Electron spectrum of a one-dimensional quasicrystal

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The electron spectrum of a one-dimensional quasicrystal is considered. It is shown that the measure of allowed states is zero and the density of states is strongly singular. The existence of an analog of the momentum is demonstrated; it is represented by a fraction n of the states of energy less than a given value. The dependence of the energy on n exhibits gaps for $n = a + b\varphi$ [a and b are integers; $\varphi = (5^{1/2} - 1)/2$] and scaling behavior for $n = c + d\varphi$ (c and d are rational numbers). An exact solution in the tight-binding limit is obtained by the renormalization group method.

1. INTRODUCTION

The properties of the Schrödinger operator with a quasiperiodic potential are of considerable interest in the physics of incommensurate systems. It is known that any quasiperiodic function can be derived from a periodic function in a space with a large number of dimensions when the latter is limited to a certain subspace:

$$U(\mathbf{x}) = F(\mathbf{x}, \mathbf{y}(\mathbf{x})). \qquad (1)$$

Here, U is a quasiperiodic function in k-dimensional space with $k + l$ periods; F is a periodic function in $(k + l)$-dimensional space; $y_i(x_j)$ $(j = 1,..., k, i = 1,..., k + l)$ is the embedding of a k-dimensional space in a space of $k + l$ dimensions.

The case of a smooth function $F(k = 1, l = 1)$ has been studied thoroughly.[1] However, it has recently become clear that in certain situations which are physically important the function F is discontinuous. These situations include the spectrum of surface states of electrons on a crystal face with sufficiently large ("irrational") Miller indices ($k = 2$, $l = 1$), the problem of electrons on a dislocation the direction of which is incommensurate with the lattice periods ($k = 1, l = 2$), and finally the problem of electron properties of recently discovered quasicrystalline substances ($k = 3$, $l = 3$).

In all these cases a discontinuous quasiperiodic distribution of atoms can be described by the tube model[2]: a certain set T is selected in an orthogonal complement to a k-dimensional space and all the points are taken on an integer-valued lattice in a k-dimensional tube of cross section T. The positions of atoms are given by the projections of these points on a k-dimensional subspace.

We shall consider an example of a potential of this type which is quite easy to analyze. We shall assume that an irrational number α and a band $\lambda < y - \alpha x < \lambda + 1 + \alpha$ on a two-dimensional lattice are given. The lattice points in such a band are joined by a broken line drawn along the edges of the lattice. Moreover, there are two smooth functions in a unit segment (two types of atom) such that $U_1(0) = U_2(0) = U_1(1) = U_2(1)$. The function U for each of the integer-valued segments coincides with one of the functions U_1 and U_2, and U_1 and U_2 alternate in the same order as the vertical and horizontal parts of the broken line (Fig. 5 below).

The results of numerical calculations carried out using such a potential have been reported on several occasions.[3,4] It has been established that for any value of the incommensurate potential the measure of the spectrum is zero. This shows that perturbation theory cannot be applied.

In fact, if we were to carry out calculations for a weak potential using perturbation theory we would have to assume that each harmonic of the potential opens up (independently of others) a gap in the spectrum of free particles and this gap would be proportional to the harmonic. The Fourier transform of such a potential can be calculated by a method described in Ref. 2. It consists of δ peaks with positions which are obtained by projection from lattice points on a straight line and because of the sharp edge of the tube the intensity of the peaks falls slowly (as $1/q^*$) on increase in q^*, which is the distance from a lattice point to its projection. Therefore, the sum of absolute values of the harmonics (i.e., the sum of the gaps which are opened up in the spectrum) diverges logarithmically for any potential no matter how weak. Therefore, our problem cannot be solved by perturbation theory methods and requires a special approach described below.

2. RECURSION FOR TRANSFER MATRICES AND THEIR TRACES

We shall consider a sequence of letters A and B describing the alternation of segments of a broken line corresponding to $\lambda = -1$ (A is a vertical segment and B is a horizontal segment). There is an effective algorithm for calculating this sequence and it involves expansion of the number α as a continued fraction. Let $\alpha = 1/(n_1 + 1)/(n_2 + ...$ and that kth suitable fraction is P_k/Q_k (P_k and Q_k are corprime numbers). Then, a segment I_k of a broken line consisting of the first $P_k + Q_k$ letters is obtained from the segments I_{k-1} and I_{k-2} as follows:

$$I_k = I_{k-1} \ldots I_{k-1} I_{k-2} \qquad (2)$$

(I_{k-1} is repeated n_k times). The effectiveness of this algorithm is manifested by the fact that it can be used to calculate a segment of length N in $\sim \ln N$ steps.[5]

We shall now deal with the problem of calculating the spectrum. We shall consider a segment I_k and the potential in this segment. We shall periodically continue the potential from a segment over the whole line and we shall be interested in the band structure of the resultant crystal with a unit cell of $P_k + Q_k$ atoms. It is given by the condition $|\mathrm{tr}\, T_k(\varepsilon)| < 2$, where $T_k(\varepsilon)$ is a real unimodular 2×2 matrix describing the variables at the right end of the segment in terms of the variables at the left end.

The problem thus reduces to a calculation of a transfer matrix or, more exactly, of its trace. The above property of a broken line readily yields the following recurrence relationship for T_k:

$$T_k = T_{k-2}(T_{k-1})^{n_k}. \qquad (3)$$

Since it is not the transfer matrices but their traces that are important, we shall rewrite the mapping (3) for traces. We shall introduce the variables $x_k = (\mathrm{tr}\, T_{k-1} T_k)/2$, $y_k = (\mathrm{tr}\, T_k)/2$, $z_k = (\mathrm{tr}\, T_{k-1})/2$. These variables transform as follows:

$$\begin{gathered} x_{k+1} = S^{n_k+1}(y_k)\, x_k - S^{n_k}(y_k)\, z_k, \\ y_{k+1} = S^{n_k}(y_k)\, x_k - S^{n_k-1}(y_k)\, z_k, \quad z_{k+1} = y_k, \end{gathered} \qquad (4)$$

where $S^n(t) = \sin(n \arcos t)/\sin(\arccos t)$ is Chebyshev polynomial. This mapping has an integral:

$$J(x, y, z) = x^2 + y^2 + z^2 - 2xyz = \mathrm{tr}(T_k T_{k-1} T_k^{-1} T_{k-1}^{-1})/2. \qquad (5)$$

Since the Jacobian (4) is -1, the mapping (4) transforms the surface $J = \mathrm{const}$ into itself by one-to-one correspondence.

The problem is therefore reduced to the following. There is a curve $x_1(\varepsilon), y_1(\varepsilon), z_1(\varepsilon)$. It has to be iterated by the mapping (4) and we have to find the band structure, set ε, for which $|y_k(\varepsilon)| < 1$. We shall now give the quantities under discussion calculated for a specific potential of the tight-binding problem:

$$\begin{gathered} \varepsilon\psi_n = \psi_{n+1} + \psi_{n-1} + V_n \psi_n, \\ V_n = \lambda, \text{ if the } n\text{th letter is} - A, \\ V_n = -\lambda, \text{ if the } n\text{th letter is} - B, \\ x_0(\varepsilon) = \varepsilon - \lambda/2, \quad y_0(\varepsilon) = \varepsilon + \lambda/2, \quad z_0(\varepsilon) = 1, \quad J = 1 + \lambda^2. \end{gathered} \qquad (6)$$

In this case the initial curve lies completely on a certain invariant surface. However, this is not generally true and the invariant J may depend on ε. However, we can say that in the case of allowed values of the energy we have $J \geqslant 1$. We can easily check that if $|\mathrm{tr}\, T_1 T_2 T_1^{-1} T_2^{-1}| < 2$, then $|\mathrm{tr}\, T_1| > 2$ and $|\mathrm{tr}\, T_2| > 2$.

Although some of the results obtained below are valid for all values of α, we shall consider only the case when $\alpha = \varphi = (5^{1/2} - 1)/2$. The mapping and the invariant were obtained for the golden section in Ref. 3. The mapping (2) becomes

$$M: x \to 2xy - z, \quad y \to x, \quad z \to y. \qquad (7)$$

2. GEOMETRY OF THE SURFACE J=const

If $J = 1$ (when the matrices T_1 and T_2 commute) this surface consists of five parts: the first is a curvilinear tetrahedron with vertices at the points $P(1,1,1)$, $Q(1, -1, -1)$, $R(-1,1,-1)$ and $S(-1,-1,1)$, parametrized by angles θ_1 and θ_2: $x = \cos(\theta_1 + \theta_2)$, $y = \cos\theta_1$, $z = \cos\theta_2$; the second is a funnel with its vertex at the point P: $x = \cosh(\theta_1 + \theta_2)$, $y = \cosh\theta_1$, $z = \cosh\theta_2$; the third, fourth, and fifth are similar funnels with vertices at Q, R, and S.

For J differing from unity the conical singularities at P, Q, R, and S are replaced by four necks.

We shall now consider the behavior of mapping near the neck P. If $|J - 1| \ll 1$, its behavior can be linearized (P is a fixed point) and the eigen-numbers can be obtained: -1, φ^2, φ^{-2}. We can see that a neck has two points P' and P'' which are transformed into one another and which are fixed relative to the mapping square. In the case of an arbitrary value of J, P' and P'' are described by

$$\begin{gathered} x = t \pm (t^2 - t)^{1/2}, \quad y = t \mp (t^2 - t)^{1/2}, \quad z = t \pm (t^2 - t)^{1/2}, \\ J = 4t^2 - 3t, \quad t > 1. \end{gathered} \qquad (8)$$

The eigen-numbers of the square M are

$$[8t - 1 \pm [(8t - 1)^2 - 4]^{1/2}]/2. \qquad (9)$$

The positions of the separatrices beginning at the points P' and P'' are shown in Fig. 1a.

The distribution of the separatrices shows that if some initial point lies in the region 1 of the neck, it is displaced to the funnel and does not return. Its coordinates will then increase and the corresponding energy is forbidden.

Therefore, the forbidden energies correspond to points

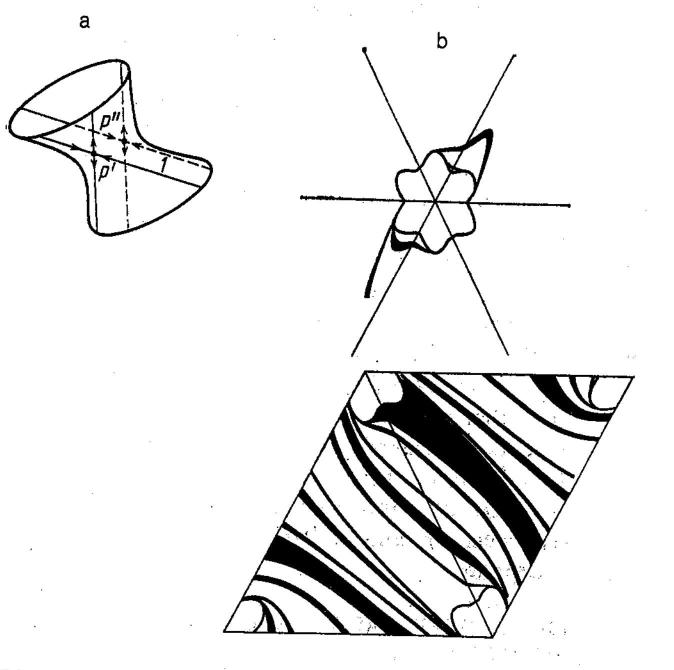

FIG. 1. a) Separatrices in the vicinity of a neck P. b) Part of the forbidden region between the initial segments of two separatrices (shown black): the lower part applies to a torus θ_1, θ_2, and the upper part to a funnel.

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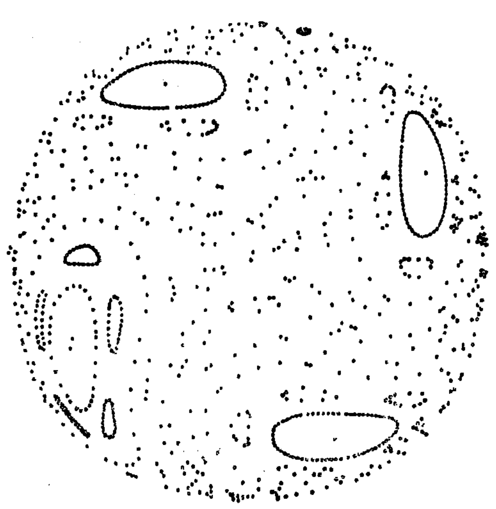

FIG. 2. Mapping orbits on the $J = 0.3024$ surface demonstrating nonintegrability of the mapping M. The projection on the yz plane is shown.

inside the forbidden region, i.e., the region between the pairs of separatrices drawn to reach the points P' and P'', Q' and Q'', S' and S'', and R' and R''; these points appear as a result of bifurcation of the conical singularities at P, Q, S, and R. The forbidden region has a fairly complex structure because separatrices appear in the funnels an infinite number of times and then return. We can calculate the whole forbidden region by continuing the separatrices without limit. The initial parts of the separatrices and the corresponding forbidden region are shown in Fig. 1b. A quantitative determination of the spectrum is not possible by this method because the mapping M is not integrable (Fig. 2).

If $J = 1$, the mapping M becomes simple in terms of the coordinates θ_1 and θ_2: $(\theta_1, \theta_2) \to (\theta_1 + \theta_2, \theta_1)$. This is an integer-valued hyperbolic mapping of the torus (eigennumbers-φ and φ^{-1}). Such mapping mixes strongly the points and after a large number of iterations converts any curve into a thick winding on a torus. Therefore, almost any point on the curve passes an infinite number of times in the vicinity of the necks. We therefore conclude that if $J > 1$, almost all the energies are forbidden. The energy spectrum is then a Kantor set of measure zero. This is in agreement with the numerical calculations reported in Refs. 3 and 4. Since the total number of states in a chain is proportional to its length (and equal to the number of atoms in the case of tight binding), the density of states considered as a function of the energy is strongly singular. A natural explanation of this behavior is that identical configurations are encountered very frequently in a chain. For a certain sequence of N letters A and B in a chain, another identical sequence is encountered no further than cN letters from any given point. Therefore, the energy levels are almost degenerate and the density of states is singular.

4. NUMBER OF STATES AS AN ANALOG OF QUASIMOMENTUM

We shall now show that the number of states with an energy less than a given value has a clear geometric meaning and is equal to the "number of revolutions" of the $C_{\varepsilon_0}[x_k(\varepsilon), y_k(\varepsilon), z_k(\varepsilon), \varepsilon < \varepsilon_0]$ curve about the surface $J = \text{const}$.

We shall now project the surface on the yz plane. The bounding curve of the projection is described by the equation $(1 - y^2)(1 - z^2) = 1 - J$ and it is shown in Fig. 3. The energy bands for the k-iteration chain are obtained from the condition $|y_k(\varepsilon)| < 1$, and their number is the same as the number of times that a curve C varies from values > 1 to values < -1 or vice versa. Any curve C such that after the k th iteration its terminal point has become displaced to a neck and has not returned can be made to correspond to an element of a group of one-dimensional homologies of the surface, $n_1\Gamma_1 + n_2\Gamma_2$, where n_1 and n_2 are numbers defined below, whereas Γ_1 and Γ_2 are the contours shown in Fig. 3. The integer n_1 is equal to the number of intersections of the curve C in the region $|y| < 1$, where topologically removable intersections are ignored, and n_2 is defined similarly but with y replaced with z. A study of the action of mapping on a group of homologies gives

$$M\colon\ \Gamma_1 \to \Gamma_1 + \Gamma_2, \quad \Gamma_2 \to \Gamma_1. \tag{10}$$

Moreover, it is clear that the number of intersections of the curve C in the region $|y| < 1$ is not less than the first coefficient of its expansion in terms of Γ_1 and Γ_2. Since this is true for any part of the curve with its ends at holes and the number of times that the curve intersects the region $|y| < 1$ is equal to the total number of the energy bands (number of atoms in a chain), we can formulate the following conclusion. If after a certain number of iterations the energies ε_1 and ε_2 become forbidden (because the corresponding points have been displaced to necks), then the number of states between ε_1 and ε_2 (or the number of the energy bands for a periodic continued potential) is equal to the first cofficient of the expansion of the curve $C_{\varepsilon_1\varepsilon_2}$ in terms of Γ_1 and Γ_2.

We shall now show that in spite of the nonperturbative nature of the problem in the absence of quasimomentum, there is a quantity analogous to the quasimomentum. This quantity is the number of states. In the case of a weak smooth quasiperiodic potential we find that gaps appear in the $\varepsilon(p)$ spectrum at values of p equal to integer-valued linear combinations of the wave vectors of the harmonics of the potential. In our case a similar conclusion applies to the function $\varepsilon(n)$ $(0 < n < 1)$, which is defined as follows: $\varepsilon(n_0) = \varepsilon$ if the ratio of the number of states with energies less than ε to the total number of states in a chain is n_0. Although in our problem there is no quasimomentum, the positions of the gaps in the spectrum $\varepsilon(n)$ are described by the same rule as in the usual case: the values of n at which there is a gap are described by the formula

$$n = (a + b\varphi)/(a_0 + b_0\varphi), \tag{11}$$

where a and b are arbitrary integers; a_0 and b_0 are certain integers fixed for a given chain.

We can demonstrate the validity of Eq. (11) by considering a curve the end of which is located in a neck after the k th interaction (i.e., the energy ε_0 has become forbidden). We shall assume that $C_{\varepsilon_0} = n_1\Gamma_1 + n_2\Gamma_2$ and $C_\infty = m_1\Gamma_1 + m_2\Gamma_2$. It follows from Eq. (10) that after further iterations we find that

$$n_1' = F_l n_1 + F_{l-1} n_2, \quad n_2' = F_{l-1} n_1 + F_{l-2} n_2$$

(F_l is the l th Fibonacci number). In the limit $l \to \infty$ the fraction n of states with energies less than ε is

$$\lim_{l\to\infty} [(F_l n_1 + F_{l-1} n_2)/(F_l m_1 + F_{l-1} m_2)].$$

It follows from the properties of the Fibonacci numbers and those of the golden section that $n = (n_1 + n_2\varphi)/(m_1 + m_2\varphi)$, where m_1 and m_2 are the coefficients of the expansion of the curves $x_1(\varepsilon)$, $y_1(\varepsilon)$, $z_1(\varepsilon)$ in terms of Γ_1 and Γ_2. Bearing in mind the tight-binding case, we obtain $m_1 = 1$ and $m_2 = 0$. This proves the assertion described by Eq. (11).

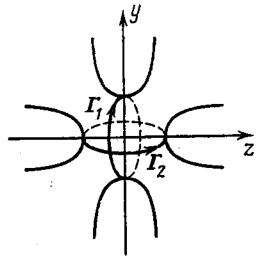

FIG. 3. Projections of the surface $J = \text{const}$ on the yz plane. The contours Γ_1 and Γ_2 are shown.

5. SCALING PROPERTIES OF THE SPECTRUM

We shall now consider points on the $J = \text{const}$ surface which are fixed for a certain degree of mapping M: $M^n(x) = x$. The minimum n for which this is true will be called the order of a fixed point. At a point of order n we can linearize M^n and find the eigen-numbers Λ^n and Λ^{-n} of the resultant linear mapping $(\Lambda > 1)$.

There is a simple relationship between fixed points on a factorized torus $J = 1$ and other surfaces $(J > 1)$. Each fixed point for $J = 1$ corresponds to a fixed point for $J > 1$ with two exceptions.

1) The first-order point P corresponds to second-order points P' and P''.

2) An orbit of the third-order points Q, R, and S corresponds to an orbit of six points Q', Q'', R', R'', S' and S'' of sixth order, which play a role similar to that of P' and P'' on necks Q, R, and S. We shall list several other fixed points.

1) The second-order points are described by the formulas of Eq. (8) for $t < -1/4$ and we shall call them O_2^1 and O_2^2.

2) Six points $(\pm c,0,0)$ $(0,\pm c,0)$ and $(0,0,\pm c)$ form an orbit of sixth-order points O_6^i $(i = 1,2,\ldots,6)$.

All fixed points of the mapping corresponding to scaling points of the spectrum. In fact, if in the case of iterations of the k th degree of mapping M a certain point $x_0(\varepsilon)$, $y_0(\varepsilon)$, and $z_0(\varepsilon)$ tends to a fixed point x_0 of k th order [eigennumbers of the linearization of M^k at x_0 or Λ^k and $-\Lambda = {}^{-k}$], the region in the vicinity of the point of the spectrum has the following property: after repeated dilatation by a factor of φ on the n scale and by a factor of Λ on the ε scale, the graph ceases to vary. This follows the properties of a fixed point and from the fact that each iteration increases the density of states by a factor of φ^{-1} (asymptotically, i.e., after a large number of iterations). We can easily show that $n = c + d\varphi$ (c and d are rational numbers) and that k is the period of the expansion of the number n as a Fibonacci code (see the Appendix).

Therefore, in addition to the gaps in the dependence of ε and n, which occur at $n = a + b\varphi$ (a and b are integers), at points of the $p + q\varphi$ type (p and q are rational numbers), the dependence exhibits a scaling behavior. It should be noted that the band edges (where p and q are integers) are also among the scaling points (and the corresponding fixed points are P', P'', Q', Q'', R', and R''). Figure 4 shows the average coefficients of the dilation Λ for orbits of length less than 14 considered as a function of $\ln J$. Since fixed points everywhere fill densely the allowed region, it is likely that for any orbit on the surface the dilatation coefficient is greater than φ^{-1}. For low values of J the smallest dilatation coefficient corresponds to the orbit O_6^i:

$$\Lambda = \{(8J^2+1) + [(8J^2+1)^2 - 1]^{1/2}\}^{1/6}. \tag{12}$$

Hence, we can estimate the Hausdorff dimension of the spectrum in the case of low values of $J - 1$:

$$d \leqslant \log_\Lambda(\varphi^{-1}) = 1 - (2/3\cdot 5^{1/2})(J-1) + O[(J-1)^2]. \tag{13}$$

These are the general properties of the spectrum independent of the properties of the atoms and of the force of the incommensurate potential. All these properties can be generalized to the case of an arbitrary irrational number which describes the slope (apart from the scaling points, which exist only for the slopes that are quadratic irrationalities: $\alpha = p + qr^{1/2}$). The scaling coefficients are not universal, since in general J depends on ε (the curve representing the initial data intersects invariant surfaces). This applies also to the widths of the forbidden bands, although (as discussed below) the forbidden band with a coordinate $n = p + q\varphi$ on the scale of states decreases in width on increase in p (or q).

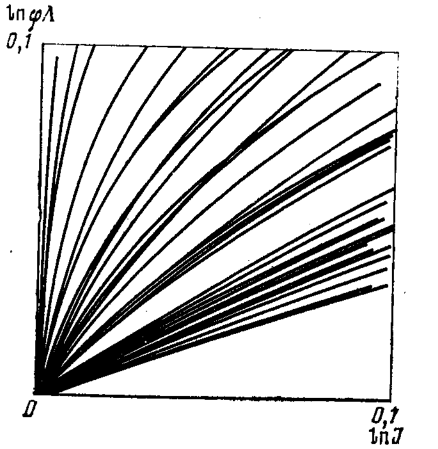

FIG. 4. Multipliers Λ of fixed point orbits of length less than 14. The dependence on J is shown.

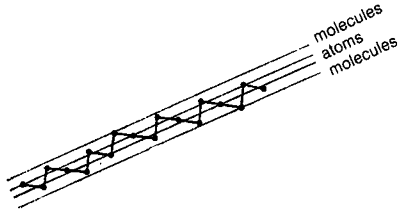

FIG. 5. Geometry of the distribution of atoms and molecules in a band $-1 < y - \varphi x < \varphi$. The upper band of width φ^2 can be regarded as corresponding nominally to even levels, and the lower band to odd levels.

6. RIGOROUS SOLUTION IN THE TIGHT-BINDING CASE

We shall now consider the case of a strong potential $J \gg 1$ for which we can calculate vigorously the positions of gaps in the spectrum on the energy scale. If $J \gg 1$, the situation is dominated by fixed points O_2^i and O_6^j $(i = 1,2;$ $j = 1,2,\ldots, 6)$, for which the dilatation coefficients are the largest.

We shall consider the following model:

$$\varepsilon\psi = t_n(\psi_{n+1} - \psi_n) + t_{n-1}(\psi_{n-1} - \psi_n),$$
$$t_n = V, \quad \text{if the } n\text{th segment of a broken line is vertical,} \tag{14}$$
$$t_n = \varkappa V, \text{ if the } n\text{th segment of a broken line is horizontal,} \quad \varkappa \ll 1.$$

This means that a particle may jump from one site of a broken line to a neighboring one (Fig. 5) and that the amplitudes of the jumps along the vertical are large, whereas along the horizontal they are small. We shall use perturbation theory in terms of $\varkappa$. In the first approximation we shall assume $\varkappa = 0$ (when the horizontal bonds or segments are broken). There remain pairs of sites connected by vertical bonds (molecules) and single sites (atoms). An atom has a level with zero energy and a molecule has two levels, one even and one odd with the energies V and $-V$, respectively. In the next orders of perturbation theory each of these levels splits into a band and the width of the band decreases on reduction in $\varkappa$. We can easily demonstrate that all the atoms are located in a band which is φ^3 times narrower than the initial band and the sites forming molecules are outside this band (Fig. 5). This makes it possible to calculate the fractions of states in the first, second, and third bands. These fractions are φ^2, φ^3, and φ^2, respectively.

We shall now consider atoms. Their positions are obtained from the positions of all the points in a band by the application of the matrix M^3, where

$$M = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}.$$

In this case a horizontal segment transforms into a broken line containing all the molecules and a vertical segment into a broken line containing one molecule. The Hamiltonian for the atoms is the same as the initial Hamiltonian, except that instead of V and $\varkappa V$ we now have an amplitude of jumps via one and two molecules. The amplitude of a jump via one molecule is given by the formula

$$V' = \langle a|H|+\rangle\langle +|V|a\rangle/(-V_+) + \langle a|H|-\rangle\langle -|H|a\rangle/(-V_-), \tag{15}$$

whereas the interaction via two molecules looks similar but a bit more complex. Calculations demonstrate that $V' = -\varkappa^2 V$ and $\varkappa' = -\varkappa$.

We shall now consider molecules. The positions of the upper ends of the molecules coincide with the positions of integer points in a band $0 < y - \varphi x < -\varphi^{-1}$ (after application of the mapping M^{-2} to the points in this band). The bonds between molecules may be direct or via one atom and a direct bond corresponds to a vertical segment in this band, whereas a bond via an atom corresponds to a horizontal segment. The initial broken line and the broken line in a band $0 < y - \varphi x < \varphi^{-1}$ differ by a phason shift, but the corresponding energy spectra are identical. Therefore, splitting of the levels $\pm V$ occurs in the same way as the splitting described earlier. Only the amplitudes of the jump become renormalized: $V' = \varkappa V/2$, $\varkappa' = \varkappa$.

Therefore, the level splitting pattern is described by a tree shown in Fig. 6. The product of the degrees φ given alongside the branches of the tree which begin from the root and end at a vertex describes the fraction of the states corresponding to this vertex. If we count the sequence of zeros and ones along the branches of the tree following a path corresponding to the upper edge of a gap, we obtain a Fibonacci code expansion of an analog of the quasimomentum of the state at the edge of the gap. The paths along the tree which are periodic from a certain point correspond to the scaling points in the spectrum (Sec. 4). As expected, their Fibonacci code taken along the branches of the path is periodic beginning from a certain point. Each such path corresponds to a fixed point of the mapping M^k for a certain value of k. For example, paths down, down, down,...correspond to the points O_6^i $(i = 1,2,\ldots,6)$; the paths left, right, left, right,...correspond to the points O_2^i $(i = 1,2)$, and the paths left, left, left,...and right, right, right,...correspond to the points P' and P''.

7. FORM OF THE WAVE FUNCTION

We shall now describe the properties of the eigenfunctions in the tight-binding case. It is clear from Sec. 6 that in this case each wave function is concentrated mainly at a finite set of sites. For each state this fraction is described in an obvious manner by its Fibonacci code. Simple calculations give the following result.

The fraction of states in a chain of length L, concentrated at L^x sites, is proportional to $\exp[-(x-\alpha)^2/2D]$, where

$$\alpha = c/\log_2 \Phi = 0.4921,$$
$$D^{-1} = (\log_2 \Phi \log_2 L)/[c(c+1)(1-2c)] = 4.781 \log_2 L, \tag{16}$$
$$\Phi = \varphi^{-1}, \quad c = (^6/_5)\varphi - {}^2/_5,$$

i.e., a typical wave function is large at $L^{0.492}$ sites (this should be compared with the two-dimensional case discussed in Ref. 6). It should be stressed that these sites are distributed quasiperiodically in a segment, i.e., the eigenfunction is not localized or delocalized in the usual sense.

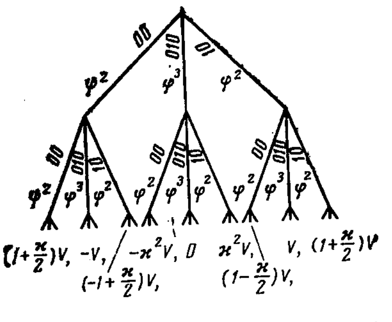

FIG. 6. Tree showing the splitting of levels. The energies of the bands obtained after two splittings are shown.

We shall now consider the case of an arbitrary binding. Let us assume that we know the wave function corresponding to a scaling point in the spectrum, i.e., to an orbit of a period n of the mapping M. In this case there is such a matrix S that $T_{k+n} = S^{-1} T_k S$. There is a simple relationship between the wave function at an arbitrary point and its value at the first two sites. We can expand the number N of a site of interest to us as a series in terms of the Fibonacci numbers:

$$N = \sum_{i, F_i \leqslant n} \alpha_i F_i, \quad \alpha_i(1-\alpha_i) = 0, \quad \alpha_i \alpha_{i+1} = 0. \tag{17}$$

Then, the transfer matrix linking the beginning of a chain to a site N is

$$T_N = \prod_i [\alpha_i T_i + (1-\alpha_i)E] \tag{18}$$

(E is a 2×2 unit matrix) and we correspondingly have

$$T_N = S^{-\{N/n\}} \prod_{p=0}^{\{N/n\}} (R_p S), \quad R_p \prod_{j=1}^{n} [\alpha_{np+j} T_j + (1-\alpha_{np+j})E]; \tag{19}$$

R_p can assume also a finite number of values and in general the different values of R_p do not commute. We can determine the properties of such a product of matrices using familiar results on the localization in a one-dimensional random potential. Applying them in our case, we find that the wave functions are localized in logarithmic space. This means that a typical wave function increases exponentially on increase in the number of nonzero terms in the Fibonacci-number expansion for the site in question.

8. CONCLUSIONS

The properties of the electron spectrum of a quasicrystal differ considerably from the spectrum obtained in a smooth quasiperiodic potential. There is no localization–delocalization transition typical of this case. The Hausdorff dimension of the spectrum is always less than unity and it decreases monotonically to zero on increase in the strength of the potential. The wave functions are critical, i.e., they are concentrated mainly at L^α atoms (L is the number of atoms in a chain). We should mention here the treatment in Ref. 8, where it is shown mathematically that localization does not occur.

Naturally, solutions of the one-dimensional problem are insufficient for the description of electronic properties of real quasicrystals. However, calculations of the spectra of two-dimensional quasicrystalline lattices reported in Ref. 6 show that they have much in common with the one-dimensional case. For example, they are characterized by anomalously short distances between neighboring levels that are not described by the Dyson statistics (attraction between levels or quasidegeneracy). The wave functions are also critical.

Since the measure of the spectrum is zero, the density of states is also zero for almost any position of the Fermi level (in the one-dimensional case). Therefore, it is particularly interesting to note the report[7] of an experimental observation of a strong reduction in the density of states at the Fermi level in a quasicrystalline alloy of the composition $U_{20}Pd_{60}Si_{20}$, compared with crystalline and amorphous alloys of the same composition.

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APPENDIX

Fibonacci code

The number x $(0 < x < 1)$ can be represented in the form

$$x = \sum_{i=1}^{\infty} c_i \varphi^i,$$

where $c_i = 0$ or 1, and we have $c_i c_{i+1} = 0$. The sequence of zeros and ones $\{c_i\}$ is known as the code of the number x.

The properties of this code are as follows: 1) for numbers of the $a + b\varphi$ type (a and b are integers), beginning from a certain point the code consists of zeros alone; 2) for numbers of the $p + q\varphi$ type (p and q are rational) beginning from a certain point the code becomes periodic.

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