Quantization rules for quasistationary states

V.S. Popov, V.D. Mur and A.V. Sergeev
Institute of Theoretical and Experimental Physics, Moscow, USSR

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The modification of the Bohr–Sommerfeld quantization rules, which is due to the barrier penetrability, is found. The equation obtained is valid for an arbitrary analytical potential $U(x)$, obeying the quasiclassical conditions. It determines both the position E_r and the width Γ of the quasistationary state. A generalization of the Gamow formula for multidimensional systems with separable coordinates is derived. A comparison with exactly solvable models as well as with numerical solutions of the Schrödinger equation for the Stark problem is performed.

1. Introduction

The Bohr–Sommerfeld quantization rules determine the discrete energy spectrum (see, e.g., refs. [1,2]). In many physical problems, however, the potential has a barrier which gives rise to quasistationary states, instead of discrete levels. The calculation of the resonance energy E_r and its width Γ is an actual problem for atomic and nuclear physics, scattering theory, etc.

We will consider this problem in the quasiclassical approximation which yields formulae convenient for calculations and are valid for an arbitrary smooth potential $U(x)$. These formulae derived for $n \gg 1$ are often valid up to small quantum numbers, $n \sim 1$.

2. Generalization of quantization rules

We use the parabolic approximation near the barrier summit, $x \approx x_m$,

$$p(x) = (\tfrac{1}{4}\rho^2 - a)^{1/2}, \quad a = (U_m - E)/\omega, \tag{1}$$

where $\rho = 10^{1/2}(x - x_m)$, $\omega = [-U''(x_m)]^{1/2}$ and $\hbar = m = 1$. The Schrödinger equation in this case has an exact solution,

$$\psi(x) = \text{const} \times D_{-(1/2+ia)}(\rho \exp(-\tfrac{1}{4}i\pi)),$$

which corresponds to a quasistationary state (outgoing wave at $x \to \infty$). If this function is matched at $\rho < 0$ with the semiclassical wave function, we obtain the following quantization condition [#1],

$$\int_{x_0}^{x_1} p(x,E)\,dx = (N + \tfrac{1}{2})\pi, \quad N = n - \frac{1}{2\pi}\varphi(a). \tag{2a}$$

where $n = 0, 1, 2, \ldots$

$$\varphi(a) = \frac{1}{2i}\ln\left(\frac{\Gamma(\frac{1}{2}+ia)}{\Gamma(\frac{1}{2}-ia)[1+\exp(-2\pi\omega)]}\right) + a(1-\ln a), \tag{2b}$$

$$a = \frac{1}{\pi}\int_{x_1}^{x_2} (-p^2)^{1/2}\,dx \tag{3}$$

($x_1 < x < x_2$ is the subbarier region). The parameter a which for a parabolic barrier is defined in (1), is written here in a more general form applicable for any potential. If the integral (3) can be evaluated explicitly, its analytical continuation is of no difficulty. For an arbitrary potential $U(x)$ the values of a for the complex energy E can be found numerically, which together with eq. (2a) determine the spectrum of quasistationary states.

[#1] See ref. [3]. A formula equivalent to eq. (1) has been obtained by Connor [4]. However, in ref. [4] the attention was restricted to the case of a sharp resonance ($\Gamma_n \ll E_n$) and the region $E \approx U_m$ was not considered.

There are also equations of the type of (2a) for multidimensional problems with separable variables $q_1, q_2, ..., q_f$ (f is the number of degrees of freedom):

$$\int_{q_i^{(0)}}^{q_i^{(1)}} p_i\, \mathrm{d}q_i = (N_i + \tfrac{1}{2})\pi\,, \quad i = 1, 2, ..., f, \tag{4}$$

Here $q_i^{(0,1)}$ are the turning points limiting the classically allowed region along the coordinate q_i, p_i is the quasiclassical momentum, $N_i = n_i - (1/2\pi)\varphi/a_i$, if tunneling along q_i is possible; otherwise, $a_i = \infty$ and $N_i = n_i = 0, 1, 2, ...$ is integer. The solution of eqs. (4) determines the resonance energy $E = E_r - \frac{1}{2}\mathrm{i}\Gamma$ and the separation constants β_i which are also complex.

3. Consequences of the basic equations

Let us consider some consequences of the basic equations (2) and (4).

(a) Since

$$\varphi(a) = \frac{1}{24a} + \frac{7}{2880a^3} + ... + \tfrac{1}{2}\mathrm{i}\exp(-2\pi a)\,,$$

$$a \to +\infty\,, \tag{5}$$

if we set

$$p(r) = \{2[E_r - \tfrac{1}{2}\mathrm{i}\Gamma - U(r)]\}^{1/2}\,,$$

we find from (2a) the well-known Gamow formula [5] for the width of the quasistationary state:

$$\Gamma = \frac{1}{T}\exp\left(-2\int_{r_1}^{r_2}[-p^2(r)]^{1/2}\,\mathrm{d}r\right), \quad T = 2\int_{r_0}^{r_1}\frac{\mathrm{d}r}{p(r)} \tag{6}$$

(T is the period or radial oscillations of a particle, $r_0 < r < r_1$).

(b) If the barrier penetrability is exponentially small, tunneling occurs mainly along a single coordinate, say q_f (if $\exp(-2\pi a_f) \gg \exp(-2\pi a_i)$, $1 \leqslant i \leqslant f-1$). Then one can obtain from eqs. (4) a generalization of the Gamow formula:

$$\Gamma = cT_f^{-1}\exp(-2\pi a_f)\,, \tag{7a}$$

which differs from eq. (6) by the preexponential factor c. Here [#2]

$$c = \left[\alpha\left(1 + \sum_{i=1}^{f-1}\frac{\bar{v}_f}{\bar{v}_i}\right)\right]^{-1}\,,$$

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

$$\sum_{i=1}^{f}\beta_i = \mathrm{const}\,, \tag{7b}$$

where the β_i are the separation constants, and we denote by $\bar{v}_i$ the mean value of $v_i(q)$ over the quasiclassical wave function,

$$\bar{v}_i = \int_{q_i^{(0)}}^{q_i^{(1)}}\frac{v_i(q)}{p_i(q)}\,\mathrm{d}q\left(\int_{q_i^{(0)}}^{q_i^{(1)}}\frac{\mathrm{d}q}{p_i(q)}\right)^{-1}\,. \tag{7c}$$

In the above equations $u_i(q_i) + \beta_i v_i(q_i)$ is the potential for the coordinate q_i, so that the action

$$S = \sum_{i=1}^{f}\int p_i(q_i)\,\mathrm{d}q_i\,,$$

and the value of α is determined in the process of separation of variables (if $f=1$, then $\alpha = c = 1$ and eq. (7a) reduces to (6)). The explicit form of the functions u_i, v_i depends on the problem considered. For instance, for the Stark problem in hydrogen we have: $f=2$, $\alpha = \frac{1}{4}$, $\beta_1 + \beta_2 = 1$,

$$u_i(q_i) = \tfrac{1}{8}[m^2 q_i^{-2} + (-1)^{i-1}\mathcal{E}q_i]\,,$$

$$v_i(q_i) = -1/2q_i\,,$$

where $\mathcal{E}$ is the electric field, m is the magnetic quantum number, $i = 1$ or 2, $q_1 = \xi$, $q_2 = \eta$ (ξ, η are parabolic coordinates [1]) and $\hbar = e = m_e = 1$. Contrary to value of α, the values of the separation constants β_i can be determined only together with the energy E.

(c) Let $\Delta_n = \Gamma_n/\Delta E_n$, where ΔE_n (the spacing) is the distance between neighbouring rresonances. In the subbarrier region $\Delta_n \approx (2\pi)^{-1}\exp(-2\pi a_n)$ and thus the resonances are isolated at $a_n \gtrsim 1$. When the level ($n = n_*$) crosses the boundary $\mathrm{Re}\,E = U_m$, the following equation holds,

[#2] Eq. (7b) does not define the most general case of separation of variables in the Schrödinger equation, but many important physical problems belong to it (e.g., a hydrogen atom in a uniform electric field $\mathcal{E}$, the problem of two Coulomb centres, etc. [1]).

$$\Delta_{n*}=\frac{\ln 2}{2\pi}(1+k_1/L^2+...) \quad (8)$$

($L=\log n_*+4.50\gg 1$, $k_1=3.32$), which is asymptotically exact ($n\to\infty$) for an arbitrary potential [6]. So, at $E=U_m$ the resonances do not overlap yet, and a few resonances can be observed in the above-barrier region [#3].

Eqs. (2a), (4) and (7a) may have various physical applications. We shall discuss here only a few examples.

4. Exactly solvable models

(a) A parabolic barrier: $l=0$,

$$V(r)=-\tfrac{1}{2}\omega^2(r-R)^2\equiv-\frac{g}{2R^2}(1-x)^2, \quad (9)$$

where $v(x)=(1-x)^2$, $x=r/R$ and $g=\omega^2R^4$ is a dimensionless coupling constant. The boundary conditions for the wave function of the quasistationary state are $\chi(0)=0$ and

$$\chi(r)\sim r^{-(1/2-ia)}\exp(\tfrac{1}{2}i\omega r^2)$$

at $r\to\infty$ (the Sommerfeld radiation condition). Finally, the energy spectrum is determined from the equation

$$D_\nu(-2^{1/2}\exp(-\tfrac{1}{4}i\pi)g^{1/4})=0,$$
$$\nu=-\tfrac{1}{2}+iE/\omega \quad (10)$$

($a=-E/\omega$), where $D_\nu(z)$ is the parabolic cylinder function. Eq. (2a) in the case of ns levels can be written as

$$g^{1/2}-a[\tfrac{1}{2}\ln(g/a^2)+1+\ln 2]+\varphi(a)$$
$$=2\pi(n-\tfrac{1}{4}), \quad (11)$$

where $n=n_r+1=1, 2, ...$.

These equations were solved numerically. Denote by g_n the value of the coupling g at which Re $E_n=0$. The ratios g_{cl}/g_n and $\tilde{g}_{cl}/g_n$ (where $g_{cl}(n\text{s})=[2\pi(n-\tfrac{1}{4})]^2$ follows from the Bohr–Sommerfeld quantization condition and $\tilde{g}_{cl}$ follows from eq. (11)) are given in table 1. Table 1 contains also the "reduced widths" $\gamma_n=\Gamma_n/2(n-\tfrac{1}{4})\omega$ and the quantities $\eta_n=\tilde{\gamma}_n/\gamma_n-1$ which characterize the accuracy of eq. (11) for the level widths. The quasiclassical approximation has a high accuracy in this case. Note that eq. (11), which was obtained assuming $n\gg 1$, remains valid also for small quantum numbers [#4]. Inclusion of the barrier penetrability correction $\varphi(a)$ allows one to calculate the widths Γ_n and considerably improves the accuracy of the calculation of g_n (at $n\geq 2$).

The validity of the asymptotic relation (8) was also

[#3] However, their widths quickly grow when the energy E_r increases, $E_r>U_m\equiv U(x_m)$.

[#4] Just as in problems referring to the discrete energy spectrum with physically meaningful potentials [7].

Table 1
g_{cl}/g_n, $\tilde{g}_{cl}/g_n$, γ_n and η_n. All numbers correspond to the moment when the ns level enters the continuous spectrum, that is, Re $E_n=U_m=0$.

$n_r=n-1$	g_{cl}/g_n	$\tilde{g}_{cl}/g_n$	γ_n	η_n
0	1.020150	0.967219	0.1038047	1.299(−2)
1	1.012862	0.993747	3.7837(−2)	2.316(−3)
2	1.008655	0.997462	2.2234(−2)	8.885(−4)
3	1.006416	0.998636	1.5484(−2)	4.579(−4)
4	1.005058	0.999151	1.1770(−2)	2.760(−4)
5	1.004155	0.999421	9.4392(−3)	1.833(−4)
10	1.002142	0.999835	4.6068(−3)	4.890(−5)
20	1.001049	0.999956	2.1848(−3)	1.185(−5)
30	1.000681	0.999980	1.4032(−3)	5.14(−6)
40	1.000500	0.999989	1.0235(−3)	2.83(−6)
50	1.000393	0.9999926	8.0092(−4)	1.78(−6)
100	1.000185	0.9999981	3.7374(−4)	4.19(−7)
200	1.000087	0.9999995	1.7462(−4)	9.85(−8)
1000	1.000015	$1-2\times10^{-8}$	3.0166(−5)	3.42(−9)

checked and completely confirmed.

(b) In the case of potential

$$V(r)=-\alpha^2/2r^2-\tfrac{1}{8}\omega^2r^2 \tag{12}$$

an exact solution can be obtained for an arbitrary angular momentum l,

$$\chi_\ell(r)=\text{const}\times r^{-1/2}W_{\kappa\mu}(-\tfrac{1}{2}\mathrm{i}\omega r^2)\,, \tag{13}$$

where $\kappa=\mathrm{i}E/\omega$, $\mu=\frac{1}{2}\mathrm{i}g$,

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

and $W_{\kappa\mu}(z)$ is the Whittaker function. When $\alpha>l+\frac{1}{2}$, the effective potential $U(r)$ which includes the centrifugal energy has a barrier and thus the quasistationary states exist. Here we discuss this case.

If $\alpha>l+\frac{1}{2}$, the condition $\chi_l(0)=0$ is fulfilled for any energy E and does not define the energy spectrum. As for other problems with "collapse to the centre" [8–10], to obtain the quantization rule we impose the orthogonality condition of wave functions corresponding to energy E_n and to some fixed energy E_0. It can be easily shown that the integral entering the orthogonality condition is determined by the behaviour of the Whittaker function in eq. (13) at $r\to0$. It leads to the equation

$$Q(E_n,g)-Q(E_0,g)=-n\pi/g\,, \tag{14}$$

which determines the energy spectrum. Here

$$Q(E,g)=\frac{1}{2\mathrm{i}g}\ln\left(\frac{\Gamma(\frac{1}{2}+\mathrm{i}g(\epsilon+1))}{\Gamma(\frac{1}{2}+\mathrm{i}g\epsilon)}\right), \tag{15}$$

$$\epsilon=\frac{E-U_m}{2U_m}\,,\quad U_m=-\tfrac{1}{2}g\omega\,,\quad a=\frac{U_m-E}{\omega}=g\epsilon\,.$$

(c) Similar results were obtained for the potential

$$V(r)=-\alpha^2/2r^2+\tfrac{1}{2}\zeta\quad(\alpha>l+\tfrac{1}{2},\zeta>0)\,, \tag{16}$$

for which the exact solution of the Schrödinger equation is also expressed in terms of the Whittaker function.

Let us briefly discuss the quantum correction to the Gamow formula. If $g\gg1$, one can use in eqs. (14) and (15) the asymptotic expansion for $\ln[\Gamma(z+\frac{1}{2})]$ as $z\to\infty$. It gives, for both potentials (12) and (16), that

$$\Gamma=T^{-1}\exp(-2\pi a)\,[1+g^{-2}\Phi(\epsilon)+O(g^{-4})]\,, \tag{17}$$

where

$$\Phi(\epsilon)=\frac{1+2\epsilon}{24\epsilon^2(1+\epsilon)^2\ln(1+\epsilon^{-1})}$$

for the potential (12), $0<\epsilon<\infty$;

$$\Phi(\epsilon)=-\frac{(1-\epsilon)^{3/2}}{12\epsilon^2[\operatorname{arth}(1-\epsilon)^{1/2}-(1-\epsilon)^{1/2}]}$$

for (16), $\epsilon=(U_m-E)/U_m$ $(0<\epsilon<1)$. Since $\Phi\sim[\epsilon^2\ln(1/\epsilon)]^{-1}$ at $\epsilon\to0$, the Gamow formula begins to lose validity near the barrier summit. The corresponding energy region is, however, rather narrow due to the condition $g\gg1$, and also because the functions $\Phi(\epsilon)$ are numerically small at $\epsilon\sim1$.

5. The Stark effect for a hydrogen atom

Application of the Bohr–Sommerfeld conditions leads to a system of two transcendental equations (see eq. (6) in ref. [11]), the solution of which involves either dropping the terms proportional to $F/8n^2$ or solving them in their entirety (the $1/n$ and $1/n^2$ approximations, respectively). Here we shall present only a few results of the calculations [#5].

Table 2 contains the values of the reduced energy, taken with opposite sign, e.g., $-\epsilon_n'=-2n^2E_r^{(n_1n_2m)}$. The values of $-\epsilon_n'$, obtained by the $1/n$ and $1/n^2$ approximations, as well as the results of the summation of perturbation series with the help of the HPA are presented [#6]. The influence of the barrier penetrability on the resonance energy E_r is rather small for the same F (see table 2), though it grows to some degree with increasing F.

The corresponding results for the width ($\epsilon_n''=n^2\Gamma^{(n_1n_2m)}$) are given in fig. 1. In this case the barrier

[#5] See also refs. [11–13] and references therein. In this section we use atomic units, $F=n^4\mathcal{E}$, $\epsilon=2n^2(E_r-\frac{1}{2}\mathrm{i}\Gamma)$ ($\mathcal{E}=1$ a.u. corresponds to 5.142×10^9 V/cm), $n=n_1+n_2+|m|+1$, n_1, n_2, m are parabolic quantum numbers.

[#6] Nowadays there exist precise numerical calculations of the Stark resonance energies E_r and their widths Γ performed by different numerical methods, see e.g. refs. [11–15] and references therein. We used the $1/n$ and $1/n^2$ approximations, as well as summation of divergent perturbation series (in powers of $\mathcal{E}$) by means of Hermite–Padé approximants (HPA). For details of these calculations see refs. [11,13].

Table 2
The reduced energies for the $(n-1, 0, 0)$ Stark resonances, with $\varphi(a)\equiv 0$ and with barrier penetrability included.

	$F=n^4\mathcal{E}$	$1/n$		$1/n^2$		HPA
		$\varphi(a)\equiv 0$	with $\varphi(a)$	$\varphi(a)\equiv 0$	with $\varphi(a)$	
$n=20$	0.10	0.72994		0.73000		0.7300
	0.20	0.48280	0.48301	0.48309	0.48309	0.4831
	0.25	0.36628	0.36677	0.36692	0.36695	0.367
	0.30	0.25489	0.25619	0.25696	0.25663	0.256
	0.35	0.1502	0.1490	0.1498	0.1488	0.149
	0.40	0.0432	0.0421	0.0425	0.0413	0.042
	0.45	−0.0643		−0.0652		−0.065
	0.50	−0.1716		−0.1727		−0.173
	0.60	−0.3842		−0.3855		−0.386
	0.70	−0.5923		−0.5936		−0.596
	1.00	−1.1896		−1.1907		−1.19
$n=50$	0.20	0.46304	0.46307	0.46309	0.46309	0.463
	0.30	0.22169	0.22186	0.22192	0.22193	-
	0.35	0.1079	0.1077	0.1083	0.1078	-

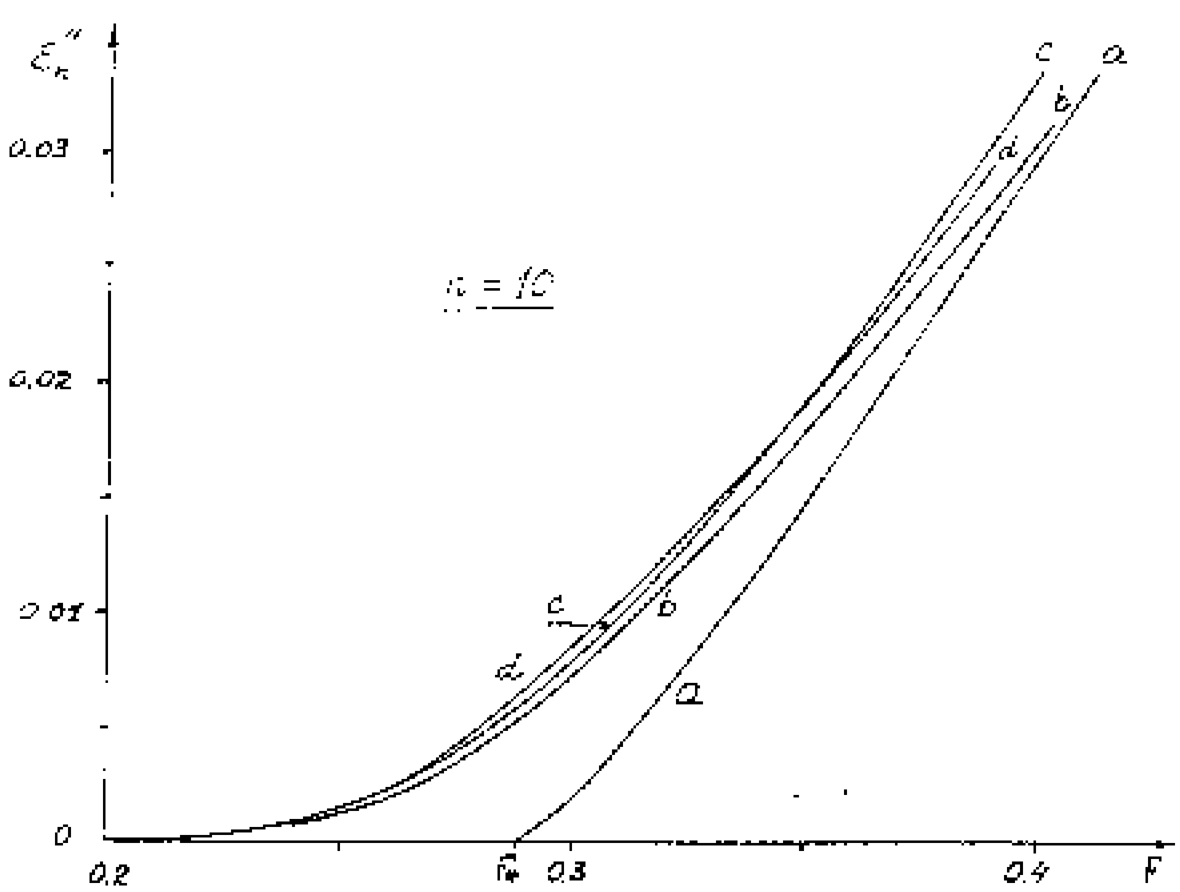

Fig. 1. The effect of barrier penetrability on the calculation of the width of the (9, 0, 0) state. (a) Calculation with the barrier penetrability neglected, i.e. $\varphi(a)\equiv 0$; (b) the same with the function $\varphi(a)$ included; (c) HPA method; (d) improved WKB approximation, see eq. (18).

penetrability correction is very essential at $F\lesssim 0.3$, but with the further increase of F its role diminishes. At $n\gtrsim 20$, in most cases one can restrict oneself to the $1/n$ approximation.

The quasiclassical approximation can be improved so that at $F\to 0$ the level widths would coincide with their exact asymptotics [1,14]. For this purpose it is sufficient to introduce a correction to the parameter a (3): $a\to a-\Delta a$,

$$\Delta a=\alpha(n_2)+\alpha(n_2+m)\,, \tag{18}$$

which depends on quantum numbers of the state, but not on the value of F. Here

$$\alpha(x)=\frac{1}{2\pi i}\varphi(-i(x+\tfrac{1}{2}))=0.0115, \qquad x=0\,,$$
$$=(48\pi x)^{-1}, \quad x\gg 1\,, \tag{19}$$

where the function φ is defined in (2b). It can be seen from fig. 1, that with the barrier penetrability correction included, the quantization rules not only ensure the correct asymptotical behaviour of $\Gamma(F)$ at $F\to 0$, but also lead to the numerical results practically coinciding with the HPA at $F\leqslant 0.4$.

In conclusion we discuss the question of applicability of the generalized Gamow formula. For the states with $m=0$ the integrals entering eq. (7a) are calculated analytically. The results for the $(n-1, 0, 0)$ states are presented in fig. 2. The solid curve is calculated using the HPA and agrees with the calculation by Kolosov [15] performed by a different method; the dashed curve corresponds to eq. (7a). It follows from fig. 2 that eq. (7a) has a high accuracy when $a\gtrsim 1$, and is qualitatively applicable even up to $a\approx 0.05$.

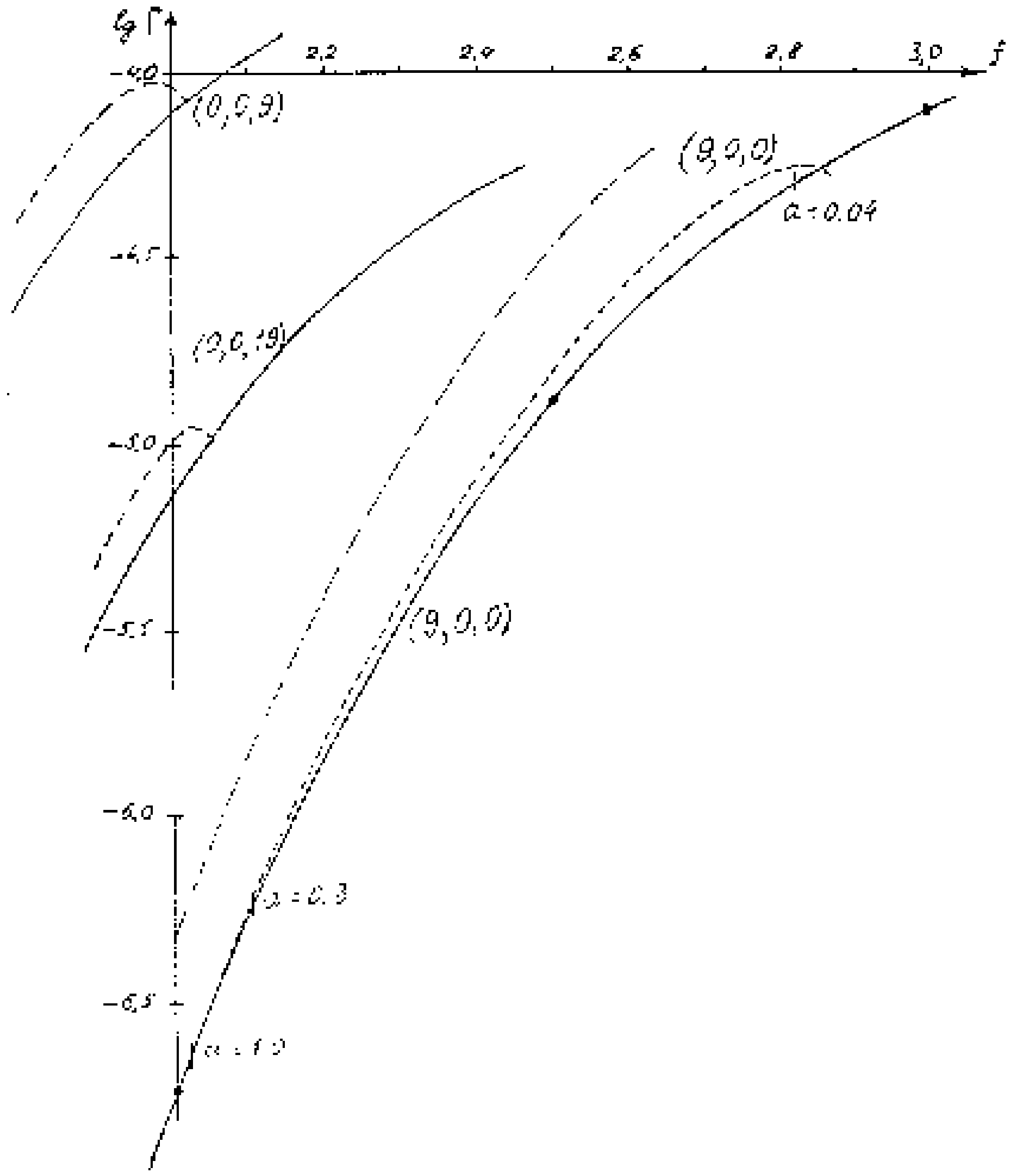

Fig. 2. Width Γ of the (n_1, n_2, m) states with $n=10$ and 20 in an electric field $\mathscr{E}$ (atomic units). Solid curves are the exact values of $\lg \Gamma^{(n_1,n_2,m)}$ (full dots are results from ref. [15], (- - - -) and (– · – · –) correspond to eqs. (7) and (6), respectively; $f=10n^4\mathscr{E}$.

Similar results were obtained for the other states (n_1, n_2, m). It can be shown that eq. (7a) is applicable if

$$a \gtrsim a_m = \{2\pi[\ln(n_2+\tfrac{1}{2})+b]\}^{-1}, \qquad (20)$$

where $b=\ln(48\pi^2)-4\approx 2.16$ (the numerical value of b depends on the problem considered). Since $a_m \ll 1$ not only for $n_2 \gg 1$, but even at $n_2 \sim 1$, the Gamow formula, as well as its generalization (7), ceases to be applicable only in the narrow energy region near the barrier summit ($E \approx U_m$).

Note that the preexponential factor c in (7a), which is due to multidimensionality of the problem considered, differs essentially from 1. For example, at $F \to 0$

$$c(F)=2(1-\kappa)+3(1-\kappa^2-1/2n^2)F+O(F^2), \qquad (21)$$

where $\kappa=(n_1-n_2)/n$, $-(1-n^{-1}) \leqslant \kappa \leqslant 1-n^{-1}$. So, the difference between eq. (7a) and the one-dimensional formula (6) is significant (see also fig. 2).

6. The analytic continuation of the quantization rules

When the energy $E \to U_m$, the turning points $x_{1,2}$ get closer and the Bohr–Sommerfeld quantization rule ceases to be applicable. At a further increase of the energy E, x_1 and x_2 diverge in the complex plane and the applicability conditions of the WKB method are again fulfilled. At $|a| \gg 1$ we have

$$\varphi(a)=-2\pi i a+1/24a+\ldots, \quad \tfrac{1}{2}\pi < \arg a < \pi. \qquad (22)$$

Taking into account that $E=E_r-\frac{1}{2}i\Gamma$ and $\Gamma>0$, we find

$$\int_{x_0}^{x_1} p\,dx=(n+\tfrac{1}{2}+ia)\pi$$

$$=(n+\tfrac{1}{2})\pi+i\int_{x_1}^{x_2}(-p^2)^{1/2}\,dx.$$

Since $(-p^2)^{1/2}=ip(x)$, we finally obtain

$$\oint_C [p^2(x)]^{1/2}\,dx=2\pi(n+\tfrac{1}{2}), \qquad (23)$$

where the integration contour C encloses the complex turning points x_0 and x_2. Unlike this, in the usual case of a discrete spectrum [2] the contour C encloses the points x_0 and x_1 which are on the real axis.

The validity of eq. (23) is illustrated in fig. 1, where curve (a) is obtained from analytic continuation of the usual quantization rules and corresponds to eq. (23), and curve (c) is calculated using the HPA and, up to the accuracy in the figure, coincides with the exact solution. Although in the subbarier region, $F<F_*=0.289$, the given approximation (a) does not determine the width of the level, at $F>F_*$ the curve comes close to the exact solution.

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