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Quantization rules with barrier penetrability

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Abstract. A correction to the quasiclassical quantization rules that allows for the presence of a barrier factor is found. The equation obtained in the process determines both the position of the quasistationary level E_r and the level width Γ. The results are compared with numerical solutions of the Schrödinger equation and with those obtained from an exactly solvable model. Finally, a generalization of the Gamow formula for systems with separable variables is derived.

1. Introduction

The Bohr–Sommerfeld quantization rules determine a discrete energy spectrum [1, 2], and integrals of the $\int p\,dx$ type are evaluated over the classically allowed region $x_0 < x < x_1$ (see figure 1), while the behaviour of the potential outside of this region is insignificant. (Actually, it is assumed that $U(x) > E$ as $x \to \pm\infty$.)

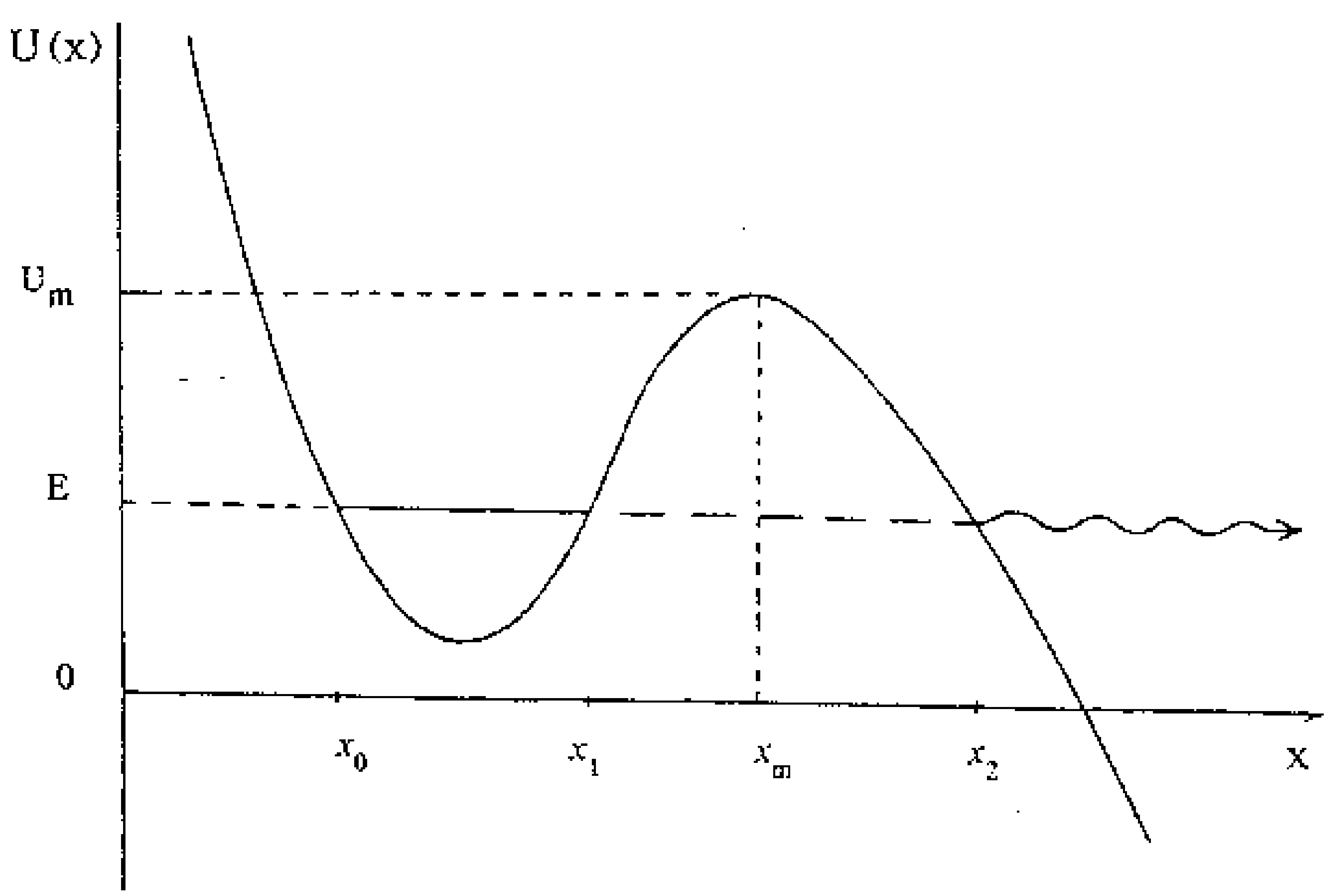

Figure 1.

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In many physical problems, however, the potential is in the form of a barrier, as a result of which the levels are quasistationary ($E = E_r - i\Gamma/2$). Since the Gamow wave function grows exponentially as $r \to \infty$, a numerical calculation of the position of level E_r and the level's width Γ poses certain difficulties.

We will consider this problem in the quasiclassical approximation, which yields formulae valid for an arbitrary smooth potential $U(x)$. The region where these formulae, derived for $n \gg 1$, are valid often "extends" to small quantum numbers $n \approx 1$ (just as in problems referring to the discrete spectrum with physically meaningful potentials; e. g., see [2, 3]).

A brief discussion of the main results of this work has been published in [4].

2. Generalization of the Bohr–Sommerfeld quantization rules

Near the top of the barrier, $x \approx x_m$, the parabolic approximation holds true:

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

where $\rho = (x - x_m)/\xi$, and $\xi_0 = (\hbar/m\omega)^{1/2}$ and $\omega = [-U''(x_m)]^{1/2}$ are the amplitude and frequency of the zero-point vibrations of the particle about the equilibrium point (from now on we assume that $\hbar = m = 1$). In this case the Schrödinger equation has the exact solution

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

which satisfies Sommerfeld's radiation condition (the $D_\nu(z)$ are parabolic cylinder functions [5]). To the left of the barrier ($\rho < 0$, $|\rho| \gg a$) this solution is matched with the quasiclassical solution

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

As usual, the quantization condition emerges from the requirement that the phases of functions (2) and (2′) coincide (to within $n\pi$) in the overlap region $a \ll |\rho| \ll x_m/\xi_0$, which always exists for large n. Knowing the asymptotic behaviour of $D_\nu(z)$ as $z \to \infty$, we obtain (see also [6, 7])

$$\int_{x_0}^{x_1} p(x)\,dx = \left(N + \frac{1}{2}\right)\pi \qquad N = n - \frac{1}{2\pi}\varphi(a) \tag{3}$$

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

$$\varphi(a) = \frac{1}{2i}\ln\left\{\Gamma\left(\frac{1}{2} + ia\right)\Big/\Gamma\left(\frac{1}{2} - ia\right)\left(1 + e^{-2\pi a}\right)\right\} + a(1 - \ln a) \tag{3'}$$

and

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

(the notation is given in figure 1). Parameter a, which for a parabolic barrier is defined in (1), is written here in a more general form, applicable for an arbitrary potential that meets the quasiclassical requirements. For quasistationary states this parameter is complex-valued, as are the turning points $x_{1,2}$.

In the simplest cases, integral (3″) can be evaluated explicitly, so there is no difficulty in continuing it analytically. For an arbitrary potential $U(x)$ the values of a for complex-valued E can be found numerically, which together with equation (3) determine the spectrum of quasistationary states.

Let us now analyze the main equations.

(a) The case where $a \ll 1$ corresponds to low barrier factors. Bearing in mind that

$$\varphi(a) = \frac{1}{24a} + \frac{7}{2880a^3} + \cdots + \frac{\mathrm{i}}{2}\mathrm{e}^{-2\pi a} \qquad a \to +\infty \tag{4}$$

(the properties of function $\varphi(a)$ have been studied extensively in [8]) and assuming that the radial momentum (in the spherically symmetric case) is

$$p = \{2[E_r - \mathrm{i}\Gamma/2 - U(r)]\}^{1/2} \qquad U(r) = V(r) + \left(l + \frac{1}{2}\right)^2 \Big/ 2r^2$$

we find that equation (3) yields

$$\Gamma = T^{-1}\exp\left(-2\int_{r_1}^{r_2}|p|\,\mathrm{d}r\right) \qquad T = 2\int_{r_0}^{r_1}p^{-1}\mathrm{d}r \tag{5}$$

where T is the period of radial oscillations of the particle inside the well (the Gamow formula for the width of a quasistationary state). Thus, equation (3) leads to meaningful results not only for small a but also for the opposite case, $a \gg 1$. It is, therefore, reasonable to expect that for intermediate values $a \approx 1$ it also provides a correct interpolation for the exact solution. Later on we will see that is is indeed the case (see sections 3 and 4).

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

$$\int_{q_i^{(0)}}^{q_i^{(1)}} p_i\,\mathrm{d}q_i = \left(N_i + \frac{1}{2}\right)\pi \tag{6}$$

where $N_i = n_i - \frac{1}{2\pi}\varphi(a_i)$ if tunnelling in coordinate q_i is possible ("an open channel"); otherwise $N_i = n_i = 0, 1, \ldots$. Solving this system of equations yields the complex-valued energies $E = E_r - \mathrm{i}\Gamma/2$ and the separation parameters β_i. When the barrier factor is low, tunnelling occurs practically in a single coordinate, say, q_f. (Note that the other "decay channels" are either closed or $\exp(-2\pi a_i) \ll \exp(-2\pi a_f)$. Systems satisfying special symmetry conditions may prove to be an exception.) For Γ we then arrive at the following formula (see appendix A):

$$\Gamma = \frac{c}{T}\exp(-2\pi a_f) \tag{7}$$

where

$$c = \left\{\alpha\left(1 + \sum_{i=1}^{f-1} \overline{v_f}/\overline{v_i}\right)\right\}^{-1} \qquad T = 2\int_{q_f^{(0)}}^{q_f^{(1)}} p_f^{-1}\,\mathrm{d}q_f$$

which is the generalization of the Gamow formula (5) and for $f = 1$ transforms into it. Here the p_i are the quasiclassical momenta

$$p_i(q) = \{2[\alpha E - U_i(q)]\}^{1/2} \qquad U_i(q) = u_i(q) + \beta_i v_i(q), \tag{8}$$

the β_i are the separation parameters $\left(\sum_{i=1}^{f}\beta_i = \text{constant}\right)$, and the $\overline{v_i}$ stand for the averages over the quasiclassical wave function:

$$\overline{v_i} = \int_{q_i^{(0)}}^{q_i^{(1)}} \frac{v_i(q)}{p_i(q)}\,\mathrm{d}q \Bigg/ \int_{q_i^{(0)}}^{q_i^{(1)}} \frac{\mathrm{d}q}{p_i(q)} \tag{9}$$

with $q_i^{(0,1)}$ the turning points.

In the particular case of the Stark effect in the hydrogen atom ($f = 2$), equation (7) transforms into a formula that earlier was found in [8] by direct calculation (considerably more complex) of the flux of particles leaving for infinity.

(c) The above formulae can be refined by allowing for a term of the order of $\hbar^2$ that is a correction to the ordinary quasiclassical scheme [9, 10]. Then the phase $\theta(r)$ in (2′) is given by the formula

$$\theta(r) = \int_{r_0}^{r} \mathrm{d}r\left\{p - \frac{1}{4}\left(\frac{p'}{p^2}\right)' - \frac{1}{8}\frac{(p')^2}{p^3} + \frac{1}{8rp^2}\right\} \tag{10}$$

(here $p' = \mathrm{d}p/\mathrm{d}r$), while the exact solution (2) yields, for $\tau = -\rho \gg |a|$, the following:

$$\theta(r) = \frac{1}{4}\tau^2 - \frac{a}{2}\ln\frac{\tau^2}{a} + \frac{1}{2}[\varphi(a) - a] + \frac{1}{2}\left(a^2 - \frac{3}{4}\right)\tau^{-2} + O(\tau^{-4}). \tag{10′}$$

By applying the parabolic approximation (1) for momentum $p(r)$ and evaluating the integrals in $\theta(r)$ we see that (10) can be matched with (10′). This again brings us to the quantization condition (3) in which, however, the function φ of (3′) is replaced with φ_2:

$$\varphi_2(a) = \varphi(a) - \frac{1}{24a}. \tag{11}$$

Comparison with (4) shows that what is subtracted from $\varphi(a)$ is the first term of its asymptotic expansion as $a \to \infty$. As is known (see [2]), the formal parameter $\hbar^2$ in the quasiclassical expansion transforms into $1/n^2$ in the final formulae. Since $\varphi_2(a) = O(a^{-3})$, the substitution of φ_2 for φ ensures that the resonance energy is calculated with a relative accuracy of the order of n^{-4}.

The same approach can be used to take into account the higher-order corrections to the quasiclassical scheme (see [10–12]), but the complexity of the calculations grows very rapidly. Apparently, allowing for corrections up to $\hbar^{2K}$ inclusive leads to a quantization condition (3) with the function

$$\varphi_K(a) = \varphi(a) - \sum_{j=1}^{K-1} c_j a^{-(2j-1)} \tag{11'}$$

where

$$c_j = (-1)^{j-1}\left[1 - 2^{-(2j-1)}\right] B_{2j}/2j(2j-1)$$

are the expansion coefficients of the asymptotic expansion (4), and the B_{2j} are Bernoulli numbers. Since $\varphi_K(a) = O\big(a^{-(2K-1)}\big)$ as $a \to \infty$, the accuracy with which E_r is calculated rises to n^{-2K} in the process. (In what follows we do not consider approximations corresponding to functions φ_K with $K > 2$.)

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

$$\varphi(a) = \mathrm{i}\ln(a - a_k) + O(1) \qquad a \to a_k. \tag{12}$$

One can easily see that the singularities correspond to the poles of the scattering amplitude for a parabolic barrier $U(x) = -\frac{1}{2}\omega^2 x^2$. Indeed, in this case the amplitude of the forward wave [1, 13],

$$B = (2\pi)^{-1/2} 2^{-\mathrm{i}a} \mathrm{e}^{-\pi a/2} \Gamma\left(\frac{1}{2} + \mathrm{i}a\right) \qquad a = -E/\omega, \tag{13}$$

has simple poles at points $a = a_k$. A pole in the scattering amplitude corresponds to a logarithmic singularity in $\varphi(a)$, since the latter is directly related to the scattering phase.

The respective wave functions exhibit the following asymptotic behaviour:

$$\psi_k(x) \sim x^k \exp(\mathrm{i}\omega x^2/2) \qquad x \to \pm\infty$$

and are not square-integrable. On the other hand, B and $\varphi(a)$ are regular at the mirror-symmetric points $a = a_k^*$:

$$\varphi(-\mathrm{i}(k+1/2)) = \mathrm{i}\ln\left[(2\pi)^{1/2}\left(\frac{2k+1}{2\mathrm{e}}\right)^{k+1/2} \Big/ k!\right].$$

(The amplitude B at the point $a = a_k^*$ cannot have a pole because this would contradict the hermiticity of the Hamiltonian, that is, there could exist square-integrable wave functions $\psi_k(x) \sim x^{-(k+1)} \exp(\mathrm{i}\omega x^2/2)$, $x \to \pm\infty$ $(k \geq 0)$ that would correspond to complex-valued energies $E = \mathrm{i}(k + 1/2)\omega$.)

(e) If the energy of a level approaches the top of the barrier, the quantization integral $J = \int_{x_0}^{x_1} p(x, E)\, \mathrm{d}x$ has a logarithmic singularity:

$$J(a) = J_0 + \frac{1}{2} a \ln a - J_1 a + J_2 a^2 + \cdots \qquad a \to 0. \tag{14}$$

The coefficient of this singularity is independent of $U(x)$, and for the next coefficient J_1 we can easily obtain a formula (see appendix B). When the level crosses the boundary $E = U_{\mathrm{m}}$, the following formula holds true:

$$\frac{\Gamma_n}{\mathrm{d}E_n/\mathrm{d}n} = \frac{\ln 2}{2\pi} = 0.1103 \tag{15}$$

which is asymptotically exact $(n \to \infty)$ for an arbitrary potential. Thus, at $E = U_{\mathrm{m}}$ the resonances do not yet overlap. Hence, in the region of energies $E > U_{\mathrm{m}}$ several above-the-barrier resonances can be observed although their widths rapidly grow with E:

$$\begin{aligned} \Gamma_n &= \Gamma_{n_0} + A(n - n_0)\omega \\ A &= \frac{\pi^2}{2}\left[(J_1 + b)^2 + \left(\frac{\pi}{4}\right)^2\right]^{-1} \qquad b = 0.482 \end{aligned} \tag{16}$$

($n = n_0$ corresponds to the energy $E = U_{\mathrm{m}}$; see equation (B.6)).

(f) Here is a remark concerning the connection between equations (3) and (11) and the results obtained previously by other researchers. The effect of the barrier factor on the quasiclassical quantization rules has been studied by Rice and Good [14], Connor [6], Drukaryov [7], and Kondratovich and Ostrovski [15]. The expressions for the corrections to the quantization rule that were obtained in [7, 14] correspond to the function $\varphi(a) = \arg \Gamma(\frac{1}{2} + \mathrm{i}a) + a(1 - \ln a)$, which is practically no different from (3′) if a is real and $a \gg 1$, that is, the barrier factor is small. This approximation, however, determines only the level's shift but not its width (to obtain (5) one must allow for $\mathrm{Im}\,\varphi(a)$). As the level approaches the top of the barrier, $|a| \approx 1$ and this approximation loses all meaning. A formula equivalent to (3′) has been obtained by Connor [6]. Note that in the cited papers no allowance was made for above-the-barrier resonances, when the parameter a becomes complex-valued, and for correction (11) of the order of $\hbar^2$.

Quantization rules (3) and (6) can have various applications. Let us consider some examples.

3. Model with exact solution

Let us consider states with $l = 0$ in the potential

$$V(r) = -\frac{1}{2}\omega^2 (r - R)^2 \qquad 0 < r < \infty. \tag{17}$$

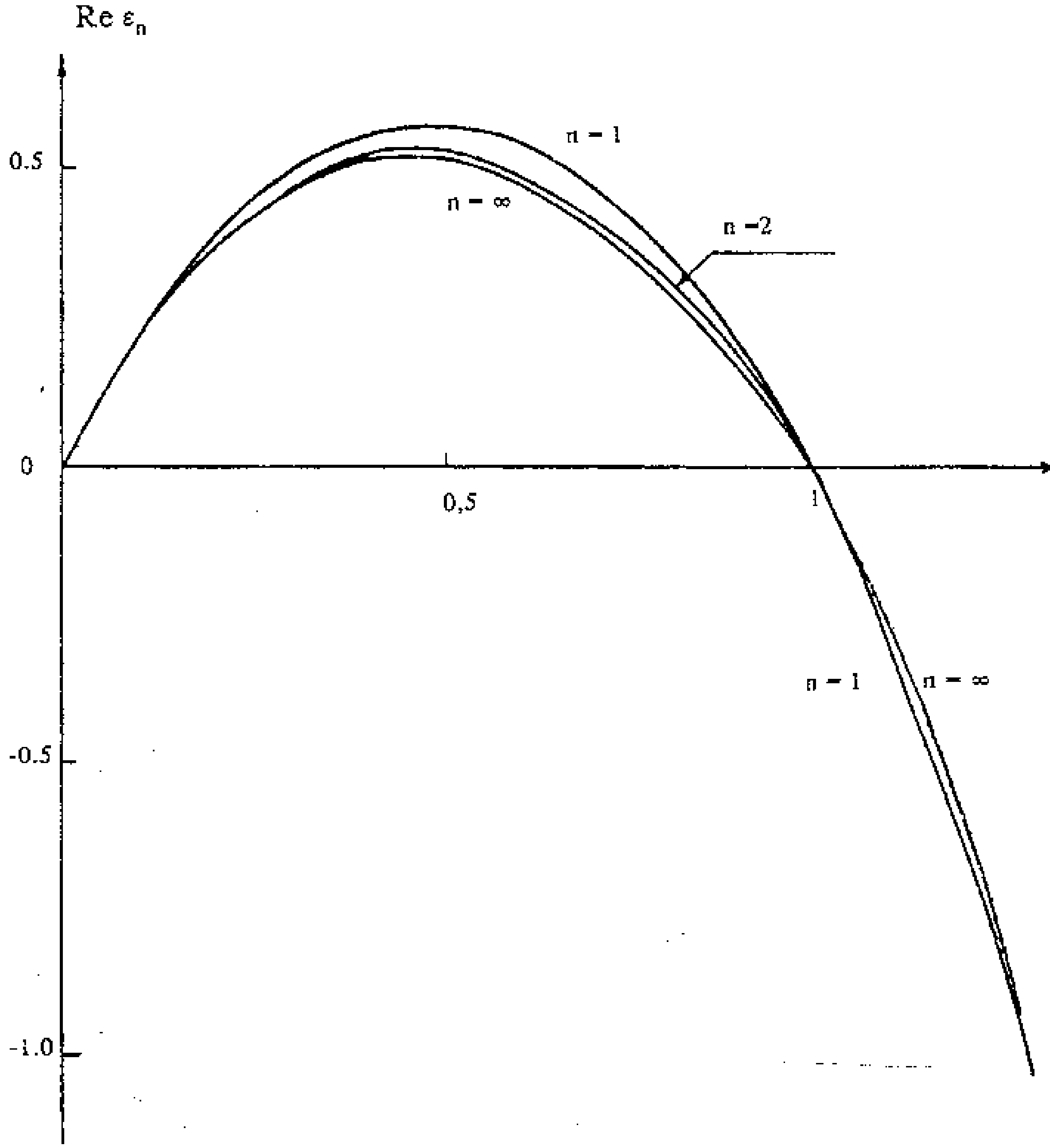

Figure 2. The real part of the ns-level energies in terms of the reduced variables (22).

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

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

with $\nu = -(\frac{1}{2} + ia)$ and $a = -E/\omega$. The spectrum of quasistationary states is determined from the condition that χ is regular at zero, $\chi(0) = 0$, which yields

$$D_{-\frac{1}{2}-ia}(-2^{1/2}e^{-i\pi/4}s) = 0 \tag{18}$$

where $s = (2J_0)^{1/2} = \omega^{1/2}R$. Assuming that $n \gg 1$ and $|E| \ll V_0 = -V(0)$ and taking into account the asymptotic behaviour of parabolic cylinder functions [5], from the exact equation (18) we get

$$s^2 - a\left(\ln\frac{s^2}{a} + 1 + \ln 2\right) + \varphi(a) = 2\pi\left(n - \frac{1}{4}\right). \tag{19}$$

On the other hand in this case $r_0 = 0$ and

$$\int_0^{r_1} p(r)\,\mathrm{d}r = J_0\phi(\varepsilon)$$

where $\varepsilon = E/V(0)$, and

$$\begin{aligned}\phi(\varepsilon) &= (1-\varepsilon)^{1/2} - \varepsilon\tanh^{-1}(1-\varepsilon)^{1/2} \\ &= \begin{cases} 1 + \frac{1}{2}\varepsilon\ln\varepsilon - \left(\frac{1}{2} + \ln 2\right)\varepsilon + \frac{1}{8}\varepsilon^2 + \frac{1}{32}\varepsilon^3 + \cdots & \text{as } \varepsilon \to 0 \\ \frac{2}{3}(1-\varepsilon)^{3/2} + O\left((1-\varepsilon)^{5/2}\right) & \text{as } \varepsilon \to 1. \end{cases}\end{aligned} \tag{20}$$

Hence, the common Bohr–Sommerfeld quantization rule assumes the form

$$J_0\phi(\varepsilon) = \left(n - \frac{1}{4}\right)\pi \qquad n = n_r + 1 = 1, 2, \ldots \tag{21}$$

which agrees with equation (19) for $\varepsilon \ll 1$ (highly excited levels). However, (19) contains an additional term $\varphi(a)$, in full accordance with (3).

If we ignore the barrier factor, the discrete spectrum occupies the interval $0 < \varepsilon < 1$. Putting $\varepsilon = 0$ in (21), we find the total number of s-levels in potential (17):

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

The results of the numerical calculations are depicted in figures 2 and 3.

It is expedient to go over to the scaled variables

$$\sigma = \left[s^2 \Big/ 2\pi\left(n - \frac{1}{4}\right)\right]^{1/2} \qquad \varepsilon_n = E_n \Big/ \left(n - \frac{1}{4}\right)\omega \qquad \gamma_n = -\operatorname{Im}\varepsilon_n \tag{22}$$

since this makes it possible to depict curves for different ns-levels in a single diagram.

The quantization rule (21) suggests that when a level enters the continuous spectrum, σ becomes equal to 1 (provided that $n \to \infty$ and the barrier factor is ignored). The quasiclassical approximation with the barrier factor included has sufficiently good accuracy even for the ground state, $n = 1$. A more detailed understanding of this can be gained from table 1, which lists the values of σ_n and γ_n corresponding to the moment when an ns-level enters the continuous spectrum.

The above example shows the range of applicability of equation (3), obtained under the condition that $n \gg 1$ (a common assumption in the WKB method), may extend to moderate values of quantum numbers.

We have also checked whether the asymptotic formula (15) is valid. The derivative $(\mathrm{d}E_n/\mathrm{d}n)_{E=0}$ is replaced with $\delta E_n = \frac{1}{2}\operatorname{Re}\{E_{n+1}(\tilde{R}_n) - E_{n-1}(\tilde{R}_n)\}$, where $\tilde{R}_n$ is determined by the condition that $\operatorname{Re} E_n(\tilde{R}_n) = 0$. The ratio $\Delta_n = \Gamma_n/\delta E_n$ tends to limit (15) as $n \to \infty$, although fairly slowly (for example, $\Delta_n = 0.1084$ at $n = 100$).

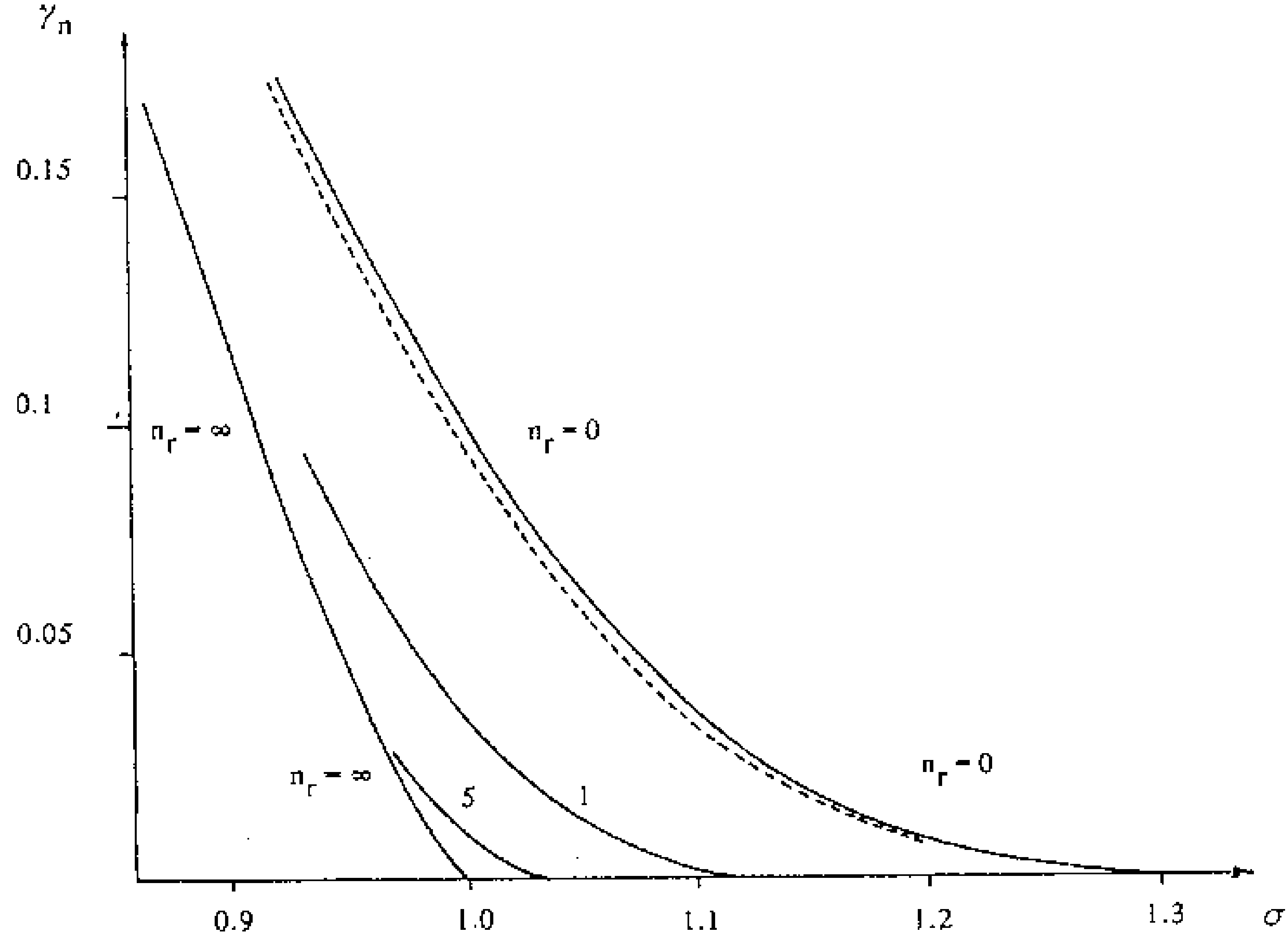

Figure 3. The width of ns-states for potential (17). The solid curves represents the results of calculations using the exact equation (18) and the dashed curve corresponds to approximation (3). Variables (22) are used here, too.

Table 1.

n_r	σ_n exact	WKB	δ_n	γ_n, exact	δ_n	Δ_n
0	0.995025	0.986768	0.83%	0.103805	1.30%	0.1000
1	0.996810	0.995248	0.16%	3.784(-2)	0.23%	0.1039
2	0.997848	0.997214	6.3(-4)	2.223(-2)	0.09%	0.1052
3	0.998403	0.998062	3.4(-4)	1.548(-2)	4.6(-4)	0.1059
5	0.998964	0.998819	1.5(-4)	9.439(-3)	1.8(-4)	0.1063
10	0.999465	0.999424	4.2(-5)	4.607(-3)	4.8(-5)	0.1071
50	0.999902	0.999900	2.0(-6)	8.009(-4)	$< 10^{-5}$	0.1081

Note: The above figures correspond to the moment when an ns-level enters the continuous spectrum, that is, $\mathrm{Re}\, E_n = 0$, and δ_n is the error of the WKB approximation (19). The quantity inside the parentheses stands for the order of the respective figure, $(n) \equiv 10^n$.

4. The Stark effect in a strong field

We will now use the quantization rule (3) to calculate the Stark effect in a strong field. (See also the papers [16, 17] and the citations given there.) The energy $E^{n_1 n_2 m}(\mathcal{E})$ can be close to the top of the barrier or even exceed it (sub-barrier and above-the-barrier resonances, respectively).

Among all the sublevels $|n_1 n_2 m\rangle$ with a given n of the greatest interest (from the experimental viewpoint) are, apparently, the $|n-1, 0, 0\rangle$ states and the adjacent ones (in quantum number values) as being the most stable. This can easily be seen by observing the following asymptotic formula ($\mathcal{E} \to 0$) [1]:

$$\Gamma^{(n_1 n_2 m)}(\mathcal{E}) \approx \text{const} \times \mathcal{E}^{-(2n_2+m+1)} \exp(-2/3n^3\mathcal{E}).$$

It is these states that manifest themselves (see [16, 18]) as peaks in the atomic photoionization cross sections near $E = 0$.

For states with $n \gg 1$ and $m \approx 1$, the quantization conditions in the hydrogen atom assume the form

$$\beta_i(-\varepsilon)^{-1/2} f(z_i) + (-1)^i \frac{F}{8n^2}(-\varepsilon)^{-3/2}\left[g(z_i) - m^2 h(z_i)\right] = \nu_i \qquad (23)$$

$$\beta_1 + \beta_2 = 1$$

where $z_i = (-1)^i 16\beta_i F\varepsilon^{-2}$ ($i = 1$ or 2),

$$\nu_1 = \left(n_1 + \frac{m+1}{2}\right)\Big/ n \qquad \nu_2 = \left(n_2 + \frac{m+1}{2} - \frac{1}{2\pi}\varphi(a)\right)\Big/ n \qquad (24)$$

and

$$a = \frac{n(-\varepsilon)^{3/2}}{2^{7/2}F}(1-z_2) f(1-z_2) + \mu^2 \frac{nF^2}{2^{1/2}(-\varepsilon)^{3/2}} F(3/4, 5/4; 1; 1-z_2) + O(\mu^4). \qquad (25)$$

Here we use atomic units, $\hbar = m_e = e = 1$, and the reduced variables ($\mu = m/n$)

$$\varepsilon = 2n^2 E^{(n_1 n_2 m)} = \varepsilon' - i\varepsilon'' \qquad F = n^4\mathcal{E} \qquad (26)$$

where n_1, n_2, and m are the parabolic quantum numbers [1] ($m \geq 0$), $n = n_1 + n_2 + m + 1$ is the principal quantum number, $\mathcal{E}$ the strength of the constant electric field in units of $\mathcal{E}_{at} = m_e^2 e^5 \hbar^{-4} = 5.142 \times 10^9$ V/cm, β_i are the separation parameters, and f, g, and h are expressed in terms of hypergeometric functions as follows:

$$f(z) = F(1/4, 3/4; 2; z)$$

$$g(z) = \frac{1}{3}F(3/4, 5/4; 2; z) + \frac{2}{3}F(3/4, 5/4; 1; z)$$

$$h(z) = F(3/4, 5/4; 2; z).$$

Note that in (23) the correction term that allows for the barrier factor is present only in the second equation, $i = 2$, because an electron tunnels along the coordinate $\eta = r - z$ and the effective potential $U_1(\xi)$, $\xi = r + z$, is always of a confining type [1].

When these equations are solved numerically, either the terms of the order of $F/8n^2$ must be discarded (the $1/n$-approximation) or the system must be solved in complete form (the $1/n^2$-approximation). We have calculated the values of E_r and Γ in the hydrogen atom for different states $|n_1 n_2 m\rangle$ using equations (23)–(25) as well as an independent method, the summing of divergent series of ordinary perturbation

Table 2. Stark-resonance calculations for the hydrogen atom performed by various methods.

$\|n_1, n_2, m\rangle$	$\|2,2,0\rangle$		$\|5,5,0\rangle$		$\|7,7,0\rangle$	
$\mathcal{E}$	1.8(−4)		1.0(−5)		3.0(−6)	
F	0.1125		0.1464		0.1519	
Method	ν	Γ	ν	Γ	ν	Γ
$1/n$	4.92385	2.22(−6)	10.7128	2.82(−6)	14.5767	1.347(−6)
$1/n^2$	4.92406	2.19(−6)	10.7127	2.80(−6)	14.5766	1.338(−6)
PHA	4.92402	2.283(−6)	10.713	2.83(−6)	14.577	1.35(−6)
[19]	4.9240	2.282(−6)	10.688	2.815(−6)	14.5771	1.338(−6)

Note: Here $n_1 = n_2 = (n-1)/2$, and the values of $\mathcal{E}$, ν, and Γ are expressed in terms of atomic units.

theory by the Padé–Hermite Approximation (PHA) scheme. Here we list only some of the results obtained; the reader interested in technical details can refer to [17].

We start with the case of moderate fields, $F < 0.2$. For the hydrogen atom, the numerical calculations of positions and widths of resonances have been calculated by Damburg and Kolosov [19]. We calculated $\nu = (-2E_r)^{-1/2}$ and Γ both in the $1/n$- and $1/n^2$-approximations in equations (23) and in the PHA scheme. The results for states with $n_1 = n_2 = (n-1)/2$ are listed in table 2 (note that $\nu = n = 1, 2, \ldots$ in the case of unshifted Coulomb levels). The results of our calculations agree well with each other and with the result obtained in [19].

In the case of strong fields let us first consider the positions of the Stark resonances $|n_1, 0, 0\rangle$. Table 3 lists the values of $\varepsilon'_n = -2n^2 \operatorname{Re} E^{(n-1,0,0)}$ for $n = n_1 + 1 = 20$ (similar results have been obtained for $n = 50$). Clearly, the barrier factor has little effect on the position of resonance E_r (compare lines (a) and (b) for a single value of F), although the effect grows somewhat with field strength.

Table 3. The energy of the $|19,0,0\rangle$ state in electric field $\mathcal{E}$.

		Method		
$F = n^4\mathcal{E}$		$1/n$	$1/n^2$	PHA
0.10	(a)	0.72994	0.73000	0.7300
0.20	(a)	0.48280	0.48309	0.4831
	(b)	0.48301	0.48309	
0.30	(a)	0.25489	0.25696	0.256
	(b)	0.25619	0.25663	
0.35	(b)	0.1490	0.1488	0.149
0.40	(a)	0.0432	0.0425	0.042
	(b)	0.0421	0.413	
0.45	(a)	−0.0643	−0.0652	−0.065
0.50	(a)	−0.1716	−0.1727	−0.173
0.60	(a)	−0.3842	−0.3855	−0.386
1.00	(a)	−1.1896	−1.1907	−1.19

Note: The energies $-\varepsilon'_n = -2n^2 \operatorname{Re} E^{(n-1,0,0)}$ are listed as multiplied by −1. *Notation:* (a) calculations using equation (23) without barrier factor, that is, $\varphi(a) \equiv 0$, and (b), with barrier factor.

The corresponding results for $\gamma_n = n^2\Gamma^{(n-1,0,0)}$ are shown in figure 4. Clearly, the barrier-factor correction to the level width is essential in the region where $F < F_0$, but as the field strength grows, the role of this correction diminishes. (Here F_0 corresponds to the case where $\varepsilon = 0$, that is, the level crosses the ionization limit $E = 0$. For the $|19,0,0\rangle$ state we have $F_0 \approx 0.42$.) For $n \geq 20$ one can limit oneself to the solution of equations (23) in the $1/n$-approximation, and in the majority of cases the accuracy proves sufficient for comparison with experimental data.

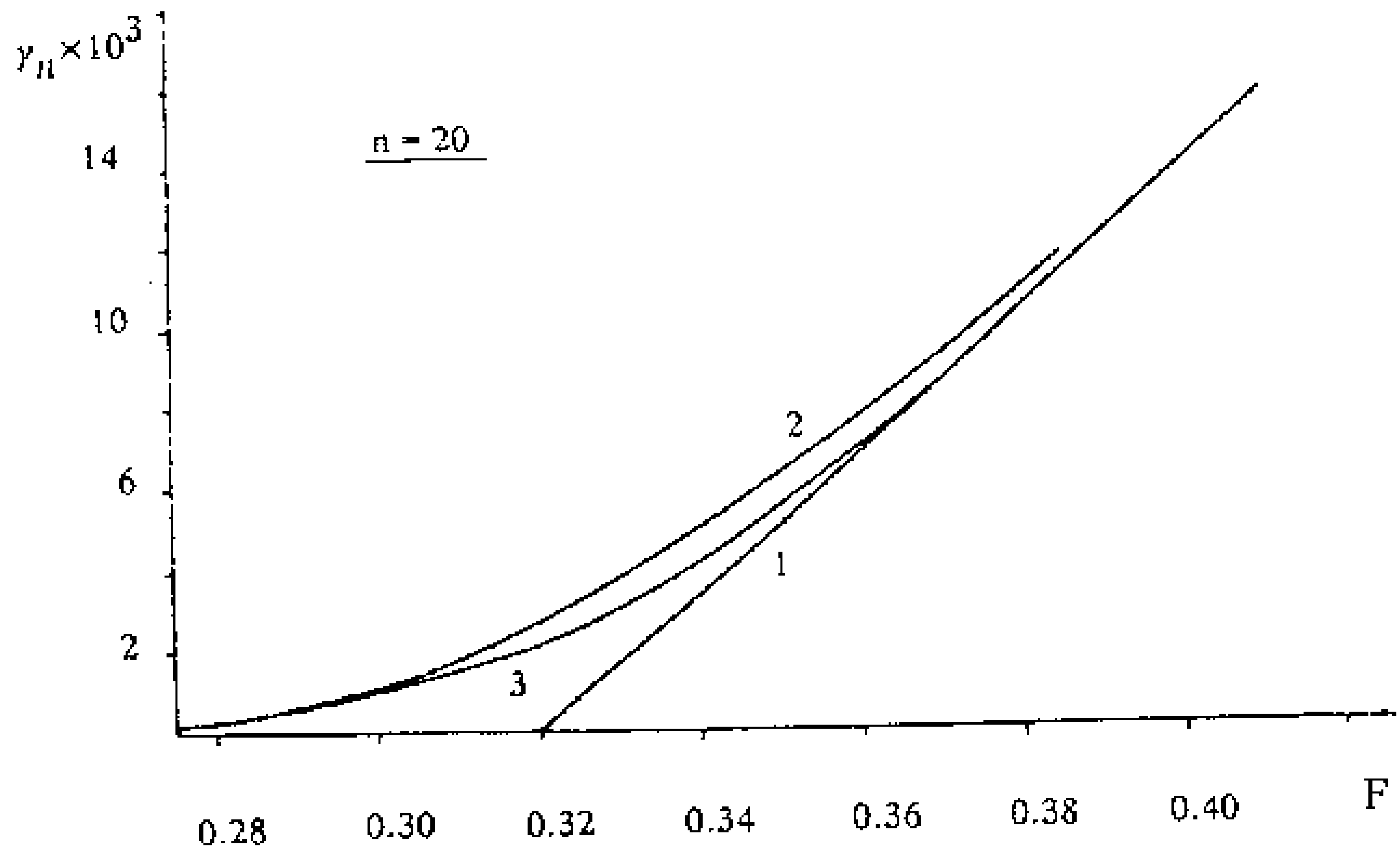

Figure 4. The effect of the barrier factor on the width of the $|19,0,0\rangle$ state. Curve *1* corresponds to the $1/n$-approximation without barrier factor, and curves *2* and *3* to the $1/n$- and $1/n^2$- approximation with barrier factor.

In figure 5 the calculated values of the Stark-resonance energies are compared with the experimental data on the hydrogen-atom photoionization spectrum taken from [20]. Clearly, the positions of the peaks correspond to ε'_n, while the peak widths agree qualitatively with the values of ε''_n for Stark resonances (other examples of this kind are discussed in [16, 18]). Level widths grow rapidly when $E > 0$, even for $|n-1,0,0\rangle$ states, which have the lowest ionization probability.

Thus, the use of quasiclassical quantization conditions that allow for barrier penetrability makes it possible to explain quantitatively the hydrogen-atom photoionization spectrum both in the sub-barrier region and above the barrier.

The generalization of the above theory to highly excited states of other atoms can be found in [16, 17], where, for one thing, scaling relations for near-threshold Stark resonances are established.

5. Conclusion

The quantization conditions (3) may be generalized to the relativistic case and applied to the Dirac equation. This, for one thing, would simplify the calculation of the positions and widths of positron resonances, corresponding to states that have dived into the lower continuum. Basically, with exponential accuracy, the formulae of the quasiclassical approximation for scalar and spinor particles coincide, but for thorough

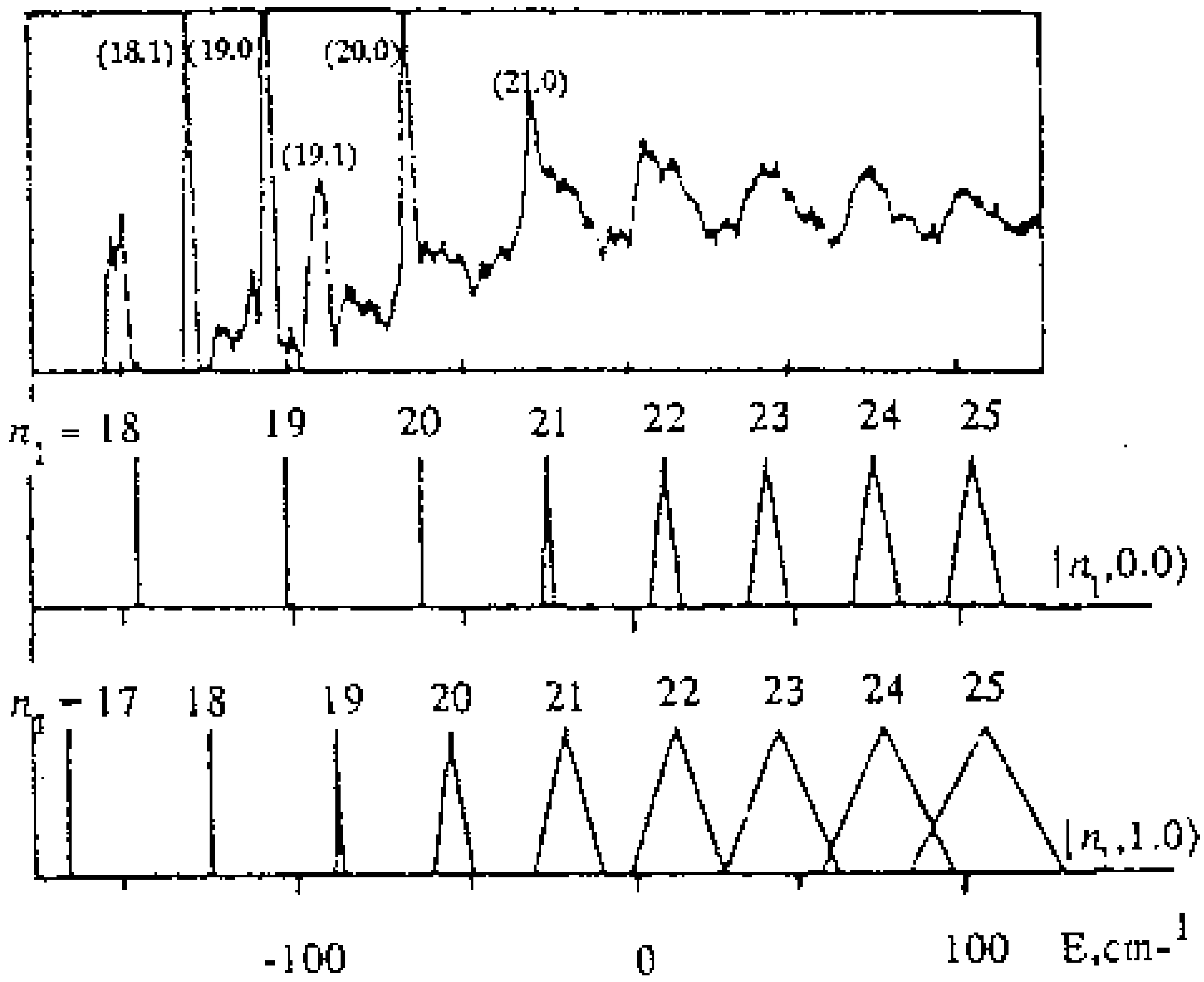

Figure 5. The experimental hydrogen-atom photoionization spectrum at $\mathcal{E}$ = 8.0 kV/cm. The results of our calculations for the $|n_1,0,0\rangle$ and $|n_1,1,0\rangle$ states are also shown. The top vertex of a triangle indicates the resonance energy E_r and the length of the base is equal to width Γ.

calculations of the pre-exponential factor certain difficulties emerge (see [21] for the case of fermions). We hope to return to this question in the future.

Acknowledgments

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Appendix A. Generalization of the Gamow formula to the case of several degrees of freedom

We assume that the quasiclassical momenta p_i ($i = 1, 2, \ldots, f$) can be represented in form (8). This is not the most general case of variable separation, but many problems interesting from the standpoint of physics belong to this case. For instance, the Schrödinger equation for the case of the Stark effect in the hydrogen atom separates in the parabolic coordinates $\xi = r + z$, $\eta = r - z$, and φ ($0 \le \varphi \le 2\pi$), with (see [1])

$$U_1(\xi) = -\frac{\beta_1}{2\xi} + \frac{m^2}{8\xi^2} + \frac{1}{8}\mathcal{E}\xi$$
$$U_2(\eta) = -\frac{\beta_2}{2\eta} + \frac{m^2}{8\eta^2} - \frac{1}{8}\mathcal{E}\eta. \tag{A.1}$$

(Here $\beta_1 + \beta_2 = 1$, $v_{1,2}(q) = -1/2q$, and $\alpha = 1/4$.) Electron tunnelling proceeds along coordinate η, and $U_1(\xi)$ is a confining potential for all $\mathcal{E} > 0$.

Another example is the nonrelativistic problem of two centres. Here

$$v_1(\xi) = \frac{\beta_1}{\xi^2 - 1} \qquad v_2(\eta) = \frac{\beta_2}{1 - \eta^2} \qquad \alpha = \frac{1}{2}R^2 \qquad \beta_1 + \beta_2 = 0 \tag{A.2}$$

where $\xi = (r_1 + r_2)/R$ and $\eta = (r_1 - r_2)/R$, and R is the distance between the fixed centres (nuclei).

Putting $E = E_r - \mathrm{i}\Gamma/2$ and $\beta_j = \beta_j' + \mathrm{i}\beta_j''$ in (6) (both Γ and β_j'' are exponentially small), we arrive at the following equations:

$$\frac{1}{2}\alpha\Gamma + \beta_j''\overline{v_j} = 0 \quad (1 \le j \le f-1) \qquad \sum_{j=1}^{f}\beta_j'' = 0 \tag{A.3}$$

where notation (9) has been employed. At $j = f$ one must allow for function $\varphi(a)$ on the right-hand side, which yields

$$\alpha\Gamma T\left(1 + \sum_{j=1}^{f-1}\overline{v_f}/\overline{v_j}\right) = \exp(-2\pi a_f). \tag{A.4}$$

This yields

$$\begin{aligned} \beta_i'' &= -\alpha\Gamma/2\overline{v_i} \qquad i = 1, 2, \ldots, f-1 \\ \beta_f'' &= \frac{1}{2}\alpha\Gamma\sum_{i=1}^{f-1}(\overline{v_i})^{-1} \end{aligned} \tag{A.5}$$

and for Γ we get formula (7).

As an illustration let us take the Stark effect. Performing the scaling transformation $\xi = n^2x$, $\eta = n^2y$, we find that

$$\begin{aligned} p_\xi &= \frac{1}{2n}k_1(x) \qquad p_\eta = \frac{1}{2n}k_2(y) \\ k_{1,2}(q) &= \left(\varepsilon \mp Fq + \frac{4\beta_{1,2}}{q} - \frac{\mu^2}{q^2}\right)^{1/2} \end{aligned} \tag{A.6}$$

where $\mu = m/n$ and the reduced variables (26) are employed. Whence,

$$\begin{aligned} c &= \frac{4\sigma_1\tau_2}{\sigma_1\tau_2 + \sigma_2\tau_1} \\ T &= 2\int_{\eta_0}^{\eta_1}\frac{\mathrm{d}\,\eta}{p_\eta} = 4n^3\tau_2 \end{aligned} \tag{A.7}$$

and equation (7) yields

$$\Gamma = \frac{\sigma_1}{n^3(\sigma_1\tau_2 + \sigma_2\tau_1)}\exp(-2\pi a) \tag{A.8}$$

where

$$\sigma_i = \int_{q_0}^{q_1}\frac{\mathrm{d}q}{qk_i(q)} \qquad \tau_i = \int_{q_0}^{q_1}\frac{\mathrm{d}q}{k_i(q)}$$

$$a = \frac{n(-\varepsilon)^{3/2}}{2\pi F}\int_{u_1}^{u_2}\frac{\mathrm{d}u}{u}\left(t - \frac{1}{4}z_2u + u^2 - u^3\right)^{1/2} \qquad t = \frac{\mu^2F^2}{(-\varepsilon)^3}.$$

Formula (A.8) was obtained earlier in [16] by an independent method without using equation (7).

Appendix B

Let us consider the quantization condition (3) in the energy range near the barrier's top ($a = (U_{\rm m} - E)/\omega \to 0$). If we introduce the notation

$$J(a) = \int_{x_0}^{x_1} p(x, E)\,{\rm d}x \tag{B.1}$$

we can show that expansion (14) is valid, with

$$J_0 = \int_{\overline{x_0}}^{x_{\rm m}} \overline{p}\,{\rm d}x \qquad J_1 = \frac{1}{2}\ln J_0 + I \tag{B.2}$$

$$I = \frac{1}{2}\left[1 + \ln\frac{2\omega(x_{\rm m} - \overline{x}_0)^2}{J_0}\right] + \int_{\overline{x_0}}^{x_{\rm m}} {\rm d}x\left(\frac{\omega}{\overline{p}} - \frac{1}{x_{\rm m} - x}\right) \tag{B.3}$$

and $\overline{p} = p(x, E = U_{\rm m})$ and $\overline{x_i}$ are the quasiclassical momentum and turning points at $E = U_{\rm m}$ ($\overline{x_1} = x_m$; see figure 1). Since $\overline{p}(x) = \omega|x - x_{\rm m}| + \cdots$ as $x \to x_{\rm m}$, the poles of the integrand cancel out and the integral is always convergent.

To prove this we note that

$$\frac{{\rm d}J}{{\rm d}a} = -\frac{1}{2}\omega T \qquad \omega = \left[-U''(x_{\rm m})\right]^{1/2} \tag{B.4}$$

with the oscillation period T of the particle diverging logarithmically as $a \to 0$. Isolating the singular part of the integral, we get

$$\frac{1}{2}T = \omega^{-1}\ln\frac{x_{\rm m} - x_0}{x_{\rm m} - x_1} + \int_{x_0}^{x_1} {\rm d}x\left[\frac{1}{p(x, E)} - \frac{1}{\omega(x_{\rm m} - x)}\right]$$

with $x_{\rm m} - x_1 = \omega^{-1}[2(U_{\rm m} - E)]^{1/2} + \cdots = (2a/\omega)^{1/2} + \cdots$. Whence,

$$\begin{aligned} \omega T &= \ln\frac{1}{a} + c_0 - c_1 a - c_2 a^2 - \cdots \\ c_0 &= 2J_1 - 1 \qquad c_k = (k+1)J_{k+1} \quad \text{for} \quad k \geq 1 \end{aligned} \tag{B.5}$$

and, allowing for equation (B.4), we arrive at equations (14) and (B.2). If we ignore the barrier factor, the number of bound states is

$$n_0 = \frac{1}{\pi}J_0 + \frac{1}{4} + O(J_0^{-1}) \tag{B.6}$$

(for $J_0 \gg 1$). Equation (3) assumes the form $\varphi(a) + a\ln a - 2Ia = 2\pi(n - n_0)$. Using the expansion

$$\varphi(a) = \frac{{\rm i}}{2}\ln 2 - a\ln a + \left(1 - 2\ln 2 - C - {\rm i}\frac{\pi}{2}\right)a + O(a^2) \tag{B.7}$$

with $|a| \ll 1$ and $C = 0.5772\ldots$ the Euler constant, we see that terms proportional to $a \ln a$ cancel out and the equation assumes the form

$$\left(\Lambda + \mathrm{i}\frac{\pi}{2}\right)a + O(a^2) = 2\pi(n_0 - n) + \mathrm{i}\frac{\ln 2}{2} \tag{B.8}$$

where $\Lambda = J_0 + \beta$, with $\beta = 2b + 1 = C + 2\ln 2 = 1.964$. Assuming here that $E = E_r - \mathrm{i}\Gamma/2$, at $E_r = 0$ we arrive at equations (15) and (16). Note that E_r equals U_m not at $n = n_0$ (as was the case when we ignored the barrier factor) but at a somewhat greater value $n = n_0 + \ln 2/8\Lambda$ (however, this correction is small).

Note that both J_1 and c_0 in equations (14) and (B.5) are anomalously large since they contain $\ln \Lambda$, while the subsequent factors J_k rapidly decrease as k grows. This is easily seen if we turn to potential (17) (see equation (B.10)).

Let us illustrate these formulae by the following examples.

(a) For the parabolic barrier (17) we have

$$J_0 = \frac{V_0}{\omega} = \frac{1}{2}\omega R^2 \qquad I = \frac{1}{2} + \ln 2$$

where $V_0 = -V(0)$ is the depth of the potential well at zero. (In the case at hand the characteristic points are $r_0 = 0$, $r_{1,2} = R(1 \mp \varepsilon^{1/2})$, and $r_m = R$. Note that $\ln \varepsilon$ is contained only in the second term of expansion (20), which is followed by a series of integral powers of ε.) The integrals J and T can be calculated analytically:

$$J(a) = J_0\phi(\varepsilon) \qquad T = 2\omega^{-1}\tanh^{-1}(1-\varepsilon)^{1/2} \tag{B.9}$$

where $\varepsilon = -E/V_0$, and $\phi(\varepsilon)$ has been defined in (20). As $\varepsilon \to 0$, that is, for levels close to the top of the barrier, we arrive at expansion (14) in which

$$J_1 = \frac{1}{2}\ln J_0 + 1.193 \qquad J_n = a_n J_0^{1-n} \quad \text{for} \quad n \geq 2 \tag{B.10}$$

where the a_n are the expansion coefficients in (20) when $\varepsilon \to 0$.

(b) Let us consider the s-levels in the potential

$$V(r) = -\zeta r^{-1} - \mathcal{E} r \tag{B.11}$$

(the spherically symmetric model of the Stark effect). Here $V_m = -2(\zeta\mathcal{E})^{1/2}$, $r_m = (\zeta/\mathcal{E})^{1/2}$, $r_{1,2} = r_m\left[\varepsilon \mp (\varepsilon^2 - 1)^{1/2}\right]$, $\omega = 2^{1/2}\zeta^{-1/4}\mathcal{E}^{3/4}$, and $\overline{p}(r) = \omega r_m(\rho^{-1/2} - \rho^{1/2})$, with $\varepsilon = E/V_m$ and $\rho = r/r_m$, where

$$J_0 = \frac{4}{3}\omega r_m^2 = 2^{5/2} \times 3^{-1}(\zeta^3/\mathcal{E})^{1/4} \qquad I = \frac{1}{2}(\ln 24 - 3).$$

(c) Generalizing the above examples, we put $\overline{p} = \omega r_m(\rho^{\alpha-1} - \rho^{\alpha})$, $0 < \alpha \leq 1$. From (B.2) we find that $J_0 = \omega r_m^2/\alpha(\alpha+1)$ and

$$I = \frac{1}{2}[1 + \ln 2\alpha(\alpha+1)] - C - \psi(2-\alpha) = \begin{cases} 1.193 & \text{if } \alpha = 1 \\ 0.089 & \text{if } \alpha = 1/2 \\ \ln\alpha + 0.193 & \text{if } \alpha \to 0 \end{cases}$$

(the previous cases are obtained if we put $\alpha = 1$ and $\alpha = 1/2$). Thus, the values of I are of the order of unity (except for the case when $\alpha \to 0$, which corresponds to "falling to the centre" [1]) and J_1 contains a large logarithm. As equation (B.10) implies, the subsequent coefficients J_n fall off rapidly with increasing n. In view of this we can keep only the three first terms in the expansion.

We note in conclusion that the coefficients of the leading singularity in $J(a)$ and T are independent of the shape of the potential.

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