# QUASICLASSICAL PARTICLES IN A ONE-DIMENSIONAL PERIODIC POTENTIAL

A. M. DYKHNE

Institute for Radiophysics and Electronics, Siberian Section, Academy of Sciences, U.S.S.R.

Submitted to JETP editor, December 13, 1960

J. Exptl. Theoret. Phys. (U.S.S.R.) **40**, 1423-1426 (May, 1961)

The widths of the energy gaps in the spectrum of a quasiclassical particle in a one-dimensional periodic potential are calculated. The widths are found to be exponentially small. The factor in front of the exponential and the energy spectrum near the edge of the band are determined.

THE energy spectrum of a particle in a periodic field cannot be determined in the general case. Any specific computation can be carried out using perturbation theory only when the period potential is much smaller than the particle energy. The purpose of the present paper is to find the spectrum in the quasiclassical approximation.

We shall treat the one-dimensional case. The potential U is a periodic function of x with period L. The condition for quasiclassical behavior, $kL \gg 1$, where k is the quasimomentum of the particle, is assumed to be satisfied. If the energy of the particle E is less than the maximum value $U_{max}$ of the potential, the dispersion can be determined by the usual WKB method.

However, if $E > U_{max}$, the usual WKB method leads to an incorrect result. In fact, the quasiclassical wave function ($\hbar = 1$)

$$\psi(x) = p^{-1/2} \exp\left(i\int^{x} p\,dx\right) \tag{1}$$

has the form of a Bloch wave, and the dependence of the energy on quasimomentum is given by the equation

$$kL = \int_0^L p\,dx. \tag{2}$$

The spectrum thus obtained is continuous. However, we know very well that in the spectrum there actually are energy gaps which cannot be found by using the ordinary WKB method. In fact, as we shall see from the following, the width of the energy gaps is an exponentially small quantity and cannot be found by expansion in powers of a small parameter.

The method developed below is analogous to one proposed by Pokrovskii and Khalatnikov[1] for finding the amplitude for reflection at a barrier. The method enables one to determine the energy gaps with a relative accuracy 1/kL. We choose as our two linearly independent solutions of the Schrödinger equation two complex conjugate functions. When they are displaced by an amount equal to the period, these functions are transformed as follows:

$$f(x+L) = Df(x) + Rf^*(x),$$
$$f^*(x+L) = D^*f^*(x) + R^*f(x), \tag{3}$$

where R, D are certain constants.

From the condition of constancy of the Wronskian for f and f*, we have

$$|D|^2 = 1 + |R|^2. \tag{4}$$

Forming the general solution $\psi(x)$ from the functions (3), and writing the condition $\psi(x+L) = \lambda\psi(x)$, we get the dispersion equation in the usual way. It has the form

$$\lambda^2 - 2\lambda\,\mathrm{Re}\,D + 1 = 0. \tag{5}$$

So far we have not used the quasiclassical approximation. We now use it for calculating the quantity D. For this purpose we consider the behavior of the functions f(x) and f*(x) in the complex x plane. [U(x) is assumed to be an analytic function on the real axis.] Let us assume that the quantity $E - U(x)$ has simple zeros in the upper half plane at the points $x_n = x_0 + nL$ (where n is integral). We consider the behavior of the solutions f(x) and f*(x) on the line ($l$) along which $\mathrm{Im}\int_{x_0}^{x} p\,dx = 0$ and the line conjugate to it in the lower half plane. The approximate appearance of these curves is shown in the figure. At the points $x_n$ these curves make an angle equal to $2\pi/3$.

As the function f(x) we choose a solution which behaves like $p^{-1/2}\exp[i(\tau - \tau_0)]$ on the segment $l_1$ ($\tau = \int^{x} p\,dx$, $\tau(x_0) \equiv \tau_0$). Since the point $x_0$ is the "turning point," to find the solution in the region $l_2$ we must join the quasiclassical solution with the solution of the Airy equation. Using the well-known formulas for joining at the turning point (cf., for example, reference 2), we find the solution over the region $l_2$ in the form

$$f(x+L)=p^{-1/2}\{\exp[i(\tau(x+L)-\tau_0)]$$
$$-i\exp[-i(\tau(x+L)-\tau_0)]\}. \quad (6)$$

This expression can be written as

$$f(x+L)=p^{-1/2}\{e^{i\varphi}\exp[i(\tau(x)-\tau_0)]$$
$$-ie^{-i\varphi}\exp[-i(\tau(x)-\tau_0)]\},$$
$$\varphi=\int_0^L p\,dx. \quad (7)$$

On the level line $\mathrm{Im}(\tau-\tau_0)=0$ both exponents in (7) are of the same order, so that this form is correct. Furthermore we note that the function $f^*(x)$ on the curve $l^*$ behaves like $p^{-1/2}\times\exp[-i(\tau-\tau_0^*)]$. In extending it from the line $l^*$ to $l$ it increases. Therefore on the line $l$ the function $f^*(x)$ will behave like

$$f^*(x)=p^{-1/2}\{\exp[-i(\tau-\tau_0^*)]+A\exp[i(\tau-\tau_0)]\}. \quad (8)$$

The coefficient A in the decreasing exponential remains undetermined in this continuation, but the coefficient in the increasing exponential is not changed.

Comparing (7) and (8) we can find the coefficient R which enters in (3). It is equal to

$$R=i\exp[i(\tau_0-\tau_0^*)](1+O(1/kL)). \quad (9)$$

The modulus of the quantity D is determined from (4) and (8). As we see from (7),

$$\arg D=\varphi(1+O(1/kL)). \quad (10)$$

The forbidden energy bands are determined from the condition of reality of $\lambda$ in equations (5). Thus we have

$$|\cos\varphi|\geqslant 1-|R|^2/2. \quad (11)$$

For the center of the n-th energy gap $E_n$, we find from (11) and (7) the well-known expression

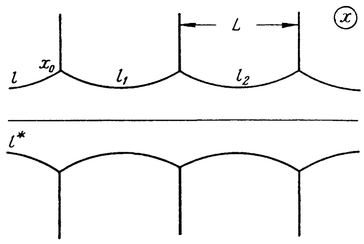
$$\int_0^L \sqrt{2m(E_n-U)}\,dx=\pi n(1+O(1/kL)).$$

For the width of the gap we get

$$\Delta_n=\frac{2}{T_n}\exp\left[i\int_{x_0^*}^{x_0}\sqrt{2m(E-U)}\,dx\right](1+O(1/kL)). \quad (12)$$

Here $T_n$ is the time of passage of a classical particle with energy $E_n$ through one period of the potential.

As we see from (12), the widths of the energy gaps are actually exponentially small. As for the positions of the energy gaps, they are determined only to within the accuracy of a power.




The expressions obtained above correspond to the case

$$U_{max}kL/E\gg 1,\qquad (1-U_{max}/E)kL\gg 1. \quad (13)$$

In similar fashion we can also treat other cases

$$\frac{U_{max}}{E}kL\lessapprox 1,\qquad \left(1-\frac{U_{max}}{E}\right)kL\lessapprox 1.$$

In the first of these cases the zeros of the function $p^2(x)$ are located near the poles of the function $U(x)$. Then for the determination of the quantities R, D one must use the hypergeometric equation in place of the Airy equation.

In the second case, the zeros $x_0$ and $x_0^*$ of the function $p^2(x)$ are close to one another. Then for the joining of the quasiclassical wave functions one must use parabolic cylinder functions. However, as it is easy to show, the value arg D in both cases can be taken from equation (10), while the value of R formally coincides with the amplitude for reflection of the particle from the potential field, vanishing as $x\to\pm\infty$.

Using the results of references 3 and 4, where the calculation of R was done respectively for the first and second cases, we obtain the following expressions for the widths of the energy gaps. In the first case

$$\Delta_n=\frac{2}{T_n}|F(\mu_n)|\exp\left[i\int_{x_0^*}^{x_0}\sqrt{2m(E-U)}\,dx\right],$$
$$\left(1-\frac{U_{max}}{E}\right)kL\gg 1. \quad (14)$$

Here $\mu_n=\sqrt{2m/E_n}\,U_0$, $U_0$ is the residue of the function $U(x)$ at the pole which is nearest to the zero of $x_0$,

$$F(\mu)=\frac{2\pi\exp[i\mu\ln(i\mu/2e)]}{\Gamma(i\mu/2)\Gamma(1+i\mu/2)}. \quad (15)$$

In the second case we have

$$\Delta_n=\frac{2}{T_n}\left[2\,\mathrm{ch}\left(2i\int_{x_0^*}^{x_0}\sqrt{2m(E-U)}\,dx\right)\right]^{-1/2},\qquad \frac{U_{max}}{E}kL\gg 1. \quad (16)$$

It is not difficult to see that formula (12) is obtained from (14) and (16) for the case when both inequalities (13) are satisfied.

In all the cases treated, the energy spectrum near the edges of the zones differs markedly from (2). Relatively simple computations lead to the rule

$$E = E_n \pm \sqrt{(\Delta_n / 2)^2 + v_n^2 (\Delta k_n)^2}, \qquad L\Delta k_n \ll 1, \quad (17)$$

where $v_n$ is the velocity of a classical particle with energy $E_n$; $\Delta k_n = k - \pi n/L$; and the quantity $\Delta_n$ is taken from (12), (14), or (16).

The author is grateful to V. L. Pokrovskii for valuable comments.

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Translated by M. Hamermesh
242