Quantization rules with allowance for barrier penetration

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The semiclassical quantization rules are corrected with allowance for barrier penetration. The resulting equation determines both the position E_r and the width Γ of the quasistationary level. A comparison is made with numerical solutions of the Schrödinger equation and with exactly solvable models. The generalization of the Gamov formula for systems with separating variables is found. The possibility of generalizing the results obtained to the relativistic case is discussed.

The Bohr–Sommerfeld quantization rules determine discrete energy spectra (see, e.g., Refs. 1 and 2). Integrals of the form $\int p\,dx$ are taken over the classically allowed region $x_0 < x < x_1$ (see Fig. 1 in Ref. 3), and it is assumed that the behavior of the potential outside this region is unimportant.

At the same time, in many physical problems the potential possesses a barrier, as a consequence of which the levels are quasistationary ($E = E_r - i\Gamma/2$). In view of the exponential increase of the Gamov wave function as $r \to \infty$ the numerical calculation of the position and width of the level presents certain difficulties.

We shall consider this problem in the semiclassical approximation; this leads to analytical formulas that are valid for an arbitrary smooth potential (see Sec. 1). An analysis of these formulas is contained in Sec. 2, in which a generalization of the well known Gamov formula to the case of systems with separating variables is also given. In Sec. 3 we give a comparison of this approximation with exact solutions of the Schrödinger equation for several model potentials, and in Sec. 4 we compare the approximation with numerical calculations for the Stark effect in a strong field. Section 5 is devoted to an analysis of the relativistic case (for the example of spin-0 particles). Approximate analytical formulas for near-threshold resonances, and also some details of the calculations, have been placed in the appendices.

1. GENERALIZATION OF THE BOHR–SOMMERFELD QUANTIZATION RULES

Near the top of the barrier ($x \approx x_m$) we use the parabolic approximation:

$$p(x) = \left(\frac{1}{4}\rho^2 - a \right)^{1/2}, \qquad a = \frac{U_m - E}{\omega}, \tag{1.1}$$

where $\rho = (x - x_m)/\xi_0$, and $\xi_0 = (\hbar/m\omega)^{1/2}$ and $\omega = [-U''(x_m)]^{1/2}$ are the amplitude and frequency of the zero-point oscillations of the particle about the point of (unstable) equilibrium; below, $\hbar = m = 1$. The Schrödinger equation then has the exact solution

$$\psi(x) = \text{const}\, D_{-1/2-ia}(\rho e^{-i\pi/4}), \tag{1.2}$$

which satisfies the radiation condition [$D_\nu(z)$ is a parabolic-cylinder function[4]]. To the left of the barrier ($\rho < 0, |\rho| \gg a$) this function joins with the semiclassical solution

$$\psi(x) = \text{const} \cdot [p(x)]^{-1/2} \sin'\left(\theta(x) + \frac{\pi}{4} \right) \qquad \theta = \int_{x_0}^{x} p\,dx.$$

$$\tag{1.2'}$$

As usual, the quantization condition arises from the requirement that the phases of the functions (1.2) and (1.2') coincide (modulo $n\pi$) in the region of overlap $a \ll |\rho| \ll x_m/\xi_0$, which always exists for large n. Using the asymptotic form of the function $D_\nu(z)$ for $z \to \infty$, we obtain (see also Refs. 5 and 6)

$$\int_{x_0}^{x_1} p(x,E)\,dx = \left(N + \frac{1}{2} \right)\pi, \qquad N = n - \frac{1}{2\pi}\varphi(a), \tag{1.3}$$

$$\varphi(a) = \frac{1}{2i}\ln\left\{ \Gamma\left(\frac{1}{2} + ia \right) \middle/ \right.$$
$$\left. \Gamma\left(\frac{1}{2} - ia \right)(1 + e^{-2\pi a}) \right\} + a(1 - \ln a), \tag{1.4}$$

$$a = \frac{1}{\pi}\int_{x_1}^{x_2} (-p^2)^{1/2}\,dx, \tag{1.5}$$

where $n = 0,1,2,\ldots$, $\Gamma(z)$ is the gamma function, $x_1 < x < x_2$ is the sub-barrier region, and the notation is as in Fig. 1 of Ref. 3. Here the parameter a, which for a parabolic barrier is defined in (1.1), is written in a more general form applicable for an arbitrary smooth potential $U(x)$ satisfying the conditions of applicability of the semiclassical approximation. For quasistationary states this parameter is complex, as are the turning points $x_{1,2}$.

In the simplest cases the integral (1.5) can be calculated explicitly so that its analytic continuation does not present difficulties. For an arbitrary potential the values of a for complex values of E can be found numerically, and, together with Eq. (1.3), determine the spectrum of the quasistationary states.

For multidimensional problems with separable variables $q_1,\ldots,q_f$ (f is the number of degrees of freedom) the quantization conditions have the form

$$\int_{q_i^{(0)}}^{q_i^{(1)}} p_i\,dq_i = \left(N_i + \frac{1}{2} \right)\pi. \tag{1.6}$$

Here $q_i^{(0,1)}$ are the turning points bounding the classically accessible regions of motion along the corresponding coordinates, and p_i is the semiclassical momentum [see (2.4) below]. Here, in (1.6),

$$N_i = n_i - \frac{1}{2\pi}\varphi(a_i), \qquad (1.7)$$

holds if tunneling along the coordinate q_i is possible (an "open channel"); otherwise, we have $a_i = \infty$ and $N_i = n_i = 0,1,\ldots$. The solution of this system of equations determines the energy $E = E_r - i\Gamma/2$ and the separation constants β_i, which are also complex.

2. ANALYSIS OF THE BASIC EQUATIONS

Equations (1.3) and (1.6) give the generalization of the Bohr–Sommerfeld quantization rules to the case of potentials with a barrier. We list some consequences.

a) The case $a \gg 1$ corresponds to small barrier penetrability. Taking into account the expansion $(a \to +\infty)$

$$\varphi(a) = \frac{1}{24a} + \frac{7}{2880a^3} + \ldots + \frac{i}{2}e^{-2\pi a}, \qquad (2.1)$$

which follows from (1.4), and [in a spherically symmetric problem with potential $V(r)$] taking the radial momentum to be equal to

$$p_r = \{2[E_r - i\Gamma/2 - U(r)]\}^{1/2}, \qquad U(r) = V(r) + (l+1/2)^2/2r^2,$$

we obtain from (1.3) the Gamov formula for the width of a quasistationary state:

$$\Gamma = T^{-1}\exp\left(-2\int_{r_1}^{r_2}|p(r)|\,dr\right), \qquad T = 2\int_{r_0}^{r_1}\frac{dr}{p(r)}, \qquad (2.2)$$

where T is the period of the radial oscillations of the particle inside the well $(r_0 < r < r_1)$. Thus, Eq. (1.3) leads to correct results not only for small a, when the parabolic approximation is valid, but also in the opposite case $a \ll 1$. Therefore, it may be expected that for intermediate values $a \sim 1$ as well it will give a correct interpolation of the exact solution. Later we shall see that this is so (see Secs. 3 and 4 below).

b) We shall consider Eqs. (1.6) in the case when the penetration of the barrier is exponentially small. In this case the tunneling occurs in practice along one particular coordinate,[1] e.g., q_f. In this case for the width Γ we obtain

$$\Gamma = cT_f^{-1}\exp(-2\pi a_f), \qquad (2.3)$$

where

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

$$p_i = \{2[\alpha E - U_i(q)]\}^{1/2}, \qquad U_i(q) = u_i(q) + \beta_i v_i(q), \qquad (2.4)$$

in which the β_i are the separation constants $\Sigma_{i=1}^f\beta_i = \text{const}$, and the $\bar{v}_i$ denote averages over the semiclassical wave function:

$$\bar{v}_i = \int_{q_i^{(0)}}^{q_i^{(1)}}dq\,\frac{v_i(q)}{p_i(q)}\Bigg/\int_{q_i^{(0)}}^{q_i^{(1)}}\frac{dq}{p_i(q)}. \qquad (2.5)$$

To obtain these formulas one must substitute

$$E = E_r - i\Gamma/2, \qquad \beta_i = \beta_i' + i\beta_i''$$

into (1.6), and, assuming the width Γ and β_i'' to be exponentially small, expand all the integrals in them (details of the calculations can be found in Ref. 7).

We note that Eq. (2.4) does not specify the most general case of separation of variables, but it applies to many physically interesting problems. For example, the Schrödinger equation for the hydrogen atom in a uniform electric field $\mathscr{E}$ admits separation of variables in the parabolic coordinates $\xi = r + z$, $\eta = r - z$, $\varphi(0 \leqslant \varphi \leqslant 2\pi)$, with[1]

$$u_{1,2}(q) = \frac{m^2}{8q^2} \pm \frac{1}{8}\mathscr{E}q, \qquad (2.6)$$

$$v_1(q) = v_2(q) = -1/2q, \qquad \alpha = 1/4$$

(here $q = \xi$ or η).

Another example is the nonrelativistic two-center problem:[1,8]

$$v_1(\xi) = \frac{\beta_1}{\xi^2 - 1}, \qquad v_2(\eta) = \frac{\beta_2}{1 - \eta^2}, \qquad \alpha = \frac{1}{4}R^2, \qquad \beta_1 + \beta_2 = 0, \qquad (2.7)$$

where ξ and η are elliptic coordinates:

$$\xi = (r_1 + r_2)/R, \qquad \eta = (r_1 - r_2)/R,$$

and R is the distance between the fixed centers (nuclei). From the examples given the origin of the constant α in (2.4) is clear; its numerical value depends on the specific problem and is determined in the process of the separation of variables.

The multidimensional problem differs from the one-dimensional problem in the factor c that appears in the pre-exponential factor in (2.3); the factor c takes into account, as it were, the change in the frequency of collisions of the particle with the barrier wall $(q_f = q_f^{(1)})$ as a consequence of its motion along the other coordinates q_i $(i \neq f)$. Below we shall see that this factor can differ substantially from unity. If $f = 1$, (2.3) goes over into the usual Gamov formula (2.2).

c) The preceding formulas can be made more precise by including in the analysis a correction of order $\hbar^2$ to the usual semiclassical approximation.[9,10] In the case the phase θ in (1.2') is equal to

$$\theta(r) = \int_{r_0}^{r}\left\{p + \frac{1}{4}(p^{-1})'' - \frac{1}{8}\frac{p'^2}{p^3} + \frac{1}{8p^2r}\right\}dr \qquad (2.8)$$

(here, $p' = dp/dr$), and from the exact solution (1.2) for $\tau = -\rho \gg |a|$ we obtain

$$\theta(r) = \frac{1}{4}\tau^2 - \frac{a}{2}\ln\frac{\tau^2}{a}$$
$$+ \frac{1}{2}[\varphi(a) - a] + \frac{1}{2}\left(a^2 - \frac{3}{4}\right)\tau^{-2} + O(\tau^{-4}). \qquad (2.9)$$

Using for the momentum $p(r)$ the parabolic approximation (1.1) and calculating the integrals appearing in $\theta(r)$, we can convince ourselves that the expressions (2.8) and (2.9) can be joined. We then arrive again at the quantization condition

(1.3), in which, however, the function (1.4) is replaced by φ_2:

$$\varphi_2(a) = \varphi(a) - 1/24a. \tag{2.10}$$

Comparison with (2.1) shows that from $\varphi(a)$ we subtract the first term of its asymptotic expansion for $a \to \infty$. As is well known, the formal parameter $\hbar^2$ of the semiclassical approximation (for the energy) goes over in the final formulas into $1/n^2$. Since $\varphi_2(a) = O(a^{-3})$, the replacement $\varphi \to \varphi_2$ in (1.3) ensures that the resonance energy is calculated to terms of order n^{-4}.

In the same way, it is possible to take into account also the next corrections to the semiclassical approximation,[10-12] but the calculations become considerably more complicated. It is evident that allowance for corrections up to $\hbar^{2K}$ inclusive leads to the quantization condition (1.3) with a function φ_K:

$$\varphi_K(a) = \varphi(a) - \sum_{j=1}^{K-1} c_j a^{-(2j-1)}, \tag{2.11}$$

where

$$c_j = (-1)^{j-1}(1 - 2^{-(2j-1)})B_{2j}/2j(2j-1)$$

are the coefficients of the asymptotic series (2.1) and B_{2j} are the Bernoulli numbers.[4] Since $\varphi_K(a) = O(a^{-(2K-1)})$ for $a \to \infty$, the accuracy of the calculation of the resonance energy E_r is then increased to n^{-2K} (approximations corresponding to functions $\varphi_K(a)$ with $K > 2$ are not considered further in this article).

d) The function $\varphi(a)$ has singularities at the points $a = a_k = (k + \frac{1}{2})$ ($k = 0, 1, \ldots$) in the upper half-plane:

$$\varphi(a) = i \ln(a - a_k) + O(1), \quad a \to a_k, \tag{2.12}$$

which correspond to poles of the scattering amplitude for scattering by the parabolic barrier $U(x) = -\frac{1}{2}\omega^2 x^2$. Here, a pole in the scattering amplitude corresponds to a logarithmic singularity of the function $\varphi(a)$, since the latter is directly related to the phase shift.

e) If the energy of the level approaches the top of the barrier, the quantization integral

$$I = \int_{x_0}^{x_1} p(x, E) dx$$

has a logarithmic singularity:

$$I(a) = I_0 + \frac{1}{2}a \ln a - I_1 a + I_2 a^2 + \ldots, \quad a \to 0, \tag{2.13}$$

where[7]

$$I_0 = \int_{\bar{x}_0}^{x_m} \bar{p}\, dx, \tag{2.14}$$

$$I_1 = \frac{1}{2}[1 + \ln 2\omega (x_m - \bar{x}_0)^2] + \int_{\bar{x}_0}^{x_m} dx \left(\frac{\omega}{\bar{p}} - \frac{1}{x_m - x}\right),$$

in which $\omega = [-U''(x_m)]^{1/2}$ and $\bar{p} = p(x, E = U_m)$ and $\bar{x}_i$ are the semiclassical momentum and turning point for $E = U_m$ [we note that $\bar{x}_1 = x_m$ ius the point of the maximum of the potential $U(x)$]. Since $\bar{p}(x) = \omega|x - x_m|$ for $x \to x_m$,

the poles in the integrand of (2.14) cancel completely and the integral converges.

For resonance levels in the neighborhood of $E \approx U_m$ we can obtain the following formulas (see Appendix A):

$$E_n = U_m + 2\pi\omega \frac{L}{L^2 + \pi^2/4}(n - n_*) + \ldots,$$
$$\frac{\Gamma_n}{\omega} = \frac{\ln 2}{L} + \frac{2\pi^2}{L^2 + \pi^2/4}(n - n_*) + \ldots \tag{2.15}$$

Here,

$$L = (\ln n_* + k) \gg 1, \quad k = C + \ln 16\pi \approx 4.50, \quad C = 0.577 \ldots,$$

and $n = n_*$ corresponds to the number of the level at the point at which it intersects the boundary $\mathrm{Re}\, E = U_m$. Hence, for the ratio $n_n = \Gamma_n/\Delta E_n$ we obtain

$$\eta_n = \Gamma_n \left(\frac{dE_n}{dn}\right)^{-1}\Big|_{n=n_*} = \frac{\ln 2}{2\pi}[1 + O(L^{-2})]. \tag{2.16}$$

This relation is asymptotically exact ($n \to \infty$) for an arbitrary potential. Thus, when $\mathrm{Re}\, E = U_m$ the resonances still do not overlap: $n_\infty = (\ln 2)/2\pi = 0.1103$. Hence in the region of energies $E > U_m$ as well several sub-barrier resonances can be observed (although their widths increase rapidly with increase of E; see Eq. (A8) in Appendix A).

f) The main parameter of this theory is a; see (1.5). In the parabolic approximation we have $a \equiv J$, but this is valid, generally speaking, only for small a [here, $J = (U_m - E)/\omega$ is an adiabatic invariant for a harmonic oscillator with frequency ω]. The next terms of the expansion of $a(J)$ in powers of J can be found by taking into account that

$$\frac{da(J)}{dJ} = \frac{\omega}{\pi} \int_{x_1}^{x_2} [2(U(x) - E)]^{-1/2} dx, \quad a(0) = 0,$$

and using the Newcomb-Lindstedt formula for the period of the oscillations of an anharmonic oscillator.[13] Finally we obtain

$$a = J + c_2 J^2 + c_3 J^3 + \ldots,$$
$$c_2 = -\frac{3}{4}(u_2 - \frac{5}{4}u_1^2), \tag{2.17}$$
$$c_3 = -\frac{5}{4}(u_4 - \frac{7}{2}u_3 u_1 - \frac{7}{4}u_2^2 + \frac{63}{8}u_2 u_1^2 - \frac{231}{64}u_1^4),$$

where u_k are the coefficients in the expansion of $U(x)$ about the point of the maximum:

$$U(x) = U_m - \frac{1}{2}\omega^2(x - x_m)^2[1 + u_1\rho + u_2\rho^2 + u_3\rho^3 + \ldots],$$

and $\rho = (x - x_m)/\xi_0 = \omega^{1/2}(x - x_m)$ is the dimensionless coordinate.

As an example we consider

$$U(r) = \frac{g^2}{\alpha}r^\alpha - \frac{1}{2(2-\alpha)}\omega^2 r^2, \quad \alpha < 2. \tag{2.18}$$

This potential has a maximum at $r = r_m$:

$$r_m = \left[(2-\alpha)\frac{g^2}{\omega^2}\right]^{1/(2-\alpha)}, \quad U_m = \frac{1}{2\alpha}\left[(2-\alpha)\frac{g^2}{\omega^\alpha}\right]^{2/(2-\alpha)},$$

with $U''(r_m) = -\omega^2$ for an g and α. For energies E close to U_m, we have

$$r_{1,2}=r_m\{1\mp[(U_m-E)/\alpha U_m]^{1/2}\}+O(U_m-E),$$

$$a=J-(\alpha-1)(\alpha+2)bJ^2+O(J^3),\qquad(2.19)$$

where

$$b=\omega^{(2+\alpha)/(2-\alpha)}[(2-\alpha)g^2]^{-2/(2-\alpha)}>0.$$

For $E=U_m$ the two turning points $r_{1,2}$ collide, and for $E>U_m$ they emerge into the complex plane.

As can be seen from (2.19), the coefficient of J^2 vanishes for $\alpha=1$ or $\alpha=-2$. These values of α in (2.18) correspond to exactly solvable models, which are considered in the next subsection. Here, all the subsequent coefficients of the expansion (2.17) are identically equal to zero, i.e., $a(J)\equiv J$ for all $E>U_m$. This implies that for the potential $U_m-U(x)$ the period T of the oscillations does not depend on the amplitude. In particular, this property is possessed by the potential

$$U(r)=\frac{g^2}{2r^2}+\frac{1}{8}\omega^2r^2,\qquad(2.20)$$

for which $T=2\pi/\omega$ irrespective of the values of E and g.

g) We make a comment concerning the relationship of Eqs. (1.3) and (2.1) to the results of previous authors. The influence of barrier penetration on the semiclassical quantization rules has been considered previously by Rice and Good,[14] Connor,[5] Drukarev,[6] and Kondratovich and Ostrovskiĭ.[15] The expressions obtained in Refs. 6 and 15 for the correction to the quantization rule correspond to the function

$$\varphi(a)=\arg\Gamma(\tfrac{1}{2}+ia)+a(1-\ln a),$$

which is practically the same as (1.4) if a is real and $a\gg1$, i.e., if the penetration of the barrier is small. However, this approximation determines only the shift and not the width of the level [to obtain Eqs. (2.2) and (2.3) it is necessary to take Im $\varphi(a)$ into account]. As the energy of the level approaches the top of the barrier, when $|a|\lesssim1$, this approximation loses it validity. A formula equivalent to (1.5) was obtained by Connor.[5] We note that in the papers indicated above there was no consideration of the solution of Eq. (1.3) for above-barrier resonances, when the parameter a is complex, and the correction of order $\hbar^2$ to the semiclassical approximation was also not taken into account.

The theory of the penetration of multidimensional potential barriers without the assumption of spherical symmetry has been stimulating considerably interest recently. Usually, separation of variables is not assumed in this case, and the penetration of the barrier is assumed to be small. In this case the problem reduces to the determination of the most probable sub-barrier trajectory, as has been demonstrated for the example of the two-dimensional anisotropic anharmonic oscillator[16] (see also Refs. 17 and 18). It is evident that (for potentials with separable variables) Eq. (2.3) can be obtained in this way, although this result is not contained in the papers indicated above. For a specific problem (the Stark effect in the hydrogen atom, $f=2$) such a formula was obtained in Ref. 19.

The quantization rules (1.3) and (1.6) can have various physical applications. We turn to the consideration of some examples.

3. EXACTLY SOLVABLE MODELS

First of all, we consider several potentials with spherical symmetry, for which the Schrödinger equation can be solved analytically.

1) The rectangular barrier:

$$V(r)=\begin{cases}U_0,&L<r<L+R,\\0,&0<r<L\ \ \text{or}\ \ r>R+L.\end{cases}$$

We have the following equation for the energy E of the quasistationary states:

$$\frac{(\varkappa-ik)(\varkappa+k\ \text{ctg}\ kL)}{(\varkappa+ik)(\varkappa-k\ \text{ctg}\ kL)}=e^{-2\varkappa R},\qquad(3.1)$$

where $l=0,\ k^2=2E,\ \varkappa^2=2(U_0-E),\ k^2+\varkappa^2=2U_0$, and $\hbar=1$.

Assuming $\exp(-2\varkappa R)\ll1$, from this we obtain[20,21]

$$\frac{\Delta E_r}{E_0}=\frac{4\varepsilon(1-2\varepsilon)}{1+\varkappa_0L}e^{-2\varkappa_0R},$$

$$\frac{\Gamma}{E_0}=\frac{16\varepsilon^{1/2}(1-\varepsilon)^{1/2}}{1+\varkappa_0L}e^{-2\varkappa_0R},\qquad(3.2)$$

where $\varepsilon=(U_0-E_0)/U_0(0<\varepsilon<1),\ E=E_0+\Delta E_r-i\Gamma/2$, and the values of $\varkappa_0$ and $E_0=k_0^2/2$ are calculated with neglect of the penetrability of the barrier, i.e., $k_0\cot k_0L=-\varkappa_0$. Since the coefficient of transmission through a rectangular barrier is equal to[1]

$$D=\frac{4k^2\varkappa^2}{(k^2+\varkappa^2)\text{sh}^2\ \varkappa R+4k^2\varkappa^2}=16\varepsilon(1-\varepsilon)e^{-2\varkappa_0R}+O(e^{-4\varkappa_0R}),$$

and the period of the oscillations is $T=2L/k_0$, we have

$$\Gamma=\frac{\varkappa_0L}{1+\varkappa_0L}T^{-1}D+O(D^2),\qquad(3.3)$$

which coincides with the Gamov formula for $L\gg1/\varkappa_0$. The difference from (2.2) in the pre-exponential factor is due to the fact that the potential under consideration is not smooth. Note that the level shift ΔE_r is exponentially small, and changes sign at $\varepsilon=\frac{1}{2}$ (i.e., at $E_f=\frac{1}{2}U_0$).

2) The parabolic barrier ($l=0$):

$$V(r)=-\tfrac{1}{2}\omega^2(r-R)^2,\quad0<r<\infty.\qquad(3.4)$$

The substitution $x=(2\omega)^{1/2}e^{-i\pi/4}(r-R)$ brings the Schrödinger equation to the standard form

$$\frac{d^2\chi}{dx^2}+\left(v+\frac{1}{2}-\frac{x^2}{4}\right)\chi=0,$$

where $v=-(1/2+ia)$ and $a=-E/\omega$. The spectrum of quasistationary states is determined from the condition of regularity at zero: $\chi(0)=0$, whence

$$D_v(-2^{1/2}e^{-i\pi/4}s)=0,\qquad(3.5)$$

where $s=\omega^{1/2}R$. Assuming $n\gg1$ and $|E|\ll1/2\omega^2R^2$, and using the asymptotic form of the parabolic-cylinder functions,[4] from the exact equation (3.5) we obtain

$$s^2-a\left(\ln\frac{s^2}{a}+1+\ln2\right)+\varphi(a)=2\pi(n-\tfrac{1}{4}).\qquad(3.6)$$

On the other hand, in this case

$$r_0=0, \qquad r_1=R(1-\varepsilon^{1/2}), \qquad \int_0^{r_1} p\,dr = {}^1\!/_2 s^2 \Phi(\varepsilon),$$

where $\varepsilon = -E/V_0 = 2a/s^2$ and

$$\Phi(\varepsilon) = (1-\varepsilon)^{1/2} - \varepsilon\,\mathrm{arth}(1-\varepsilon)^{1/2}$$

$$= \begin{cases} 1 + {}^1\!/_2\varepsilon \ln\varepsilon - ({}^1\!/_2 + \ln 2)\varepsilon + {}^1\!/_8\varepsilon^2 + \ldots, & \varepsilon\to 0, \\ {}^2\!/_3(1-\varepsilon)^{1/2} + O((1-\varepsilon)^{5/2}), & \varepsilon\to 1. \end{cases}$$

The usual Bohr–Sommerfeld quantization condition and the Gamov formula take the following form:

$$s^2\Phi(\varepsilon) = 2\pi(n - {}^1\!/_4), \qquad n=1,\,2,\,\ldots, \tag{3.7}$$

$$\Gamma = {}^1\!/_2\omega\,[\mathrm{arth}\,(1-\varepsilon)^{1/2}]^{-1}\exp(-\pi s^2\varepsilon). \tag{3.8}$$

Equation (3.5) can be rewritten in the following form:

$$\left. {}_2F_0\!\left(\frac{1}{4} - \frac{ia}{2}, \frac{3}{4} - \frac{ia}{2};\, is^{-2}\right) \right/$$

$${}_2F_0\!\left(\frac{1}{4} + \frac{ia}{2}, \frac{3}{4} + \frac{ia}{2};\, -is^{-2}\right)$$

$$= (2\pi)^{-1/2}\Gamma\!\left(\frac{1}{2} + ia\right)\exp\left\{\frac{1}{2}\pi a\right.$$

$$\left. + i\left[s^2 - a\ln 2s^2 - 2\pi\left(n - \frac{1}{4}\right)\right]\right\}, \tag{3.9}$$

which is convenient for numerical calculation. Here the ratio of hypergeometric functions ${}_2F_0$ has been replaced by a Padé approximant $[N/N]$, and this, for $N = 5$, already ensures an accuracy of the order of 10^{-8} in the calculation of the energy. The results of the calculation are collected in Table I. Writing the potential (3.4) in the standard form

$$V(r) = -\frac{g}{2R^2}\,v(x), \qquad x = \frac{r}{R},$$

we have

$$v(x) = (1-x)^2\theta(1-x), \qquad g = \omega^2 R^4 \equiv s^4,$$

where g is the dimensionless coupling constant. We have denoted by g_n that value of the coupling constant for which the level "touches" the top of the barrier (i.e., $\mathrm{Re}\,E_n = U_m = 0$). In the first two columns of Table I we give the ratios g_{cl}/g_n and $\tilde{g}_{cl}/g_n$, which characterize the accuracy of the semiclassical approximation. Here, $g_{cl}(sn) = 4\pi^2(n - 1/4)^2$ is the value that follows (for $\varepsilon = 0$) from (3.7), and $\tilde{g}_{cl}$ is the value that follows from (3.6), including the function $\varphi(a)$. It can be seen that g_{cl} and $\tilde{g}_{cl}$ approach the exact values g_n from opposite sides, and that, starting from $n = 2$, the $\tilde{g}_{cl}$ have a higher accuracy than the g_{cl}. Thus, allowance for the penetration of the barrier considerably improves the accuracy of the semiclassical approximation.

Table I also contains the "reduced" widths

$$\gamma_n = [\Gamma_n/2(n - {}^1\!/_4)\,\omega]_{g=g_n} \tag{3.10}$$

and the quantities $\delta_n = \tilde{\gamma}_n/\gamma_n - 1$ [γ_n have been calculated using the exact equation (3.9), and $\tilde{\gamma}_n$ have been calculated from (3.6)]. As follows from Table I, the semiclassical equation (3.6), obtained under the condition $n \gg 1$, also remains applicable for small quantum numbers, including the ground state.[2] The introduction of the correction for the penetration of the barrier makes it possible to calculate both the position and the width of the resonance level, and in a wide range of energies.

We have also checked that the asymptotic relation (2.16) is fulfilled. The derivative dE_n/dn at $n = n_*$ was replaced by $1/2\,\mathrm{Re}\,\{E_{n+1}(R_n^*) - E_{n-1}(R_n^*)\}$, where the value R_n^* is determined from the condition $\mathrm{Re}\,E_n(R_n^*) = 0$. Although n_n tends to the limit η_∞ rather slowly, the form of the expansion (2.16) is fully confirmed (in view of the large numerical value of the constant k it is necessary to incorporate it in the expansion parameter L^{-2}).

3) For

$$V(r) = -\frac{\alpha^2}{2r^2} - \frac{1}{8}\omega^2 r^2, \tag{3.11}$$

it is possible to find the exact solution for arbitrary angular momentum l. The effective potential U, including the centrifugal energy, has the same form, but with the replacement

TABLE I.

n_r	g_{cl}/g_n	$\tilde{g}_{cl}/g_n$	γ_n	δ_n
0	1,020 150	0,967 219	1,0380 (—1)	1,299 (—2)
1	1,012 862	0,993 747	3,7837 (—2)	2,316 (—3)
2	1,008 655	0,997 462	2,2234 (—2)	8,885 (—4)
3	1,006 416	0,998 636	1,5484 (—2)	4,579 (—4)
4	1,005 058	0,999 151	1,1770 (—2)	2,760 (—4)
5	1,004 155	0,999 421	9,4392 (—3)	1,833 (—4)
10	1,002 142	0,999 835	4,6068 (—3)	4,890 (—5)
20	1,001 049	0,999 956	2,1848 (—3)	1,185 (—5)
30	1,000 681	0,999 980	1,4032 (—3)	5,14 (—6)
40	1,000 500	0,999 989	1,0235 (—3)	2,83 (—6)
50	1,000 393	0,999 9926	8,0092 (—4)	1,78 (—6)
100	1,000 185	0,999 9981	3,7374 (—4)	4,2 (—7)
200	1,000 087	0,999 9995	1,7462 (—4)	9,8 (—8)

Note. The figures in brackets denote the order of the number, i.e. $(-k) \equiv 1)^{-k}$. The reduced widths γ_n correspond to the coupling constant $g = g_n$ at which, in the potential (3.4), an ns level appears (i.e., $\mathrm{Re}\,E_n = 0$). The quantities $\delta_n = \tilde{\gamma}_n/\gamma_n - 1$ determine the error in the semiclassical equation (3.6) for the width of the level.

$$\alpha \to g = [\alpha^2 - (l + \tfrac{1}{2})^2]^{1/2}. \tag{3.12}$$

If $\alpha > 1 + \tfrac{1}{2}$ (the condition for "collapse to the center"[1]), the potential $U(r)$ possesses a barrier. Let us consider this case.

Cutting off $U(r)$ at some $r = r_0 \ll r_1$, we obtain

$$\int_0^{r_1} p\, dr = \frac{g}{2}\left(\ln\frac{r_m}{r_0} - 1\right) - gQ_{cl}(\varepsilon) + \gamma' = (n - \tfrac{1}{4})\pi,$$

where

$$r_m = (2g/\omega)^{1/2}, \quad r_{1,2} = r_m[(\varepsilon+1)^{1/2} \mp \varepsilon^{1/2}],$$

$r_{1,2}$ are the turning points, $\varepsilon = (E - U_m)/2U_m$ ($\varepsilon > 0$ for $< U_m$, since $U_m = -\tfrac{1}{2}g\omega < 0$),

$$Q_{cl}(\varepsilon) = \tfrac{1}{2}[(\varepsilon + 1)\ln(\varepsilon + 1) - \varepsilon \ln \varepsilon],$$

and the phase γ' (which is independent of the energy) is the contribution from the region $0 < r < r_0$.

As usual in problems with collapse to the center, to eliminate the dependence of the spectrum on the region of short distances it is convenient to fix the energy of one of the levels ($n = n_0$). This leads to the quantization condition

$$Q_{cl}(\varepsilon_n) - Q_{cl}(\varepsilon_0) = -n\pi/g, \tag{3.13}$$

($n = 0, \pm 1, ...$). From this, in the case $\varepsilon \gg 1$, we obtain

$$E_n = E_0 \exp(-2\pi n/g), \tag{3.14}$$

which is characteristic[23] for an attractive potential $U \propto -1/r^2$ (near the top of the barrier this approximation is inapplicable). In the given case,

$$a = g\varepsilon = \frac{U_m - E}{\omega}, \quad T = \omega^{-1}\ln(1 + \varepsilon^{-1})$$

and the Gamov formula takes the form

$$\Gamma_n = \omega b_n e^{-2\pi a_n}, \quad b_n = \left[\ln\left(1 + \frac{g}{a}\right)\right]^{-1} = \left[\ln\left(1 + \frac{1}{\varepsilon_n}\right)\right]^{-1}. \tag{3.15}$$

Let us compare these results with the exact solution. The substitution

$$\chi_l(r) = \xi^{-1/4} w(\xi), \quad \xi = -\tfrac{1}{2}i\omega r^2$$

brings the Schrödinger equation to the form

$$\frac{d^2 w}{d\xi^2} + \left\{-\frac{1}{4} + i\frac{E}{\omega\xi} + \frac{1 + \alpha^2 - (l + \tfrac{1}{2})^2}{4\xi^2}\right\}w = 0,$$

whence

$$\chi_l(r) = \text{const } \xi^{-1/4} W_{\varkappa,\mu}(\xi), \tag{3.16}$$

where $W_{\varkappa,\mu}$ is the Whitaker function, with $\varkappa = iE/\omega$ and $\mu = ig/2$. This solution corresponds to a quasistationary state, since, for $r \to \infty$,

$$\chi_l(r) \propto \exp\left(\frac{i}{4}\omega r^2 + 2\varkappa \ln r\right) \propto \exp\left(i\int^r p\, dr\right)$$

(the radiation condition). For $\alpha > 1 + \tfrac{1}{2}$ the wave function oscillates for $r \to 0$:

$$\chi_l(r) = \text{const } \xi^{1/4}(A\xi^{-ig/2} + B\xi^{ig/2}),$$
$$A = \Gamma(ig)/\Gamma(\tfrac{1}{2} + ig(\varepsilon+1)), \quad B = \Gamma(-ig)/\Gamma(\tfrac{1}{2} + ig\varepsilon), \tag{3.17}$$

and the boundary condition $\chi_l(0) = 0$ does not determine the energy spectrum, since it is fulfilled for arbitrary ε.

Following Ref. 23, to obtain the quantization condition we impose the requirement that the wave functions corresponding to the energy E_n and to a certain (fixed) energy E_0 be mutually orthogonal. It follows directly from the Schrödinger equation that

$$(E_n - E_0)\int_0^\infty \chi_n\chi_0\, dr$$
$$= \left(-\frac{i}{2}\omega\xi\right)^{1/2}(\chi_0'\chi_n - \chi_n'\chi_0)\big|_0^\infty, \quad \chi' = \frac{d\chi}{d\xi}.$$

As $R \to \infty$ the right-hand side vanishes, since

$$\xi^{1/2}(\chi_0'\chi_n - \chi_n'\chi_0) \propto \xi^{\varkappa_n + \varkappa_0 - 1}e^{-\xi} \propto r^\lambda \exp(\tfrac{1}{4}i\omega r^2)$$
$$\lambda = -1 + i(E_n + E_0)/\omega.$$

On the other hand,

$$\xi^{1/2}(\chi_0'\chi_n - \chi_n'\chi_0)\big|_{\xi=0} = \text{const }(A_n B_0 - A_0 B_n).$$

When (3.17) is taken into account the orthogonality condition takes the previous form (3.13) if in place of $Q_{cl}(\varepsilon)$ we substitute

$$Q(\varepsilon, g) = \frac{1}{2ig}\ln\frac{\Gamma(\tfrac{1}{2} + ig(\varepsilon+1))}{\Gamma(\tfrac{1}{2} + ig\varepsilon)}. \tag{3.18}$$

Thus, we have obtained the exact quantization condition for the potential (3.11).

For $g \gg 1$, we can use the asymptotic expansion for $\ln \Gamma(z + 1/2)$, which gives

$$Q(\varepsilon, g) = Q_{cl}(\varepsilon) + c - \frac{1}{48g^2(\varepsilon^2 + \varepsilon)} + \frac{3(\varepsilon^2 + \varepsilon) + 1}{5760g^4(\varepsilon^2 + \varepsilon)^3} + \dots, \tag{3.19}$$

where $c = c(g)$ is a constant that does not depend on ε and so is important in (3.13). The quantum corrections to the Bohr–Sommerfeld quantization rule [the third and fourth terms in the right-hand side of (3.19)] increase without limit as $\varepsilon \to 0$, and therefore Eq. (3.13) is not applicable near the top of the barrier. Allowance for the correction for the penetration of the barrier reduces to the replacement

$$Q_{cl} \to \tilde{Q} = Q_{cl} - \varphi(a)/2g.$$

Then

$$Q(\varepsilon, g) = \tilde{Q} + c + \frac{1}{48g^2(\varepsilon+1)} + \dots . \tag{3.19'}$$

In this case the quantum correction remains bounded for all $\varepsilon > 0$ (or $E \leqslant U_m$), and therefore Eq. (3.13), with Q_{cl} replaced by $\tilde{Q}$, can be used for $E \approx U_m$ as well. This is the

advantage of (1.3) in comparison with the usual Bohr-Sommerfeld quantization rule.

If we substitute $a = a_n + i\Gamma_n/2\omega$ into (3.18) and assume $\Gamma_n \ll \omega a_n$, it is not difficult to obtain a refinement of the Gamov formula. As we should expect, this differs from (3.15) only in the pre-exponential factor:

$$b_n = \left[\ln \beta_n + \frac{1-\beta_n^2}{24a^2} + O(a^{-4}) \right]^{-1}, \qquad (3.20)$$

where $\beta_n = 1 + g/a = 1 + \varepsilon_n^{-1}$ (in the sub-barrier region, $\beta_n > 1$).

4) For the potential

$$V(r) = -\frac{\alpha^2}{2r^2} + \frac{\zeta}{r}, \quad \alpha > l + \frac{1}{2}, \qquad (3.21)$$

the exact solution can also be expressed in terms of the Whitaker function:

$$\chi_l(r) = \text{const} \, W_{\varkappa,\mu}(2\lambda r), \quad \varkappa = -\zeta/\lambda, \quad \mu = ig, \qquad (3.22)$$

where $\lambda = (-2E)^{1/2}$ and g has the previous value (3.12). The wave function corresponding to a quasistationary state is obtained from this with $\lambda = -ik$. We arrive at the following equation for the spectrum of the quasistationary states:

$$\frac{\Gamma(\frac{1}{2}+i(\zeta k_n^{-1}+g))\Gamma(\frac{1}{2}+i(\zeta k_0^{-1}-g))}{\Gamma(\frac{1}{2}+i(\zeta k_n^{-1}-g))\Gamma(\frac{1}{2}+i(\zeta k_0^{-1}+g))} = \left(\frac{k_0}{k_n}\right)^{2ig} e^{-2\pi i n}, \qquad (3.23)$$

which can also be written in the form (3.13) if we replace the function $Q_{cl}(\varepsilon)$ by Q:

$$Q(k,g) = \ln k + \frac{1}{2ig} \ln \left\{ \Gamma\left(\frac{1}{2} + i\left(\frac{\zeta}{k}+g\right)\right) \right/$$

$$\Gamma\left(\frac{1}{2} + i\left(\frac{\zeta}{k}-g\right)\right) \right\}, \qquad (3.24)$$

with $k = (2E)^{1/2}$. The given potential can be considered without difficulty in the semiclassical approximation. In particular, here

$$r_{1,2} = r_m (1 \pm \varepsilon^{1/2})^{-1}, \quad r_m = g^2/\zeta, \quad U_m = \zeta^2/2g^2,$$

$$a = g[(1-\varepsilon)^{-1/2} - 1] = 2J_0 \left[\left(1 - \frac{J}{J_0}\right)^{-1/2} - 1 \right], \qquad (3.25)$$

$$T = \frac{2}{\omega(1-\varepsilon)^{1/2}} [\text{arth}(1-\varepsilon)^{1/2} - (1-\varepsilon)^{1/2}],$$

where $\varepsilon = (U_m - E)/U_m$ (the quasistationary levels lie at $0 < \varepsilon < 1$), and $J_0 = g/2$ is the value of the invariant J at $E = 0$. Hence, for $E \to U_m$,

$$a(J) = J + \frac{3}{4J_0} J^2 + \frac{5}{8J_0^2} J^3 + \ldots, \qquad (3.26)$$

$$T = \omega^{-1} \left[\ln \frac{1}{\varepsilon} - 2(1 - \ln 2) + \ldots \right]$$

($\omega = \zeta^2/g^3$). On the other hand,

$$a \propto (1 - J/J_0)^{-1/2} \to \infty \text{ as } E \to 0,$$

and, therefore, the barrier penetration and the width Γ van-

ish, and for $\varepsilon > 1$ the spectrum is discrete.

In the latter two examples we have obtained for the quasistationary states comparatively simple analytical solutions, which, however, so far as we know, have not been considered in the literature. It is evident that this is due to the collapse to the center that occurs in such potentials. We note that Eqs. (3.18) and (3.23) cannot be obtained by analytic continuation of the known[1] solutions for the discrete spectrum. In fact, the latter follow from the condition of regularity of the wave function at zero ($A_n = 0$), whereas the spectrum of the quasistationary levels is determined from the condition $A_n/B_n = A_0/B_0$, where A and B are the coefficients for $r \to 0$; see (3.17).

4. STARK EFFECT IN A STRONG FIELD: CONDITIONS FOR APPLICABILITY OF THE GAMOV FORMULA

We apply the quantization condition (1.3) to the calculation of the Stark effect in a strong field.[3] Here the energy of the level can be close to the top of the barrier or even above the top (sub-barrier and above-barrier resonances, respectively). Below we use atomic units ($\hbar = e = m_e = 1$) and reduced variables

$$\varepsilon = 2n^2 E^{(n_1 n_2 m)} = \varepsilon' - i\varepsilon'', \quad \varepsilon'' = n^2 \Gamma^{(n_1 n_2 m)},$$

$$F = n^4 \mathscr{E}, \quad \mu = m/n, \qquad (4.1)$$

where $E^{(n_1 n_2 m)} = E_r - i\Gamma/2$ is the energy of the quasistationary state $|n_1 n_2 m\rangle$, $\mathscr{E}$ is the electric-field intensity in atomic units $m_e^2/\hbar^4 = 5.142 \times 10^9$ V/cm, n_1, n_2, and m are parabolic quantum numbers ($m \geqslant 0$), and $n = n_1 + n_2 + m + 1$ is the principal quantum number of the level.

Among all the sublevels $|n_1 n_2 m\rangle$ with a given n the states of greatest interest from the experimental point of view are the states $|n-1,0,0\rangle$ and those close to them in their quantum numbers, as these are the most stable. Such states are manifested[24,25] as peaks in the photo-ionization cross sections of atoms near the energy $E = 0$ (the ionization limit in the absence of an external field).

For the states with $m = 0$ in the hydrogen atom the integrals in the quantization conditions can be calculated analytically (see Appendix B). As a result we arrive at Eqs. (B10), in which[4]

$$\nu_1 = \left(n_1 + \frac{m+1}{2}\right) \bigg/ n, \quad \nu_2 = \left[n_2 + \frac{m+1}{2} - \frac{1}{2\pi}\varphi(a)\right] \bigg/ n, \qquad (4.2)$$

$$a = \frac{1}{\pi} \int_{\eta_1}^{\eta_2} (-p_\eta^2)^{1/2} d\eta = \frac{n(-\varepsilon)^{1/2}}{2\pi F} \int_{u_1}^{u_2} \frac{du}{u} (A - Bu + u^2 - u^3)^{1/2}, \qquad (4.3)$$

where

$$A = \mu^2 F^2/(-\varepsilon)^3, \quad B = z_2/4 = \beta_2 \mathscr{E}/E^2,$$

p_η is the semiclassical momentum for the coordinate η, and $\eta_{1,2}$ are the turning points ($\eta = r - z = -n^2 \varepsilon u/F, \varepsilon < 0$). For $m = 0$ we have $u_{1,2} = 1/2[1 \mp (1 - z_2)^{1/2}]$, so that the barrier in $U_2(\eta)$ vanishes at $z_2 = 1$ [which is a singular point

for the hypergeometric functions appearing in (B10)]. For $m \ll n$ we obtain from (4.3)

$$a = \frac{n(-\varepsilon)^{1/2}}{2^{1/2}F}\{(1-z_2)F(^1/_4,^3/_4; 2; 1-z_2)$$

$$+ \mu^2 \frac{8F^3}{(-\varepsilon)^3}F(^3/_4,^5/_4; 1; 1-z_2)+O(\mu^4)\}. \qquad (4.4)$$

Thus, all the quantities appearing in the quantization conditions have been calculated explicitly in terms of the hypergeometric functions $F(...; z) \equiv {}_2F_1(...; z)$. Therefore, the procedure for analytic continuation to arbitrary complex values of ε, β_1, and β_2 does not present difficulties in the present case.

In solving the system (B10) numerically it is possible either to discard the terms $\propto F/8n^2$ or to solve the complete system of equations (we call these two variants of the calculation the $1/n$ and $1/n^2$ approximations, respectively). We have calculated E_r and Γ for various states $|n_1 n_2 m\rangle$ of the hydrogen atom, using these equations and also an independent method—summation of the divergent perturbation-theory series in powers of $\mathscr{E}$ by means of Padé-Hermite approximants (PHA); for details of the latter method, see Ref. 21. We give some results.

We consider first the positions of the Stark resonances $|n_1,0,0\rangle$ with $n_1 = n - 1$. Table II gives the values of $-\varepsilon'_n = -2n^2 E_r^{(n-1,0,0)}$ for $n = 20$ (analogous results have also been obtained for $n = 10$ and $n = 50$). It can be seen that the effect of barrier penetration on the position E_r of the resonance is not great [compare rows (a) and (b) for the same F], although with increase of the field it increases slightly (the PHA method is very accurate in the weak-field region, but for $F \gtrsim 0.3$ it already has a lower accuracy than the semiclassical equations).

The corresponding results for the imaginary part of the energy are given in Fig. 1. It follows from this figure that the penetration correction to the width of the levels is very important in the region $F \lesssim F_*$, but with further increase of F its role is reduced. For $n \gtrsim 20$, with an accuracy sufficient for
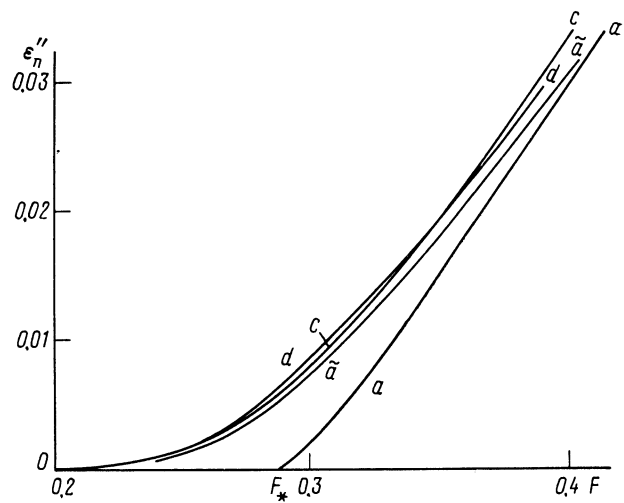

FIG. 1. Reduced width $\varepsilon_n'' = n^2\Gamma_n$ for the $|9,0,0\rangle$ with $n = 10$. Curve a: $1/n$ approximation without allowance for barrier penetration, i.e., $\varphi(a) \to 0$; curve $\tilde{a}$: $1/n$ approximation with allowance for barrier penetration [see (4.2)]; curve c: result of the PHA method (Ref. 21); curve d: $1/n$ approximation improved as in (4.7).

experiment, in most cases we can confine ourselves to the $1/n$ approximation.

We note that this approximation has entirely acceptable accuracy even for small n. For example, from (4.3) and (b.10) it is not difficult to obtain an approximate asymptotic form $\tilde{\Gamma}(\mathscr{E})$ of the width of a level in a weak field:

$$\Gamma^{(n_1 n_2 m)}(\mathscr{E}) \approx \mathrm{const} \cdot F^{-(2n_2+m+1)} \exp(-2n/3F). \qquad (4.5)$$

It differs from the exact[1] asymptotic form $\Gamma(\mathscr{E})$ for $\mathscr{E} \to 0$ only by a numerical factor close to unity:

$$\tilde{\Gamma}^{(n_1 n_2 m)}(\mathscr{E})/\Gamma^{(n_1 n_2 m)}(\mathscr{E}) = \omega(n_2)\omega(n_2+m), \qquad (4.6)$$

where

$$\omega(x) = (2\pi)^{-1/2}\Gamma(x+1)[(2x+1)/2e]^{-(x+1/2)}.$$

TABLE II. Position of the Stark resonance $|19,0,0\rangle$ in an electric field $\mathscr{E}$.

$F = n^4\mathscr{E}$	$1/n$		$1/n^2$	PHA
0,10	(a)	0,72 994	0,73 000	0,7300
0,20	(a)	0,48 280	0,48 309	0,4831
	(b)	0,48 301	0,48 309	
0,25	(a)	0,36 628	0,36 692	0,367
	(b)	0,36 677	0,36 695	
0,30	(a)	0,25 489	0,25 696	0,256
	(b)	0,25 619	0,25 663	
0,35	(a)	0,1502	0,1498	0,149
	(b)	0,1490	0,1488	
0,40	(a)	0,0432	0,0425	0,042
	(b)	0,0421	0,0413	
0,45	(a)	−0,0643	−0,0625	−0,065
0,50	(a)	−0,1716	−0,1727	−0,173
0,60	(a)	−0,3842	−0,3855	−0,386
0,70	(a)	−0,5923	−0,5936	−0,596
1,00	(a)	−1,1896	−1,1907	−1,19

Note. The table gives the reduced energies $-\varepsilon'_n$, taken with the opposite sign. (a) indicates the calculations using Eqs. (B10) without barrier penetration [i.e., we set $\varphi(a) \equiv 0$]; (b) indicates the calculations with allowance for barrier penetration.

In particular, $\tilde{\Gamma}/\Gamma = e/\pi = 0.865$ in the case of the ground level, $\tilde{\Gamma}/\Gamma = 0.94$ for the state $|0,1,00\rangle$, $\tilde{\Gamma}/\Gamma = (e/\pi)^{1/2}(1 - 1/24n + ...)$ for the states $|0,0,n-1\rangle$ corresponding to circular electron orbits, and so on. The difference of $\tilde{\Gamma}$ from Γ is connected with the fact that the semiclassical approximation is not applicable for small quantum numbers. Nevertheless, for all n_1, n_2, and m the dependence of $\tilde{\Gamma}$ and Γ on the field is the same.

The semiclassical approximation can be improved in such a way that in the weak-field region the width of the levels coincides with the exact asymptotic form. For this it is sufficient to introduce a correction to the parameter a (a correction that depends on the quantum numbers of the state but does not depend on $\mathscr{E}$):

$$a \to a - \Delta a,$$

$$\Delta a = \alpha(n_2) + \alpha(n_2 + m), \tag{4.7}$$

where $\alpha(x) = -(1/2\pi)\ln\omega(x)$. This correction is numerically very small: $\alpha(0) = 0.0115$, $\alpha(1) = 0.0043$, and $\alpha(x) = (48\pi x)^{-1}$ for $x \gg 1$. It is interesting to note that

$$\alpha(x) = (i/2\pi)\varphi(-i(x+^{1}/_{2})), \tag{4.8}$$

where φ is the function introduced in (1.4).

We note first of all that the PHA have high accuracy ($\sim 10^{-5} - 10^{-6}$ for the energies of the levels) for $F \leqslant 0.3$. Therefore, in the region $F < 0.4$ curve c coincides, to within the accuracy of the figure, with the exact solution. For curve a at $F < F_*$ we have[5] $\Gamma \equiv 0$, and this is a defect of this approximation. Allowance for the penetration of the barrier removes this defect, while the introduction of the correction (4.7) not only restores the correct asymptotic form $\Gamma(\mathscr{E})$ for $\mathscr{E} \to 0$ but also leads to results that practically coincide with those obtained by the PHA method.

A detailed comparison of the various approximations is contained in Table III, which pertains to the state $|0,1,0\rangle$, for which, with increase of the field, the resonance energy E_r decreases monotonically and the width Γ increases. Here we have given the results of the $1/n$ and $1/n^2$ approximations and the PHA method; some results have been taken from the recent paper by Telnov.[26] The agreement between the different calculations is good. We note the following:

1) The position E_r of the resonance is calculated in the $1/n$ and $1/n^2$ approximations more accurately than is the width Γ. As already noted above, for $F < F_*$ these approximations without the correction $\varphi(a)$ do not determine the width of a level.

2) Although the semiclassical approximation is valid, generally speaking, for $n \gg 1$, its region of applicability is "stretched out" to small quantum numbers.

3) In very strong fields ($F \gtrsim 1$) the quantities E_r and Γ can be calculated without allowance for the penetration, especially in the $1/n^2$ approximation (this tendency is noticeable even in Fig. 1). Thus, analytic continuation of the Bohr–Sommerfeld quantization conditions into the above-barrier region makes it possible to calculate both the position and the width of a quasistationary level.

The equations (B10) can be generalized to the Rydberg states of an arbitrary atom.[19,21] They have already been applied to the calculation of the Stark resonances in the atoms H, Na, and Rb, and good agreement with the experimental photo-ionization spectra has been obtained.

We turn to the question of the region of applicability of the Gamov formula. The period T of the oscillations tends to infinity as $E \to U_m$, and therefore the Gamov formula ceases to work near the top of the barrier. For the model (3.11), comparing Eqs. (3.15) and (3.20) we find this condition in the form $a^1 \gg [24 \ln (1/\varepsilon)]^{-1}$, which excludes only a narrow region of energies near the top of the barrier (compare

TABLE III. Stark resonance $|0,1,0\rangle$ in the hydrogen atom.

$\mathscr{E}$ (F)	$-E_r$	$\Gamma/2$	$\mathscr{E}$ (F)	$-E_r$	$\Gamma/2$
3,125 (—3) (0,05)	(a) 0,13505	—	0,03 (0,48)	(a) 0,243	6,01 (—2)
	(ã) 0,13540	1,58 (—8)		(ã) 0,239	5,87 (—2)
	(b) 0,135270	—		(c) 0,240	6,01 (—2)
	(b̃) 0,135275	1,61 (—8)		(e) 0,2401	5,982 (—2)
	(c) 0,135276	1,72 (—8)	0,05 (0,80)	(a) 0,2937	0,124
5,03 (—3) (0,08)	(a) 0,14184	—		(ã) 0,2938	0,121
	(ã) 0,14275	4,956 (—5)		(b) 0,2943	0,127
	(b) 0,14251	—		(e) 0,2960	0,1232
	(b̃) 0,142606	4,949 (—5)	0,1 (1,6)	(a) 0,3828	0,276
	(c) 0,142619	5,297		(b) 0,3866	0,283
	(e) 0,142619	5,2972		(e) 0,3927	0,2861
0,01 (0,16)	(ã) 0,166094	5,28 (—3)	0,2 (3,2)	(a) 0,5021	0,547
	(b) 0,162654	—		(b) 0,5120	0,566
	(b̃)			(e) 0,5107	0,5727
	(c) 0,166094	5,443 (—3)	0,4 (6,4)	(a) 0,6600	1,026
	(e) 0,166094	5,4426		(b) 0,6728	1,060
0,02 (0,32)	(ã) 0,2063	2,98 (—2)		(e) 0,6676	1,056
	(c) 0,2067	3,040			
	(e) 0,2067	3,039			

Note. The values of $\mathscr{E}$, F, E_r, and $\Gamma/2$ are given in atomic units. The rows (a) and (ã) give the results of the $1/n$ approximation in Eqs. (B10), with and without allowance for barrier penetration, respectively; the rows (b) and (b̃) are the same for the $1/n^2$ approximation; the rows (c) give the results of the calculation by the PHA method; the rows (e) are results from Ref. 26.
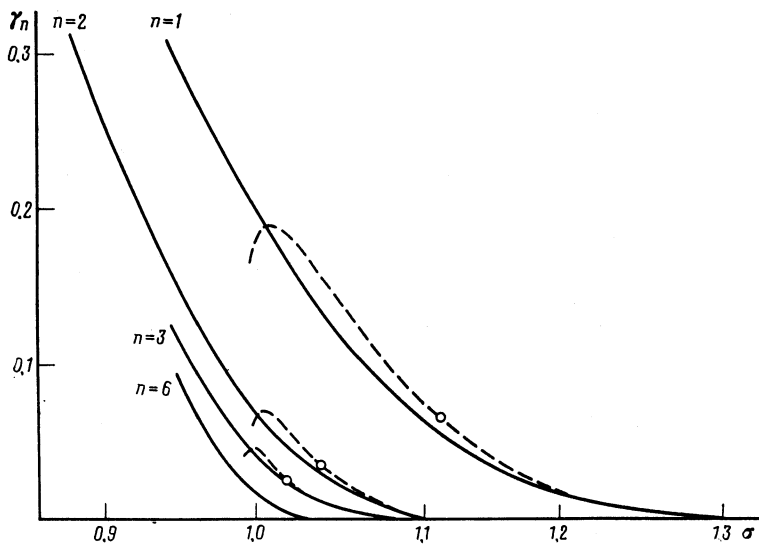
FIG. 2. Reduced width γ_n [see (3.10)] for ns levels in the potential (3.4). The points for which $a = 1$ are denoted by 0. The solid curves are from an exact calculation using (3.9), and the dashed curves are obtained from the Gamov formula (3.8); $\sigma = (g/g_n)^{1/4}$.

with the curves in Fig. 2).

We now consider the Stark effect that corresponds to the multidimensional problem with $f = 2$ degrees of freedom. Taking (2.6) into account, we find

$$c = \frac{4\sigma_1\tau_2}{\sigma_1\tau_2 + \sigma_2\tau_1}, \qquad T_\eta = 2 \int_{\eta_0}^{\eta_1} \frac{d\eta}{p_\eta} = 4n^3\tau_2, \qquad (4.9)$$

$$\Gamma^{(n_1 n_2 m)} = \frac{\sigma_1}{n^3(\sigma_1\tau_2 + \sigma_2\tau_1)} \exp(-2\pi a), \qquad (4.10)$$

where, according to (2.5) and (2.6),

$$\sigma_i = \int_{q_0}^{q_1} \frac{dq}{q k_i(q)}, \qquad \tau_i = \int_{q_0}^{q_1} \frac{dq}{k_i(q)}, \qquad (4.11)$$

and the $k_i(q)$ are defined in (B1).

The results of the calculation for the state $|9,0,0\rangle$ in the hydrogen atom are presented in Fig. 3. The solid curve is calculated by means of PHA and agrees well with the results of Kolosov;[27] the dashed curve is calculated from Eqs. (4.10) and (4.11) with $\mu = 0$. It follows from the figure that the generalized Gamov formula (2.3) has a high accuracy if $a \geqslant 1$, and is qualitatively applicable down to $a \approx 0.04$. Analogous results have been obtained for the states with $n = 15$ and 20.

5. THE RELATIVISTIC CASE

We shall discuss the question of the possibility of generalizing the previous approach to the relativistic region. Here we shall confine ourselves to the case of scalar particles and consider the Klein-Gordon equation in an external electrostatic field with spherical symmetry [$V(r) = eA^0(r)$, $\mathbf{A} = 0$]. The quantization condition retains the form (1.3), with

$$a = \frac{1}{\pi} \int_{r_1}^{r_2} (-p_r^2)^{1/2} dr = \frac{1}{\pi} \int_{r_1}^{r_2} dr \{1 - [E - V(r)]^2 + (l + 1/2)^2 r^{-2}\}^{1/2}$$

$$(5.1)$$

($p_r^2 < 0$ for $r_1 < r < r_2$). Here and below, $\hbar = m = c = 1$, m is the mass of the particle, E is the energy of the particle in units of mc^2, and l is the orbital angular momentum (the Langer correction has been taken into account).

Consider the case of a Coulomb field ($\zeta = Z\alpha \sim Z/137$, where Z is the charge of the nucleus). For
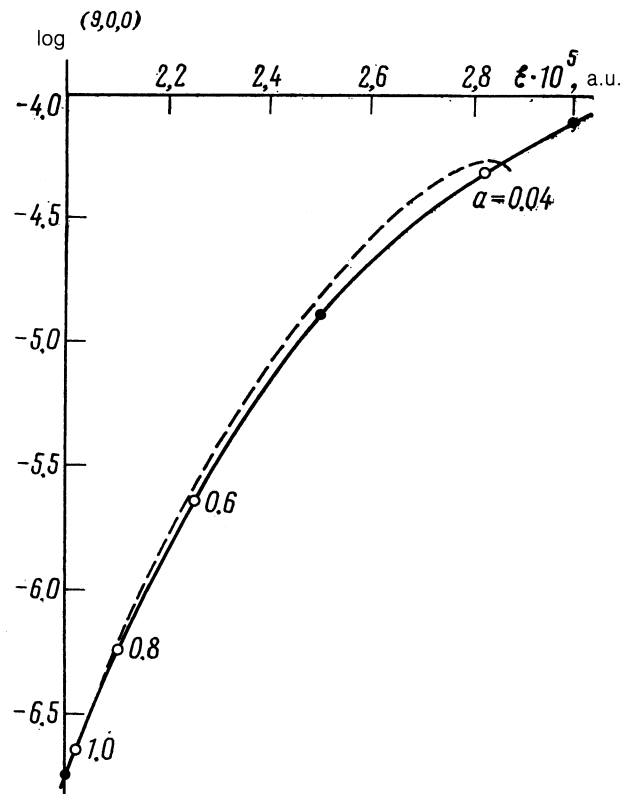

FIG. 3. Width of the level $|9,0,0\rangle$ in an electric field $\mathscr{E}$ ($n = 10$; O) points corresponding to the parameter values $a = 1.0$, 0.8, 0.6, and 0.04; ●) points corresponding to the results of Kolosov.[27] The solid curve is the result of the calculation by the PHA method; the dashed curve is obtained from Eqs. (4.10) and (4.11) with $\mu = 0$.

$\zeta > \zeta_{cr}^{(0)} = l + 1/2$, it is necessary to take the finite size of the nucleus into account.[28-31] We set

$$V(r) = \begin{cases} -\zeta/r, & r > r_N, \\ -(\zeta/r_N)f(r/r_N), & 0 < r < r_N, \end{cases} \qquad (5.2)$$

where r_N is the radius of the nucleus, and the cutoff function $f(x)$ is determined by the distribution of electric charge over the volume of the nucleus ($x = r/r_N, f(1) = 1, f(0) < \infty$). For $\zeta > \zeta_{cr}$ and $E < -1$ there is a barrier in the effective potential. So long as $|E| < \zeta/r_N$ holds the turning points $r_{1,2}$ lie outside the nucleus; their position does not depend on the model of the cutoff (see Appendix C), and

$$a = \zeta[(1 + k^{-2})^{1/2} - (1 - \rho^2)^{1/2}], \qquad (5.3)$$

where

$$k = (E^2 - 1)^{1/2}, \quad \rho = (l + 1/2)/\zeta, \quad 0 < \rho < 1.$$

For $k \to 0$, i.e., near the boundary $E = -1$, the quantity $\exp(-2\pi a)$ determines the exponentially small penetration of the Coulomb barrier for slow antiparticles. On the other hand, for deep ($|E| \gg 1$) levels the parameter a is almost independent of the energy, and therefore the correction for the barrier penetration in (1.3) reduces to a constant.

The equation determining the complex energies of the states with $\mathrm{Re}\, E \leqslant -1$ in the Coulomb field takes the following form:

$$g\left[\ln\left(\frac{r_1}{r_N}\right) - H(u)\right] + \mathrm{arcctg}\,\frac{\xi - 1/2}{g} + \frac{1}{2}\,\varphi(a) = \left(n - \frac{1}{4}\right)\pi, \qquad (5.4)$$

where $r_1 \gg r_N$, $n = n_r + 1 = 1, 2, ...,$

$$g = \zeta(1 - \rho^2)^{1/2}, \quad u = (1 - \rho^2)(1 - E^{-2}),$$

a is defined in (5.3), r_1 is defined in (C.1), the function $H(u)$ is defined in (C10), and ξ is the logarithmic derivative of the wave function at the edge of the nucleus [see (C4)]. The value of ξ depends on ζ, l, and the form of the cutoff $f(x)$, but does not depend on the energy (for $kr_N \ll 1$). Thus, for $f(x) \equiv 1$ we have

$$\xi = (2l + 1)\frac{\Lambda_{l-1/2}(\zeta)}{\Lambda_{l+1/2}(\zeta)} - l, \qquad (5.5)$$

where $\Lambda_\nu(\zeta)$ is a function closely related to the Bessel functions [see Eq. (C5)]. For an arbitrary model of the cutoff we have $\xi(\zeta = 0) = l + 1$, and ξ decreases with increase of ζ.

It is not difficult to solve Eq. (5.4) numerically. However, in the boson case, for $E \to -mc^2$ strong vacuum polarization arises,[32] leading to screening of the external potential $V(r)$. For $\zeta > \zeta_{cr}$ the one-particle Klein-Gordon equation ceases to be applicable, and the problem becomes an essentially many-particle problem. For this reason, this solution for spinless particles is only of methodological interest.

A different situation obtains for fermions. Owing to the Pauli principle, unrestricted increase of the vacuum polarization when a level intersects the boundary $E = -mc^2$ of the lower continuum is impossible,[31] and allowance for the vacuum polarization leads only to relatively small corrections to the numerical values of Z_{cr} and other physical quantities (see, e.g., Refs. 33 and 34). In this case the one-particle

approach remains applicable even for $Z > Z_{cr}$, by virtue of which the derivation of an equation analogous to (5.4) is of undoubted interest: Such an equation would simplify considerably the calculation of the positions and widths of positron resonances corresponding to states that have dropped into the lower continuum. In their basic features (with exponential accuracy) the formulas of the semiclassical approximation for the Klein-Gordon and Dirac equations do not differ from each other, although in an accurate calculation of the pre-exponential factor certain technical difficulties arise (in the case of fermions); see Ref. 35. We hope to return to this question in the future.

APPENDIX A

Consider the solution of Eq. (3.6) under the condition $s = \omega^{1/2}R \gg 1$, which ensures that the semiclassical approximation is applicable. In this case the total number of ns levels in the potential (3.4) is large:

$$n_0 = \frac{s^2}{2\pi} + \frac{1}{4} + O(s^{-2}) \qquad (A1)$$

[this follows from (3.7) with $\varepsilon = 0$]. Henceforth we assume that $|\varepsilon| \ll 1$, where $\varepsilon = -E/V_0 = 2a/s^2$ ($V_0 = 1/2\omega^2 R^2$).

1) In the sub-barrier region ($E_n < 0$, $a \ll 1$) Eq. (3.6), with the expansion (2.1) taken into account, takes the form

$$\varepsilon[\ln \varepsilon - (1 + 2\ln 2)] + \frac{i}{s^2}\,e^{-2\pi a} = -2\nu, \qquad (A2)$$

where $\nu = |n - n_0|/n_0$, and terms of order $1/\varepsilon s^2$ have been discarded (therefore, the condition for applicability of (A2) is $s^{-2} \ll \varepsilon \ll 1$, i.e., shallow levels, but not too close to the threshold $E = U_m$). Solving (A2) by iterations, we find

$$\varepsilon_n' = -\frac{E_r}{V_0} = 2\nu\left[\ln\frac{1}{\nu} + \ln\ln\frac{1}{\nu} + 1 + \ln 2 + ...\right]^{-1}, \qquad (A3)$$

$$\varepsilon_n'' = \frac{1}{s^2}\left(\ln\frac{1}{\varepsilon'} + 2\ln 2\right)^{-1}e^{-2\pi a},$$

whence ($n < n_0$)

$$E_n = 2\pi\omega(n - n_0)\left\{\Lambda + \ln\Lambda + O\left(\frac{\ln\Lambda}{\Lambda}\right)\right\}^{-1},$$

$$\Lambda = \ln\frac{2}{\nu} + 1,$$

$$\Gamma_n = \omega\left(\ln\frac{2\omega^2 R^2}{|E_n|}\right)^{-1}\exp\left(-\frac{2\pi|E_n|}{\omega}\right). \qquad (A4)$$

The expression for Γ_n agrees with Eq. (2.2), but the period of oscillations of a particle in the classically allowed region $0 < r < r_1 = R(1 - \varepsilon^{1/2})$ is equal to

$$T = 2\omega^{-1}\,\mathrm{arth}\,(1 - \varepsilon)^{1/2} = \omega^{-1}[\ln(4/\varepsilon) - 1/2\varepsilon + ...]. \qquad (A5)$$

As can be seen from (A4), the width of the levels here is exponentially small, with

$$\eta_n = \frac{\Gamma_n}{\Delta E_n} = \frac{1}{2\pi} \exp(-2\pi |E_n|/\omega) \ll 1. \tag{A6}$$

2) The region of energies near threshold: $E \approx 0$, $|a| \ll 1$. Taking into account the expansion

$$\varphi(a) = \tfrac{1}{2} i \ln 2 - a \ln a - (\alpha + i\beta) a + O(a^2), \tag{A7}$$

where $\alpha = C - 1 + 2 \ln 2$, $\beta = \pi/2$, and $C = 0.577$ is the Euler constant, it is not difficult to see that the terms $\propto a \ln a$ in (3.6) cancel altogether, and for E_n and Γ_n we arrive at Eqs. (2.15). For the ratio η_n we obtain

$$\eta_n = \frac{\Gamma_n}{\Delta E_n} = \frac{\ln 2}{2\pi} + \frac{E_n}{2\omega} + \dots , \tag{A8}$$

which, for $E_n = 0$, gives (2.16). For $E_n \sim \omega > 0$ neighboring resonances begin to overlap.

3) Finally, we consider the sub-barrier region: $E_n > 0$, $|a| \gg 1$, and $\varphi(a) = -2\pi i a + O(a^{-1})$; see Ref. 19. From this we have

$$\varepsilon [\ln \varepsilon - (1 + 2 \ln 2 + 2\pi i)] = 2\nu,$$

and for correct analytic continuation it is necessary to make the replacement $\ln \varepsilon \to \ln(-\varepsilon) + i\pi$. Finally, we arrive at the equation

$$\varepsilon [\ln(-\varepsilon) - (1 + 2 \ln 2 + i\pi)] = 2\nu, \tag{A9}$$

the solution of which (with logarithmic accuracy) is

$$\varepsilon_n' = -2\nu [\Lambda + \ln \Lambda + \dots]^{-1},$$

$$\varepsilon_n'' = \frac{2\pi\nu}{[\Lambda + \ln \Lambda + O(1)]^2}, \tag{A10}$$

where Λ is defined in (A4). In this region of energies,

$$\Gamma_n/E_n \sim \pi/\Lambda \ll 1, \qquad \Gamma_n/\Delta E_n \sim \varepsilon_n'' (d\varepsilon_n'/dn)^{-1} \sim \pi \Lambda^{-1} (n - n_*).$$

Since $|\varepsilon_n| \sim 2\nu/\Lambda = 2|a|s^{-2}$ and $|a| \gg 1$, we have $\nu \gg \Lambda/s^2$, or $n - n_* \gg \Lambda/2\pi$. Thus, every resonance is still rather narrow, but neighboring resonances already overlap.

Let us make a few concluding remarks.

a) The formulas (A3) and (A10) for ε_n' are analogous to each other, but the corresponding expressions for ε_n'' differ fundamentally: In the sub-barrier region [see (A3)] the widths are exponentially small, but in (A10) the width is only logarithmically smaller ($\sim 1/\Lambda$) than the energy of the level.

b) Consider the threshold behavior of the reduced widths (3.10) for $n \to \infty$. Taking into account that $s^2/2\pi(n - 1/4) = (g/g_n)^{1/2}$ and that the term $\exp(-2\pi a)$ in (A2) "dies out", we obtain

$$\tfrac{1}{2} \varepsilon [\ln \varepsilon - (1 + 2 \ln 2)] = (g_n/g)^{1/2} - 1. \tag{A11}$$

For $g > g_n$ the solution is real and corresponds to a bound state. In the above-barrier region ($g < g_n$), making in (A11) the replacement $\ln \varepsilon \to \ln(-\varepsilon) - i\pi$ we find

$$\gamma_n = \frac{\Gamma_n}{2(n - \tfrac{1}{4})\omega} = \begin{cases} 0, & \varkappa < 0, \\ \dfrac{\pi^2 \varkappa}{(\ln \varkappa)^2} \left[1 + O\left(\dfrac{\ln \ln \varkappa}{\ln \varkappa}\right) \right], & \varkappa > 0, \end{cases} \tag{A12}$$

where $\varkappa = (g_n - g)/g(|\varkappa| \ll 1)$. Thus, the limit curve $\gamma_{n = \infty}$ has a weak singularity on the threshold.

Since in (A11) there is no term $\infty \exp(-2\pi a)$ associated with barrier penetration, it may be concluded that the usual Bohr–Sommerfeld quantization condition, analytically continued into the above-barrier region, determines not only the position but also the width of levels with large n. This fact was discovered previously[36] during construction of a $1/n$ expansion for quasistationary states.

c) Finally, we note that the formulas of this appendix, although they have been obtained for the model (3.4), are in fact applicable to an arbitrary potential $U(x)$, since in the region of energies close to U_m ($|\varepsilon| \ll 1$) the potential can be approximated by a parabola.

APPENDIX B

Here we outline the derivation of the equations determining the Stark shifts and widths of the levels of the hydrogen atom in the case $n \gg 1$.

The semiclassical quantization conditions, with allowance for corrections of order $\hbar^2$ and $\hbar^4$, have been obtained by Bekenstein and Krieger.[10] Confining ourselves to corrections of order $\hbar^2$ in these conditions, and going over to the scaled variables

$$\varepsilon = 2n^2 E, \quad F = n^4 \mathscr{E}, \quad \mu = m/n, \quad x = n^{-2}\xi, \quad y = n^{-2}\eta$$

(ξ and η are parabolic coordinates), we have

$$p_\xi = \frac{1}{2n} k_1(x), \qquad p_\eta = \frac{1}{2n} k_2(y), \tag{B1}$$

$$k_i(q) = (\varepsilon + 4\beta_i q^{-1} - \mu^2 q^{-2} \mp Fq)^{1/2}$$

($q = x, y$ for $i = 1, 2$), and

$$\oint dy \left(k_2 - \frac{(k_2')^2}{8k_2^3} + \frac{1}{8k_2 y^2} \right) = \frac{2\pi (n_2 + \tfrac{1}{2})}{n}, \tag{B2}$$

where the integration contour encloses the turning points y_0 and y_1. For $\mu \to 0$,

$$y_0 = \frac{\mu^2}{4\beta_2} + O(\mu^4),$$

$$y_1 = -\frac{\varepsilon}{2F} \left[1 - \left(1 - \frac{16\beta_2 F}{\varepsilon^2} \right)^{1/2} \right] + O(\mu^2)$$

($\varepsilon < 0$). The quantization condition in the variable x is obtained from (B2) by the replacements $n_2 \to n_1$, $\beta_2 \to \beta_1$, and $F \to -F$.

For $m = 0$, all the integrals in (B2) can be calculated analytically. Going over to the new integration variable t:

$$y = -\frac{\varepsilon z_-}{2F} t, \quad k_2(y) = 2^{-1/2} (-\varepsilon z_+)^{1/2} k(t),$$

$$k(t) = [(1 - t)(1 - \zeta t)/t]^{1/2},$$

where

$$\zeta = z_-/z_+, \quad z_\pm = 1 \pm (1 - z_2)^{1/2}, \quad z_2 = 16\beta_2 F \varepsilon^{-2},$$

we obtain

$$\beta_2 (-\varepsilon)^{-1/2} f(z_2) + \frac{F}{8n^2} (-\varepsilon)^{-3/2} g(z_2) = \frac{n_2 + \tfrac{1}{2}}{n}, \tag{B3}$$

where

$$f(z_2) = \frac{(1+\zeta)^{1/2}}{\pi} \oint k(t)\,dt, \tag{B4}$$

$$g(z_2) = \frac{(1+\zeta)^{1/2}}{\pi\zeta} \oint dt \left[\frac{1}{t^2 k(t)} - \frac{(k')^2}{k^3} \right]. \tag{B5}$$

Here $k' = dk/dt$, and the integration contour encloses the branch points $t = 0$ and $t = 1$. The integral (B4) is easily calculated if we use an integral representation for the hypergeometric function and the quadratic Kummer transform [see formulas 2.12(4) and 2.1(26) in Ref. 37]. Taking into account the identity $k'^2 k^{-3} = \frac{1}{3}[(k^2)''/2k^3 + (k^{-1})'']$ and discarding the total derivative in the contour integral, we have

$$g(z_2) = h(z_2) - \hbar(z_2),$$
$$h(z_2) = \frac{(1+\zeta)^{1/2}}{\pi\zeta} \oint \frac{dt}{t^2 k}, \qquad \hbar(z_2) = \frac{(1+\zeta)^{1/2}}{3\pi\zeta} \oint \frac{dt}{t^3 k^3}. \tag{B6}$$

In the calculation of these integrals we use the same devices, and also the relation

$$F(\tfrac{7}{4}, \tfrac{3}{2}; 3; z) = \frac{8}{15z}\{F(\tfrac{3}{4}, \tfrac{3}{2}; 1; z) - F(\tfrac{3}{4}, \tfrac{1}{2}; 2; z)\},$$

the validity of which is easily seen by comparing coefficients of equal powers of z. Finally, we obtain

$$f(z) = F(\tfrac{1}{4}, \tfrac{3}{4}; 2; z),$$
$$g(z) = \tfrac{1}{3}F(\tfrac{3}{4}, \tfrac{5}{4}; 2; z) + \tfrac{2}{3}F(\tfrac{3}{4}, \tfrac{5}{4}; 1; z), \tag{B7}$$
$$h(z) = F(\tfrac{3}{4}, \tfrac{5}{4}; 2; z).$$

If the magnetic quantum number is nonzero (but $m \ll n$), in (B2) we can expand in the small parameter μ; here it is sufficient to consider only $\oint k_2 dy$. Introducing the joining point $\bar{y}$ such that $\mu^2 \ll \bar{y} \ll 1$, expanding $k_2(y)$ for $\bar{y} < y < y_1$ in powers of μ^2, and, in the region $y_0 < y < \bar{y}$, using the smallness of y, we find

$$\frac{1}{2\pi} \oint k_2\, dy = n\beta_2 (-\varepsilon)^{-1/2} f(z_2)$$
$$-m\pi - \frac{m^2 F}{8n(-\varepsilon)^{1/2}} h(z_2) + O(m^3) \tag{B8}$$

(the arbitrary point $\bar{y}$ drops out of the final answer). Introducing the notation

$$z_i = (-1)^i 16\beta_i F\varepsilon^{-2} = (-1)^i 4\beta_i \mathscr{F} E^{-2}, \quad i = 1, 2, \tag{B9}$$

we obtain the quantization conditions

$$\beta_1(-\varepsilon)^{-1/2}f(z_1) - \frac{F}{8n^2}(-\varepsilon)^{-1/2}[g(z_1) - m^2 h(z_1)] = \nu_1, \tag{B10}$$

$$\beta_2(-\varepsilon)^{-1/2}f(z_2) + \frac{F}{8n^2}(-\varepsilon)^{-1/2}[g(z_2) - m^2 h(z_2)] = \nu_2,$$

$$\beta_1 + \beta_2 = 1, \quad \nu_i = (n_i + \tfrac{1}{2})/n$$

(β_i are the separation constants). These equations have been solved numerically.[19] Here it is possible either to discard the terms $\propto F/8n^2$ (the $1/n$ approximation) or to solve this system in complete form (the $1/n^2$ approximation).

We note that Eqs. (B10) in the $1/n$ approximation were given in Ref. 38, and in the $1/n^2$ approximation were given in Ref. 19, and were used in calculations of the Stark levels and also in the derivation of scaling relations for near-threshold resonances. However, their derivation has not been published before.

APPENDIX C

For $E = -(k^2+1)^{1/2} < -1$ there is a sub-barrier region $r_1 < r < r_2$, where r_1 and r_2 are the turning points:

$$r_1 = \zeta(1-\rho^2)[(1+k^2)^{1/2} + (1+\rho^2 k^2)^{1/2}]^{-1}, \tag{C1}$$
$$r_2 = \zeta k^{-2}[(1+k^2)^{1/2} + (1+\rho^2 k^2)^{1/2}].$$

For $k \to 0$,

$$r_1 = \tfrac{1}{2}\zeta(1-\rho^2)[1 - \tfrac{1}{4}(1+\rho^2)k^2 + \ldots],$$
$$r_2 = \frac{2\zeta}{k^2} + \tfrac{1}{2}\zeta(1+\rho^2) + \ldots$$

and the turning point r_2 goes away to infinity. In the opposite limiting case the width of the barrier decreases:

$$r_{1,2} = \zeta(1 \mp \rho)/k, \quad |k| \gg 1.$$

However, the turning points $r_{1,2}$ lie outside the nucleus so long as $|E| < (1-\rho)\zeta/r_N$ (we assume that $r_N \ll \hbar/mc = 1$).

For $E = -1$

$$p_r = \frac{g}{r}\left(1 - \frac{r}{r_1}\right)^{1/2},$$

$$\int_{r_N}^{r_1} p_r\, dr = 2g[\mathrm{arth}\,(1-x)^{1/2} - (1-x)^{1/2}]$$
$$= g\left[\ln\frac{1}{x} - 2(1-\ln 2) + \tfrac{1}{2}x - \tfrac{1}{16}x^2 + \ldots\right] \tag{C2}$$

($x = r_N/r_1 \ll 1$), and in (5.4) we have $u = 0$, $a = \infty$, and $\varphi(a) = 0$. The quantization condition takes the form

$$g\left[\ln\frac{g^2}{2\zeta r_N} - 2(1-\ln 2)\right] + \gamma' = (n - \tfrac{1}{4})\pi, \tag{C3}$$

where

$$g = [\zeta^2 - (l + \tfrac{1}{2})^2]^{1/2}$$

and the constant γ' is determined from the condition for joining at the edge of the nucleus. Denoting by ξ the logarithmic derivative of the inner ($r \to r_N - 0$) wave function, we have

$$\gamma' = \mathrm{arcctg}\,\frac{\xi - \tfrac{1}{2}}{g}, \qquad \xi = \frac{r}{\chi}\frac{d\chi}{dr}\bigg|_{r=r_N}. \tag{C4}$$

For example, for $f(x) \equiv 1$ (the simplest cutoff model, corresponding to charge concentrated on the surface of the nucleus) ξ is given by Eq. (5.5), in which

$$\Lambda_\nu(z) = \Gamma(\nu+1)(z/2)^{-\nu}J_\nu(z), \tag{C5}$$
$$\Lambda_\nu(z) = \Lambda_\nu(-z) = 1 - z^2/4(\nu+1) + \ldots, \quad z \to 0.$$

From this follows the rapidly convergent expansion

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$$\xi = c_0 - c_1 \zeta^2 - c_2 \zeta^4 - \dots , \qquad (C6)$$

where

$$c_0 = l+1, \quad c_1 = \frac{1}{2l+3}, \quad c_2 = \frac{1}{(2l+3)^2(2l+5)},$$

$$c_3 = \frac{2}{(2l+3)^3(2l+5)(2l+7)}, \dots \qquad (C7)$$

and $c_k \sim \zeta_l^{-2k}$ for $k \to \infty$, where ζ_l is the first positive zero of the Bessel function $J_{l+1/2}(\zeta)$: $\zeta_0 = \pi$, $\zeta_1 = 4.493$, ..., $\zeta_l = l + 1.8561^{1/3} + 0(1)$ for $l \gg 1$. Thus, the coefficients c_k decrease rapidly with increase of k (especially for large l), owing to which, for the calculation of the logarithmic derivative ξ up to $\zeta \sim 1$, it is convenient to use the series (C6).

In the general case [an arbitrary form of the cutoff $f(x)$] these coefficients can be calculated using formulas given in Ref. 39. For example, for $f(x) = (3 - x^2)/2$ (which corresponds to a uniform distribution of charge over the volume of the nucleus) we have

$$c_0 = l+1, \quad c_1 = \frac{1}{2l+3}\left[1 + \frac{l+4}{(l+^5/_2)(l+^7/_2)}\right], \dots \quad (C8)$$

The solution of Eq. (C3) makes it possible to calculate for each model of the cutoff the value $Z = Z_{cr}$ at which the nl level drops down to the boundary $E = -1$ (the so-called critical charge of the nucleus[28–30]).

For $E > -1$ we obtain

$$\int_{r_N}^{r_1} p_r\, dr = g\left\{\ln\frac{r_1}{r_N} - H(u) + \frac{1+k^2}{g^2}\zeta r_N + O((\zeta r_N)^2)\right\},$$

$$(C9)$$

where

$$H(u) = {}^1/_2 u^{-1/2}[(1+u^{1/2})\ln(1+u^{1/2}) - (1-u^{1/2})\ln(1-u^{1/2})]$$

$$+ 1 - \ln 2[1 + (1-u)^{1/2}]$$

$$= \begin{cases} 2(1-\ln 2) + {}^1/_{12}u + \dots , & u \to 0, \\ 1 - t^{1/2} - {}^1/_4 t\ln t + O(t), & u = 1-t \to 1. \end{cases} \quad (C10)$$

Here, the contribution γ' to the quantization condition from the region inside the nucleus has the same magnitude (C4) as in the case $E = -1$.

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1) The other "decay channels" either are closed ($a_i = \infty$ and (a_i) = 0) or in them $\exp(-2\pi a_i) \ll \exp(-2\pi a_f)$. Systems satisfying special symmetry properties may constitute an exception.

2) The same is also true (for physically reasonable potentials) in the case of the discrete spectrum (see, e.g., Ref. 22).

3) See also Refs. 19 and 21 and the references indicated therein.

4) A correction for barrier penetration is introduced only in the second of Eqs. (B10). This is because the electron tunneling occurs along the coordinate η, while the effective potential $U_1(\xi)$ is a blocking potential.

5) This follows from the fact that solution of system (B10) remains valid at $F < F_*$ (or $0 < z_2 < 1$). The $z_2 = 1$ value corresponds to the classic threshold of F ionization. Numerically $F_* = 0.2895$ and 0.3155 for states $|9, 0, 0\rangle$ and $|19, 0, 0\rangle$.

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