Anomalous transparency for near-top Bloch states of periodic potential

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Abstract

In the paper are considered stationary (Bloch) states of a particle, in the field of periodic biparabolic type potential. It is shown that while the particle’s energy decreases in limits of a single energy band, the probability of the particle to be in barrier-type region of periodic potential increases, in contrary to the expected decreasing. This "anomalous" behavior is more pronounced for the near-top bands and monotonically decreases for the higher or lower ones.

I. INTRODUCTION

Bloch functions are the basis of periodic system theory, particularly of crystalline solid physics [1] and optical lattices [2]. For a high-precision approximation of a standing wave (sinusoidal potential), by one of the authors was suggested a biparabolic form for the potential [3], Bloch functions of which are expressed by confluent hypergeometric functions. The approximation for the potential has been used to calculate the spontaneous emission in the field of resonant standing wave, the presence of light-induced anisotropy in that emission was shown [4]. Also it was used for calculating the temperature of ideal gas BEC in a periodic field and was shown that the critical temperature decreases with the deepening of the potential [5].

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In this paper the biparabolic periodic potential is used to investigate the Bloch states themselves, more concretely, for identifying the behavior of modulo wave function as a function of energy in the limits of a specific energy band. Specially we are interested in so-called "underbarrier" (classically forbidden) states.

The way of dependance of underbarrier states on energy is well-known for a single potential barrier and for transitions from one energy band to the neighboring ones: the underbarrier wave function decreases conjointly with the decreasing of energy of a particle. But what is the kind of dependance in the limits of a sole (definite) energy band? Surprisingly this question has slipped from investigators sight; at least in scientific literature available to us we did not find works concerning this question. As a formal argument for examining this question, for us appears the fact that Bloch states are generated through the interference of particle de Broglie waves transmitted and deflected from many (infinite in the limit) potential barriers, and hence interference, besides the energy, also will play an essential role in establishment of regularities. Of course, the deflection and interference of underbarrier states take place in case of a single-barrier potential too, but they are small there and as a dominating behavior will appear the energetic behavior. Consequently, the inter-band regularity is not under necessity to be repeated for intra-band states too. Really, in case of periodic potential, when from different barriers multiple-wave interference takes place, as a dominating one can appear the interference behavior, and the dominant role of interference will be expected for intra-band regularities. Than, if the interference behavior does not coincide with energy one, the general behavior will mimic the interference but not energy regularity. Our calculations show that indeed, when particle’s energy decreases in limits of a definite band, the modulus of the wave function of underbarrier (classically forbidden) region does not decrease, as should be expected from energy reasonings, but increases. The growth rate is the greatest for the band, nearest to the height of periodic potential.
II. BIPARABOLIC POTENTIAL AND NEAR-TOP BLOCH STATE APPROXIMATION

Stationary Schrödinger equation can be written in a standard form

\[
\left( \frac{d^2}{dz^2} + E - V(z) \right) \Psi(z) = 0,
\]

(1)

where the particle coordinate \( z \) is normalized in units of the potential period \( L \) with coefficient \( 2\pi (z = 2\pi z/L = k z, k \) is the one-dimensional reciprocal lattice constant) and the full energy \( E \) and the potential energy \( V(z) \) are normalized in units of “lattice” recoil energy quantum \( E_r = \hbar^2 k^2 / 2M \), where \( M \) is mass of the particle. Taking for convenience the zero of the energy on the level of potential energy minimums, biparabolic potential \( V(z) \) takes the form (see for more details [5] or [3])

\[
V(z) = \frac{1 + (-1)^m}{2} V - (-1)^m \chi (z - m\pi)^2,
\]

(2)

where \( V \) is the height of the periodic potential, \( \chi = 2V/\pi^2 \), \( m = 0, \pm 1, \pm 2, \ldots \), and \( z \) for each \( m \) lays in range \( (m - 1/2)\pi \leq z \leq (m + 1/2)\pi \).

The form of the potential is given in fig.1, where region I (and others similar to it) will be named well-type, and region II (and similar ones) - barrier-type.

Linearly independent solutions of Schrödinger Eq.(1) for well-type region I are written in form [3], [5]

\[
\varphi_1(z) = \exp \left( -\sqrt{\chi z_1^2} \right) \Phi \left( \alpha, \frac{1}{2}; \sqrt{\chi z_1^2} \right),
\]

(3)

\[
\varphi_2(z) = z_1 \exp \left( -\sqrt{\chi z_1^2} \right) \Phi \left( \alpha + \frac{1}{2}, \frac{3}{2}; \sqrt{\chi z_1^2} \right),
\]

(4)

where \( z_1 = z - \pi, \pi/2 \leq z \leq 3\pi/2, \Phi (\ldots, \ldots) \) is the confluent hypergeometric function and

\[
\alpha = \frac{1}{4} \left( 1 - \frac{E}{\sqrt{\chi}} \right).
\]

(5)

The total wave function in this region will be
\[ \Psi_I(z) = c_1 \varphi_1(z) + c_2 \varphi_2(z), \] (6)

where \( c_1 \) and \( c_2 \) are unknown constant coefficients.

The corresponding solutions for barrier-type region II have the form

\[ \varphi_1(z) = \exp \left( \frac{i \sqrt{\chi z^2}}{2} \right) \Phi \left( \beta, \frac{1}{2}; -i \sqrt{\chi z^2} \right), \] (7)

\[ \varphi_2(z) = z z_2 \exp \left( \frac{i \sqrt{\chi z^2}}{2} \right) \Phi \left( \beta + \frac{1}{2}, \frac{3}{2}; -i \sqrt{\chi z^2} \right), \] (8)

where \( z_2 = z - 2\pi, 3\pi/2 \leq z \leq 5\pi/2 \) and

\[ \beta = \frac{1}{4} \left( 1 - i \frac{E - V}{\sqrt{\chi}} \right), \] (9)

and the total wave function in this region will be

\[ \Psi_{II}(z) = \overline{c}_1 \varphi_1(z) + \overline{c}_2 \varphi_2(z), \] (10)

with yet arbitrary coefficients \( \overline{c}_1 \) and \( \overline{c}_2 \).

With the help of continuity requirements at boundary points \( z = 3\pi/2 \) and \( 5\pi/2 \) and Bloch periodicity we get the dispersion relation, which can be written in form

\[ \cos(2\pi P) = 1 + 2 G_{11}(E) G_{22}(E), \] (11a)

or

\[ \cos(2\pi P) = -1 + 2 G_{12}(E) G_{21}(E), \] (11b)

where \( P = p/2h \) is the normalized momentum of particle and

\[ G_{ij}(E) = \left\{ \varphi_i(z) \varphi_j'(z) + \varphi_j(z) \varphi_i'(z) \right\}_{z=\pi/2}, \quad i, j = 1, 2. \] (12)

where the prime over the function means derivative with respect to \( z \).

The same requirements, as is well known, with additional normalizing condition

\[ \int_{\pi/2}^{3\pi/2} |\Psi_I(z)|^2 \, dz + \int_{3\pi/2}^{5\pi/2} |\Psi_{II}(z)|^2 \, dz = 1, \] (13)
define the coefficients $c_{1,2}$ and $\overline{c}_{1,2}$.

The edge values of energy bands according to (11a) and (11b) are determined as solutions of transcendental equations

$$G_{ij}(E) = 0. \quad (14)$$

Analysis of these conditions shows that left- and right-side edge points on the positive-side axis of quasimomentum (expanded conception of energy bands) are determined from conditions $G_{11}(E) = 0$ and $G_{12}(E) = 0$ respectively for $n$ being even, and by conditions $G_{21}(E) = 0$ and $G_{22}(E) = 0$ for $n$ being odd. For keeping analogy with the harmonic potential the band with the smallest energy is designated $n = 0$.

For even-numbered bands it is appropriate to express the coefficients by $c_1$,

$$c_2 = \frac{G_{11}(E) e^{i2\pi P} + 1}{G_{21}(E) e^{i2\pi P} - 1} c_1, \quad (15)$$

$$\overline{c}_1 = \frac{e^{i2\pi P} + 1}{2G_{21}(E)} c_1, \quad \overline{c}_2 = \frac{e^{i2\pi P} - 1}{2G_{22}(E)} c_1, \quad (16)$$

where $c_1$ is determined from the normalizing condition. For odd-numbered bands it is appropriate to express the coefficients by $c_2$;

$$c_1 = \frac{G_{21}(E) e^{i2\pi P} - 1}{G_{11}(E) e^{i2\pi P} + 1} c_2, \quad (17)$$

$$\overline{c}_1 = \frac{e^{i2\pi P} - 1}{2G_{11}(E)} c_2, \quad \overline{c}_2 = \frac{e^{i2\pi P} + 1}{2G_{12}(E)} c_2, \quad (18)$$

and use the normalizing condition to determine $c_2$.

Let’s now consider the states, with energies near to the height $V$ of periodic potential: $E \approx V$. In fig. 1 these energies lay inside the dotted lines. For them the parameter $\beta$ (see (9)), which determines the character of Bloch wave functions in barrier-type region, possesses the value $\beta = 1/4$. The corresponding formulas (7) and (8) are simplified with help of a well known representation for Bessel functions $J_\nu(x)$ by confluent hypergeometric ones:
\[ J_\nu(x) = \frac{1}{\Gamma(\nu+1)} \left( \frac{x}{2} \right)^\nu e^{-ix} \Phi \left( \frac{1}{2} + \nu, 1 + 2\nu, 2ix \right), \] \hfill (19)

where \( \Gamma(\nu+1) \) is the gamma function. To use this formula for (7) we must choose \( \nu = -1/4 \), and for (8) - \( \nu = 1/4 \). After corresponding substitutions we arrive to

\[ \varphi_1(z) = \Gamma \left( \frac{3}{4} \right) \left( \frac{\sqrt{x}z^2}{4} \right)^{1/4} J_{-1/4} \left( \frac{\sqrt{x}z^2}{2} \right), \] \hfill (20)

\[ \varphi_2(z) = \Gamma \left( \frac{5}{4} \right) z \left( \frac{\sqrt{x}z^2}{4} \right)^{-1/4} J_{1/4} \left( \frac{\sqrt{x}z^2}{2} \right). \] \hfill (21)

To avoid misunderstandings we note, that though linearly independent solutions \( \varphi_1(z) \) and \( \varphi_2(z) \) for the considered approximation do not depend on energy of the particle, the total Bloch wave function \( \Psi_{II}(z) \) is energy dependant via the coefficients \( \bar{c}_1 \) and \( \bar{c}_2 \).

As to wave-functions \( \varphi_1(z) \) and \( \varphi_2(z) \) of well-type region, we will use the second Tricomi expansion \( \Phi \) for them,

\[ e^{-x/2} \Phi(a, \sigma + 1; x) = \Gamma(\sigma + 1) (ax)^{-\sigma/2} \sum_{n=0}^{\infty} A_n(x, \lambda) \left( \frac{x}{4a} \right)^{n/2} J_{\sigma+n}(2\sqrt{ax}), \] \hfill (22)

where \( x = \frac{(1+\sigma)}{2} - a, A_0(x, \lambda) = 1, A_1(x, \lambda) = 0, ... \), and will restrict ourselves with the first member of expansion, which corresponds to sufficiently deep potentials (\( x > 1 \)). The respective Bessel functions are expressed by elementary trigonometric functions and as a consequence

\[ \varphi_1(z) = \cos(\sqrt{E}z), \qquad \varphi_2(z) = \frac{1}{\sqrt{E}} \sin(\sqrt{E}z). \] \hfill (23)

All the coefficients and dispersion relation ((11a) or (11b)) also undergo sufficient changes. The dispersion relation, for example, takes the form

\[ \cos(2\pi P) = \frac{\pi/4}{\sin(\pi/4)} \left\{ 2u \left[ J_{-1/4}(u)J_{-3/4}(u) - J_{1/4}(u)J_{3/4}(u) \right] \cos(\pi \sqrt{E}) - J_{-1/4}(u) \times \right\}, \]

\[ J_{1/4}(u) \frac{2}{\pi \sqrt{E}} \sin(\pi \sqrt{E}) - 4u^2 J_{-3/4}(u)J_{3/4}(u) \frac{2}{\pi \sqrt{E}} \sin(\pi \sqrt{E}) \] \hfill (24)

where \( u = \pi^2 \sqrt{x}/8. \)
III. RESULTS OF NUMERICAL CALCULATIONS

To display the sought dependence, that is the behavior of Bloch wave functions due to changing of the energy in limits of a single (defined) band, we proceed from the above mentioned near-top approximation. With the help of computer simulations we first determined the depth of potential $V$, so that the last allowed inner-potential band would be found immediately near the tops of periodic potential (for fig.2), with $V = 1.4494$, the energy of mentioned band lays in limits $E_{\text{min}} = 0.3947$, $E_{\text{max}} = 1.4494$, and when $V = 18.65$, in limits $E_{\text{min}} = 13.64$, $E_{\text{max}} = 18.65$). Then with the help of formulas (9) and (11), with linearly independent solutions (7), (8) and (23), coefficients (15), (16) or (17), (18), dispersion relation (24) and normalizing condition (13), we computed the sought values of $|\Psi_I(z)|^2$ and $|\Psi_{II}(z)|^2$ as a function of coordinate $z$ along one spacial period. Repeating these calculations for all the energy values of the band, we obtain a (continuous) sequence of curves, the juxtaposition of which along the energy lines gives us the seeking behavior.

In Figs. 2a and 2b we present the results of such calculations for two different depths of potential; one (Fig.2a) for a potential depth, containing two energy bands, and the other one (Fig.2b) containing four energy bands. So, Fig. 2a illustrates the energy-space distribution of Bloch states in case of relatively shallow potential. Fig. 2b illustrates the same kind distribution for relatively deep potential. Left half of the face axis ($z$) corresponds to the well-type region of the potential, and the right half - to the barrier-type region. The energy axis is, as is seen, directed from the reader (energy grows from face to back).

As anomalous one is regarded the behavior of wave function in right-half side(s) of the figure(s), that is the dynamics of Bloch functions in the barrier-type regions (see Fig.1) as a function of energy. Obviously is seen that the moving along the energy axis from the back face to the front face, which physically means getting deeper into potential, does not decrease but, quite the contrary, increases the modulo square of the wave function. That merely means that the probability of the particle to be found deeper under the potential barrier (staying in the limits of a band) is greater than the probability to be found at smaller
depths! This kind of behavior is in contrary to the regularity for the case of deepening into the periodic potential over various energy bands, or for the case of a single potential barrier. That is why we call the behavior anomalous.

To avoid possible misunderstanding of the mentioned regularity it will be noted that there is not any strangeness or abnormality in the fact, that the wave function in barrier-type (right) space region is essentially greater in average than in well-type (left) space region; it is simply the echo of overbarrier reflecting, when velocity of the particle decreases and the wave function (probability of being) respectively increases, in “underbarrier” states.

The next question that is of interest, is how does the rate of anomalous rising depend on the location of the band relative to the height of periodic potential. For this kind of calculations the near-top energy approximation, of course, is not applicable and we had to proceed from the precise formulas. A detailed analysis of the regularities obtained for Bloch state and comparison with single-barrier case we will give in another publication. We would like only to note that while moving away from near-top energies as inside as outside the periodic potential, the rate (scaled in energy units) of anomalous growth decreases.

Finally we note that we carried out the anomalous behavior also for the Kronig-Penny’s potential, but for that case the anomaly is much weaker, than for the case of biparabolic potential (see fig.(3)). It is easy to understand since the single barrier transparency in high energy region, and hence the effectivity of matter-wave interference is bigger for biparabolic-form potential than for rectangular-form one.

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FIGURES

FIG. 1. Biparabolic potential and identification of well-type(I) and barrier-type(II) regions.

FIG. 2. Modulo square of Bloch wave functions on the plane energy (E)-coordinate (z) for a near-top (with $E_{\text{max}} = V$) energy band. The depth (height) of potential is $V = 1.4494(a)$ and $V = 18.65(b)$, scaled in units of recoil energy $E_r = (2\hbar k)^2/2M$. The mentioned feature is in detail described in the text.

FIG. 3. Modulo square of Bloch wave functions on the plane energy (E)-coordinate (z) for a Kronig-Penny potential. The depth of potential is $V = 1.668$, scaled as in Fig.2.
