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PHYSICS

1966

SovietRxiv

Abstract

Full Text

UDC 530.145

PHYSICS

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MOTION OF A QUASICLASSICAL PARTICLE IN A QUASIPERIODIC POTENTIAL

(Presented by Academician M. A. Leontovich, February 4, 1965)

In considering the motion of particles in crystalline structures, it is of great importance to take into account "defects" (deviations of the potential from periodicity). If the defects are small, then an analysis of the changes occurring in the energy spectrum and in the particle wave function can be carried out with the aid of perturbation theory (^{1}). Perturbation theory becomes inapplicable when these defects are large or "accumulate" over large distances.

It was shown by I. M. Lifshits (^{2}) that, in the first approximation, a slow change of the potential can be taken into account in a classical way. In particular, wave functions were obtained that are determined through the classical dispersion law for a purely periodic potential. On the other hand, the motion of a particle in a quasiperiodic potential, with a certain special restriction on the type of aperiodicity, was studied in James' s work (^{3}) by means of a method analogous to the WKB method. The solutions obtained in (^{2}) are the leading terms of asymptotic series for the WKB approximation of the wave functions. For a number of problems connected with a more subtle study of aperiodic structures (^{2}), it is essential to clarify in detail the behavior of the electron near the edges of bands, or, in other words, to take into account nonquasiclassical effects due to the accumulation of slow changes in the structure of the potential. A similar problem was studied in (^{4}). However, the method used in (^{4}) is rather complicated in the sense that obtaining concrete physical results is connected with overcoming considerable technical difficulties. Below, a sufficiently simple method for taking nonquasiclassical corrections into account will be proposed.

1. Let us write the Schrödinger equation:

$$d^2\psi/dx^2 + [E - U_1(x) - U(x)]\psi = 0;$$

$$U(x + L(x)) = U(x); \qquad \hbar = 2m = 1, \tag{1}$$

where $U_1(x)$, $L(x)$ have a characteristic length of variation $L_1 \gg L$. We shall begin the discussion with the case in which $U_1, L = \text{const}$. The solution in this

Fig. 1

Figure 1: Fig. 1

case with a purely periodic potential is well known. In particular, the WKB approximation was considered in (^{5}). However, it will be convenient for us to consider briefly the purely periodic case by the method that we shall use below.

The quasiclassical solution has the form

$$\psi_\pm(x) \simeq p^{-1/2} \exp\left\{\pm i \int^x p\,dx\right\}; \qquad p^2 = E - U_1 - U(x). \tag{2}$$

In Fig. 1 are shown the level lines on which $\operatorname{Im} \int^x p\,dx = 0$.

Let the wave function be given in the region $x_3 > x > x_0$:

$$\psi(x) = A\psi_+ + B\psi_-. \tag{3}$$

Then in the region $x_1 = x_3 - L > x > x_0 - L = x_2$

$$\psi(x) = \overline{A}\psi_+ + \overline{B}\psi_-, \tag{4}$$

where

$$\begin{pmatrix} \overline{A} \\ \overline{B} \end{pmatrix} = -i \begin{pmatrix} \beta e^{\delta - ia} & -e^{-\delta - ia} \\ e^{\delta + ia} & \alpha e^{\delta + ia} \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix}, \tag{5}$$

$$\delta = \left| \int_{x_1}^{x_0} p\,dx \right|, \qquad a = \int_{x_2}^{x_1} p\,dx, \tag{6}$$

and the coefficients α, β can be determined by going around the points x_0, x_1 along the contour shown in Fig. 1, analogously to how this is done in (6). This gives:

$$\alpha = -\beta^* = i e^{i\varphi} \sqrt{1 + e^{-2\delta}}, \tag{7}$$

where φ is an unknown phase*, and the first equality sign follows from the condition $\psi(x) = \psi^*(x^*)$. Writing $\psi(x + L) = \mu\psi(x)$, we obtain from (3)–(7)

$$\mu^2 - 2\sqrt{1 + e^{2\delta}} \cos(a + \varphi)\,\mu + 1 = 0. \tag{8}$$

Fig. 1

The allowed energy bands are obtained from the condition $|\mu| = 1$, or

$$1 - (1 + e^{2\delta}) \cos^2(a + \varphi) \geq 0. \tag{9}$$

In particular, the case $\delta \to 0$ corresponds to the approach of the points x_0 and x_1 in Fig. 1, i.e.,

$$E - U_1 \lesssim U_0, \tag{10}$$

where U_0 is the amplitude of the potential $U(x)$. Expanding $U(x)$ in a series near the points x_0, x_1, we arrive at an equation of the form

$$d^2\psi/d\xi^2 + (\lambda + \xi^2)\psi = 0,$$

whose solution is a parabolic-cylinder function. Using the known asymptotic expansions for them (7), we find

$$\varphi = \arg \Gamma \left(\frac{1}{2} + i \frac{\lambda}{2} \right) - i \frac{\lambda}{2} \ln 2 + \frac{i}{2} \lambda \ln |\lambda|. \tag{11}$$

Let us rewrite (1) in the form:

$$\frac{d^2\psi}{dz^2} + \left[q^2 - \frac{U}{U_0}(\Omega z) \right] \psi = 0;$$

$$q^2 = \frac{E - U_1}{U_0}; \qquad z = x\sqrt{U_0}; \qquad \Omega = \frac{2\pi}{L\sqrt{U_0}}. \tag{12}$$

Condition (10) means $q \to 1$. The condition of quasiclassicality is $\Omega \ll 1$. Hence it is not difficult to see that

$$\lambda \sim \Omega^{-1}, \qquad \varphi \sim \frac{1}{\Omega} \ln \frac{1}{\Omega}, \qquad a \sim \frac{1}{\Omega}. \tag{13}$$

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* The phase φ is connected with taking into account the next correction term to (2) and will make it possible to obtain an expression for the width of the allowed bands with sublogarithmic accuracy.

This immediately determines, according to (9), the width of the allowed energy bands*

$$\Delta \sim \frac{\pi U_0 \Omega}{\ln c/\Omega}, \tag{14}$$

where c is a number depending on the specific form of $U(x)$.

2. We shall now take into account the dependence of U_1, Ω on x. Since $L_1 \gg L$, in the first approximation one may retain formulas (3)–(6), and in calculating a and δ the dependence of U_1, L on x is not taken into account. In the second approximation we take this dependence into account. Then, instead of (5), we have

$$\begin{pmatrix} \overline{A}(x) \\ \overline{B}(x) \end{pmatrix} = -i \begin{pmatrix} \beta(x)e^{\delta(x)-ia(x)} & -e^{\delta(x)-ia(x)} \\ e^{\delta(x)+ia(x)} & \alpha(x)e^{\delta(x)+ia(x)} \end{pmatrix} \begin{pmatrix} A(x) \\ B(x) \end{pmatrix}. \tag{15}$$

We replace (15) by a system of differential equations for $A(x)$ and $B(x)$

$$L\,dA/dx = -(i\beta e^{\delta-ia} + 1)A + ie^{\delta-ia}B, \tag{15'}$$

$$L\,dB/dx = -ie^{\delta+ia}A - (1 + i\alpha e^{\delta+ia})B$$

(the discarded terms are small under the condition $e^{-\delta} \gg L_1/L$). The resulting system can be solved in the WKB approximation

$$\begin{pmatrix} A(x) \\ B(x) \end{pmatrix} \sim k^{-1/2} \exp\left\{ \pm i \int^x k(x,E)\,dx \right\}, \qquad k(x,E) \simeq \ln|\mu(x,E) - 1|. \tag{16}$$

It is seen from (16) that the eigenvalues E are determined by the form of the function $k(x,E)$, and the character of the dependence $k(x)$ may be different for different values of E.

For what follows we choose a specific form of the periodic part of the potential

$$U(z) = U_0 \cos^2 \Omega z. \tag{17}$$

From equations (6) we find

$$a = \frac{2}{\Omega}\left\{ E\left(\frac{\pi}{2}, q\right) - (1-q^2)F\left(\frac{\pi}{2}, q\right) \right\},$$

$$\delta = \frac{2}{\Omega}\left\{ E\left(\frac{\pi}{2}, \sqrt{1-q^2}\right) - q^2 F\left(\frac{\pi}{2}, \sqrt{1-q^2}\right) \right\},$$

where F, E are elliptic integrals of the first and second kind, respectively. Inequality (10) corresponds to $1 - q^2 \ll 1$. Hence

$$a \sim \frac{2}{\Omega}\left\{1 - \frac{1}{4}(1-q^2)\ln\frac{16\sqrt{e}}{1-q^2}\right\},$$

$$\delta \sim \frac{\pi}{2\Omega}(1-q^2). \tag{18}$$

From (11) we obtain:

$$\varphi \sim \frac{1-q^2}{2\Omega}\ln\left(\frac{1-q^2}{\Omega}\right) - \frac{1-q^2}{2\Omega}(\ln 2 - C), \tag{19}$$

where C is Euler' s constant, or

$$a + \varphi \sim \frac{2}{\Omega} - \frac{1-q^2}{2\Omega}\ln\Omega.$$

For $\Omega, U_1 = \text{const}$ the allowed energy bands are determined, according to (9), from the expression:

$$\frac{3\pi}{4} \gtrless \frac{2}{\Omega}\left\{1 - \frac{1}{4}(1-q^2)\ln\Omega\right\} - 2\pi n \gtrless \frac{\pi}{4}. \tag{20}$$

* The width of the forbidden bands in this case is of the same order.

The values $\pi/4$ and $3\pi/4$ correspond to the edges of the band. From (20), for the width Δ of the allowed energy band we obtain the refined expression (14)

$$\Delta \simeq \pi U_0 \Omega / \ln(16\sqrt{e}/\Omega).$$

Formulas (18)–(20), in accordance with the method described, were obtained without taking into account the dependence of q on x. Let us now take this dependence into account. According to (16), the quasimpulse of the particle $k(x, E)$ may be regarded as the "momentum" for the functions $A(x)$, $B(x)$, satisfying an equation of Schrödinger type with energy $[\ln(\mu(x) - 1)]^2$.

For going around the turning points $k(x_0, E) = 0$ we use the method set forth in Sec. 1. The transition matrix is determined in an analogous manner. The turning points correspond to the edges of the energy bands determined by equation (20), where now q must be regarded as dependent on x according to (12). Figure 2 shows the surface $k^2(x, E)$.

Fig. 2

Regions I and II correspond to allowed energy bands. The plane $E = E_0$ cuts out on the surface $k^2(x, E)$ the curve $k^2(x, E_0)$, which has "humps" between

Fig. 2

Figure 2: Fig. 2

bands and "wells" inside bands. Thus a tunneling transition between bands is possible. Points a and b are turning points. The example given is one of the possible consequences of the "inhomogeneity" associated with the presence of the field $U_1(x)$. For $x > x_0$, in the range of energies for which $k^2(x_0, E) < 0$, the bands disappear, while in the range of energies where $k^2(x_0, E) > 0$, the spectrum becomes continuous. If $k^2(x, E)$ has the form of a well in some range of energies, then the spectrum becomes discrete.

In all these cases, the nonquasiclassical corrections are determined with the help of a transition matrix of the type (5) for the coefficients A_1, B_1 of the functions

$$\psi_1(x) = A_1 A(x) + B_1 B(x),$$

where $A(x)$ and $B(x)$ are quasiclassical solutions of the system (15^1). The wave function is thus represented in the form

$$\Psi = \psi_1(x)\psi(x).$$

We note that although the energy surfaces $k^2(x, E)$ were given for $\delta \to 0$, analogous arguments are easily carried out for arbitrary δ.

In conclusion, we express our gratitude to R. Z. Sagdeev for valuable advice and discussions.

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Received
7 I 1965

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Note: Figure translations are in progress. See original paper for figures.