

# Topological restrictions on quasicrystals

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A study is made of whether there can exist quasicrystals described by continuous multidimensional structures. The conditions necessary for the existence of such quasicrystals are derived. A model is proposed for the case of icosahedral symmetry. It is shown also that two-dimensional quasicrystals with the symmetry of a rectangle cannot be described by a continuous structure.

## 1. INTRODUCTION

Quasicrystals, like other incommensurate phases, can be described by periodic structures in a space with dimensions exceeding 3 (Refs. 1–4). These structures may be continuous or discontinuous. Both cases are encountered in, for example, the Frenkel–Kontorova model.<sup>5</sup> The Hamiltonian of this model is

$$H^\omega = \sum_n \frac{1}{2} (x_{n+1} - x_n - \alpha)^2 + \lambda \cos\left(\frac{2\pi\omega}{\alpha} x_n\right). \quad (1.1)$$

Here  $x_n$  are the coordinates of the atoms,  $\omega > 1$  is an irrational number describing the quasiperiodicity, and  $\lambda$  is a coefficient which governs the coupling constant. The ground state in this model is periodic if  $\lambda = 0$ :

$$x_n^0 = \alpha(n+c), \quad (1.2)$$

whereas for small values of  $\lambda$  there is a small perturbation of the state:

$$x_n^\lambda = x_n^0 + (\lambda\pi\omega/\alpha) \sin(2\pi\omega(n+c)) + O(\lambda^2). \quad (1.3)$$

On the other hand, in the limit  $\lambda \rightarrow \infty$  the particles are concentrated at minima of the periodic potential:

$$x_n^\infty = \frac{\alpha}{\omega} \left( \frac{1}{2} + [\omega(n+c)] \right) \quad (1.4)$$

(here  $[x]$  denotes an integral part of  $x$ ). The two limiting cases are described by

$$x_n^\lambda = \alpha(n+c) + f_\lambda(\omega(n+c)), \quad (1.5)$$

where  $f_\lambda$  is a periodic function with the period 1. At low values of  $\lambda$  this function is continuous (and, moreover, smooth):

$$f_\lambda(x) = \frac{\lambda\pi\omega}{\alpha} \sin(2\pi x) + O(\lambda^2), \quad (1.6)$$

whereas at high values of  $\lambda$  it is discontinuous:

$$f_\lambda(x) = \frac{\alpha}{\omega} (\frac{1}{2} - \{x\}) + O(\lambda^2) \quad (1.7)$$

(where  $\{x\}$  describes a fractional part of  $x$ ). Therefore, Eq. (1.5) represents the ground state of  $H^\omega$  for different values of  $\lambda$  if we select  $f_\lambda(x)$  in an appropriate manner.

We shall now find the same state somewhat differently. An equation

$$x = \alpha(n+y) + f_\lambda(\omega(n+y)), \quad (1.8)$$

in which  $n$  is an integer, describes a family of curves on a  $(x,y)$  plane. Selection of this family by a straight line  $y = c$  gives the positions of the atoms which are the same as in Eq. (1.5). On the other hand, such a family of curves transforms into itself as a result of translation by vectors  $(\alpha/\omega, 1/\omega)$  and  $(0, 1)$ . Therefore, the plane  $(x,y)$  can be factored in terms of these translations, the result of which is that Eq. (1.8) describes a curve on a two-dimensional torus  $T^2$ . This curve is continuous for small values of  $\lambda$  and discontinuous for large values. There is a critical value of  $\lambda$  corresponding to the loss of smoothness, investigated by Aubry *et al.*<sup>6,7</sup>

In general, quasicrystals differ from the above model only by a special symmetry (icosahedral or pentagonal), which determines the incommensurability. Therefore, quasicrystals could still be described by periodic structures in a space of higher dimensions. In all the models proposed so far such structures resemble that shown in Fig. 1b, i.e., they are discontinuous. It is reasonable to ask whether a model with a continuous structure similar to that shown in Fig. 1a can be constructed. It has been suggested that this is impossible because of the special symmetry restrictions which forbid continuous structures.<sup>8</sup> However, we shall show that a continuous model of a quasicrystal does exist and we shall find the conditions for the existence of such a model.

## 2. OVERALL PROBLEM

We consider a given quasiperiodic structure in  $d$ -dimensional space with  $d'$  incommensurate frequencies. This structure is described by a family of  $d'$ -dimensional surfaces  $\{s_i\}$  which are distributed periodically in a  $D$ -dimensional space  $R^D$ , where  $D = d + d'$ . The positions of atoms in a real space are given by the points of intersection of the surfaces

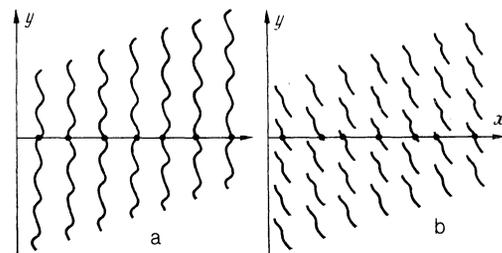


FIG. 1. a) Continuous model of a one-dimensional quasicrystal; b) model of a one-dimensional quasicrystal with discontinuous "atomic surfaces."

$\{s_i\}$  and a  $d$ -dimensional subspace  $R^d$  which is called the physical space. The dimensionality of  $d$  can be arbitrary (and not only 1, 2, or 3), because this does not affect the results of the present section.

Let us find more details of the proposed structure. We assume that  $L$  is a lattice of periods of a periodic structure in  $R^D$ . Since  $L$  contains all the translations conserving this structure, its dimensionality is  $D$ . The space  $R^D$  is a direct sum of the two subspaces  $V$  and  $V'$ :  $R^D = V \oplus V'$ . The "direction" of the  $d$ -dimensional space  $V$  determines the embedding of the physical space, whereas the  $d'$ -dimensional space  $V'$  describes the phason degrees of freedom, like the  $y$  axis in Fig. 1. We introduce coordinates in  $R^D$  in the form of a pair  $(\mathbf{x}, \mathbf{y})$ , where  $\mathbf{x} \in V$  and  $\mathbf{y} \in V'$ .

Consider an arbitrary vector  $\mathbf{a} \in V'$ . A hyperplane  $V_{\mathbf{a}}$ , obtained by a shift of  $V$  by a vector  $\mathbf{a}$ , can also be regarded as the physical space because embedding of  $V$  in  $R^D$  is completely incommensurate. The positions of the atoms are still given by the points of intersection of the system of surfaces  $\{s_i\}$  with  $V_{\mathbf{a}}$ . Moreover, real atoms cannot approach each other without any restrictions, so that the system  $\{s_i\}$  must obey an additional condition that in any section of  $V_{\mathbf{a}}$  there should be no points belonging to  $\{s_i\}$  or located near a certain value of  $h$  (which is the diameter of a "hard core").

This condition is well satisfied by both continuous and discontinuous  $\{s_i\}$  surfaces. We assume, however, that these surfaces are continuous, i.e., that they resemble that shown in Fig. 1a. This condition imposes more serious restrictions on  $\{s_i\}$ . In fact, since continuous variation of  $\mathbf{a}$  now corresponds to a continuous motion of atoms in the section  $V_{\mathbf{a}}$ , it is possible to bring in correspondence only one sheet of the  $V'$  family with a given atom. The one-to-one nature of this correspondence is ensured by the fact that  $V'$  is singly connected. Moreover, this sheet must be projected on  $V'$  in one-to-one manner without folds. This means that for each atom there is a corresponding function  $\mathbf{f}_i: V' \rightarrow V$ , for which this sheet is the graph. The "hard core" condition means in this language that for any value  $\mathbf{y} \in V'$  and any atoms  $i$  and  $j$ , we have

$$|\mathbf{f}_i(\mathbf{y}) - \mathbf{f}_j(\mathbf{y})| > h. \quad (2.1)$$

It should be noted that these restrictions correspond to the conditions 0, 1, 2, 3, and 4 in Ref. 8. Later we show that nontrivial consequences follow from these conditions and a study of these consequences is the aim of the present paper.

Consider just one sheet from the family  $\{s_i\}$  and denote this sheet by  $s$ . We can show (see Ref. 8) that the translation from  $L$  which conserves  $s$  creates a  $d'$ -dimensional sublattice  $L$  which we denote by  $l[s]$ . Then, the  $d'$ -dimensional subspace  $r[s]$  spanned by the  $l[s]$  lattice represents the "average slope" of the sheet  $s$ . More precisely, this means that there is a positive  $\delta$  such that any point on the surface  $s$  is separated from  $r[s]$  by no more than  $\delta$  (which is a direct consequence of the condition on continuity). Naturally, in the case of two parallel sheets  $s_1$  and  $s_2$  the sublattices  $l[s_1]$  and  $l[s_2]$  coincide in the same way as the subspaces  $r[s_1]$  and  $r[s_2]$ .

These structures can be understood better by considering an example from the Introduction. The family of the curves described by (1.8) is labeled by an index  $n$ . Translation from the lattice  $L$  acts on  $n$  as follows:

$$\begin{aligned} (\alpha/\omega, 1/\omega): n \rightarrow n, \\ (0, 1): n \rightarrow n+1. \end{aligned} \quad (2.2)$$

Hence, we can see that the translations  $(\alpha/\omega, 1/\omega)$  form a one-dimensional sublattice  $l[s]$ , where  $s$  denotes any of the curves described by Eq. (1.8). The subspace  $r[s]$  is the straight line  $x = \alpha y$ .

### 3. CONDITIONS FOR A NONTRANSVERSE STRUCTURE ( $d=d'$ )

The conclusions reached in the preceding section apply to all incommensurate structures. We concentrate our attention on the case when the dimensionality of the phason space  $d'$  is identical with the dimensionality of the physical space  $d$  (as is true of all real quasicrystals). We shall show that continuous atomic surfaces introduced in the preceding section exist only if the subspaces  $r[s]$  are nontransverse.

Consider two atomic surfaces  $s_1$  and  $s_2$  and find their sublattices  $l_1 = l[s_1]$  and  $l_2 = l[s_2]$ . We assume that these sublattices do not share any translations except for the zeroth. Then, their sum  $l_1 + l_2$  is a lattice of dimensionality  $2d' = D$ . For this reason the sum of the subspaces  $r[s_1] \oplus r[s_2]$  also has the dimensionality  $D$ . Consequently,  $r[s_1]$  and  $r[s_2]$  are transverse and they intersect at just one point.

The atomic surfaces  $s_1$  and  $s_2$  are close to the subspaces  $r[s_1]$  and  $r[s_2]$  (in the sense defined in Sec. 2). For this reason the surfaces  $s_1$  and  $s_2$  can be derived by a continuous uniformly confined deformation  $r[s_1]$  and  $r[s_2]$  (homotopy). Since intersection of two transverse submanifolds is topologically irremovable (see Ref. 9, Part 2, p. 522), we can see that the surfaces  $s_1$  and  $s_2$  must intersect. However, the existence of such an intersection is in conflict with the "hard core" condition. In fact, if  $\mathbf{a}$  assumes the value of the phason coordinate of the point of intersection, the separation between two atoms in the section  $V_{\mathbf{a}}$  vanishes. Hence we can conclude that the assumption about the absence of nonzero general translations of the sublattices  $l[s_1]$  and  $l[s_2]$  is in conflict with the conditions of continuity of the atomic surfaces.

This yields the necessary conditions for the existence of continuous nonintersecting atomic surfaces: *for any two atomic surfaces  $s_1$  and  $s_2$  an intersection of the corresponding sublattices  $l[s_1]$  and  $l[s_2]$  contains a nonzero sublattice*. Since this condition is very important in the subsequent treatment, we consider it in greater detail and show that if it is satisfied, there are no topological reasons why atomic surfaces should intersect.

Denote the common vector of the sublattices  $l[s_1]$  and  $l[s_2]$  by the letter  $\mathbf{z}$ . Since the spaces  $r[s_1]$  and  $r[s_2]$  also contain the vector  $\mathbf{z}$ , their sum  $r[s_1] \oplus r[s_2]$  has the dimensionality less than  $2d = D$ . Therefore, there is a vector  $\mathbf{g} \in R^D$  which does not belong to  $r[s_1]$  and  $r[s_2]$ . Let  $\delta$  be the maximum distance from the surfaces  $s_1$  and  $s_2$  to the corresponding subspaces  $r[s_1]$  and  $r[s_2]$  (see Sec. 2). Since displacement of the subspace  $r[s_1]$  by  $\mathbf{g}$  converts it into a hyperplane which does not intersect with  $r[s_2]$ , there is a minimum distance between this hyperplane and  $r[s_2]$ . If the vector  $\mathbf{g}$  is increased the required number of times, we can make this distance greater than  $2\delta$ . We can easily see that after such translation the surface  $s_1$  does not intersect  $s_2$ .

We can see that, in general, the condition of nontrans-

versality is not only necessary, but also sufficient for existence of nonintersecting continuous atomic surfaces. However, the additional symmetry of these surfaces may prevent suppression of intersections. We should consider this obstacle separately, because the symmetry group of real quasicrystals is very "rich."

We shall assume that our periodic system of surfaces  $\{s_i\}$  is invariant relative to a  $D$ -dimensional space symmetry group  $H$  acting on  $R^D$ :

$$h: x \rightarrow g(x) + \mathbf{a}_g, \quad \mathbf{a}_g \in R^D, \quad g \in G, \quad h \in H, \quad (3.1)$$

where  $G$  is a given point symmetry group  $R^D$ . Since a translation by  $L$  leaves  $\{s_i\}$  unaffected, the vector  $\mathbf{a}_g$  is defined only modulo  $L$ . In particular, the vector  $\mathbf{a}_E$  corresponding to a unit element  $E$  from the group  $G$  is contained by  $L$ .

The transformation of Eq. (3.1) applies also to atomic surfaces. We shall select for two given sheets  $s_1$  and  $s_2$  an element  $h$  of Eq. (3.1) so that

$$s_2 = h(s_1). \quad (3.2)$$

Then, in the case of sublattices  $l_1 = l[s_1]$  and  $l_2 = l[s_2]$ , we have

$$l_2 = g(l_1). \quad (3.3)$$

Thus, the action of the space group  $H$  on atomic surfaces creates the action of the point  $G$  on the corresponding sublattices. This may be useful later because the set of sublattices  $l[s_i]$  looks much simpler than  $\{s_i\}$ . First of all, we have a finite number of sublattices. This is due to the fact that two surfaces which transform into one another as a result of translation from  $L$  are characterized by the same sublattice. Therefore, we need consider only the surfaces intersecting a given unit cell; we shall find a finite number of these because of the "hard core" condition.

We have therefore to answer the following question: can there be finite sets of sublattices  $l[s_i]$  which are invariant under the action  $G$  and such that any pair of sublattices contains a shared nonzero translation? We shall tackle this question in Sec. 4 in the case of two point symmetry groups of quasicrystals (icosahedral and pentagonal). We shall show that in the case of the icosahedral group the required sublattice sets do exist, but not in the case of the pentagonal group. In Sec. 5 we shall use these sets to derive a model of an icosahedral quasicrystal with continuous atomic surfaces.

#### 4. ICOSAHEDRAL AND PENTAGONAL SYMMETRIES

We first consider the case of an icosahedral quasicrystal. The corresponding  $D$ -dimensional ( $D = 6$ ) structure with a  $d$ -dimensional embedding of the physical space ( $d = 3$ ) has been discussed on many occasions (see, for example, Refs. 2-4). We recall that the fundamental vectors of the lattice of  $L$  translations in  $R^6$  are selected in the structure so that when projected on the physical space they form vectors directed from the center to the vertices of a regular icosahedron. We determine explicitly the set of three-dimensional sublattices of the lattice  $L$ , which will be shown to satisfy the condition of transversality formulated in Sec. 3.

We assume that the vector triplet  $[\mathbf{e}_\alpha, \mathbf{e}_\beta, \mathbf{e}_\gamma]$  ( $\alpha, \beta, \gamma = 1..6$ ) from the basis of  $L$  is such that their projections (possibly with reversal of the sign for some of them) onto the physical space form vectors directed to the vertices of one

face of the icosahedron. We can easily show that sets of such triplets are invariant under the action of the symmetry group  $Y$  of the icosahedron or on the vectors  $\mathbf{e}_\alpha, \mathbf{e}_\beta$ , and  $\mathbf{e}_\gamma$ . Therefore, the set of sublattices of the lattice  $L$  spanned by these triplets

$$l[\alpha, \beta, \gamma] = z_1 \mathbf{e}_\alpha + z_2 \mathbf{e}_\beta + z_3 \mathbf{e}_\gamma, \quad z_i \in Z, \quad (4.1)$$

is invariant under the action  $Y$ . It remains to show that any pair of such sublattices contains a nonzero shared translation. However, a simple examination of all the variants shows that if two triplets  $[\mathbf{e}_\lambda, \mathbf{e}_\mu, \mathbf{e}_\nu]$  and  $[\mathbf{e}_\alpha, \mathbf{e}_\beta, \mathbf{e}_\gamma]$  are related by a symmetry transformation from  $Y$ , they include two vectors which are identical apart from the sign (Fig. 2). These vectors obviously belong to  $l[\alpha, \beta, \gamma]$  and  $l[\lambda, \mu, \nu]$ , i.e., these two sublattices have a shared nonzero vector.

Our results thus show that the icosahedral symmetry does not prevent satisfaction of the necessary condition from Sec. 3. However, it does not guarantee that the resultant sublattices have any nonintersecting atomic planes. A more detailed analysis shows that this depends on the space symmetry group of the structure in  $R^6$ . However, we shall consider the example of nonintersecting atomic planes only for the case of symmorphic space groups without inversion.

We now consider the symmetry of a pentagon ( $D = 4$  and  $d = 2$ ) and show that in this case the nontransversality condition cannot be satisfied. The symmetry group of a pentagon is generated by one element  $A$  and one relationship  $A^5 = E$  ( $E$  is a unit element). The four-dimensional space  $R^4$  separates into a direct sum of two-dimensional subspaces  $V$  and  $V'$ :  $R^4 = V \oplus V'$ . The action of the symmetry group on them is as follows: a)  $V$  and  $V'$  are invariant; b)  $A$  acts on  $V$  by rotation through an angle  $2\pi/5$  and on  $V'$  by rotation by an angle  $4\pi/5$ .

We assume that there is a symmetric system of atomic planes  $\{s_i\}$  such that the  $l[s_i]$  lattices are nontransverse. We shall consider the corresponding subspaces  $r[s_i]$  discussed in Sec. 2. This will be done by introducing coordinates in  $R^4$  in the form of a pair  $(\mathbf{x}, \mathbf{y})$ , where  $\mathbf{x} \in V$  and  $\mathbf{y} \in V'$ . Since  $s_i$  are projected in a one-to-one manner on  $V'$ , it follows that  $r[s_i]$  are also projected on  $V'$  in the same manner. Therefore, the coordinates of a set of points  $r[s_i]$  can be

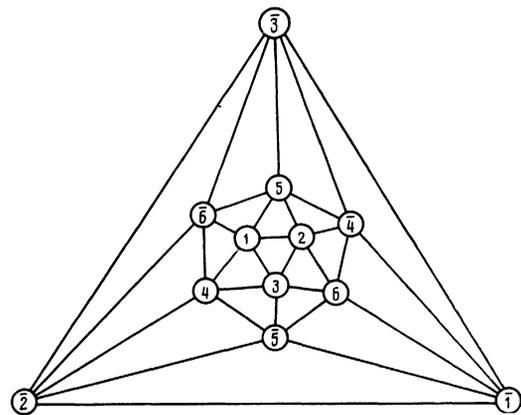


FIG. 2. Vertices and edges of an icosahedron shown in the form of a plane picture. The end of a fundamental vector  $\mathbf{e}_i$  from a lattice  $L$  is projected onto the vertex  $i$ , whereas the end of  $-\mathbf{e}_i$  is projected onto the vertex  $\bar{i}$ .

written as follows:

$$(B_i(\mathbf{y}), \mathbf{y}), \quad (4.2)$$

where  $B_i$  is a linear operator for conversion of  $V'$  to  $V$ . In other words,  $r[s_i]$  is a graph of the equation  $\mathbf{x} = B_i(\mathbf{y})$ , which relates the vectors  $\mathbf{x}$  and  $\mathbf{y}$ .

We now consider a sheet  $s_1$ . The corresponding matrix  $B_1$  can be written in terms of the orthogonal coordinates  $V$  and  $V'$ :

$$B_1 = \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \quad (3)$$

The subspace  $r[A(s_i)]$  obtained from  $r[s_1]$  by the transformation of  $A$  is described by

$$\mathbf{x} = B_1'(\mathbf{y}), \quad B_1' = C^{-1}B_1D. \quad (4.4)$$

Here,  $C$  is the matrix representing rotation in the  $V$  space by the angle  $2\pi/5$ , and  $D$  is the matrix describing rotation in  $V'$  by the angle  $4\pi/5$ .

We now write down the condition of nontransversality with the aid of the matrices  $B_1$  and  $B_1'$ . The nontransverse nature of  $r[A(s_i)]$  and  $r[s_1]$  means that there is a vector  $\mathbf{y} \neq 0$  in  $V'$  such that the points  $[B_1(\mathbf{y}), \mathbf{y}]$  and  $[B_1'(\mathbf{y}), \mathbf{y}]$  coincide, i.e.,

$$B_1(\mathbf{y}) = B_1'(\mathbf{y}). \quad (4.5)$$

This can be written in the form of the condition on the matrices:

$$\det(B_1 - B_1') = 0. \quad (4.6)$$

Bearing in mind that in terms of the orthogonal coordinates  $D = C^2$ , we obtain

$$\det(B_1 - C^{-1}B_1C^2) = 0, \quad (4.7)$$

where  $B_1$  is given by Eq. (4.3) and  $C$  is the matrix of rotation by  $2\pi/5$ . We shall introduce a new basis  $(1+i, 1-i)$  in which the matrix  $C$  is diagonal:

$$C = \begin{pmatrix} \varepsilon & 0 \\ 0 & \bar{\varepsilon} \end{pmatrix}, \quad B_1 = \begin{pmatrix} p & q \\ \bar{q} & \bar{p} \end{pmatrix}, \quad (4.8)$$

where

$$p = (a+d+i(b-c))/2, \quad q = (a-d+i(b+c))/2,$$

$\varepsilon = \exp(2\pi i/5)$ , and the bar represents complex conjugates. Equation (4.6) becomes

$$\det \begin{pmatrix} (\varepsilon-1)p & (\varepsilon^{-3}-1)q \\ (\varepsilon^3-1)\bar{q} & (\varepsilon^{-1}-1)\bar{p} \end{pmatrix} = 0 \quad (4.9)$$

or

$$|(\varepsilon-1)p|^2 = |(\varepsilon^3-1)q|^2. \quad (4.10)$$

By analogy with the transformation  $A$ , an element  $A^2$  creates a subspace

$$\mathbf{x} = B_1''(\mathbf{y}), \quad (4.11)$$

where  $B_1'' = C^{-2}B_1C^4$ . The conditions of nontransversality of the subspace and of the subspaces  $\mathbf{x} = B_1(\mathbf{y})$  can also be written in the form of Eq. (4.10):

$$|(\varepsilon^2-1)p|^2 = |(\varepsilon^{-6}-1)q|^2. \quad (4.12)$$

We shall now compare Eqs. (4.10) and (4.12) bearing in mind that  $\varepsilon^6 = \varepsilon$ ,  $\varepsilon^{-3} = \varepsilon^2$  and  $\varepsilon^{-1} = \bar{\varepsilon}$ . Since  $|\varepsilon^2 - 1| \neq |\varepsilon - 1|$ ,  $p$  and  $q$  vanish in Eq. (4.8). It then follows from Eq. (4.8) that  $a$ ,  $b$ ,  $c$ , and  $d$  all vanish, i.e., that the subspace  $r[s_1]$  coincides with  $V'$ . It follows that the sublattice  $l[s_1]$  belongs to the subspace  $V'$ . However, this lattice must transform into itself as a result of rotation by  $72^\circ$  (as an intersection of  $L$  and  $V'$  conserved under the action of the symmetry group of the pentagon). This is clearly impossible because the symmetry group of the pentagon is not crystallographic.

We have thus shown that quasicrystals with pentagonal symmetry cannot be described by continuous atomic surfaces.

## 5. EXAMPLE OF CONTINUOUS ATOMIC PLANES

In this section we use the nontransverse subspaces constructed above to derive an example of continuous atomic planes satisfying the "hard core" condition in the icosahedral symmetry. We first determine the spatial symmetry group. It will be assumed to be symmorphic with the simple cubic six-dimensional Bravais lattice (SC) and a point symmetry group of the icosahedron without inversion ( $Y$ ).<sup>10</sup> Therefore, the system of atomic surfaces which we construct should be invariant under transformations of the type

$$\mathbf{x} \rightarrow g(\mathbf{x}) + \mathbf{a}, \quad g \in G, \quad \mathbf{a} \in L, \quad (5.1)$$

$$G = Y, \quad L = \text{SC}.$$

In other words, in Eq. (3.1) we have  $\mathbf{a}_g = 0 \pmod L$ .

A set of sublattices  $l[\alpha, \beta, \gamma]$  of the lattice  $L$ , transforming into itself under the interaction of the group  $Y$  and satisfying the nontransversality condition from Sec. 2, is derived in Sec. 4. The corresponding three-dimensional subspaces  $r[\alpha, \beta, \gamma]$  intersect in pairs along straight lines or along planes. Our aim is to deform the subspaces  $r[\alpha, \beta, \gamma]$  in such a way as to remove all the intersections and obtain a system of atomic surfaces that retains the symmetry under the action of the group  $Y$  and the periodicity. We carry out this deformation in two stages. We first try to remove mutual intersections  $r[\alpha, \beta, \gamma]$  by parallel translation. We shall see that this can remove a considerable proportion, but not all the intersections. The remaining small fraction be removed during the second stage by slight bending of the surfaces obtained in the first stage.

### First stage

We note first of all that the family of subspaces  $r[\alpha, \beta, \gamma]$  consists of just 10 elements, whereas the symmetry group of the icosahedron consists of 60 elements. This is a consequence of the circumstance that each of these subspaces is transformed into itself by a subgroup of the group  $Y$  and this subgroup consists of six elements. In general, this symmetry is disturbed by translations and the number of surfaces linked by the group  $Y$  transformation increases (to 20, 30, or 60). All these surfaces can be obtained by the action of the group  $Y$  on any one of them. We therefore initially consider only one surface obtained by translation from  $r[\alpha, \beta, \gamma]$ .

We number fundamental vectors of the lattice  $L$  as shown in Fig. 2. We consider a subspace  $r[1, 2, 3]$  and a

hyperplane  $s[1, 2, 3]$  derived from the subspace by translation:

$$s[1, 2, 3] = r[1, 2, 3] + \mathbf{a}. \quad (5.2)$$

Henceforth the hyperplane parallel to  $r[\alpha, \beta, \gamma]$  will be denoted by  $s[\alpha, \beta, \gamma]$ , but because generally the number of such hyperplanes is larger than that the number of the corresponding subspaces, the order of the indices is important. We shall also use  $\mathbf{e}_\alpha$ , which will represent the vector  $-\mathbf{e}_\alpha$ . We can easily see that the addition to the vector  $\mathbf{a}$  of any vector belonging to  $r[1, 2, 3]$  does not alter  $s[1, 2, 3]$ , so that we can assume that  $\mathbf{a}$  is orthogonal to  $r[1, 2, 3]$ :

$$\mathbf{a} = (0, 0, 0, \xi, \eta, \zeta). \quad (5.3)$$

We can show that no matter what are the values of  $\xi, \eta$ , and  $\zeta$ , there is a surface which is generated from  $s[1, 2, 3]$  by the  $Y$  group and which intersects  $s[1, 2, 3]$ . In fact let us consider a surface  $s[6, 5, 1]$  obtained from  $s[1, 2, 3]$  by the action of an element of  $Y$  corresponding to rotation by  $72^\circ$  about the axis 4 in the space  $V$ . We can easily see that the straight line  $(x, \xi, -\eta, \xi, \eta, \zeta)$  belongs to both surfaces. Therefore, simple translations do not remove completely the intersections of atomic planes.

However, we note that the number of intersections can be minimized by this method. In fact, we can easily show that if none of the quantities  $|\xi - \eta|$ ,  $|\eta - \zeta|$  and  $|\zeta - \xi|$  are identical, all the other intersections are close to those already described. Namely, the hyperplane  $s[1, 2, 3]$  intersects the other hyperplanes along the following straight lines:

$$\begin{aligned} \text{intersecting with } s[6, 5, 1] & \text{ along } (x, \xi, -\eta, \xi, \eta, \zeta), \\ \text{intersecting with } s[5, 4, 2] & \text{ along } (\xi, x, -\eta, \xi, \eta, \zeta), \\ \text{intersecting with } s[2, 4, 6] & \text{ along } (-\xi, x, \xi, \xi, \eta, \zeta), \\ \text{intersecting with } s[3, 6, 5] & \text{ along } (-\xi, \eta, x, \xi, \eta, \zeta), \\ \text{intersecting with } s[4, 3, 5] & \text{ along } (\eta, -\xi, x, \xi, \eta, \zeta), \\ \text{intersecting with } s[6, 1, 4] & \text{ along } (x, -\xi, \zeta, \xi, \eta, \zeta) \end{aligned} \quad (5.4)$$

( $x$  is an arbitrary number). This completes the list of all the  $s[\alpha, \beta, \gamma]$ , hyperplanes intersecting  $s[1, 2, 3]$ . We now consider triple intersections of the surfaces. We can readily show that such intersections occur because the hyperplanes of Eq. (5.4) intersect in pairs:

$$\begin{aligned} s[6, 5, 1] \text{ intersecting with } s[5, 4, 2] & \text{ along } (\xi, \xi, -\eta, \xi, x, \zeta), \\ s[2, 4, 6] \text{ intersecting with } s[3, 6, 5] & \text{ along } (-\xi, \eta, \xi, \xi, \eta, x), \\ s[4, 3, 5] \text{ intersecting with } s[6, 1, 4] & \text{ along } (\eta, -\xi, \zeta, x, \eta, \xi). \end{aligned} \quad (5.5)$$

We thus find that 60  $s[\alpha, \beta, \gamma]$  hyperplanes intersect one another along 180 straight lines. We can readily show that the same straight lines can be divided into 60 triplets such that the lines belonging to one triplet pass through the same point and the lines from three points do not intersect. Since the 60 triplets form one orbit of the  $Y$  group, none of the two lines in any triplet are related by a symmetry transformation. We shall need this in the next stage of our procedure.

### Second stage

Our task is now to deform slightly the hyperlines  $s[\alpha, \beta, \gamma]$  in the vicinity of the straight lines where they intersect and to remove these intersections. Since, as shown above, these straight lines are grouped in 60 triplets linked by the symmetry transformation, it is sufficient to remove only the

intersections in one triplet. Let us assume that this triplet is formed by the straight lines [see Eqs. (5.4) and (5.5)]

$$\begin{aligned} (x, \xi, -\eta, \xi, \eta, \zeta), \quad (\xi, x, -\eta, \xi, \eta, \zeta), \\ (\xi, \zeta, -\eta, \xi, x, \zeta), \end{aligned} \quad (5.6)$$

which intersects at the point  $(\xi, \zeta, -\eta, \xi, \eta, \zeta)$ . If we consider a region  $\varepsilon$  in the vicinity of the straight lines described by Eq. (5.6) and assume that this region is so small that it does not contain any other intersections with their own regions  $\varepsilon$ , we find that there are no limitations on the deformation of hyperplanes within the region  $\varepsilon$ . Therefore, the problem of removal of intersections again becomes topological and can be solved, as in Sec. 3, by parallel translation (but in this case it applies only to the part of the surface within the region  $\varepsilon$ ), for example:

$$\begin{aligned} s[6, 5, 1] & \text{ is shifted by } \varepsilon'(1, 1, 1, 1, 1, 1), \\ s[5, 4, 2] & \text{ is shifted by } -\varepsilon'(1, 1, 1, 1, 1, 1) \\ s[1, 2, 3] & \text{ remains in place} \end{aligned} \quad (5.7)$$

( $\varepsilon'$  must be selected to be much smaller than  $\varepsilon$ ). Then, at the edge of the region  $\varepsilon$  we have to match smoothly the inner and outer parts of the atomic surfaces and retain their transversality to the direction of the physical space. If this deformation of atomic planes is replicated by symmetry transformations, all the other intersections are removed.

In the procedure described above we have ignored the periodicity of the system of atomic planes. However, all the steps can be repeated if we replace the space  $R^6$  with a torus  $T^6 = R^6/L$  and the subspace  $r[\alpha, \beta, \gamma]$  with the corresponding three-dimensional tori. Then, if the values of  $\xi, \eta, \zeta$ , and  $\varepsilon$  are selected to be much smaller than the lattice constant, there is no need to change the above procedure. We have thus derived a periodic system of continuous nonintersecting atomic surfaces with the symmetry of the icosahedron.

## 6. CONCLUSIONS

We have constructed above an example of an icosahedral quasicrystal with continuous atomic planes. We now ask the question: how are the atoms distributed in this model? We consider first all the surfaces linked by translation from  $L$  to any one of the surfaces  $s[\alpha, \beta, \gamma]$ . If in the construction of  $s[\alpha, \beta, \gamma]$  we had remained in the first stage, the resultant system of parallel hyperplanes would have given a rhombohedral lattice in the section formed by the physical space. However, deformation of the atomic surfaces results in a weak distortion of the lattice in which the atoms are shifted by finite distances. Since there is a total of 60  $s[\alpha, \beta, \gamma]$  surfaces, the real space contains 60 nesting slightly distorted rhombohedral lattices and the distance between any two atoms is limited from below by the value of  $h$  (when the "hard core" condition is obeyed). It should also be noted that because of the complete icosahedral symmetry of the structure, its deformation properties are the same as that of the standard and discontinuous model.

The main difference between quasicrystals with continuous and discontinuous atomic surfaces is the nature of the additional phason modes. An inhomogeneous phason shift in quasicrystals, described by continuous surfaces, relaxes to zero (naturally, if the quasicrystalline state is stable). However, in the case of discontinuous surfaces such relaxation would require finite atomic jumps. Therefore, frozen phason

deformations should exist in such substances.

It should also be pointed out that the above procedure still leaves some unanswered questions such as the possibility of existence of sets of nontransverse sublattices  $l [s_i]$ . We can show that the example given above does not exhaust all the possibilities. We need to consider also the question of existence of quasicrystals described by continuous atomic surfaces in the case of other space symmetry groups. Clearly, such crystals are not possible for every space group. In particular, an important factor is the nonsymmorphic nature of a group and the occurrence of inversion.

We conclude with some comments about the validity of our results. An analysis carried out for the icosahedral symmetry case simply demonstrates the absence of purely geometric obstacles for the existence of quasicrystals described by continuous atomic surfaces. However, we can say nothing on whether the value of  $h$ , representing the lower limit of the interatomic distance in the structure obtained, corresponds to real interatomic distances. Moreover, the Aubry transition mentioned in the Introduction demonstrates how the interaction between incommensurate subsystems may destroy the initial continuity. Therefore, the question of the influence of the interatomic interaction on the continuity of atomic surfaces requires additional study.

In the case of the symmetry of the pentagon we have to

remember that our discussion applies only to the purely two-dimensional case. However, in the three-dimensional problem the condition  $d = d'$  is not satisfied and continuous atomic surfaces are not forbidden. The example is a stack of slightly distorted two-dimensional crystals in which each layer is rotated by  $72^\circ$  relative to the preceding one. The phason shift then corresponds to a glide of layers relative to one another.

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