# Quantization with allowance for the barrier penetration

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The correction to the Bohr-Sommerfeld quantization rules, which is associated with the barrier penetration, has been determined. The equation which has been obtained determines the position and width of the quasi-steady-state levels.

**1**. The Bohr-Sommerfeld quantization rules determine the discrete energy spectrum.[1] In many physical problems, however, the potential has a barrier which gives rise to quasi-steady states, instead of discrete levels ($E = E_r - i\Gamma/2$). Because the Gamow wave function increases exponentially as $r \to \infty$, a numerical calculation of $E_r$ and $\Gamma$ poses some difficulties.

We will consider this problem in a semiclassical approximation which gives analytic expressions that can be used for a smooth random potential.

**2**. *Generalization of quantization rules.* We use the following parabolic approximation near the barrier vertex ($x \approx x_m$; see Fig. 1):

$$p(x) = (\frac{1}{4}\rho^2 - a^2)^{1/2}, \qquad a = [U(x_m) - E]/\omega,$$

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

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

which satisfies the radiation condition. If this condition is joined with the semiclassical wave function near $x_0 < x < x_1$ (Fig. 1), we obtain the quantization condition

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

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

  

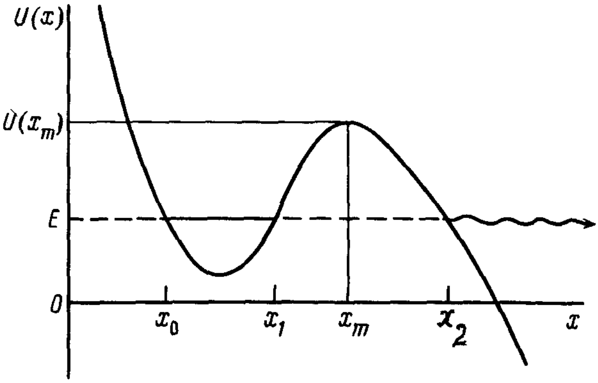


FIG. 1

$$\varphi(a)=\frac{1}{2i}\ln[\Gamma(\frac{1}{2}+ia)/\Gamma(\frac{1}{2}-ia)(1+e^{-2\pi a})]+a(1-\ln a), \qquad (1')$$

$$a=\frac{1}{\pi}\int_{x_1}^{x_2}[-p^2(x)]^{1/2}dx \qquad (1'')$$

(the notation is clear from Fig. 1).

The case $a \gg 1$ corresponds to a slight barrier penetration. Since

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

if we set $p(r)=\{2[E_r-(i/2)\Gamma-U(r)]\}^{1/2}$, we find from (1)

$$\Gamma=T^{-1}\exp(-2\int_{r_1}^{r_2}|p|dr), \quad T=2\int_{r_0}^{r_1}p^{-1}dr \qquad (3)$$

the Gamow formula for the width of a quasi-stationary level. Equations (1) generalize this formula to the case in which the level energy is close to the barrier vertex, so that the exponentially small value of $\Gamma$ vanishes. The parameter $a$ in this case is complex (just as the reversal points $r_{1,2}$). In the simplest cases integral (1″) is evaluated explicitly and its analytic continuation does not run into difficulties. For a random potential $U(r)$ the values of $a$ for complex $E$ can be determined numerically from (1″), which, along with Eq. (1), determines the spectrum of the quasi-stationary states.

There are also equations such as (1) for multidimensional problems with separable variables $q_1, \ldots q_s$ ($s$ is the number of degrees of freedom). If $2\pi a_i \gg 1$ ($1 \leqslant i \leqslant s$), the Gamow formula for the level width can be generalized. This generalization differs from (3) in the coefficient of the exponential function.

We note that $\varphi(a)$ has logarithmic singularities at the points $a=a_k$

$$a_k=(k+1/2)i,\quad k=0,1,\ldots,$$

$$\varphi(a)=i\ln(a-a_k)+O(1)\quad\text{as}\quad a\to a_k, \tag{4}$$

which correspond to the poles of the amplitude of the scattering by a parabolic barrier [the function $\varphi(a)$ is related to the scattering phase].

3. *Higher-order corrections to the Wentzel-Kramers-Brillouin approximation*. The preceding expressions can be refined by taking into account the correction of order $\hbar^2$ (Refs. 2 and 3). Equation (1) in this case retains its form, but the function $\varphi(a)$ should be replaced by $\varphi_2(a)=\varphi(a)-(1/24)a$. The first term of the asymptotic expansion in $\varphi(a)$ can thus be subtracted from it [cf. Eq. (2)]. The formal parameter $\hbar^2$ of the semiclassical expansion in the final expressions becomes $1/n^2$. Since $\varphi_2(a)=O(a^{-3})$, the substitution $\varphi\to\varphi_2$ in the quantization rule makes it possible to calculate the energy within an error[2] on the order of $n^{-4}$.

4. The quantization rule (1) has various applications. We will discuss only two examples.

a) The Schrödinger equation with $l=0$ in the potential

$$V(r)=-\frac{1}{2}\omega^2(r-R)^2,\quad 0<r<\infty \tag{5}$$

admits an exact solution. The energy spectrum is determined from the equation

$$D_\nu(-2e^{-i\pi/4}s^{1/2})=0, \tag{6}$$

where $\nu=-1/2+iE/\omega$ and $s=\frac{1}{2}\omega R^2$ ($s=V_0/\omega$, where $V_0$ is the depth of the potential well when $r=0$). On ther other hand, Eq. (1) in this case can be written as follows:

$$s\phi(\epsilon)+\frac{1}{2}\varphi(s\epsilon)=(n-{}^1\!/_4)\pi\ , \tag{7}$$

where $n=n_r+1=1,2,\ldots,$

$$\epsilon=-E/V_0,\qquad \phi(\epsilon)=(1-\epsilon)^{1/2}-\epsilon\,\mathrm{Ar\ tan}(1-\epsilon)^{1/2}\ .$$

These equations were solved numerically. The real parts of the energy calculated from (6) and (7) are approximately equal, especially in the tunneling region ($\epsilon>0$). The accuracy of the calculation of the widths (Fig. 2) is satisfactory even for the ground state. In Fig. 2 the variable $\sigma=[s/\pi(n-1/4)]^{1/2}$, so that $\sigma=1$ when the level enters the continuum (if $n\to\infty$ and the barrier penetration is ignored). This example shows that the range of applicability of Eq. (1), which was obtained under the condition that $n\gg 1$, can be extended to small quantum numbers.

b) The Stark effect in a strong field (see, for example, Refs. 4 and 5 and the bibliography cited there). For the states with $n\gg 1$ and $|m|\ll n$ the quantization conditions are

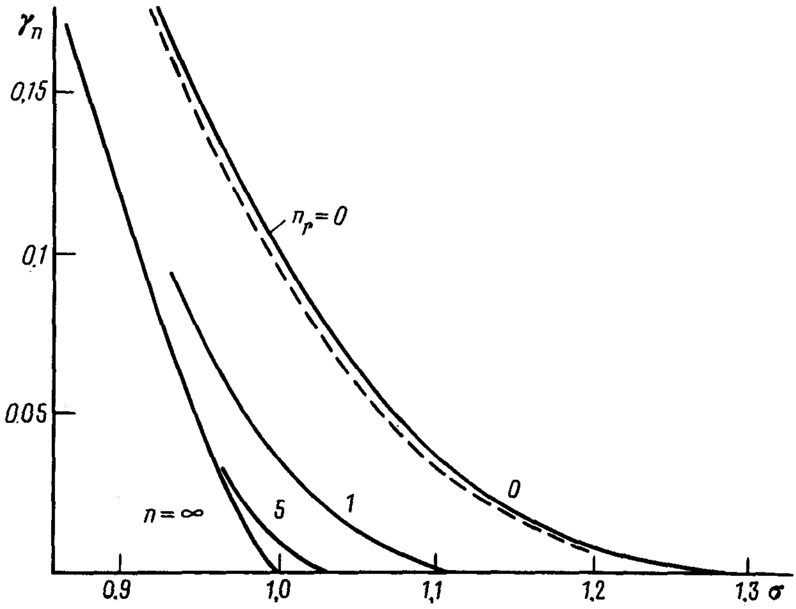


FIG. 2. The width of the $ns$ levels in potential (5) vs the parameter $\sigma$. Solid curves—Calculations based on Eq. (6); dashed curves—approximation (7). The curves have the values $n_r = n-1$; the ordinate has $\gamma_n = \Gamma_n/2(n-1/4)\omega$.

$$\beta_i(-\epsilon)^{-1/2} f(z_i) + (-1)^i \frac{F}{8n^2}(-\epsilon)^{-3/2}[g(z_i) - m^2 h(z_i)] = \nu_i , \tag{8}$$

where $\beta_1 + \beta_2 = 1$, $z_i = (-1)^i 16\beta_i F\epsilon^{-2} (i = 1 \text{ or } 2)$,

$$\nu_1 = (n_1 + \frac{|m|+1}{2}) / n, \qquad \nu_2 = (n_2 + \frac{|m|+1}{2} - \frac{\varphi(a)}{2\pi}) / n , \tag{9}$$

$$a = \frac{n(-\epsilon)^{3/2}}{2^{7/2}F}(1-z_2) f(1-z_2) + \mu^2 \frac{nF^2}{2^{1/2}(-\epsilon)^{3/2}}$$

$$\times F(3/4, 5/4; 1; 1-z_2) + O(\mu^4) . \tag{10}$$

Here $\hbar = m_e = 1$, $\epsilon = 2n^2 E^{(n_1 n_2 m)} \equiv \epsilon' - i\epsilon''$, $\mu = m/n$, $F = n^4 \mathscr{E}$ ($\mathscr{E}$ is the electric field strength), $n_1$, $n_2$, and $m$ are the parabolic quantum numbers,[1] $n = n_1 + n_2 + |m| + 1$, and $f$, $g$, and $h$ are expressed in terms of the hypergeometric functions: $f(z) = F(1/4, 3/4; 2; z)$, etc. The solution of Eq. (8) involves either dropping the terms proportional to $F/8n^2$ or solving this equation in its entirety ($1/n$ and $1/n^2$, respectively, are approximations). The real part of the reduced energy, $\epsilon_n'$ (evaluated using the inverse square law) for the states of the hydrogen atom with $n_1 = n-1$ and $n_2 = m = 0$ is given in Table I. Also given in Table I are the values of

TABLE I.

| $F$ | $n = 20$: $1/n$ | $n = 20$: $1/n^2$ | $n = 20$: PHA | $n = 50$: $1/n$ | $n = 50$: $1/n^2$ | $n = 50$: PHA |
|---|---|---|---|---|---|---|
| 0,20 | 0,48301 | 0,48309 | 0,4831 | 0,46307 | 0,46309 | 0.4631 |
| 0.25 | 0,36677 | 0,36695 | 0,3670 | 0.34054 | 0,34057 | 0,3406 |
| 0,30 | 0,2562 | 0,2566 | 0,256 | 0,22186 | 0,22193 | 0.222 |
| 0,35 | 0,1490 | 0.1488 | 0,149 | 0,10768 | 0,10775 | 0.108 |
| 0,40 | 0,0421 | 0,0413 | 0,042 | – | – | – |

$\epsilon_n'$ which were found by summing the perturbation theory series (in powers of $\mathscr{E}$) using the Padé-Hermite approximants[5] (PHA). The results of these two (independent) methods are in complete agreement with each other.

Of particular importance for the Stark level widths is the incorporation of the barrier penetration in Eq. (8). A comparison with other calculations and with the experimental data on the Stark resonances shows the $E_r$ and $\Gamma$ for the tunneling and above-the-barrier resonances can be determined by taking into account the barrier penetration in the quantization rules. These results will be discussed in a future, more detailed paper.

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[1)]Here $D_\nu(z)$ is the parabolic cylinder function.

[2)]Correspondingly, allowance for the corrections up to and including $\hbar^{2K}$ in the WKB method gives rise to the replacement $\varphi \to \varphi_K$: here $\varphi_K(a) = O(a^{-(2K+1)})$ as $a \to \infty$. Accordingly, the accuracy of calculating the energy increases to $n^{-2K}$.

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