Local rules for quasicrystals

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The cases are considered when the onset of long-range quasicrystalline order can be explained on the basis of the short-range order, i.e., the cases in which the structure is completely defined if all the local configurations are known. It is proved that such local rules exist for a two-dimensional quasicrystal only when its incommensurability is described by quadratic irrational numbers $a + bD^{1/2}$ (a and b are rational numbers, and D is an integer). Local rules exist for a three-dimensional quasicrystal with icosahedral symmetry. It follows therefore that it is possible to find a Hamiltonian with a finite interaction radius, for which such a structure will be a configuration with minimum energy. This means that quasicrystals with thermodynamic equilibrium exist.

I. INTRODUCTION

Quasicrystals, discovered by Shechtman *et al.*,[1] have their atoms arranged in an unusual long-range order. To explain the diffraction properties of these substances one usually invokes a whole-number lattice in multidimensional space and a three-dimensional subspace, the atom being located at latice sites close to the subspace. The locations of the atoms in the three-dimensional space can be determined by the projection method.[2–5] Although constructions of this kind explain well the coherence of the scattering, they have a substantial shortcoming, viz., existence of long-range order is postulated from the very outset, but it is not explained how this order stems from the short-range ordering of the atoms. However, if the crystal grows, for example, from a melt the attachment of the atoms to an already formed seed follows already certain laws that are local in character. Which of the atoms will occupy a certain space is determined by the first, second, and perhaps a few other coordination spheres. When speaking of quasicrystal growth, it can be said that the atoms sticking to the surface of the seed "do not know at all" that the structure increases in a certain incommensurate direction in multidimensional space. All that the atoms "know" is which local configuration can be formed and which cannot. This raises a question, which is the main topic of this paper: is it possible to specify a quasicrystalline structure by describing the local configurations that are encountered in it?

For a periodic crystal, an affirmative answer to a similar problem is obvious. It suffices to describe the structure of one unit cell and explain that its neighbors are identical unit cells. There is no complete answer for quasicrystals, and the available results are by way of models. Structures are considered which are called coverings or tilings of a plane or space.[6,7]

Let us define the tiling of a plane by parallelograms. Let n nonparallel vectors $\mathbf{e}_i$ ($i = 1,...,n$). be specified on a plane. We consider all the parallelograms formed by the vector pairs $\langle \mathbf{e}_i,\mathbf{e}_j \rangle$ $(i \neq j)$. A tiling is defined as a breakup of the plane into parallelograms from this set, such that the different parallelograms either do not intersect or have a common vertex or a common edge. The tilling of a space by parallelograms can be defined by introducing n vectors $\mathbf{e}_i$ ($i = 1,...,n$) and considering the parallelepipeds generated by the triads $\langle \mathbf{e}_i,\mathbf{e}_j, \mathbf{e}_k \rangle$ $(i \neq j, k \neq i)$. Tiling on a space with more dimensions is similarly defined. Tiling of a straight line is defined as breakup of the line into segments from a specified set.

From among the tilings obtained in this manner, a class called semicrystalline is singled out. These tilings have remarkable properties[6] that permit their use to simulate real quasicrystalline structures. In particular, it is reported[8] that quasicrystalline tiling, by parallelepipeds, on a three-dimensional space having icosahedral symmetry, has been successfully used as a framework for the arrangement of the atoms in the analysis of the structure of an Al–Zn–Mg alloy. There are many equivalent methods of defining quasicrystalline tiling. The best known is the following. We choose a two-dimensional subspace V in an n-dimensional space R^n containing a whole-number lattice Z^n, such that the coordinate on V is an n-component linear function of two arguments. We consider a set, called a "duct" which is a union of all the cubes that coincide in form, size, and orientation with the unit cube of the lattice Z^n, and the centers of the cubes are located on the subspace V. We consider next all the integer points of this lattice, which land inside this duct. It turns out that there exists a single two-dimensional surface consisting of two-dimensional facets of the cubes of the Z^n lattice, contained entirely in the duct, and passing through all the lattice points inside the tube (see, e.g., Ref. 2). When the surface is orthogonally projected on the subspace V, the latter breaks up into parallelograms that are projections of two-dimensional facets of the lattice cubes. This plane is tiled by parallelograms strung on the pair of vectors $\langle \mathbf{e}_i \mathbf{e}_j \rangle$ where $\mathbf{e}_i$ are the projections of the basis vectors of the n-dimensional lattice. The quasicrystalline tiling of the plane, obtained in the this manner, is of particular interest if the subspace v is incommensurate with the lattice Z^n (there are no vectors with integer components and parallel to the subspace V). This tiling is not periodic. A three-dimensional space can be similarly tiled by parallelepipeds.

These tilings are of interest for the investigated quasicrystals primarily because of the properties of their Fourier transform.[7] The Fourier transform of such a structure has much in common with the diffraction patterns obtained in scattering of electrons and x-rays. Another reason why these tilings are of interest is that they have short-range order, just as in real quasicrystals, i.e., there exists a fixed number of types of neighborings of one parallelogram. This corresponds to local order in solids, where the interaction between the atoms leads to a fixed number of atom configurations in the first and several additional coordination spheres.

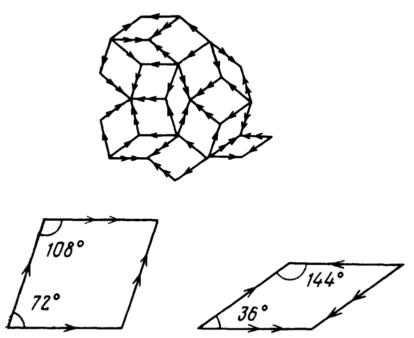

FIG. 1. Local de Bruijn rules for a Penrose lattice. The rhombs must be arranged so that the arrow orientations and their multiplicities are the same on congruent edges.

We are interested in knowing whether it is possible to impose a limit on the local order, i.e., require that only configurations of a definite type be encountered in the tiling, and to ensure that this condition determine the long-range quasicrystalline order. The first nontrivial result in this direction was obtained by de Bruijn,[6] who showed that if tilings of a plane by rhombs of two types (with arrows on the edges) are considered (see Fig. 1), and if it is stipulated that the arrows on overlapping sections of the boundaries of neighboring rhombs be of the same type and of the same direction, then the tilings discovered by Penrose,[7] and none other, are obtained. Beenker[9] has shown later that quasicrystalline tiling of a plane with eightfold symmetry does not have such properties, i.e., it cannot be reconstituted from its local configurations. Unfortunately, nothing but these results is known concerning the local rules for two-dimensional quasicrystals. Nor is there any information at all for the three-dimensional case, which is of principal interest from the experimental viewpoint.

In Sec. 2 of this paper we write down for tiling a definition that will be of importance subsequently, and use it to describe more accurately quasicrystalline tilings. We present also the needed variants of the statement that "a quasicrystal is reconstructed in accordance with its local configurations." in Sec. 3 we consider quasicrystals of unity codimensionality ($n = d + 1$) and show that it is impossible in this case to determine the local order from a set of local configurations. We explain the main idea of this proof by using as the example two-dimensional quasicrystal tiling. We fix an arbitrarily large number R and single out a set of parallelogram configurations encountered in a specified quasicrystalline tiling and having a dimension smaller than R. It turns out that, no matter the type of hyperplane V contained in the definition of the quasicrystalline tiling, it is possible to change the slope of this hyperplane in such a way that in the new quasicrystalline tiling the set of configurations with dimension smaller than R remains the same. This means that no matter how large R, the local order over scales smaller than R does not fix the long-range quasicrystalline order in the case of unity codimensionality. In Sec. 4, which is auxiliary in character, we discuss dual graphs of tilings and their properties. It contains one other useful definition, using dual graphs, of quasicrystalline tilings. This section contains no new results. In Sec. 5 we study two-dimensional crystals with codimensionality two and more (meaning that the dimensionality of the auxiliary multidimensional space exceeds three). It turns out that long-range order can be established in these quasicrystals from the short-range order only if the quasicrystal is described by quadratic irrational numbers $a + bD^{1/2}$, where a, b, and D are rational numbers. We have in mind the following. Assume a given embedding $V: R^2 \to R^n$ of a two-dimensional plane in an n-dimensional space described by n linear functions $V_i(x)$ on a plane ($i = 1,...,n$). We represent this linear dependence in the following fashion: we choose any two functions, say $V_1(x)$ and $V_2(x)$, and express the remaining functions in their terms:

$$V_i(x) = a_i V_1(x) + b_i V_2(x) + c_i \quad (i=3, \ldots, n).$$

This is possible because only two out of any number of linear functions on a plane are linearly independent. The main result of Sec. 5 can be formulated as follows. If the semicrystalline long-range order can be reconstructed from a finite set of local configurations, the coefficients a_1 and b_1 of the expansion are quadratic irrational numbers. It is shown in Sec. 6. that this condition is sufficient (see the more exact formulation in Sec. 6). In Sec. 7 are obtained analogs of certain statements of Secs. 5 and 6 for three-dimensional space, and it turns out that cubic irrational numbers, $a + bD^{1/3} + cD^{2/3}$, are allowed besides the quadratic ones. It is proved, in particular, that quasicrystalline tiling of a three-dimensional space with icosahedral symmetry is reconstructed from its local configurations. We note an interesting circumstance which may have a bearing on the results of the present paper. Quasicrystalline alloys with three types of symmetry, having point groups Y, D_{10}, and D_{12}, are known at present. All three structures are described by quadratic irrational numbers (the radicals produced are $5^{1/2}$ and $3^{1/2}$ respectively).

We note one related question of importance to the physics of quasicrystals. Consider Hamiltonians specified on different tilings and having finite interaction radii. Does a Hamiltonian of a type such that its minimum energy corresponds to a quasicrystal exist? It can be verified that the answer to this question is closely related to the presence or absence of local rules. Thus, for examples, the rules introduced by de Bruijn for the joining of rhombs specify in effect some Hamiltonian on the tilings of a plane by two types of rhombs with arrows on the edges (see Fig. 1), including nearest-neighbor interaction equal to zero if the arrows on the congruent edges are oriented in accordance with the rules, and is large if the arrows are misoriented. The de Bruijn rules in this formulation mean the configurations with minimum energy are Penrose tilings and no other. On the other hand, in many cases where the structure cannot be reconstructed from local configurations, it can be shown that there is no Hamiltonian with a finite interaction radius. It appears that only those two-dimensional quasicrystals which are connected with quadratic irrational numbers can be minimum-energy configurations for physical Hamiltonians. For three-dimensional tilings, both quadratic and cubic irrational numbers are admissible.

2. BASIC DEFINITIONS

We introduce the concept, which will be important in the sequal, of the rise of a tiling. Assume an arbitrary tiling of a plane by parallelograms strung on pairs of vectors $\langle e_i, e_j \rangle$ ($i \neq j$). We designate the "rise of a tiling" by the function $W: R^2 \to R^n$, defined as follows: We choose the vertex x of one of the parallelograms of the tiling as the origin. If y is the vertex of some other parallelogram, then the vector $y-x$ can be uniquely represented in the form $z_1e_1 + ... + z_ne_n$ (z_i are integers). We now define a rise on the vertices of parallelograms: $W(x) = (0,...,0)$, $W(y) = (z_1,...,z_n)$. The values of the function W at other points of the plane are determined from the following conditions: the functions W is linear inside and on the boundary of each parallelogram. Thus, the lifting W maps the tiling of the plane R^2 into a two-dimensional surface in R^n, consisting of unit squares with vertices at integer points.

Consider a two-dimensional linear subspace V and R^n and a standard duct around it, viz., the union of all the unit n-dimensional cubes whose centers belong to V. The subspace must be chosen such that there is not a single integer point on the duct boundary. This nondegeneracy condition can always be met by using parallel transfer of the subspace. It is easy to verify that there exists a unique surface made up of unit squares (two-dimensional facets of an n-dimensional cube), contained inside the standard duct. The tiling, whose rise is this surface, will be called a quasicrystalline tiling or a V-quasicrystal. Note that tilings obtained in this manner can be periodic as well as quasiperiodic, depending on the choice of the subspace V. To generalize the definition of a quasicrystalline tiling to other dimensionalities, we must replace the two-dimensional space by a d-dimensional one, and the unit squares by d-dimensional facets of a unit n-dimensional cube.

We define now an atlas and maps for an arbitrary tiling, and will refer for the sake of argument to tiling on a plane. We designate as the $(r, \mathbf{x})$ map of a given tiling any configuration of parallelograms of this tiling, contained in a circle with center $\mathbf{x}$ and radius r. We designate as the r-atlas of a given tiling the set of all $(r_1, \mathbf{x})$ maps, where $\mathbf{x}$ is arbitrary and $r_1 < r$. Since the number of different configurations contained in a circle of fixed radius is finite, the r-atlas is a finite set of maps. With the aid of these concepts we can formulate more accurately the question of interest to us: In which cases is the quasicrystalline tiling reconstructed if its r-atlas is known for a certain r?

We refine now the statement "a tiling is reconstructed from its r-atlas." We introduce to this end the concept of r-rules. We define r-rules as an arbitrary set of configurations of parallelograms that can be contained in a circle of radius r. Clearly, the set of all r-rules is finite for a given r.

If certain r-rules are specified, we shall say that a given tiling satisfies these rules if all its r_1-atlases $(r_1 < r)$ are subsets of these r-rules.

Assume some given two-dimensional subspace V in R^n. We shall say that strong local rules exist for the V-quasicrystal if there exist r-rules such that: a) they are satisfied by at least one tiling: b) all the tilings that satisfy these rules are quasicrystals; c) if a U-quasicrystal satisfies the rules, than the subspace U has the same dimensionality as V, and is parallel to it.

Strong local rules fix the structure almost completely, allowing only the leeway connected with parallel transfer of the duct. The Fourier transform of such a structure does not contain an arbitrary component and consists of only σ-peaks.

We shall say that for a V-quasicrystal there exist weak local rules if one can find r-rules such that a) they are satisfied by at least one tiling; b) there exists a positive number C such that for any tiling satisfying these r-rules there exists a two-dimensional subspace U such that $U \| V$, and the distance from any rise point of this tiling to the subspace U does not exceed C.

In other words, the rise of any tiling satisfying the weak local rule is almost parallel to the subspace V, deviating from it by not more than a constant. It can be stated that weak local rules specify a quasicrystal apart from a structural disorder. It is easy to verify that this structural disorder does not broaden the σ-peaks of the diffraction pattern, although it does decrease their intensity. In this sense it is similar to the substitutional disorder in ordinary crystals. We shall use hereafter the convenient abbreviations LR for local rules and (V, r)-atlas for the r-atlas of a V-quasicrystal.

We consider by way of example an arbitrary one-dimensional V-quasicrystal ($V{:}R^1 \to R^n$, $V(x) = (a_1x + b_1,..., a_nx + b_n)$) and verify that weak LR exist only if there is no incommensurability (all (a_i/a_j) are rational). Indeed, assume that weak LR exist. We denote by r the maximum radius of the maps contained in these LR. In any tiling satisfying the LR one can find two nonintersecting maps with dimensions larger than r and with tilings that coincide. It is now easy to construct a periodic tiling that satisfies the same LR, using for the period the region between these two maps. Since a periodic tiling can rise to an arbitrary distance from any incommensurate subspace, all the ratios a_i/a_j are rational, and consequently the V-quasicrystal is periodic.

Note that from the existence of strong LR follows the existence of weak LR, and the absence of weak LR means the absence of strong LR.

3. QUASICRYSTALS WITH UNITY CODIMENSIONALITY

Consider a quasicrystalline tiling of a $(d-1)$-dimensional space, obtained with the aid of a d-dimensional space and a $(d-1)$-dimensional hyperplane in it. Of physical interest are the cases $d = 3$ and 4. The first corresponds to a plane in three-dimensional space, i.e., describes the facet of a three-dimensional periodic crystal.

To prove this fact it is necessary to find for any hyperplane V that is not rational, and for an arbitrary r, a hyperplane U close in slope and such that the (V, r)-atlas coincides with the (U, r)-atlas.

Consider the plane $G(d,1)$ of all $(d-1)$-dimensional hyperplanes passing through the origin. We set in correspondence with any configuration k of a finite number of parallelotopes that can be encountered in some tiling R^{d-1} a subset $\Gamma(k)$ of the space $G(d,1)$, consisting of hyperplanes V such that the V-quasicrystal contains the configuration k an infinite number of type.

Let now strong LR be specified for the hyperplane V. We choose a certain positive r, and consider the configurations k_i $(i = 1,...,N)$ contained in the (V,r)-atlas. Clearly, the point V of the space $G(d, 1)$ is internal for all the $\Gamma(k_i)$ sets, since there are no integer points on the boundary on the tube. Therefore the (U,r)-atlas for any hyperplane U of slope sufficiently close to that of V contains all the maps of the (V, r)-atlas. We shall see that if the hyperplane V is not rational we can choose a close hyperplane U such that the (U,r)-atlas coincides with the (V,r)-atlas. The existence of a hyperplane with another slope and the same r-atlas means indeed the absence of r-rules.

A configuration k not belonging to the (V, r) atlas will be called dangerous to V if $\Gamma(k)$ intersects an arbitrarily small vicinity of V in $G(d, 1)$. Let us see the location of the rise of a dangerous configuration relative to the duct. The duct for a hyperplane specified by the equation k_i $(i = 1,...,N)$ is a layer between two hyperplanes:

$$a_1x_1+\ldots+a_dx_d=c\pm(|a_1|+\ldots+|a_d|)/2. \quad (1)$$

It follows readily from the definition of a dangerous configuration that its rise can be placed in the duct (1) if a certain choice of c is made, and the points of this rise will lie on both boundary hyperplanes. We transfer all these points to one of the hyperplanes (1), effecting it necessary a parallel transfer by the vector (sign (a_1),...,sign(a_d)) joining the hyperplanes (1). We obtain a certain set of points (at least two) on one of the hyperplanes (1). Note that all the vectors joining the points of this set have integer coordinates. Consider the rational subspace generated by these vectors. It is at the very least one-dimensional, since our set consists of not less than two points. Thus, each dangerous configuration corresponds to a certain rational subspace of the hyperplane:

$$a_1x_1+\ldots+a_dx_d=0. \quad (2)$$

We call the configuration k dangerous to V if there exists in $G(d, 1)$ such a vicinity of the point V which does not intersect with (k). It is clear from the foregoing that if we choose the hyperplane U in a sufficiently small vicinity of the point V in $G(d, 1)$, all the configurations dangerous to V will be dangerous also to U, and furthermore all the configurations contained in the (V, r) atlas will belong to the (U, r) atlas. It remains to verify that U can be chosen such that the configurations dangerous to V be dangerous also to U. Let us consider all the configurations dangerous to V, and the corresponding rational subspaces of the hyperplane (2). We take the sum of these subspaces. This is also a rational subspace of the hyperplane (2), and it is easy to verify that if r is large enough this rational subspace coincides with the maximum rational subspace of the hyperplane (2). We can now choose U in a sufficiently small vicinity of V in $G(d, 1)$, such that the maximum rational subspaces of the hyperplanes U and V coincide, but not these hyperplanes themselves. This can be done only if the maximum rational subspace of V does not coincide with V itself, i.e., if the hyperplane V is not rational. By choosing U in this manner, we obtain different hyperplanes U and V with identical r-atlases. Since the number r can be made arbitrarily large, there are no strong LR for the nonrational hyperplane V.

The arguments used in this proof do not apply to a codimensionality larger than unity. It was important for our purposes that the duct boundary consisted of hyperplanes connected by an integer vector, so that it was possible to transfer all the extreme points of the dangerous configuration to a single hyperplane. When the codimensionality exceeds unity, different sections of the duct boundary are not parallel, and the procedure is inapplicable.

4. DUAL GRAPHS OF TILINGS

Let us define the dual graph of a tiling, a construction which plays the main role in Secs. 5, 6, and 7. A dual graph of the tiling of a plane consists of n sets of line, one for each $\mathbf{e}_i$ $(i = 1,...,n)$, satisfying the following conditions: a) two lines from one set do not intersect; b) any two lines from two different sets intersect only once, and each such intersection can be set in correspondence with a tiling parallelogram $\langle \mathbf{e}_i,\mathbf{e}_j \rangle$ with vectors $\mathbf{e}_i$ and $\mathbf{e}_j$ corresponding to these two sets; c) only paired line intersections are allowed in a dual graph.

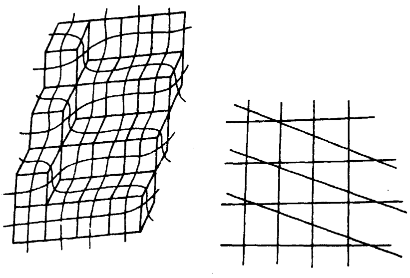

FIG. 2. Dual graph of quasicrystalline tiling, drawn on the tiling (left) and rectified (right).

The dual graph of plane tiling with $n = 3$ is shown in Fig. 2. It is clear that if a dual graph is drawn for a certain tiling, and the tiling itself is erased, the tiling can be restored if we know the relation between the n sets of the nonintersecting lines and the vectors $\mathbf{e}_i$. We assume hereafer that such a relation is fixed once and for all. It is clear also that a tiling corresponding to a graph does not change if the graph is deformed without changing the topology of the intersections. Graphs obtained from one another by such a deformation are called equivalent.

We consider now a dual graph of a quasicrystalline tiling. De Bruijn has shown in his remarkable paper[6] that the dual graph of the Penrose tiling is equivalent to a graph consisting of five sets of nonequidistant parallel lines having fivefold symmetry. It was shown later that analogous statements are valid also for an arbitrary quasicrystalline tiling.[10] Note that a dual graph of the tiling of a plane can be deformed in such a way that two sets of lines are transformed into two sets of parallel equidistant straight lines. A nontrivial property of quasicrystalline tilings is that such a deformation straightens also the remaining sets of line. Each set of parallel equidistant straight lines corresponds to a linear function $f(\mathbf{x}) = ax_1 + bx_2 + c$, $\mathbf{x} = (x_1,x_2)$, with the aid of which the points of the straight lines are written in the form $f(\mathbf{x}) = k$ (k runs through all the integers). Thus a dual graph of a quasicrystalline tiling is uniquely connected with some set $f_i'(i = 1,..,n)$ of linear functions of a plane. The points of the dual graph are given by the equations $f_i = k_i$ (k_i are integers).

It is important that all the constructions considered in Secs. 1 and 2 can be formulated in terms of dual graphs. In place of the tilings we shall speak of graphs satisfying the conditions a), b) and c) indicated above. We define the functions $W:R^2 \rightarrow R$, called the rise of the graph. We choose a point $\mathbf{x}$ not belonging to the graph, and erase all the sets of lines except the ith set. We consider the function W_i, the value of which at a point y not belonging to the graph is equal to the number of ith-set lines that separate $\mathbf{y}$ from $\mathbf{x}$. The value of W on the graph line can be determined, for example, from the semicontinuity on the right or on the left (see Fig. 3). Using the functions W_i $(i = 1,...,n)$, we determine the

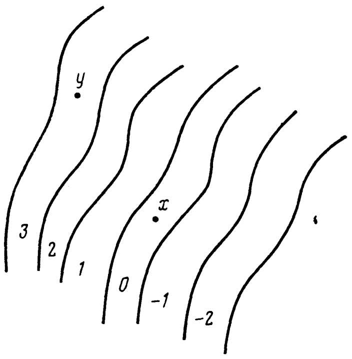

FIG. 3.

function W: $W(\mathbf{x}) = W_i(\mathbf{x}),..., W_n(\mathbf{x}))$. The connections between the rise of a graph and that of a tiling is obvious. To each graph-line region in which all the functions W_i $(i = 1,...,n)$ take on constant values there corresponds the vertex of a parallelogram. Therefore the lift of a graph defines a function that takes on integer values on the vertices of the tiling. After an aditional definition inside the parallelogram with the aid of the linearity condition (see Sec. 1), we obtain a function that coincides with the rise of the tiling. Conversely, a rise of a tiling determines a rise of a dual graph. We designate these two rises by one and the same letter W, since the rise referred to will always be clear. We present an expression for the rise W of a dual graph of a quasicrystal, specified with the aid of the linear functions f_i $(i = 1,...,n)$:

$$W_i=[f_i] \tag{3}$$

(the square brackets denote the integer part).

We introduce maps and atlases for the graphs. We take an arbitrary point $\mathbf{x}$ of the plane, specify a number r, and consider the set of points $\mathbf{y}$ such that $|W_i(\mathbf{y}) - W_i(\mathbf{x})| < r$ $(i = 1,...,n)$. The part of the graph belonging to this region will be called the $(r, \mathbf{x})$-map. The definitions of the r-atlas, r-rules, and strong and weak LR coincide verbatim with those in Secs. 1 and 2.

Let us discuss in detail the properties of quasicrystal atlases. Assume a given set of linear functions f_i $(i = 1,...,n)$ that give the lines of the dual graph. The functions of f_i are called linearly dependent on the field Q of the rational numbers if they are connected by the relation $a_1 f_1 + ... + a_n f_n = \text{const}$ (a_1 belongs to Q). We separate from the set f_i $(i = 1,...,n)$ the maximum set of functions linear on Q. We assume them to be numbered from 1 to m. The remaining functions f_i $(i = m + 1,...,n)$ are represented (apart from a constant) by linear combinations of independent functions f_i $(i = 1,...,m)$ with rational coefficients:

$$f_i = \sum_j a_{ij} f_j + b_i \tag{4}$$

$(i = m + 1,...,n; j = 1,...,m; a$ are rational numbers). The incommensurability of the quasicrystal structure is connected only with the independent functions f_i' $(i = 1,...,m)$, while the remaining functions correspond to decoration of the lattice.

We call the two set of functions f_i and f_i' $(i = 1,...,n)$ satisfying (4) equivalent if the functions of f_i' differ from f_i by constants:

$$f_i' = f_i + c_i \quad (c_i = \text{const}; \ i = 1, \ldots, n),$$
$$c_j = \sum_k a_{jk} c_k, \quad j = m+1, \ldots, n; \quad k = 1, \ldots, m, \tag{5}$$

a_{jk} are rational numbers from (4). The quasicrystals obtained from these two sets differ by a parallel displacement of the duct in the incommensurate direction, or by a so-called phase shift. It is easy to verify that any r map of the graph $f_i = k_i$ $(i = 1,...,n; k_i$ are integers) is present also in the graph $f_i' = k_i$ $(i = 1,...,n; k_i$ are integers). Using this fact, we can check the validity of a statement which we shall need in Sec. 5.

If two quasicrystalline tilings correspond to equivalent sets of linear functions [in the sense of Eq. (5)], their r-atlases also coincide at all r.

5. TWO-DIMENSIONAL QUASICRYSTALS

The main result of this section is proof of the absence of local rules for a large class of quasicrystalline tilings. The main idea of this proof is the following.

Assume the numbers s and q given $(s > 0, q > 0)$ and that we have found two points $\mathbf{x}$ and $\mathbf{y}$ in a two-dimensional crystal such that the tilings of the rings $s < |\mathbf{z} - \mathbf{x}| < s + 2q$ and $s < |\mathbf{z} - \mathbf{y}| < s + 2q$ coincide, and the $(s,\mathbf{x})$ and $(s,\mathbf{y})$ maps are different. If strong r-rules exist for a certain $r < 1$, we proceed as follows: We prepare a new tiling of the plane, replacing the configuration in the $(s, \mathbf{x})$ map by the configuration of the $(s, \mathbf{y})$ map. The resultant tiling also satisfies these r-rules and is quasicrystalline, since, by assumption, the r-rules are strong. We have obtained two different quasicrystalline tilings the coincide everywhere except in a circle with center at the point $\mathbf{x}$ and with a radius s. This is impossible, and we find thus that there are no r-rules with $r < q$.

We show now how to apply these premises to prove the absence of local rules. Assume a given set of straight lines $f_i = k_i$ $(i = 1,...,n; k_i$ are integers) of a dual graph of a quasicrystalline tiling. Any three straight lines of this graph (from different sets) form a triangle when intersecting, since ternary intersections are forbidden. The equivalence transformation (5) displaces these sets of straight lines (each set has a different displacement vector) and the traingles change shape (see Fig. 4). Clearly, if all the parameters c_i in (5) are smaller in absolute value than a certain small l, only sufficiently small triangles, of size not larger than const$\cdot l$, can be restructured. Let us formulate these simple premises in the form of two statements that follow directly from (5).

a) There exists a constant C such that the equivalence transformation (5) with $|c_i| < l$ $(i = 1,...,m)$ does not restructure triangles with area larger than Cl^2.

b) if a triad of functions f_1, f_2, and f_3 is linearly indepen-

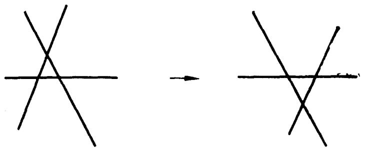

FIG. 4. Triangle restructuring under equivalence condition (5).

dent over the field Q, there exists a constant C such that under one of the two equivalence transformations (5) with $c_i \pm l$, $c_i = 0$ ($i = 2,...,m$) any (k_1, k_2, k_3) triangle of the form $f_1 = k_1, f_2 = k_2, f_3 = k_3$ and with area smaller than Cl^2 becomes restructured.

Assume now that we have found a circle with center at the point $\mathbf{x}$ and of radius r containing traingles of size smaller than l, and that all the triangles in the ring $s < |\mathbf{z} - \mathbf{x}| < s + 2q$ are much larger. In this case we can find an equivalence transformation (5) under which the triangles are restructured in the circle but not in the ring. Under this transformation, any $(s + 2q, \mathbf{x})$ map is transformed in some other map from the atlas of the same tiling. From the arguments presented above we find that there are no strong r-rules with $r < q$. Let us show how to make this heuristic reasoning rigorous.

We introduce the following definition. We saw that the three linear functions ($f_i = a_i x_1 + b_i x_2 + c_i$ ($i = 1,2,3$) meet the condition for the presence of a second intersection (the SI condition) if there exist integers n_1, n_2, and n_3 that do not vanish simultaneously and for which

$$\det \begin{vmatrix} n_1 & n_2 & n_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = 0. \tag{6}$$

This means that if for at certain c_i in (5) the three sets of the straight lines $f_i = k_i$ have one triple intersection point $\mathbf{x}$, they have also a second one $\mathbf{y}$, with $f_i(\mathbf{y}) = f_i(\mathbf{x}) + n_i$ ($i = 1,2,3$).

We can now formulate the main statement of the present section. If strong local rules exist for a quasicrystalline tiling of a plane, and the dual graph of the tiling is obtained with the aid of the linear functions f_i ($i + 1,...,n$), then the SI condition is met for any triad of functions $f_j f_k$ ($i,j,k = 1,...,n$).

To prove this we must examine how the dual-graph small triangles are distributed over the plane, and we shall find it more convenient to speak of triangles not of small size l but of small area h. Let all the sets of straight lines of the dual graph be erased except for three, see the first, second and third. Each triad of lines $f_1 = k_1$, $f_2 = k_2$, $f_3 = k_3$ produces a triangle on intersection, and all such (k_1, k_2, k_3) triangles are similar. Three situations are possible.

a) The functions f_1, f_2, and f_3 are linearly dependent on Q. In this case the lines $f_i = k_i$ ($i = 1, 2,3$: k_i are integers) form a periodic structure, and if h is small enough there are no triangles with area smaller than h at all.

b) The functions f_1, f_2, and f_3 are linearly independent of the field of Q, but they meet the SI condition. In this case the triangles with area smaller than h are distributed as shown in Fig. 5a (if h is small enough). The triangles are located at a fixed (independent of h) distance from one another. The distribution of the triangles over the plane has an average density of order $h^{1/2}$. It follows from the foregoing that the average distance between the lines on which the small triangles lie is of the order of $h^{1/2}$.

c) The SI condition is not met for the functions f_1, f_2 and f_3. In this case triangles with areas smaller than h are uniformly distributed over the plane at an approximate density $h^{1/2}$ and are far from one another (see Fig. 5b). If we introduce a function $d(h)$ equal to the minimum distance be-

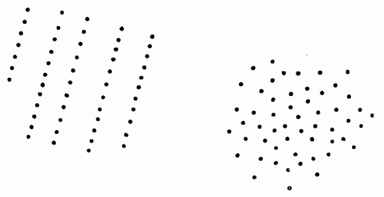

FIG. 5. Distribution of small-area triangles over a plane: a—the SI condition is met; b—the SI condition is not met.

tween triangles of area smaller than h, then $d(h)$ tends to infinity when h tends to zero. All these statements follow readily from the equation for the area of the triangle made up of the three straight lines ($a_i x_1 + b_i x_2 = c_i$ ($i = 1,2,3$):

$$S = \frac{|\Delta_{123}|^2}{2|\Delta_{12}\Delta_{23}\Delta_{31}|}, \quad \Delta_{123} = \det \begin{vmatrix} a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \\ c_1 & c_2 & c_3 \end{vmatrix},$$

$$\Delta_{ij} = \det \begin{vmatrix} a_i & a_j \\ b_i & b_j \end{vmatrix} \quad (i, j = 1, 2, 3). \tag{7}$$

Clearly, if the sets of straight lines f_i ($i = 1,...,n$) includes three for which the SI condition is not met, there are no other triangles formed by the lines of these three sets around any of the small triangles formed by the lines of the same sets. It can be verified that there exists a small triangle surrounded by a broad ring that contains no other small triangle made up by triads of the lines of the other sets. We find that if strong LR do exist, the SI condition is met for any triad of straight line.

Assume that an arbitrary qusicrystalline plane tiling exists, that it satisfies some strong local rules, and that its dual graph is described by the linear functions described by the linear functions f_i ($i = 1,...,n$). We consider first a situation when only three of the functions f_i are linearly independent on Q. If $n - 3$ we find, using the statment of Sec. 3, that the tiling of the plane is periodic. This does not hold if $n > 3$. As shown above, however, the SI condition is met by all triads of functions. If all the functions are represented as linear combinations of two, say f_1 and f_2, we obtain

$$f_i = a_i f_1 + b_i f_2 + c_i g(a_0 f_1 + b_0 f_2), \quad i = 3, \ldots, n. \tag{8}$$

Here a_i, b_i, and c_i are rational numbers, different for each i; a_0 and b_0 are rational numbers and are equal at all values of i, g is not rational and does not depend on i. It can be verified, by the method used to prove the statement of Sec. 3, that for any arbitrarily large r it is possible to find a sufficiently small vicinity of the number g such that the r-atlases of all the quasicrystals (8) with fixed a_i,b_i,c_i,a_0 and b_0, and with arbitrary g that vary in this vicinity coincide. This means that there are no strong local rules.

Let the number of linearly independent functions exceed three. We choose four of them and designate them f_1, f_2, f_3, f_4. As shown above, the SI condition is met for any three out of these four functions. We write down this condition by representing f_3 and f_4 (apart from a constant) as linear combinations of f_1 and f_2 with real coefficients:

$$f_3 = af_1 + bf_2 + \text{const}, \qquad f_4 = cf_1 + df_2 + \text{const}. \tag{9}$$

We write down the SI conditions for the four triads (1,2,3), (1,2,4), (1,3,4), (2,3,4) in the form (6), introducing four triads of integers (n_1, n_2, n_3), (m_1, m_2, m_3), (p_1, p_2, p_3), (q_1, q_2, q_3):

$$\det\begin{vmatrix}1 & 0 & n_1\\ 0 & 1 & n_2\\ a & b & n_3\end{vmatrix}=0,\quad \det\begin{vmatrix}1 & 0 & m_1\\ 0 & 1 & m_2\\ c & d & m_3\end{vmatrix}=0,$$
$$\det\begin{vmatrix}1 & 0 & p_1\\ a & b & p_2\\ c & d & p_3\end{vmatrix}=0,\quad \det\begin{vmatrix}1 & 0 & q_1\\ a & b & q_2\\ c & d & q_3\end{vmatrix}=0. \tag{10}$$

We obtain a system of four equations for a, b, c, and d. It is easy to verify that its solutions are of the form

$$a=a'+a''D^{1/2},\quad b=b'+b''D^{1/2},\quad c=c'+c''D^{1/2},\quad d=d'+d''D^{1/2}, \tag{11}$$

$a', a'', b', b'', c', c'', d', d''$ are rational numbers and D is an integer. Quadratic irrational numbers of type (11) form a field designated $Q[D^{1/2}]$. It is easy to verify that not only f_2 and f_1 but also all the remaining ($i = 5,...,n$) are expressed in terms of f_1 and f_2 with coefficients $Q[D^{1/2}]$ (with the same D). This yields the following final result:

If strong local rules exist for a quasicrystalline tiling of a plane, the number of functions that are independent on the field Q can be equal to: a) two for a periodic tiling, b) four for a tiling constructed with the aid of quadratic irrational numbers. In this case it is possible to find in the set f_i ($i = 1,...,n$) two functions in terms of which all other can be expressed, with coefficient from $Q[D^{1/2}]$.

These results can be applied to quasicrystalline tilings with symmetry of order P. It is easy to verify that quadratic irrational values are obtained only for $P = 5,10$ ($Q[5^{1/2}]$), $P = 8$ ($Q[2^{1/2}]$ and $P = 12$ ($Q[3^{1/2}]$), and that at $P = 3$, 4, and 6 the structure is periodic. We find that there are no strong local rules for $P = 7$, 9, and 11 and for all P larger than 12. As for the strong local rules for the quadratic irrational values, this is apparently quite a difficult problem. The general situation has not been studied, and there only a few results for symmetric tilings. The existence of strong LR for $P = 5$ and 10 was proved in Ref. 6. It was proved in Ref. 9 that there are no strong LR for $P = 8$. No answer is known for $P = 12$.

6. TWO-DIMENSIONAL QUASICRYSTALS WITH QUADRATIC IRRATIONAL NUMBERS

The main task of this section is to prove the existence of weak local rules for quasicrystalline tilings of a plane with quadratic irrational numbers (see the preceding section). The local rules that we shall consider are very easy to define—they constitute the r-atlas of the quasicrystal for some sufficiently large r.

We take first an arbitrary quasicrystal. After fixing a large number r, we find the r-atlas of this quasicrystal and take it to be the LR. We shall need some properties of tilings with such LR. We draw the dual graph of a tiling that satisfies these LR. If r is large enough, one can find for each line of the graph a map on which is shown this line itself and two neighboring lines from the same set. Therefore the number of lines of each set in a dual graph of a tiling is infinite and they can be assigned integer numbers. We take to sets of graph lines, say the first and the second, and deform the graph in such a way that these lines are transformed into straight lines $x_1 = k_1$, $x_2 = k_2$ (k_1, k_2 are integers), and the topology of the intersections remains unchanged. For the dual graph of the initial quasicrystalline tiling this deformation can be carried out in such a way that the lines of all the remaining sets also become straight, $f_i = k_i$ (f_i are certain linear functions, k_i are integers, $i = 3, .., n$). The lines of the ith set of the dual graph of an arbitrary tiling ($i > 2$) need not necessarily become straight after this deformation. If, however, the tiling satisfies the indicated r-rules for a sufficiently large r, it can be stated that the slopes of the lines of the ith set, relative to the lattice of the lines of the first two sets, will be close to the slope of the straight lines of the ith set of the dual graph of the quasicrystal. In fact, given the r-rules, the slope is fixed apart from edge effects on boundary of the map, and since the size of the map is of the order of r, the accuracy with which the r-rules determine the slope is of the order of const/r.

This is true for an arbitrary quasicrystal, and not only for a quasicrystal with quadratic irrational values. We shall see that if the quasicrystal meets the conditions of item b) of the statement of the preceding section (four functions independent on Q and quadratic irrational numbers), then the lift of the tiling satisfying the LR differs by not more than a constant from the two-dimensional subspace of the spare R^n along which the lift of the initial quasicrystalline tiling proceeds.

In other words, the following statment is valid:

Let the quasicrystal be such that: a) the linear functions that give the dual graph of the tiling include four that are linearly independent on Q; b) it is possible to find among them two functions in terms of which the remaining ones are linearly expressed with coefficients from the field $Q[D^{1/2}]$. Weak local rules exist then in this case.

The idea of the proof can be briefly described as follows: We deform the dual graph in such a way that the first two sets become rectified, and we consider the rise W of this graph. We neglect for the time being the discontinuity of W and assume that the components of the rise W_i ($i = 1,...,n$) are smooth functions locally close to linear. The first two components of this lift are globablly close to linear functions, i.e., they differ from linear functions by not more than a constant. We consider W in a region whose size is large compared with the distance between the lines of the sets of the graph, but small compared with the scale over which the deviation of W_i from linear function manifests itself (as shown above, this scale is large if the radius of the rules is large enough). The function W can be replaced in ths region by a linear one. For each triad of functions W_i, W_j, W_h we can write an SI condition. If $n > 3$, these conditions determine completely the linearized functions W_i, leaving no leeway whatsoever. We find that the derivatives of W_i are constants, and the functions themselves are linear and therefore are equal to f_i ($i = 3,...,n$) to within a constant. Of course, the functions W_i are neither continuous nor, all the more, smoothly varying in the strict sense of the word. The proof requires therefore a more accurate analysis, which will be reported elsewhere.

7. THREE-DIMENSIONAL QUASICRYSTALS

A few words concerning the quasicrystalline tilings of a three-dimensional space. The dual graph of an arbitrary tiling of a three-dimensional space consists of a set of two-dimensional surfaces, and for a quasicrystal it consists of a set of parallel planes. All the arguments used to prove the statements of Sec. 5 can obviously be applied to the three-dimensional case, where the second-intersection condition for triads of straight lines is replaced by a second-intersection condition for tetrads of planes. We can say that the SI condition is met for the four linear functions $f_i = a_i x_1 + b_i x_2 + c_i x_3$ ($i = 1, 2, 3, 4$) in space if we can find integers n_i ($i = 1,2,3,4$), such that

$$\det \begin{vmatrix} a_1 & b_1 & c_1 & n_1 \\ a_2 & b_2 & c_2 & n_2 \\ a_3 & b_3 & c_3 & n_3 \\ a_4 & b_4 & c_4 & n_4 \end{vmatrix} = 0. \quad (12)$$

Repeating the arguments of Sec. 5 with allowance for this substitution, we verify that the following statement is true: if strong local rules exist for a three-dimensional quasicrystal, the SI condition (12) is met for any four sets of planes of its dual graph.

It is more difficult to obtain an analog of the statement of Sec. 6. It must be borne in mind that the set of tetrads of integers n_i ($i = 1,...,4$) satisfying (12) can be one-, two-, or three-dimensional. Accordingly, we can introduce conditions SI-1, SI-2, and SI-3. A complete analysis of all the ensuing possibilities is quite complicated. We point out only several obvious solutions. Let all the SI conditions be the SI-3 conditions. In this case we are dealing with a commensurate periodic structure. A case of quadratic irrational numbers is also posssible, a characteristic example of which is a quasicrysal with icosahedral symmetry. If, finally, only conditions SI-1 obtain, the solution comprises the cubic irrational numbers $a + bD^{1/3} + cD^{2/3}$. Some combined variants are apparently also possible.

We consider now in greater deail an icosahedral quasicrystal and show that the statement of Sec. 6 leads to the existence of weak local rules for this crystal. Let $\mathbf{e}_i$ ($i = 1.,,,.6$) be unit vectors directed along the symmetry axes of the icosahedron. The dual graph of the quasicrystalline tiling consists of six weeks of planes $(\mathbf{e}_i, \mathbf{x}) = c_i + k_i$ ($\mathbf{x} = (x_1, x_2, x_3)$; $i = 1,...,6$; k_i are arbitrary integers). We choose an r-atlas of this graph with sufficiently large r and take it to constitute the local rules. We consider an arbitrary tiling or, more accurately, a dual graph of an arbitrary tiling, for which these rules are satisfied. We deform this graph in such a way that three sets of two-dimensional surfaces become rectified and coincide with the three sets of parallel plane of the dual graph of the initial quasicrystal (to be specific, we shall refer to the first, second and third sets corresponding to the vectors $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$). We choose any one of the obtained planes, say $(\mathbf{e}_1, \mathbf{x}) = c_1$, and examine the lines of intersection of this plane with other surfaces of the graph. We obtain five sets of lines on the chosen plane. We note now that the three-dimensional r-rules induced two-dimensional r-rules on this plane and the latter, obviously, coincide with the rules for some two-dimensional quasicrystal and fivefold symmetry. For this quasicrystal, the number of functions independent on the field of Q is four, and all the irrationalities are contained in the quadratic field $Q[5^{1/2}]$. From the statement of Sec. 6 follows the existence of weak local rules. Since two out of the five sets of lines have already been rectified, it follows from the existence of LR that the remaining sets are also almost rectified, i.e., they deviate from the straight lines of the quasicrystal by not more than a constant. This means that the rise of the graph of our tiling differs from the rise of the graph of the quasicrystal by an amount that depends only on the coordinate along the vector $\mathbf{e}_1$. We note that we neglect everywhere, without additional stipulations, functions that are bounded in all of three-dimensional space. Thus, if the rise of the quasicrystal is equal to $(f_1, f_2, f_3, f_4, f_5, f_6)$, where $f_1 = (\mathbf{e}_1, \mathbf{x})$, and the rise of the tiling considered by us is equal to $(W_1, W_2, W_3, W_4, W_5, W_6)$, where $W_i = f_i$ ($i = 1,2,3$), are functions of the projection $f_1(\mathbf{x})$ of $\mathbf{x}$ on the vector $\mathbf{e}_1$. If we choose the plane $(\mathbf{e}_2, \mathbf{x}) = c_2$ in place of $(\mathbf{e}_1, \mathbf{x}) = c_1$ and repeat fully all the arguments, it turns out that the quantities ($i = 4,5,6$) depend only on $f_2(\mathbf{x})$. Comparing these two results, we find that $W_i = f_i$ ($i = 1,...,6$) apart from a bounded function. The existence of weak LR for an icosahedral quasicrystal is thus proved.

8. CONCLUSION

Our results show that quasicrystal with quadratic irrational numbers are "good" from the physical point of view. Their quasiperiodic structure can be fully specified by describing a finite set of maps of fixed radius. By proving the existence of weak LR for quasicrystals with quadratic irrational numbers we have actually constructed a certain Hamiltonian with a finite interaction radius between parallelograms, for which a configuration with minimum energy is a quasicrystal. In fact, assume that certain r-rules are specified. We consider a Hamiltonian with a finite interaction radius, in accord with which the configurations with radii smaller than r, contained in the r-rules, have zero energy, while the remaining ones with the same radius have a large positive energy. We have proved that any structure with a minimal energy is close to a quasicrystal. Moreover, it can be shown that, for quasicrystals with unity codimensionality, one Hamiltonian with such properties cannot have a finite interaction radius. This means that no local interaction between the parallelograms can stabilize an incommensurate quasicrystalline structure of this type. Although a proof of this statement exists only for quasicrystals with unity codimensionality, its connection with the general property of having no local rules is understood. It appears that no such Hamiltonians exist in all cases when there are no local rules.

We conclude by pointing out certain questions that call for further research. First is a complete analysis of three-dimensional LR conditions and the study of the situation with weak LR in three-dimensional space (the analogs of the statements of Sec. 6). Second, it would be of interest to generalize the constructions of Penrose and of de Bruijn (inflation-deflation procedure) to include the case of arbitrary quadratic irrationalities and to ascertain for which quasicrystals with quadratic irrational numbers do strong local rules exist.

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