Electron conductivity in incommensurate systems near the localization threshold

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A system of noninteracting electrons moving in a field of two periodic potentials with incommensurate periods is considered. An Anderson transition takes place in such a system at a certain value V_c of the potential. The conductivity of a finite sample (of length L) is $\sigma(L) \propto \exp(-L/\xi)$ in the region of localized states ($V > V_c$) and $\sigma(L) \propto L$ in the metallic phase ($V < V_c$). The quantity $g = \sigma(L)/L$ as $L \to \infty$, i.e., the total (not specific) conductivity of a macroscopic sample, vanishes at the transition point jumpwise at $T = 0$ and linearly at finite temperature.

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INTRODUCTION

In this paper, which is a direct continuation of a preceding one,[1] we consider the problem of motion of an electron in the field of two periodic potentials with incommensurate periods (irrational ratio of the periods). This problem is of interest both for the understanding of the properties of incommensurate systems,[2,3] and for the understanding of effects of localization in disordered systems.[4]

In recent papers[5–7] arguments were advanced, confirmed by numerical experiments, favoring the assumption that for the simplest model, described by the tight-binding equation with periodic modulation of the levels

$$a_{l+1}+a_{l-1}+V\cos(2\pi\beta l)\,a_l=Ea_l, \tag{1}$$

where β is an irrational parameter, the value of the potential $V = 2$ is the Anderson-transition point: at $V > 2$ all the eigenfunctions of Eq. (1) are localized, and at $V < 2$ they are delocalized. On the other hand, Azbel[3] has shown that the spectrum of an incommensurate system has the character of a "devil's staircase," and presented a method of calculating this spectrum for numbers β in whose expansion into a continued fraction

$$\beta=\frac{1}{n_1+\beta_1}=\frac{1}{n_1+\dfrac{1}{n_2+\beta_2}}=\ldots=\cfrac{1}{n_1+\cfrac{1}{n_2+\cfrac{1}{n_3+\ldots}}} \tag{2}$$

all $\beta, \beta_1, \beta_2, \ldots$ turn out to be small.

In my preceding paper,[1] by modifying somewhat Azbel's method,[3] an algorithm was obtained for constructing the wave functions of an incommensurate system for $\beta, \beta_1, \beta_2, \ldots \ll 1$, and the existence of an Anderson transition at $V = 2$ was shown in a consistent manner. In this approach there appears in natural fashion single-parameter scaling, close to that proposed in Ref. 8 for disordered systems. In addition, it is shown in Ref. 1 that the description of an incommensurate system of general form near the localization threshold reduces to Eq. (1).

In view of the great interest evinced recently in the conductivity of disordered systems near the Anderson transition, it is natural to consider the analogous problem for incommensurate systems. There is no doubt that there is no static conductivity at $T = 0$ in the region of localized states ($V > 2$); on the other hand, the existing notions concerning the conductivity of the metallic phase are rather indeterminate and frankly hypothetical in character. Sokolof f[5] suggested continuous vanishing of the conductivity as the transition is approached. Azbel[3] emphasized the non-ohmic character of the conductivity: Ohm's law $R \propto L$ (L is the length of the sample) is possible only on the average, neglecting the oscillatory dependence on L, which results from the presence of the devil's staircase.

An investigation of the conductivity of incommensurate systems is the main purpose of the present paper. The corresponding calculations, carried out for a small β_k, are described in §§ 3, 4; sufficient for their understanding is acquaintance with the physical picture given in Ref. 1 of the spectrum and of the wave function. However, the renormalization group constructed in Ref. 1 is insufficient for the purposes of the present paper, since it is not applicable in some sections of the spectrum (for more details see Ref. 1), which are precisely the ones which determine mainly the conductivity. Therefore another variant of the normalization group is proposed in § 1 below and is applicable already for all states. The result is in fact that the reasoning of Ref. 1 is applicable to the entire spectrum, despite violation of the tight-binding approximation in some of its sections. Simultaneously, the method of §1 has made it possible to consider arbitrary irrational numbers (without assuming small β_k). It turned out that the results of Ref. 1 are valid for all irrational numbers, expect for their set of zero measure, for which localization takes place only in a weak sense (§ 2).

§1. RENORMALIZATION GROUP

1. We consider an auxiliary equation obtained from (1) after approximating β by a rational fraction M/N, which we shall assume to be irreducible:

$$a_{l+1}+a_{l-1}+V\cos[2\pi(M/N)(l+\varphi)]\,a_l=Ea_l, \tag{3}$$

where φ is a constant phase. This equation describes a periodic system with a period consisting of N atoms, and its spectrum consists of N energy bands. It will be shown below that the dispersion laws of these bands $\varepsilon_s(p)$, where p is the quasimomentum, which depend on φ as a parameter, are given by

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$$\varepsilon_s(p,\varphi)=f_s[\cos Np+V(N)\cos 2\pi M\varphi],\quad s=1,2,\ldots,N, \tag{4}$$

where $f_s(x)$ is a smooth and monotonic function. Within the limits of applicability of the method of Ref. 1, the function $f_s(x)$ turned out to be linear, and the coefficient $V(N)$ played the role of a scaling parameter in scale transformations. Actually the generalization proposed here for the renormalization group consists of introducing a function $f_s(x)$ of general form and retaining $V(N)$ as the scaling parameter. We shall show that this choice of the scaling parameter is physically correct.

We put in Eq. (1)

$$\beta l\equiv(M/N)[l+\varphi(l)], \tag{5}$$

after which it goes over into (3), but with a variable phase $\varphi=\varphi(l)$. The properties of Eq. (3) with a variable $\varphi(l)$ can be explained by starting from the properties of this equation with a constant φ.

We subdivide the considered system into blocks of N atoms in each. Motion within each individual block corresponds to N energy levels and wave functions localized within an individual block (Fig. 1). At constant φ all the blocks are identical because of periodicity, and have identical systems of levels; when φ varies, all the levels vary in the same manner in all the blocks, with a characteristic amplitude W_N. The possibility of a transition for one block to another leads to broadening of all the levels into bands having a width of the order of the overlap interval of the wave functions J_N. It can be seen from (4) that, regardless of the concrete form of the functions f_s, the ratio of the characteristic value of the band shift with changing φ to the characteristic width of this band is determined by the parameter $V(N)$. Thus,

$$V(N)\sim W_N/J_N. \tag{6}$$

The foregoing reasoning is valid, strictly speaking, when the width of the bands J_N is small compared with the distance δE_N between them (tight binding). Since $W_n\lesssim\delta E_N$ (see Fig. 1b and Fig. 2 below), the estimate (6) is valid at any rate for $V(N)\gg 1$.

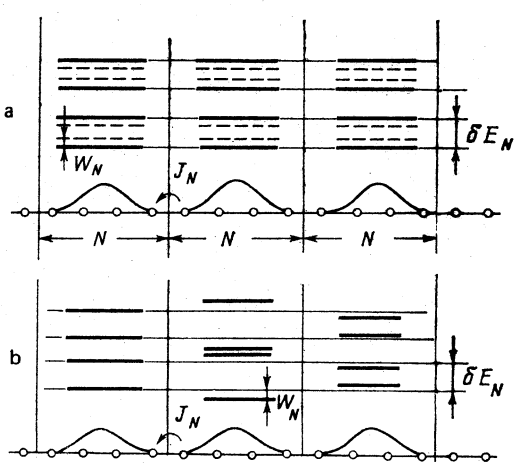

FIG. 1. Systems of energy levels and wave functions corresponding to motion inside individual blocks: a—the phase φ is constant in space, dashed—the system of levels at a different value of φ; b—φ varies linearly in space.

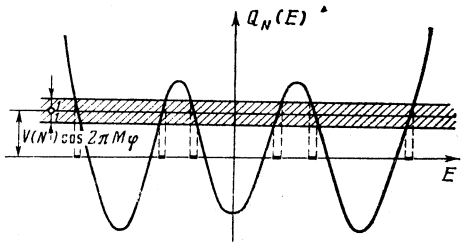

FIG. 2. Graphic solution of Eq. (20). Solid curve—the polynomial $Q_N(E)$. The separated sections of the E axis correspond to allowed bands.

Let now φ vary in space in accordance with (5), i.e., linearly. As a result, the energy levels in different blocks become different, oscillating periodically in space. If $\varphi(l)$ changes slowly enough so that the argument of the cosine in (4) does not change too rapidly within the limits of the block:

$$\delta(2\pi M\varphi)\leqslant 1 \quad \text{at} \quad \delta l\sim N, \tag{7}$$

then the amplitude of the level oscillations will be $\sim W_N$, and the overlap integrals remain $\sim J_N$. If the period T_N of the level oscillations is not too large, e.g., not larger than Q of the blocks, i.e.,

$$\delta(2\pi M\varphi)>1/Q \quad \text{at} \quad \delta l\sim N, \tag{8}$$

then the parameter $V(N)$ can be interpreted as the ratio of the "deviation" of the levels in the neighboring blocks to the overlap integral J_N. This ratio, as is well known, is indeed a good scaling parameter for the localization.[8,9]

We discuss now the restrictions (7) and (8). From the definition (5) of $\varphi(l)$ we obtain

$$\delta(2\pi M\varphi)=2\pi(\beta-M/N)N^2,\quad \delta l=N. \tag{9}$$

It is known from mathematics[10] that the inequality

$$|\beta-M/N|<1/2N^2 \tag{10}$$

can be reached only when M/N is a convergent p_k/q_k of the number β, i.e., it is obtained by terminating the continued fraction (2) at the k th step (by equating β_k to zero). Comparing (9) with (10), we see that the condition

$$\delta(2\pi M\varphi)<\pi,\quad \delta l=N$$

is reached only for a convergent. In view of (7), we are in fact forced to choose M/N only in the form of a convergent.

Let M/N be the convergent p_k/q_k. Then, using the known recurrence relations[10]

$$\begin{aligned} &p_k=n_kp_{k-1}+p_{k-2},\quad p_0=0,\quad p_1=1,\\ &q_k=n_kq_{k-1}+q_{k-2},\quad q_0=1,\quad q_1=n_1, \end{aligned} \tag{11}$$

we can show that

$$\beta=\frac{p_k}{q_k+\gamma_k},\qquad \gamma_k=\frac{(-1)^{k+1}\beta_k}{p_k+\beta_kp_{k-1}}\sim\frac{\beta_k}{p_k}. \tag{12}$$

Substituting (12) in (9) we obtain the estimate

$$\delta(2\pi M\varphi)\sim\pi\beta_k,\quad \delta l\sim N,\ \text{if}\quad M/N=p_k/q_k.$$

Assuming β_k to be bounded from below (we shall return to this question in § 2), we easily satisfy the condition (8).

Thus, the interpretation of $V(N)$ as a ratio of the value of the level deviation in the neighboring blocks to the overlap integral, at any rate, it is valid when M/N is a convergent. This is sufficient for carrying out scale transformations. We shall show that as $V(N)\to\infty$ and $N\to\infty$ localization takes place. We put $N=q_k$ and choose k such that $V(q_k)\gg Q$ [see (8)]. We combine m blocks into one large block — no collectivization will take place because $W_N\gg J_N$ — the wave functions corresponding to motion in an individual block remain localized in it. This situation is preserved when m is increased to a certain $m_{\max}$. As will be shown below, $m_{\max}N>q_k+1$. Thus, the radius of localization of the "block" wave functions is not changed when the size of the block is changed from q_k to q_{k+1}. Breaking up again into blocks of size $N=q_{k+1}$, we can repeat the same reasoning. Consequently, a finite localization radius is preserved also as $N\to\infty$.

When $m_{\max}$ is determined, two cases can be encountered.

a. If the period T_N of the level oscillations is such that T_N/N is close to an integer m_0 accurate to $\sim 1/V(N)$, we have $m_{\max}=m_0$, since the first and the (m_0+1) st blocks have close levels and resonance is possible at $m=m_0+1$. From the relation

$$T_N-q_{k+1}=\beta_{k+1}q_k,$$

which follows from (5), (11), and (12), recognizing that $V(N)\gg Q\approx\max_k(1/\beta_k)$, we see that $q_{k+1}<m_0q_k$, i.e., $q_{k+1}<m_{\max}N$.

b. If T_N/N is not close to an integer and lands in the interval $(m_0,\ m_0+1)$, no resonance takes place at $m=m_0+1$ and $m_{\max}\geqslant m_0+1$. Since $q_{k+1}<T_n$, we have $q_{k+1}<(m_0+1)N\leqslant m_{\max}N$.

If, however, $V(N)\ll 1$ as $N\to\infty$, it can be readily shown that $W_N\ll J_N$, and when several blocks are joined into one the corresponding wave functions are mixed with approximately equal weights, i.e., delocalization of the states takes place. Thus, the asymptotic behavior of $V(N)$ as $N\to\infty$ makes it possible to assess the character of the eigenfunctions of Eq. (1).

We proceed now to derive Eq. (4). After imposing on the wave functions of Eq. (3) the Bloch boundary condition

$$a_{l+N}=e^{ipN}a_l$$

the spectrum of the system is determined by the determinant of an $N\times N$ matrix

$$\Delta=\begin{vmatrix} V^{(1)}-E & 1 & 0 & 0 & \dots & e^{-ipN} \\ 1 & V^{(2)}-E & 1 & 0 & \dots & 0 \\ 0 & 1 & V^{(3)}-E & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ e^{ipN} & 0 & \dots & \dots & 1 & V^{(N)}-E \end{vmatrix}, \tag{13}$$

where

$$V^{(l)}=V\cos 2\pi(M/N)(l+\varphi). \tag{14}$$

The determinant Δ is a function of p, φ, E, and V. Its dependence on p and φ can be determined.

We note that only two elements of the matrix (13) depend on p. Expanding the determinant in terms of the upper row, and the resultant determinants in terms of the column that contains $\exp(ipN)$, we obtain the dependence of Δ on p:

$$\Delta(p)=2(-1)^{N+1}\cos pN+\text{const}(p). \tag{15}$$

To determine the dependence of Δ on φ it is convenient to introduce a new variable:

$$\psi=2\pi(M/N)\varphi$$

and use the following properties:

$$\Delta(\psi)=\Delta(-\psi), \tag{16a}$$

$$\Delta(\psi+2\pi M/N)=\Delta(\psi). \tag{16b}$$

The properties (16) follow from the fact that the substitutions $\varphi\to-\varphi$ and $\varphi\to\varphi+1$ transform the system described by Eq. (3) into a system that is physically equivalent to it: formally, the Hamiltonian is reduced to its previous form by making the respective substitutions $l\to-l$ and $l\to l-1$. The determinant Δ, however, being a polynomial in E, is determined completely by its zeros, i.e., by the spectrum of Eq. (3).

It is clear from the form of (13) that Δ is a sum of different products $V^{(1)}, V^{(2)},\dots, V^{(N)}$, and by virtue of (14) it is consequently the sum of terms of the form

$$\cos^m\psi\sin^l\psi,\quad m+l\leqslant N.$$

In view of (16a), the sine functions enter only raised to even (c) degrees; they can therefore be expressed in terms of the cosines and we can write

$$\Delta(\psi)=\sum_{k=0}^{N}A_k\cos^k\psi, \tag{17}$$

or re-expanding in a Fourier series

$$\Delta(\psi)=\sum_{k=0}^{N}B_k\cos k\psi. \tag{18}$$

From the property (16b) and from the irreducibility of the fraction M/N it follows that all the coefficients B_h in (18), except B_0 and B_N, are equal to zero. To find the coefficient B_N we note that the term containing $\cos^N\psi$ in (17) stems only from the product

$$V^{(1)}V^{(2)}\dots V^{(N)}\equiv V^N\cos\psi\cos(\psi+2\pi M/N)\dots\cos(\psi+2\pi M(N-1)/N]=(-1)^{N+1}V^N\cos^N\psi+\dots,$$

and this determines A_N. On the other hand, the connection between B_N and A_N follows from the expansion of $\cos N\psi$ in power of $\cos\psi$:

$$\cos N\psi=2^{N-1}\cos^N\psi+\dots.$$

By virtue of the foregoing, the dependence of Δ on ψ takes the form

$$\Delta(\psi)=(-1)^{N+1}\frac{V^N}{2^{N-1}}\cos N\psi+\text{const}(\psi). \tag{19}$$

Combining (15) and (19) we obtain the secular equation in the form

$$\cos Np+(V/2)^N\cos 2\pi M\varphi=Q_N(E), \tag{20}$$

where $Q_N(E)$ is a polynomial of degree N in E.

Since the matrix (13) is Hermitian, it follows that Eq. (20) has exactly N real roots at arbitrary p and φ; therefore the polynomial $Q_N(E)$ takes the form shown in Fig. 2, i.e., it has $N-1$ extrema that break up the E axis into N intervals of monotonicity $Q_N(E)$, on each of which Eq. (20) can be solved relative to E to obtain the dispersion laws of each of the N bands of Eq. (3):

$$E=\varepsilon_s(p,\varphi)=f_s(\cos pN+(V/2)^N\cos 2\pi M\varphi), \quad s=1,2,\ldots,N. \tag{21}$$

By the same token we obtain Eq. (4) with the scaling parameter

$$V(N)=(V/2)^N. \tag{22}$$

Equation (22) determines the sought transformation of the renormalization group. In the case $V>2$ we have $V(N)\to\infty$ as $N\to\infty$, meaning localization of all the states, and at $V<2$ we have $V(N)\to 0$ as $N\to\infty$, meaning their delocalization. By the same token $V=2$ is the Anderson transition point in accordance with the result of Ref. 1 for small β_k.

Substantial changes of $V(N)$ take place on the characteristic line $\xi\sim|\ln(V/2)|^{-1}$, which has at $V>2$ the meaning of the localization radius, and diverges near the threshold like

$$\xi\propto|V-2|^{-1}, \tag{23}$$

i.e., with index 1 in accordance with the results for small β_k (Ref. 1). Since an incommensurate system of general form reduces[1] to Eq. (1), this index is universal. At $V<2$, the quantity ξ has the meaning of the effective period of the system — if the size of the block N amounts to several ξ, it can be assumed that there is no level-oscillation effect, so that the incommensurate system is indistinguishable from a periodic system with period N.

2. We apply the foregoing results to the case β, β_1, $\beta_2,\ldots\ll 1$. Using for M/N the convergent p_k/q_k, the phase $\varphi(l)$ turns out to vary slowly:

$$\varphi(l)=-\frac{\gamma_k}{q_k+\gamma_k}l=\frac{(-1)^k\beta\beta_k}{p_k(p_k+\beta_k p_{k-1})}\approx(-1)^k\frac{\beta\beta_k}{p_k^2}l\approx(-1)^k\frac{\beta_k}{p_kq_k}l \tag{24}$$

[we have used (5) and (12)]; therefore the quasiclassical approach is applicable, and for each of the q_k bands into which the spectrum of Eq. (1) breaks up in this approximation, we can write down its own Schrödinger equation. The Hamiltonians of these bands are obtained from (21) by the substitutions $p\to\hat{p}=-id/dl$ and $\varphi\to\varphi(l)$. The scaling transformation

$$l/q_k\to l', \quad \hat{p}q_k\to\hat{p}', \tag{25}$$

yield (we omit the primes) the Schrödinger equation of the sth band:

$$f_s(\cos\hat{p}+V_k\cos 2\pi\beta_k l)a(l)=Ea(l), \quad V_k=(V/2)^{q_k}, \quad s=1,2,\ldots,q_k, \tag{26}$$

which corresponds to the k th stair of the devil's staircase of Ref. 1.

To establish the connection with Ref. 1, we examine how the transition takes place from one stair of the devil's staircase to another. On the first stair $p_1/q_1=1/n_1$ [see (2)], and Eq. (26) yields

$$f_s(\cos\hat{p}+V_1\cos 2\pi\beta_1 l)a(l)=Ea(l), \quad V_1=(V/2)^{n_1}, \quad s=1,2,\ldots,n_1. \tag{27}$$

For s not close to $n_1/2$, the tight-binding approximation yielded in Ref. 1 the equation

$$(\cos\hat{p}+V_1\cos 2\pi\beta_1 l)a(l)=Ea(l), \tag{28}$$

i.e., the function $f_s(x)$ is linear. For s close to $n_1/2$, the tight-binding approximation cannot be used and $f_s(x)$ is essentially nonlinear. At $\beta_1\ll 1$, however, this does not prevent a transition to the next stair of the devil's ladder. Following the method of Ref. 1, we put $\beta_1=1/n_2$ and seek the dispersion laws $\varepsilon_r(p,\varphi)$, $r=1,2,\ldots,n_2$ (we assume the index s to be fixed and leave it out) of the bands of Eq. (27). They are connected in obvious fashion with the dispersion laws $\varepsilon_r^0(p,\varphi)$ of Eq. (28):

$$\varepsilon_r(p,\varphi)=f(\varepsilon_r^0(p,\varphi)).$$

At $\beta_1\ll 1$ all the bands are narrow and the argument of the function $f(x)$ changes little; expanding it in a series, we obtain

$$\varepsilon_r(p,\varphi)=A_r+B_r\varepsilon_r^0(p,\varphi),$$

i.e., the spectra $\varepsilon_r(p,\varphi)$ and $\varepsilon_r^0(p,\varphi)$ differ only in a shift of the energy and by a constant factor, and this has no effect whatever on the succeeding iterations. Recognizing that Eqs. (27) and (28) have identical eigenfunctions and the same shapes of the phase trajectories, we can conclude that at β, $\beta_1,\beta_2,\ldots\ll 1$ we can use the reasoning of Ref. 1, without paying attention to the fact that the tight-binding approximation is not applicable in some sections of the spectrum.

§2. RAPIDLY DECREASING β_k AND WEAK LOCALIZATION

In §1 we have assumed β_k to be bounded from below, to make the period of the oscillations of the levels $T_N\sim N/\beta_k$ ($N=q_k$) not too large. At arbitrary β_k, the deviation of the levels between neighboring blocks is $\sim W_N/T_N\sim\beta_k W_N$ and the role of the scaling parameter is assumed by the quantity $V_k\beta_k$ rather than V_k. In particular, the localization condition is

$$V_k\beta_k\to\infty, \quad k\to\infty. \tag{29}$$

In view of the rapid increase of V_k at $V>2$:

$$V_k\sim(V/2)^{1/\beta\beta_1\ldots\beta_{k-1}} \text{ (for } \beta,\beta_1,\ldots\ll 1),$$

The difference between (29) and the condition $V_k\to\infty$ used above is inessential at any reasonable rate of decrease of β_k as $k\to\infty$. Nonetheless, one can always construct a sequence of β_k (meaning also find an irrational number β) such that

$$V_k\beta_k\to 0, \quad V_k\to\infty \quad \text{as} \quad k\to\infty. \tag{30}$$

Let us consider this case in greater detail.

As explained in detail in Ref. 1, an incommensurate system has an infinite sequence of characteristic lengths:

$$L_1\sim 1/\beta, \quad L_2\sim 1/\beta\beta_1,\ldots, \quad L_k\sim 1/\beta\beta_1\ldots\beta_{k-1},\ldots. \tag{31}$$

At a system length $L\sim L_k$, one Wannier function of order k

can be fitted within the limits of the system (see Ref. 1); the localization radius $\xi(L_k)$ of the function is determined by the size of the classically attainable region $\delta l \sim 1/V_{k-1}\beta_{k-1}$ for the Schrodinger equation of the $(k-1)$st stair [see (26)]. Recalling that the unit length for this equation is $L_{k-1} \sim q_{k-1}$ [see (25)], we obtain

$$\xi(L_k) \sim 1/V_{k-1}\beta\beta_1 \ldots \beta_{k-1} \sim L_k/V_{k-1}.$$

In view of (30) we have

$$\xi(L_k) \to \infty, \quad \xi(L_k)/L_k \to 0 \quad \text{as} \quad k \to \infty,$$

i.e., when the size of the system is increased the localization radius diverges, but decreases compared with the length of the system.

We consider now the normalization integral of the wave functions. At $L \sim L_1$ the wave function has a localization radius $\xi(L_1) \sim 1/V\beta$ and contains, with a substantial weight, $\sim 1/V_\beta$ initial Wannier functions; at $L \sim L_2$ it contains $\sim 1/V_1\beta_1$ Wannier functions of the first order, i.e., $\sim 1/V\beta V_1\beta$ initial Wannier functions, etc. Recognizing that the Wannier functions are orthonormal, we obtain

$$\int_0^{L_k} |\psi(x)|^2\, dx \sim \frac{1}{V\beta V_1\beta_1 \ldots V_{k-1}\beta_{k-1}} \sim \frac{L_k}{VV_1 \ldots V_{k-1}}.$$

Consequently, in the limit as $L \to \infty$ we have

$$\int_0^L |\psi(x)|^2\, dx \to \infty, \quad \frac{1}{L}\int_0^L |\psi(x)|^2\, dx \to 0,$$

i.e., the normalization integral diverges, but more slowly than the size of the system. Consequently, the wave functions are localized but weakly — with increasing distance from this localization center they decrease on the average, but not rapidly enough to ensure normalization. Since the functions are not square-integrable, they belong to the continuous spectrum; the spectrum, however, is singularly continuous, (see the terminology in Ref. 11), since the energy interval occupied by it has a measure zero (§ 3).

It is curious that at $L \sim L_{k+1}$ the values of the wave function on the edges of the system, as can be easily seen from Eq. (26) are

$$\psi(L_{k+1}) \sim V_k^{-1/\beta_k} \sim (V/2)^{-1/\beta\beta_1 \ldots \beta_k} \sim e^{-L_{k+1}/\xi}, \quad \xi \sim 1/\ln(V/2),$$

i.e., an impression is created that a constant localization radius is present, the same as for slowly decreasing β_k. For this reason, Aubry's approach,[6] based on the use of Thouless formula (which contains the values of the wave function only at the edges of the system), leads to the conclusion that the localization is the same for all the irrational numbers β.

It is clear from the foregoing that for the conclusions of § 1 and Ref. 1 to be valid it is necessary to restrict the rate of decrease of β_k (or of the increase of n_k). We assume the simplest sufficient condition:

$$n_k < Ak^2 \quad \text{for all} \quad k. \tag{32}$$

The set of numbers β that do not satisfy this condition at any A has a measure zero (Ref. 10); therefore the weakening of (32) is only of academic interest. Under the condition (32), only logarithmic corrections, which do not influence the critical exponent, can appear in the law (23).

Thus, the conclusions concerning the character of the wave functions of an incommensurate system, obtained in § 1 and in Ref. 1, are valid for practically all irrational numbers. Summarizing them, we can formulate the following theorem, which replaces for incommensurate systems the Bloch theorem.

For each small section of the spectrum of an incommensurate system there exists a critical value of the potential V_c at which a phase transition takes place. This transition is characterized by a certain length $\xi(V)$, which diverges near the transition with index 1, and has far from the transition the order of magnitude of the interatomic distance. At $V > V_c$ the wave functions are exponentially localized in a region with dimension $\sim\xi$, and at $V < V_c$ they are indistinguishable from the Bloch waves corresponding to a period $\sim\xi$.

§3. ENERGY SPECTRUM

In the subsequent calculations (§§ 3,4) we confine ourselves to irrational numbers such that $\beta, \beta_1, \beta_2, \ldots \ll 1$, since this simplifies greatly the calculations and makes the physical picture more lucid. These numbers, while constituting a set of zero measure, are, as we have seen in § 1, typical representatives of irrational numbers.

The energy spectrum of an incommensurate system has the structure of a devil's staircase[1,3]: the initial band of width ~ 1 splits in first-order approximation (on the first stair of

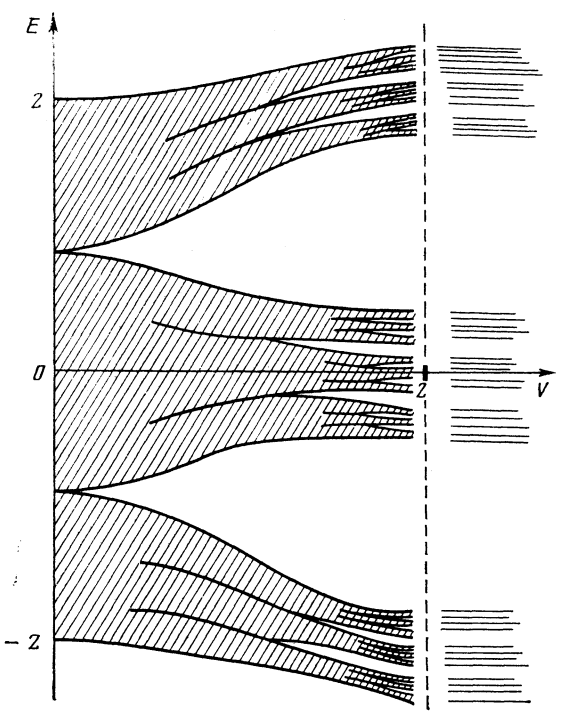

FIG. 3. Deformation of the spectrum of an incommensurate system with changing V — the allowed energy intervals are shaded. All the forbidden bands exist at arbitrarily small V, but have extremely small widths. At $V > 2$ the spectrum is discrete (or, in the case of rapidly decreasing β_k, singularly continuous).

the devil's staircase) into $n_1 \sim 1/\beta_1$ bands of first order, each of which splits into n_2 bands of second order, etc. The deformation of the spectrum with change of V is shown in Fig. 3: when V increases the widths of the forbidden bands increase, and the energy interval occupied by the spectrum Γ (i.e., the total width of the allowed bands) decreases. At $V>2$ the value of Γ becomes zero. Indeed, since Eq. (20) has exactly N real roots at all p and φ, the polynomial $Q_N(E)$ should have an oscillation amplitude not smaller than $V(N)+1$ (see Fig. 2); therefore at $V(N)\gg 1$ the total width of the allowed bands is

$$\Gamma_{(N)} \lesssim 1/V(N) \sim (V/2)^{-N}$$

and tends to zero as $N\to\infty$. This agrees with the fact that the localized states correspond to a discrete spectrum.

Let us ascertain the law according to which Γ vanishes as it approaches the threshold from the side of the metallic region. Let $V=2-\delta$, where $\delta \ll 1$. On the first stair of the devil's staircase the initial band of width $\Gamma_{(0)} \sim 1$ splits into n_1 bands; the widths of almost all these bands are exponentially small, of the order of V^{-n_1}. Exceptions are the bands located in the energy interval of width $\sim\beta$ near $E=0$, i.e., near the center of the initial band. In this interval, the tight binding approximation is violated and the band widths turn out to be of the order of the distances between them. Therefore the total width of the bands on the first stair is

$$\Gamma_{(1)} \sim \beta.$$

On the second stair, each of the first-order bands splits into n_2 second-order bands, which all are exponentially small with the exception of the central ones, so that

$$\Gamma_{(2)} \sim \Gamma_{(1)}\beta_1 \sim \beta\beta_1,$$

and in general on the k th stair

$$\Gamma_{(k)} \sim \beta\beta_1 \ldots \beta_{k-1}. \tag{33}$$

This process, however, does not go on to infinity, since the coefficients V_k in the Hamiltonian (26) for the k th stair decrease and the width of the forbidden bands decreases. Therefore, to obtain the value of Γ it is necessary to substitute for k in (33) the number of stairs in which the sequence V_k from the initial one $V_0 = V = 2-\delta$ decreases to a certain small value. Expanding (22) near the threshold and recoginizing that $N \sim 1/\beta\beta_1 \cdots \beta_{k-1}$, in the case considered, we obtain

$$V_k - 2 = (V-2)/\beta\beta_1 \ldots \beta_{k-1}.$$

Putting $V_k - 2 = \text{const}$ and comparing with (33), we obtain

$$\Gamma \propto |V-2|, \tag{34}$$

i.e., Γ tends to zero in power-law fashion with a critical exponent equal to unity.[1)]

The law (34) remains in force if Γ is taken to mean the total width of the allowed bands located inside a certain interval ΔE situated in an arbitrary section of the spectrum, since this interval contains several bands of k th order, organized in the same way as the initial band. On the other hand, the coefficient in the relation (34) depends strongly on the position of the interval ΔE in the spectrum, and ranges from unity to exponentially small values.

§4. CONDUCTIVITY

Let a system of noninteracting electrons be located in the considered incommensurable potential and let them fill the previously obtained single-electron states in accordance with the Pauli principle. We shall obtain the conductivity of such a system.

As explained in Ref. 1, an incommensurate system has a sequence of characteristic lengths

$$L_1 \sim 1/\beta, \quad L_2 \sim 1/\beta\beta_1, \ldots, L_k \sim 1/\beta\beta_1 \ldots \beta_{k-1}, \ldots,$$

which are quasiperiods of the system: in the first approximation an incommensurate system is similar to a periodic one with a period L_1, and with still higher accuracy it is approximated by a periodic system with period L_2, etc. These considerations lead directly to a simple method of calculating the conductivity.

We are interested in the conductivity of a macroscopic sample. It is convenient to take the macroscopic limit as $L\to\infty$ by a special method. We choose m such that $1 \ll m \ll \min_k(1/\beta_k)$. Let the length of the system L lie in the interval

$$mL_{k+1} \geqslant L \geqslant mL_k. \tag{35}$$

By virtue of the condition $L \geqslant mL_k \gg L_k$, the length of the system spans many periods L_k. We shall assume that the spectrum of the system is defined by this period, and the influence of the periodicity of next order, with period L_{k+1}, will be taken into account as a perturbation. Let J_k be the width of one of the bands, corresponding to the period L_k. For a sample of length L, this band consists of L/L_k individual levels; their spacing is $\sim J_k L_k/L$. The influence of the period L_{k+1} manifests itself in the form of periodic oscillation of these levels with amplitude W_k. We choose k such that

$$W_k \ll J_k L_k/L \tag{36}$$

— this is always possible in a metallic phase, since at $V<2$ the sequence $V_k = W_k/J_k$ decreases exponentially (§ 1), $V_k \sim \exp(-L_k/\xi)$, and $L_k/L \gg L_k/mL_{k+1} \sim 1/m\beta_k$ by virtue of (35) [we do not consider the rapidly decreasing β_k (see § 2)]. Under the condition (36) the periodicity of order $(k+1)$ causes only a small change in the wave functions of the system. The path length l, however, is the distance over which the scattering potential causes a substantial change in the free-motion wave functions (according to Mott[12] this is the loss of phase coherence): over this distance there should take place one collision, i.e., there should be accumulated a reflection coefficient ~ 1. Therefore under the condition (36) we have $l > L$, i.e., the scattering takes place mainly from the boundaries of the sample.

Since W_k/J_k decreases rapidly with increasing k, all the arguments presented above are valid for all k that are larger than the one indicated above. Therefore all that needs be done is to calculate the conductivity of a periodic system with period L_k of finite length L from the interval (35), and go to the macroscopic limit, letting k tend to infinity.

The conductivity of the periodic system is estimated in the usual manner, but with account taken of the fact that the spectrum has an arbitrarily sparse structure, so that even

within the limits of the thermal smearing of the Fermi distribution there exist both allowed and forbidden bands. As usual, it can be assumed that the electric field F causes a shift of the Fermi distribution by an amount

$$\delta p \sim eF\tau/\hbar,$$

where τ is the relaxation time. Therefore the nonequilibrium distribution function is

$$f_p = f^0(\varepsilon_{p+\delta p}) \approx f^0(\varepsilon_p) + \frac{\partial f^0}{\partial \varepsilon} v_p \delta p,$$

where $f^0(\varepsilon)$ is the Fermi function. The electric current is equal to

$$j \sim e\int v_p f_p dp \sim \frac{e^2}{\hbar} FL \int \frac{\partial f^0}{\partial \varepsilon} v_p dp,$$

where we have replaced τv_p by the mean free path, the latter determined by the length of the system L. The conductivity is therefore

$$\sigma(L) \sim \frac{e^2}{\hbar} L \int \frac{\partial f^0}{\partial \varepsilon} d\varepsilon, \tag{37}$$

where the integration is only over the allowed energy intervals. If there are no forbidden bands within the limits of the thermal smearing, the integral in (37) is equal to unity; in the general case, however, it is determined by the density of the allowed bands near the Fermi level:

$$\sigma(L) \sim (e^2/\hbar) L (\Delta\Gamma/\Delta E)_k, \quad mL_{k+1} \geqslant L \geqslant mL_k, \tag{38}$$

where $\Delta\Gamma$ is the total width of the allowed bands in the interval $\Delta E \sim T$ located near the Fermi level, and the index k indicates that the spectrum corresponds to the k th stair of the devil's staircase. Formula (38) yields the estimate we need. This estimate is exact at $L \lesssim \xi$ in the metallic phase, but can be used as an upper-bound estimate at $L \lesssim \xi$ also in the region of localization of the states (in this case the condition $l > L$ is not satisfied and we discard an essential scattering source).

As is clear from the preceding section

$$\left(\frac{\Delta\Gamma}{\Delta E}\right)_k \propto \begin{cases} \text{const}, & V<2 \\ e^{-L_k/\xi}, & V>2 \end{cases}, \quad k \to \infty,$$

therefore as $L \to \infty$ we have

$$\begin{aligned} &\sigma(L) \propto L, \quad V<2, \\ &\sigma(L) \leqslant L e^{-L/\xi}, \quad V>2, \end{aligned} \tag{39}$$

and consequently, for an infinite system

$$\sigma = \begin{cases} \infty, & V<2, \\ 0, & V>2. \end{cases} \tag{40}$$

Thus, the disorder connected with the incommensurability is insufficient to produce in the metallic phase in the system a proper mean free path — this agrees with the viewpoint advanced in § 1 that at $V<2$ an incommensurate system behaves like a periodic system with period $\sim\xi$; in the region of localized states, however, the conductivity, as assumed, vanishes.

It is of interest that the oscillations of σ, predicted by Azbel,[3] as have functions of L a substantial amplitude only at $L \lesssim \xi$. It is easily seen how they arise. At $L \lesssim \xi$ the inequality $l > L$ is satisfied only in the intervals

$$L_k/\beta_k^{1/2} \gg L \gg L_k \tag{41}$$

[the maximum level scatter connected with L_{k+1} has within the limits of the system a value $\sim W_k L/L_{k+1}$ and should be less than $J_k L_k/L$; recognizing that $W_k \sim J_k$ at $L \lesssim \xi$ we obtain (41)]. The estimate (38) is valid in the interval (41); with further increase of L the condition $l > L$ is violated and σ ceases to depend on L until restructuring of a spectrum with a period L_{k+1} sets in at $L \, L_{k+1}$ ($(\Delta\Gamma/\Delta E)_k$ changes to $(\Delta\Gamma/\Delta E)_{k+1}$). At $L \gg \xi$ the inequality $l > L$ is established in the entire length interval, and the sequence $(\Delta\Gamma/\Delta E)_k$ reaches its limiting value, so that the oscillations are damped and $\sigma(L)$ becomes asymptotically linear[2)].

For a more detailed study of the behavior of the conductivity near the transition we consider the quantity

$$g = \sigma(L)/L, \quad L \to \infty,$$

which is the total (not specific) conductivity of the microscopic sample, i.e., a directly observable quantity. In the metallic region, g is a constant:

$$g \sim (e^2/\hbar)(\Delta\Gamma/\Delta E).$$

The subsequent results depend on which of the limits, as $T \to 0$ or as $V \to 2$, is taken first; we consider in succession two cases.

a. $T \neq 0$, $V \to 2$. In this case the interval $\Delta E \sim T$ is constant. Since the total widths of the allowed bands in any interval ΔE decrease in accordance with (34), we have

$$g \propto (2-V).$$

b. $V \neq 2$, $T \to 0$. In this case we should let ΔE tend to zero. Since a decrease of ΔE leads us to higher and higher stairs of the devil's staircase [first ΔE contains one band of order k, then one band of order $(k+1)$, etc.], and the coefficients V_k in the Hamiltonian of the k th stair (26) decrease with increasing k, ΔE contains fewer forbidden bands, so that

$$\Delta\Gamma/\Delta E \to 1, \quad \Delta E \to 0;$$

therefore

$$g \propto \text{const}.$$

The complete picture of the dependence of g on V is shown in Fig. 4. The quantity U, which determines the distance from the threshold at which the transition from a con-

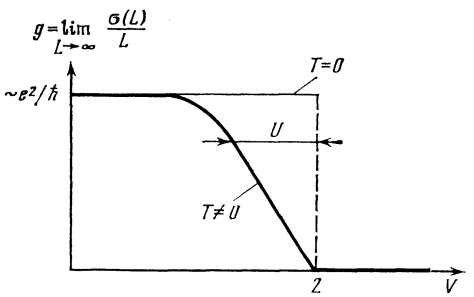

FIG. 4. Behavior of the conductivity of an incommensurate system near the localization threshold.

stant to a linear dependence takes place, is of the order of

$$U \sim \alpha T,$$

where the coefficient α depends strongly on the position of the Fermi level, and, generally speaking, is exponentially large [it is connected with the coefficient in the relation (34)]. We note that the presence of an abrupt transition at $T \neq 0$ is due to the absence of inelastic scattering processes.

A few words on the dependence of g on the position of the Fermi level ε_F. At $T = 0$ this dependence is smooth with the exception of isolated points at which g vanishes and which correspond to intersection of the Fermi level with the band boundaries. At finite but small T, the isolated points smear out into minima of finite width and the $\sigma(\varepsilon_F)$ dependence becomes oscillating; the envelope of the maxima remains smooth, however. Finally, at T larger than a certain T_0, the $\sigma(\varepsilon_F)$ dependence becomes extremely irregular — the amplitude of the oscillations varies exponentially strongly with changing ε_F. The temperature T_0 is of the order of the width J_k of the narrowest of the bands of order k, corresponding to the stairs with $L_k \sim \xi$.

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[1)] Strictly speaking, the index is obtained with logarithmic accuracy up to terms $\sim(\ln 1/\max \beta_k)^{-1}$. However, the only way it can be universal, i.e., independent of the model parameters, is to be exactly equal to unity.
[2)] For rapidly decreasing β_k (§ 2), oscillations remain also at $L \gg \xi$.

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