Quantization rules for above-barrier resonances

V. D. Mur
Moscow Engineering-Physics Institute, 115409 Moscow

V. S. Popov
Institute of Theoretical and Experimental Physics, Russian Academy of Sciences, 117259 Moscow

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The Bohr–Sommerfeld quantization condition is analytically continued into the above-barrier region. The result is used to find the asymptotic behavior of the energies of resonances under strong-coupling conditions.

1. The semiclassical approximation or WKB method is one of the most effective approximate methods of quantum mechanics. It is ordinarily used in the case of a discrete spectrum (Refs. 1–3, for example). In this letter we generalize the Bohr–Sommerfeld quantization condition for quasistationary states (resonances) with complex energies $E = E_r - i\Gamma/2$. As a result, the calculation of E_r and Γ is simplified significantly, particularly in the limiting case of strong external fields.

2. We consider a smooth (analytic) potential $U(x)$ which satisfies the conditions for semiclassical treatment. We denote by $x_0 < x < x_1$ the classically allowed region, in which the particle undergoes a finite motion, by $x_1 < x < x_2$ the above-barrier region, and by x_m the top of the barrier. We introduce $U_m = U(x_m)$. At $x > x_2$ the particle goes off to infinity. As $E_r \to U_m$, the turning points x_1 and x_2 become closer together. There is a (narrow) energy interval in which the semiclassical approximation is not valid. As E_r increases further, i.e., in the above-barrier region, these points go out into the complex plane, and the semiclassical approximation becomes valid again. It can be shown that the analytic continuation of the Bohr-Sommerfeld quantization condition is

$$\frac{1}{2\pi}\oint_C \left\{p+\frac{1}{24}\frac{U''}{p^3}+O(\hbar^4)\right\}dx=(n+\tfrac{1}{2})\hbar, \tag{1}$$

where $n=0, 1, 2, \ldots$; $p(x,E) = \{2m[E - U(x)]\}^{1/2}$; the integration contour C encloses the turning points x_0 and x_2 (which are complex under the condition $E_r > U_m$); and the corrections on the order of $\hbar^2$ to the ordinary semiclassical description have been taken into account.[2,3] In the case of a discrete spectrum, the contour C encloses the turning points x_0 and x_1, which lie on the real axis.[1–3] As we go from the below-barrier region ($E < U_m$) into the above-barrier region ($E > U_m$), the integration contour thus undergoes a reconnection.

Equation (1) is considerably simpler from the calculation standpoint than other (numerical) methods for determining E_r and Γ. Such questions have become a matter of special concern in recent years because of (in particular) experimental observations

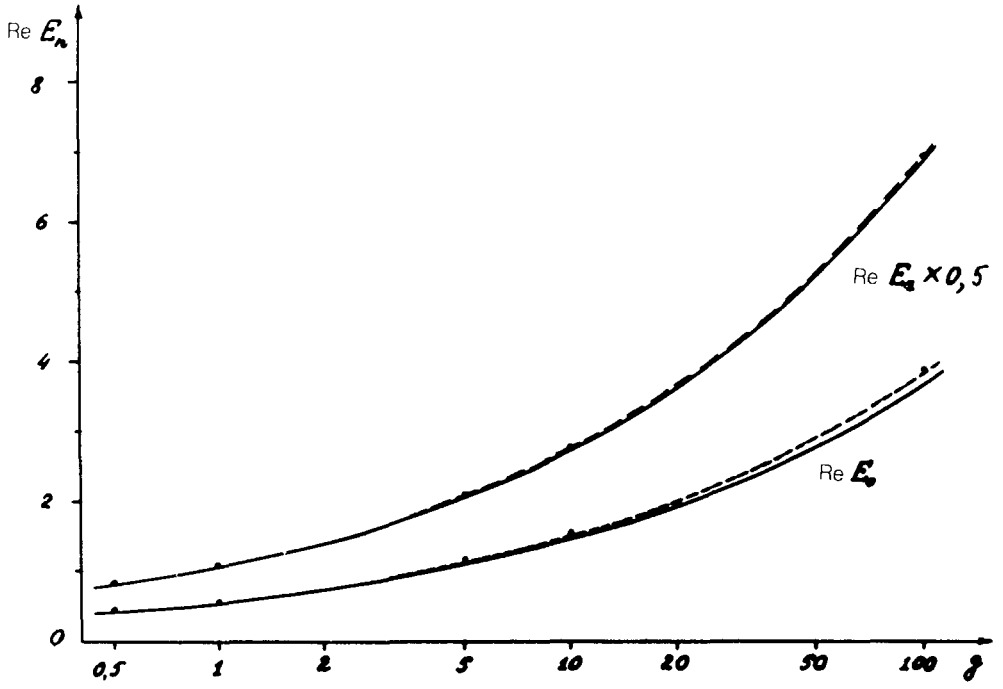

FIG. 1. Positions of the resonances with $n=0$ (the ground level) and $n=1$ for a cubic anharmonic oscillator. Solid line—Leading term of the asymptotic behavior; dashed line—two terms of series (3); points—results of a numerical calculation.[4] The abscissa scale is logarithmic.

of a complex resonance structure in the photoionization cross sections of atoms in external fields. Leaving those questions for future study, we restrict the present letter to the illustrative model in Eq. (2) below. In this case, Eq. (1) can be compared with the exact solution. We will also demonstrate (in the example of the Stark effect) that this equation can be used to find the asymptotic behavior of the resonance energies under strong-coupling conditions.

3. We consider the 1D harmonic oscillator

$$H=\tfrac{1}{2}(p^2+x^2)-gx^N, \quad N=3,5,7,\ldots . \tag{2}$$

Using (1), we can show that in the limit $g \to \infty$ we have

$$E_n(g) \approx C_N e^{-1\pi/(N+2)}[(n+\tfrac{1}{2})^N g]^{2/(N+2)} \sum_{k=0}^{\infty} d_k \lambda^{-k\alpha}, \tag{3}$$

where $\alpha = 4/(N+2)$,

$$C_N=\left\{\left(\frac{\pi}{8}\right)^{1/2}(N+2)\Gamma\left(\frac{N+2}{2N}\right)\Big/\Gamma\left(\frac{1}{N}\right)\cos\frac{\pi}{2N}\right\}^{2N/(N+2)}, \tag{4}$$

TABLE I.

g	$n=0$	$n=1$
100	0.726541	0.726542
	0.726534	0.726539
10	0.72646	0.72650
	0.72620	0.72639
5	0.72630	0.72643
	0.7255	0.7261
1	0.72323	0.72502
	0.7128	0.7206
0.5	0.71613	0.72182
	0.684	0.714

Values of ξ [see (7)] for the first two levels of the cubic oscillator. The upper line shows the result of the numerical calculation of Ref. 4 (for the given n and g), while the lower one shows the asymptotic value from (3).

$$d_k=d_k^{(0)}+d_k^{(2)}(n+1/2)^{-2}+d_k^{(4)}(n+1/2)^{-4}+\dots, \tag{5}$$

and $\lambda = (n + 1/2)^{(N-2)/2}g$ is the effective coupling constant for highly excited levels. Here we have $d_0^{(0)}=1$; the other coefficients are expressed in terms of contour integrals

$$J_k=\oint x^{2k}(1-x^N)^{1/2-k}dx$$

and can be evaluated analytically.

Potential (2) with $N=3$ (a cubic oscillator) has been analyzed by Alvarez,[4] who derived[1)] highly accurate numerical values of $E_n(g)$ for $n=0$ and 1 and $g \leqslant 100$. In this case the first few coefficients in expansions (3) and (5) have the values

$$C_3=1.6586, \quad d_1^{(0)}=0, \quad d_2^{(0)}=-0.0366\exp(-i\pi/5),$$
$$d_0^{(2)}=3^{1/2}/50\pi=0.0110, \quad d_1^{(2)}=0,\dots. \tag{6}$$

The coefficients $d_k^{(j)}$ fall off with increasing j and k, so only three terms need be retained in (3).

The results of Ref. 4 are compared with asymptotic expression (3) in Fig. 1. We see that the range of applicability of the semiclassical asymptotic expression "stretches" to values $g \sim 1$ (even for the ground level, $n=0$). A particularly high accuracy is reached (Table I) for the ratio

$$\xi=-\mathrm{Im}\,E_n(g)/\mathrm{Re}\,E_n(g). \tag{7}$$

The semiclassical quantization conditions in the above-barrier region were analyzed in the case of the Stark effect in the hydrogen atom in Ref. 5. An analytic continuation of these conditions into the above-barrier region of energies, carried out in accordance with (1), leads to the following system of equations [for $(n_1,n_2, 0)$ states]:

TABLE II. The parabolic quantum numbers n_1,n_2, and m of the Stark resonance; the reduced electric field $F=n^4$calE, and the classical ionization threshold[5,6] F_*. Cases $F > F_*$ correspond to above-barrier resonances, and $F < F_*$ to below-barrier resonances.

	$-E_r$, cm^{-1}			
n_1, n_2, m	Theory	Experiment[7]	F	F_*
16, 1, 0	106.9	103.8	0.343	0.2895
15, 1, 0	167.8	167.9	0.273	0.2626
15, 0, 0	196.5	198.5	0.214	0.3077
14, 2, 0	212.1	210.1	0.273	0.2362
13, 2, 0	273.6	275.8	0.214	0.2329
12, 3, 0	313.3	314.8	0.214	0.2143
11, 4, 0	353.8	351.4	0.214	0.2001
10, 4, 0	418.7	419.2	0.165	0.1965

Note: The parabolic quantum numbers n_1, n_2, and m of the Stark resonance; the reduced electric field $F=n^4E$, and the classical ionization threshold[5,6] F_*. Cases $F>F_*$ correspond to above-barrier resonances, and $F<F_*$ to below-barrier resonance.

$$(\beta_1/z_1)^{3/4}G(-z_1)=-2\nu_1F^{1/4},$$
$$(\beta_2/z_2)^{3/4}[G(z_2)-i\cdot 2^{1/2}G(1-z_2)]=2\nu_2F^{1/4}, \tag{8}$$

where $z_i = 16\beta_iF/\epsilon^2$,$\nu_i = (n_i + 1/2)/n$, β_i are separation constants, $\beta_1 + \beta_2 = 1$, $G(z) = z_2F_1(1/4, 3/4; 2; z)$, and ϵ and F are the reduced variables $\epsilon = 2n^2(E_r - i\Gamma/2)$ and $F = n^4\mathscr{E}$ (as in Refs. 5 and 6, we are using atomic units). In (8) we ignored corrections on the order of $\hbar^2$, but incorporation of such corrections is no problem.[6]

Analysis of Eqs. (8) reveals $\epsilon \propto F^{2/3}$ and $\beta_i \propto F^{1/3}$ as $F \to \infty$. We consider two limiting cases: (a) the longest-lived states $(n-1, 0, 0)$ and (b) short-lived states $(0, n-1, 0)$. The asymptotic expansion of the reduced energy ϵ in this case is more complex than (3). It contains, along with power-law corrections $\propto F^{-k/3}$, some logarithms:[2)]

$$\epsilon=(3\pi f)^{2/3}[1-k_1f^{-1/3}\ln f-k_2f^{-1/3}+\dots]. \tag{9}$$

Here $k_1 = (2/3)(3\pi)^{-4/3} = 0.0335$, $k_2 = 0.5402$, and $f=F$ in case (a) and $f = F\exp(-i\pi)$ in case (b). The leading term in the asymptotic behavior, $\epsilon \propto F^{2/3}$, is independent of the shape of the potential which binds the particle at short range. It is determined exclusively by the uniform field $\mathscr{E}$.

Solving system (8), we find the positions E_r and the width Γ of the Stark resonances in a strong electric field $\mathscr{E}$. Table II compares the values calculated for E_r with the experimental position of the peaks in the photoionization cross section of the hydrogen atoms (for the value[7] $\mathscr{E} = 16.8$ kV/cm). We see that the semiclassical description agrees with the experimental results within the error of the latter (1–2 cm^{-1}; Ref. 7). There is also a qualitative agreement in terms of the widths of the resonances, but this question [as well as a comparison of asymptotic expression (9) with numerical calculations] requires a discussion of certain details, so we will save it for a more comprehensive publication.

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[1)]A "complex-rotation" method was used.
[2)]Because of the Coulomb singularity of the potential at short range, as can be shown.

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