\omega_2},\qquad \text{(A24)}$$

$$A_n=\frac{2^{1/2}\pi}{n!}\left(\frac{n}{e}\right)^{n+1/2}=\begin{cases}0{,}991 & \text{for } n=1,\\ 1{,}032 & \text{for } n=2,\\ (\pi/e)^{1/2}(1-1/12n+\dots), & n\gg1.\end{cases}\qquad \text{(A25)}$$

For the states $|0, 0, n-1\rangle$ with $n\gg1$ the turning points y_0 and y_1 are close to each other, the quantities entering into D become simpler,

$$Q_0(y)=F^{1/2}(y-y_0)(y_2-y)^{1/2}y^{-1},$$
$$S_0(y)=1/2y^2+\varepsilon^{(1)}/4+\beta_2^{(1)}/y,$$

and the barrier penetrability D can be calculated explicitly [see (17)–(17b)].

We shall give explicit expressions for the quantities that appear in the above formulas. Their dependence on the field F is given in the parametric form

$$x_0=(1-\tau^2)^{-2}(1-\tau),\ y_0=(1-\tau^2)^{-2}(1+\tau),\ y_2=\tau^{-1}(1+\tau)^{-2},$$
$$\omega_1=(1+3\tau)^{1/2}/2(1+\tau),\ \omega_2=(1-3\tau)^{1/2}/2(1-\tau),$$
$$\varepsilon=\varepsilon^{(0)}+n^{-1}\varepsilon^{(1)}+\dots,$$
$$\varepsilon^{(0)}=-(1-\tau^2)^2(1+3\tau^2),$$
$$\varepsilon^{(1)}=(1-\tau^2)^3[(1+3\tau)^{1/2}+(1-3\tau)^{1/2}-2],\qquad \text{(A26)}$$

$$\beta_i=\beta_i^{(0)}+n^{-1}\beta_i^{(1)}+\dots,\qquad \beta_{1,2}^{(0)}=1/2\pm1/4(\tau-3\tau^3),$$

$$\beta_1^{(1)}=-\beta_2^{(1)}=1/4(1-\tau^2)[(1+\tau)(1+3\tau)^{1/2}-(1-\tau)(1-3\tau)^{1/2}-4\tau],$$

$$\tau(1-\tau^2)^4=F,\qquad \text{(A27)}$$

with the choice of the root $\tau=\tau(F)$ that vanishes for $F\to0$:

$$\tau=\begin{cases}F+4F^3+42F^5+\dots, & F\to0,\\ \dfrac{1}{3}-\dfrac{2^{1/2}}{9}f^{1/2}+O(f), & F\to F_*.\end{cases}\qquad \text{(A28)}$$

($f=1-F/F_*$). In the limit $F\to F_*$ the frequency behaves as $\omega_2\propto f^{1/4}\to0$; when $F>F_*$, the classical equilibrium point moves away into the complex plane, and the $1/n$ expansion determines not only the positions but also the widths of the Stark resonances,[14,16] which cease to be exponentially small.

APPENDIX 3

When $a\to0$, we have[8]

$$T=\omega^{-1}\{\ln(1/a)+c_0+O(a)\},\qquad \text{(A29)}$$

where

$$c_0=\ln J_0+\ln\frac{[2\omega(x_m-\bar{x}_0)^2]}{J_0}+2\int_{\bar{x}_0}^{x_m}\left(\frac{\omega}{\bar{p}}-\frac{1}{x_m-x}\right)dx,\qquad \text{(A30)}$$

$J_0=\int_{\bar{x}_0}^{x_m}\bar{p}\,dx$, $\bar{p}=p(x,\ E=U_m)$, x_m is the position of the maximum of the potential, $U_m=U(x_m)$, $\omega=[-U''(x_m)]^{1/2}$, and $\bar{x}_i$ denotes the positions of the turning points at $E=U_m$ (so that $\bar{x}_1=\bar{x}_2=x_m$). When $a\ll1$, we have

$$\Gamma\approx\omega(\ln(1/a)+c_0)^{-1}\exp(-2\pi a),\qquad \text{(A31)}$$

from which we obtain the equation $a[\ln(1/a)+c_0]=(2\pi)^{-1}$ for the determination of a_m. Using the fact that $J_0=(n_0+\frac{1}{2})\pi+O(1/n_0)$, we arrive at the condition (20), in which

$$b=\ln[2\pi\omega(x_m-\bar{x}_0)^2/J_0]+2\int_{\bar{x}_0}^{x_m}\left(\frac{\omega}{\bar{p}(x)}-\frac{1}{x_m-x}\right)dx.\qquad \text{(A32)}$$

Let us consider several examples.

a) For a parabolic barrier

$$V(r)=-1/2\omega^2(r-R)^2,\ 0<r<\infty\qquad \text{(A33)}$$

($l=0$), we obtain $\bar{x}_0=0$, $\bar{p}=\omega|r-R|$, and

$$J_0=1/2\omega R^2,\quad b=\ln4\pi\approx2{,}53.\qquad \text{(A34)}$$

b) Generalizing the preceding example, let us set

$$\bar{p}(r)=[\omega r_m/(\alpha-\beta)](\rho^\beta-\rho^\alpha),\ \rho=r/r_m\qquad \text{(A35)}$$

($\alpha>\beta>-1$), which corresponds to the behavior $V(r)\propto-r^{2\beta}$ for $r\to0$ and $V(r)\propto-r^{2\alpha}$ for $r\to\infty$. If $\alpha=1$

and $\beta = 0$, then we return to (A33); the case $\alpha = \frac{1}{2}$, $\beta = -\frac{1}{2}$ corresponds to the spherically symmetric ($l = 0$) model of the Stark effect, etc. In this case the quantities J_0, c_0, and b can be calculated in an analytic form:

$$J_0 = \omega r_m^2/(\alpha+1)(\beta+1),$$

$$b = \ln\left(\frac{2\pi(\alpha+1)(\beta+1)}{(\alpha-\beta)^2}\right) - 2\left(C + \psi\left(\frac{1-\beta}{\alpha-\beta}\right)\right), \quad \text{(A36)}$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$ and $C = 0.5772...$ is the Euler constant. In particular, for $\alpha = 1$ we have $b = \ln[4\pi(1+\beta)/(1-\beta)^2]$ (the condition $\beta > -1$ excludes fall to the center[11]).

c) Finally, let us consider the Stark effect for the states with $m = 0$ and $n \gg 1$. In this case the effective potential $U_2(\eta)$ possesses a barrier as long as $z_2 = 16\beta_2 F\varepsilon^{-2} < 1$. Taking into account the fact that when $z_2 = 1$ we have the relation[14]

$$\left.\frac{n(-\varepsilon)^{3/2}}{2^{1/2}F}\right|_{F=F_*} = \frac{3\pi}{16}(2n_2+1), \quad \text{(A37)}$$

from (14) we find

$$a_\eta = \frac{3\pi}{16}(2n_2+1)(1-z_2) + \ldots,$$

$$\tau_2 = \text{const}\left[\ln\frac{1}{1-z_2} + 2(3\ln 2 - 2) + \ldots\right], \quad 1 + \frac{\sigma_2\tau_1}{\sigma_1\tau_2} = O(1),$$

whence

$$b = \ln(48\pi^2) - 4 \approx 2.16. \quad \text{(A38)}$$

We note that the last coefficient is numerically close to the value of b from (A34).

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3) See, however, Refs. 1–5 and the literature quoted there. Among the numerical methods of determining the resonances we mention the method of complex scaling,[1,2] which works well for sufficiently narrow resonances.

4) Equation (5) corresponds to the case in which the variables in the Hamilton–Jacobi and Schrödinger equations separate fully. This case covers many physical problems: the hydrogen atom in a homogeneous electric field, the problem of two centers, geodesics on a triaxial ellipsoid, etc.[11-13] Note that (unlike α) the separation constants β_i can be determined only together with the energy E.

5) Here n_1, n_2, and m are the parabolic quantum numbers ($m \geq 0$), which are conserved in the presence of a homogeneous electric field $\mathscr{E}$, and $n = n_1 + n_2 + m + 1$ is the principal quantum number of the level. In (10) and (11) we have taken into account the fact that the tunneling of the electron occurs along the variable η and that the potential $U_1(\xi)$ is confining.[11]

6) I.e., by summation of the divergent series of perturbation theory (in powers of the electric field $\mathscr{E}$) with the help of Padé–Hermite approximants (for more details about this method, see Refs. 14 and 16). Note that within the accuracy of Fig. 1 the Padé–Hermite approximants coincide with the exact solution of the problem.

7) For $\nu = -1$ and 0, respectively.

8) As expected, the arbitrary matching point $\bar{u}$ drops out of the sum $J_1 + J_2$.

9) The calculation using the $1/n$ expansion gives the value $A_n = (\pi/e)^{1/2} = 1.075...$, which is independent of n. The coefficient A_n given in (A25) was chosen so that in the limit $F \to 0$ the expression (A23) coincides with the exact asymptotic formula (19) for all values $n = 1, 2, 3, \ldots$. Note that the values of A_n are numerically very close to unity; thus, (A23) has only a percentage deviation from the general formula (2).

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