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## LOCAL ISOMORPHISM, LANDAU THEORY, AND MATCHING RULES IN QUASICRYSTALS

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**Résumé:** On discute quelques différences entre les quasicristaux et les cristaux ordinaires. Les conséquences physiques d'isomorphisme local et des règles d'accordement sont présentées.

**Abstract:** Several issues which occur in quasicrystals but which are absent in ordinary crystals are discussed. The physics involved in the ideas of local isomorphism and matching rules is illustrated.

Standing as they do in such striking contrast to the structures of classical crystallography, quasicrystals [1] have generated a great deal of interest, both theoretically and experimentally. The exciting discovery of a rapidly cooled alloy of AlMn [2] exhibiting sharp diffraction peaks in an array with classically forbidden icosahedral rotation symmetry has been confirmed by many successive experiments. Should this material turn out to be a quasicrystal, as many believe, it would represent a new phase of matter.

While quasicrystals are similar to crystals in some ways, they differ in many important aspects. In this paper we shall discuss some of the features peculiar to quasicrystals which are imperative in their study. We shall briefly review the concepts of quasicrystals in the Introduction using the Penrose tilings as a prototype. In section 2 we shall discuss local isomorphism, a concept which does not apply to ordinary crystals. Section 3 briefly reviews methods for constructing quasicrystals, emphasizing the various free parameters which control the specific details of the quasicrystals. In section 4, connections to Landau theory will be indicated. Section 5 discusses the role which matching or bonding rules play in determining the nature of a quasicrystal structure. Here too we exhibit a set of matching rules which is consistent with the icosahedral quasicrystal derived from projection from a six-dimensional hypercubic lattice. In section 6 we argue that these issues are not only of mathematical interest, but are relevant to physics as well.

## 1 Introduction

Ordinary crystals are constructed out of a single unit cell repeated in a periodic array. Quasicrystals are built out of a finite number (two or more) unit cells layed face-to-face (edge-to-edge in two dimensions); these are arranged *quasiperiodically*. (A function is quasiperiodic if it can be written as the sum of periodic functions, some of whose periods are incommensurate.) Quasicrystals are characterized not only by their quasiperiodic translational order, but by their *bond-orientational-order* (BOO): all of the "bonds" connecting near neighbors are oriented along a set of star axes. That the unit cells are placed face-to-face implies that quasicrystals are *Delaunay systems*: neighboring quasicrystal sites never get closer together than some finite minimal distance.

The prototype quasicrystal is the Penrose tilings of the plane [3,4] which were constructed as examples of a non-periodic tiling. Figure 1 depicts a small portion of a Penrose tiling. As may be seen, there are two unit cells, a fat and a skinny rhombus, which are the basic building blocks of the Penrose tilings. These unit cells are laid edge-to-edge, and it may be verified by inspection that the vertices of the tiling never get closer together than some minimum distance. The Penrose tilings have pentagonal (we could equally well say decagonal) BOO: the edges of the tiles are aligned along the axes of a regular pentagon.

That the Penrose tilings have quasiperiodic translational order is less obvious; this is revealed by a construction due to R. Ammann. At the right of Figure 2 is depicted a decoration of each of the two rhombic unit cells of the Penrose tiling. A certain set of line segments has been drawn

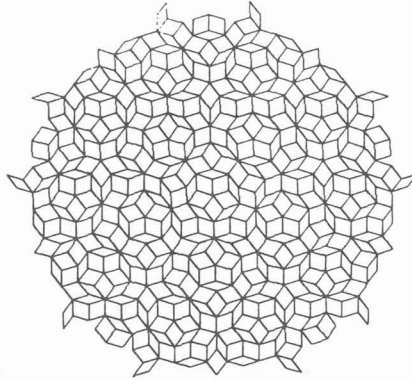


Figure 1: A portion of a Penrose tiling.

on each of the tiles. We demand that when the tiles are laid, these segments do not terminate, but continue across the edges of the tiles. (This is one manifestation of the *matching rules* which serve to guarantee legitimate Penrose tilings.) The resultant set of lines is shown superimposed on a portion of a Penrose tiling in the upper part of Figure 2. These comprise a specific *Fibonacci pentagrid*, the set of intersections of which is known as the *Ammann quasilattice* of the Penrose tilings. The lines are divided into five families (labeled by  $\mu = 1, \dots, 5$ ) oriented along the axes of a regular pentagon, and the lines in each family are spaced according to the *Fibonacci sequence*.

$$x_n^\mu = n + \alpha^\mu + \frac{1}{\tau} \left[ \frac{n}{\tau} + \beta^\mu \right], \quad (1)$$

with special choices of the parameters  $\alpha^\mu$  and  $\beta^\mu$ . Here  $\tau = \text{golden ratio} = (1 + \sqrt{5})/2$ , and  $[ ]$ 's represent the greatest integer function. The Fibonacci sequence is quasiperiodic, as has been discussed elsewhere<sup>5</sup>. It is because of this sequence that the pentagrid of Figure 2 is called a *Fibonacci pentagrid*.

The Penrose tilings also have a self-similarity transformation, called *deflation*, in which the tiles are dissected in a well-defined fashion (illustrated in Figure 3) into smaller whole and half tiles. In a legitimate Penrose tiling, the half tiles combine with other half tiles in such a way as to produce another, scaled down Penrose tiling. The inverse operation is called *inflation*, it begins with a Penrose tiling and generates another, larger scale Penrose tiling. The Ammann quasilattice itself has an inflation-deflation rule<sup>6</sup>, and this, in tandem with the decoration of Figure 2 induces the inflation-deflation rule of the Penrose tilings shown in Figure 3.

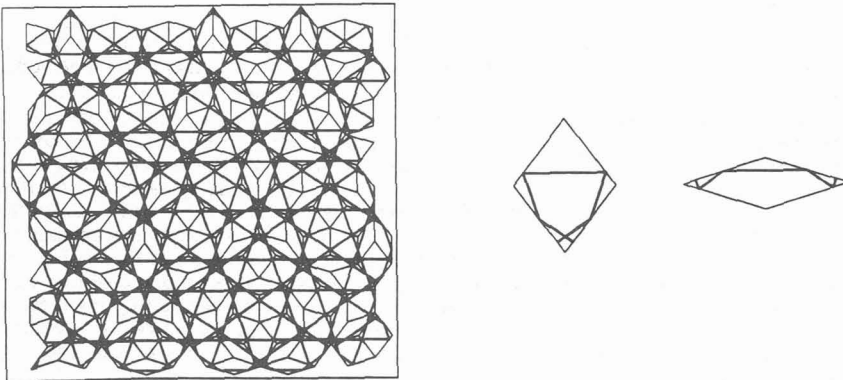


Figure 2: At right, a decoration of the Penrose tiles. When the tiles are laid in a legal fashion, a Fibonacci pentagrid results: this is shown at the top.

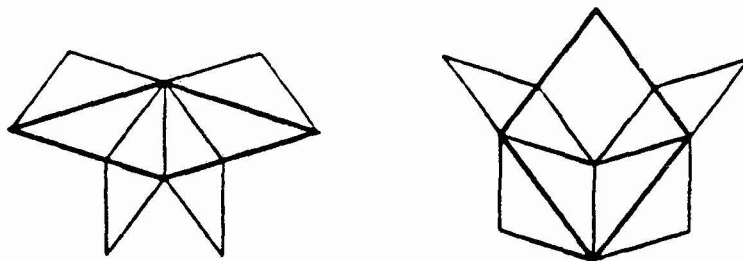


Figure 3: The inflation/deflation rules for the Penrose tiles.

## 2 Local Isomorphism

In ordinary crystals there is only a single unit cell, and there is only a single way to pack them consistent with the symmetry of the crystal. With quasicrystals the situation is much more complicated, owing to the larger number of unit cells. Using the same cells, many distinct packings may be constructed.

The set of all quasicrystal packings employing the same unit cells may be partitioned into equivalence classes known as local isomorphism (LI) classes. Within each LI class there is (generally) an infinite number of distinct packings. Two quasicrystals belonging to different LI classes are locally distinguishable: there exist motifs which appear in one packing which do not appear in the other. Three such non-locally isomorphic tilings are illustrated in Figure 4.

Two locally isomorphic quasicrystals however, are *geometrically indistinguishable*: any bounded region appearing in one appears in the other, and vice versa. To see this another way, we may think of overlaying the two packings. Then via a finite (albeit perhaps large) relative translation of the packings, they may be brought into coincidence over any arbitrary preassigned bounded region. Note that every finite region appearing in one quasicrystal packing appears in one locally isomorphic to it with the same frequency. It should be emphasized that two locally isomorphic tilings are not identical—it is not possible to bring them into perfect coincidence over their entire, infinite extent.

Note that the local isomorphism classes are indeed equivalence classes, since local isomorphism is a symmetric, reflexive, and transitive relation. Thus the LI classes are mutually exclusive. We shall argue in section 5 that the notion of local isomorphism is physically relevant, and is not just a mathematical classification.

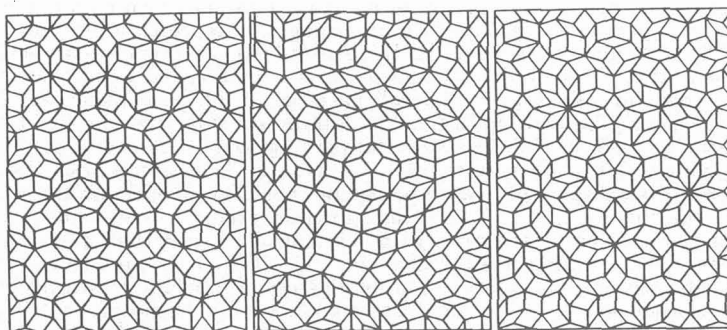


Figure 4: Three tilings built out of the same unit cells, which belong to different LI classes

### 3 Degrees of Freedom in the Construction of Quasicrystals

To date, several methods for constructing quasicrystals have been proposed. One way, in analogy with the Penrose tilings, is to attempt to matching and inflation/deflation rules with a given set of unit cells. In general this is very difficult, although we shall discuss one set of matching rules in Section 4.

Another method which has been proposed has been called the *projection* technique.<sup>[7,8,9,10]</sup> In this method, a hyperplane  $\Sigma$  (the "physical space"), whose dimension is equal to that of the desired quasicrystal, is constructed in a higher dimensional periodic lattice (generally taken to be hypercubic) and a certain subset of the lattice sites are projected orthogonally onto  $\Sigma$ ; these are the vertices of the quasicrystal packing. One advantage of this method is the elegant way in which the Fourier transforms of the packings thus obtained may be computed. It has also been suggested that the projection method can be used to produce quasicrystals with arbitrary symmetry.<sup>[11]</sup>

One may also employ a technique known as the multigrid or generalized dual method.<sup>[7,12,13]</sup> to produce quasicrystal packings. This method can be used to construct the largest set of quasicrystal packings (all LI classes) for any given orientational symmetry. The one disadvantage is that there is no direct analytic method known for finding the diffraction pattern of a general packing constructed by this technique. Although the details of the construction method are given elsewhere<sup>[7,13]</sup>, we will briefly recount the method. Given an  $N$ -grid composed of ( $N$  families of) periodically spaced straight lines (planes in 3D) in a grid-space,<sup>[14]</sup> a unique star vector,  $e_i$ , is associated with each of the  $N$  grids. The "dual" transformation associates a vertex in the quasicrystal packing with each open region (a region bounded by grid lines (planes) through which no other grid lines (planes) pass) in the grid-space. It is important to note that this procedure is not simply to place a vertex of the packing inside its associated region in the grid-space. The set of vertices is guaranteed to form a full quasicrystal packing of unit cells with orientational symmetry corresponding to the "star" vectors,  $e_i$ , and neighboring vertices are separated by one of the star vectors.

The dual transformation also associates each point of intersection of grid lines (planes) in the grid space with a unit cell in the quasicrystal packing. The nature of this unit cell is determined by the number of grid lines (planes) which intersect at the point and their angles of intersection. In the event that only two lines intersect at a point in the grid space, the associated unit cells are rhombuses (In three dimensions, if only three grid planes intersect at a point the unit cell associated with the intersection point is a rhombohedron.). If more than two (three) grid lines (planes) intersect at a point in 2D (3D) then the unit cells associated with such intersection points are more complicated, possessing more edges (faces) than does a rhombus (rhombohedron).

In any sufficiently general construction method there are free parameters determining the precise nature of the tilings produced. These may be divided into two classes: (a) those that shift packings within a given LI class, and (b) those that change the LI class of the tilings generated. These free parameters may be related to physically meaningful properties with the aid of Landau theory, as we shall see.

Let us examine a specific case, the construction of pentagonal tilings in 2D (employing the previously discussed rhombic unit cells of the Penrose tilings) by direct projection from a five-dimensional hypercubic lattice  $A$ . This construction has been described in detail in elsewhere.<sup>[9]</sup> In order to determine which plane is the "physical" plane, we note that there is a natural action of the pentagonal group on  $A$  which simply permutes its axes. This operation entails a five-dimensional representation of the pentagonal group. Decomposing this representation into representations irreducible over the real numbers, we find that there are two 2D irreducible representations, and the 1D trivial representation. The irreducible subspaces of  $A$  corresponding to these representations are used in the projection. One of the 2D subspaces is the physical plane,  $\Sigma$ , the other is the "perpendicular space",  $\Sigma'$ . Last, we have the trivial invariant subspace, the (1,1,1,1,1) direction.

In order to get the vertices of the quasicrystal packing we now project a certain subset of the points of  $A$  orthogonally onto  $\Sigma$ . The way in which this subset is chosen is described elsewhere.<sup>[9,8]</sup>

Translating the physical space in its own plane does not have an effect on the resulting tiling; it simply translates the entire pattern. This translational invariance corresponds to *phonon* degrees of freedom of the tiling. What is also true, although not obvious, is that translating  $\Sigma$  along any vector in the plane of  $\Sigma'$ , while certainly changing the tiling, only produces locally isomorphic tilings. Such translations are analogous to phason degrees of freedom present in incommensurate systems such as charge density waves<sup>[15]</sup> (Although it should be noted that if pinning effects occur, results of ordinary elasticity theory may not apply.). However, if we translate  $\Sigma$  along the (1,1,1,1,1) direction, we produce tilings which are not locally isomorphic.

One way icosahedral quasicrystal packings may be produced is by projection from a 6D hypercubic lattice to 3D. It is important to realize that this construction, in contrast to that of the pentagonal tilings, can produce only a single LI class of packings. These packings will have as

their unit cells two *rhombohedra*[16,1], one prolate, the other oblate. We shall return to these unit cells shortly to discuss a set of matching rules for them.

To make contact with the Landau theory and broken symmetry modes to be discussed in the next section, let us turn to quasicrystals generated by the multigrid or generalized dual method. We may construct the quasicrystal packing dual to any multigrid; in particular the Fibonacci pentagrids (hexagrids in 3D) may be used to obtain the pentagonal (icosahedral) packings. The free parameters  $\alpha^\mu$  and  $\beta^\mu$  in the Fibonacci sequence of Equation (1) control the specific nature of the packings dual to these penta- (hexa-) grids. In particular, if the parameters of two Fibonacci penta- (hexa-) grids  $\mathcal{F}$  and  $\mathcal{F}'$  are related by

$$\alpha'^\mu = \alpha^\mu + \mathbf{u} \cdot \mathbf{G}_\mu \quad (2)$$

$$\beta'^\mu = \beta^\mu + \mathbf{w} \cdot \mathbf{G}_{(\mu)} \quad (3)$$

for all  $i$ , where  $\mathbf{u}$  and  $\mathbf{w}$  are independent arbitrary 3-vectors and the  $\mathbf{G}_i$  are the six icosahedral (five pentagonal) star vectors, then the packings dual to  $\mathcal{F}$  and  $\mathcal{F}'$  are locally isomorphic. We shall use the " $(\cdot)$ " brackets to represent an operation on an integer argument  $n$ , ranging from 0 to 5 (1 to 5 in 2D) such that  $\mathbf{G}_{(n)} = \mathbf{G}_{(2n, \text{mod}5)}$  if  $n \neq 0$ , and  $\mathbf{G}_{(0)} = -\mathbf{G}_0$ . The vectors  $\mathbf{G}_i$  and  $\mathbf{G}_{(i)}$  are related to the two different 3D representations of the icosahedral group (or the two different 2D real representations of the pentagonal group in the case of the 2D pentagonal tilings).

#### 4 Landau Theory

Thusfar in this paper, we have described quasicrystals in a language tailored to discussions of unit cell packings. One may also use this language to describe crystals as packings of a single unit cell. There is an alternative description which is often used to describe crystals, the so-called *Landau theory*, which is especially useful for discussing stability<sup>17,18</sup> and defects.<sup>19</sup> This description is in fact applicable to any translationally ordered phase, and we shall discuss it here for the case of quasicrystals, focusing in particular on the examples of pentagonal and icosahedral quasicrystals. It should not be thought that the ideas discussed in this chapter constitute a different theory of icosahedral phases: the two descriptions, via unit cell packings and via Landau theory, are complementary approaches.

The density  $\rho(\mathbf{r})$  of any translationally ordered phase  $P$ , such as a quasicrystal, may be expanded in a Fourier series

$$\rho(\mathbf{r}) = \sum_{\mathbf{G} \in \mathcal{R}} \rho_{\mathbf{G}} e^{i\mathbf{G} \cdot \mathbf{r}}, \quad (4)$$

where  $\mathcal{R}$  is the reciprocal lattice associated with  $P$ . The set of  $\mathbf{G}$  is not linearly independent over the integers, so there exists a minimal basis set  $\{\mathbf{G}_\alpha\}$  out of which all of the reciprocal lattice vectors can be constructed. In ordinary crystals, there are  $d$  vectors in such a basis (where  $d$  is the dimension of the crystal), whereas for quasicrystals and incommensurate crystals there are  $n_id$ , where  $n_i$  is the number of incommensurate lengths. Each  $\rho_{\mathbf{G}}$  is a complex number with an amplitude  $|\rho_{\mathbf{G}}|$  and a phase  $\Phi_{\mathbf{G}}$ . The phase  $P$  is characterized by nonvanishing  $\rho_{\mathbf{G}}$ . Phase transitions to and from  $P$  may be described by a phenomenological Landau free energy density  $F$  that can be expanded in a power series in  $\rho(\mathbf{r})$ , the  $n^{\text{th}}$  term of which contains terms of the form

$$|\rho_{\mathbf{G}_1}| |\rho_{\mathbf{G}_2}| \cdots |\rho_{\mathbf{G}_n}| e^{i(\Phi_{\mathbf{G}_1} + \Phi_{\mathbf{G}_2} + \cdots + \Phi_{\mathbf{G}_n})} e^{i(\mathbf{G}_1 + \mathbf{G}_2 + \cdots + \mathbf{G}_n) \cdot \mathbf{r}} + c.c. \quad (5)$$

To obtain the free energy, we must integrate over  $\mathbf{r}$ , and terms such as these vanish identically unless  $\sum_{k=1}^n \mathbf{G}_k = 0$ . When this condition on the sum of the phases is satisfied, the corresponding term in the free energy is

$$|\rho_{\mathbf{G}_1}| |\rho_{\mathbf{G}_2}| \cdots |\rho_{\mathbf{G}_n}| \cos\left(\sum_{k=1}^n \Phi_{\mathbf{G}_k}\right) \quad (6)$$

Minimization of the free energy leads to a minimum energy state with constraints among the  $\Phi_{\mathbf{G}}$ 's. These constraints leave unspecified  $n_id$  phases  $\Phi_n$  which are the hydrodynamic variables of the theory. To understand the hydrodynamic modes of the structure, it is sufficient to consider a density

$$\rho(\mathbf{r}) = \sum_{\alpha=1}^{n_id} |\rho_{\mathbf{G}_\alpha}| e^{i\Phi_\alpha} e^{i\mathbf{G}_\alpha \cdot \mathbf{r}}. \quad (7)$$

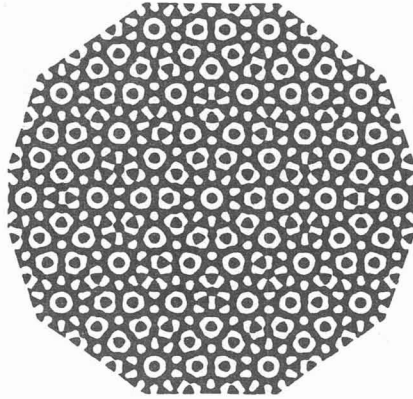


Figure 5: A density wave image obtained by summing five pentagonally oriented density waves. Regions where  $\rho(\mathbf{r}) > 0$  are indicated in black; regions where  $\rho(\mathbf{r}) \leq 0$  are white.

Let us now focus on the pentagonal quasicrystal composed out of density waves at the five fundamental reciprocal lattice vectors  $\mathbf{G}_n$ , pointing along the axes of a regular pentagon. Although, strictly speaking, only four basis vectors are necessary to characterize pentagonal quasicrystals, it is convenient to consider this redundant set of five (this is analogous to the case of the 2D triangular lattice where a redundant set of three vectors is used). Such a density is depicted in Figure 5. Where  $\rho(\mathbf{r})$  is greater than zero, a black dot is placed; white regions indicate that  $\rho(\mathbf{r})$  is less than or equal to zero. In the minimum energy state, the phases associated with these five basis vectors satisfy  $\sum_n \Phi_n = \gamma = \text{constant}$ . We may parametrize these five phases  $\Phi_n$  as

$$\Phi_n = \mathbf{G}_n \cdot \mathbf{u} - \mathbf{G}_n \cdot \mathbf{w} - \gamma \delta_n \quad (8)$$

where  $\mathbf{G}_{i/n}$  means  $\mathbf{G}_{2n \bmod 5}$ . The vector  $\mathbf{u}$  may be identified with translations of the structure, as with ordinary crystals.<sup>20</sup> The vector  $\mathbf{w}$ , however, does not occur in ordinary crystals; it corresponds to relative shifts of the density waves. By analogy to the crystalline case, we shall refer to  $\mathbf{u}$  as the *phonon* variable, and by analogy to incommensurate crystals, where this extra mode occurs, the vector  $\mathbf{w}$  shall be called the *phason* variable. It should be noted that if pinning occurs, this may make this mode behave differently from what would be predicted by the usual elasticity theory. If we vary the constant  $\gamma$ , however, this will generally change the LI class of the structure; it corresponds to translating the hyperplane  $\Sigma$  in the (1,1,1,1,1) direction as was discussed in Section 3.

Note the similarity of Equation (8) to the changes in the parameters  $\alpha$  and  $\beta$  of Equations (2) and (3), which are the most general shifts of these parameters which preserve local isomorphism class.<sup>21</sup> By this analogy, we see that an intimate connection exists between the unit cell packing picture and the density wave description detailed here. Thus, we see that changing the constant  $\gamma$  of the phases corresponds to changing the local isomorphism class of the structure (provided that  $\gamma$  itself is not of the form  $\mathbf{G}_n \cdot \mathbf{u} - \mathbf{G}_{i/n} \cdot \mathbf{w}$ ). Such changes cost energy to effect; this may be seen as follows: the quintic term in the Landau expansion for the free energy is of the form  $\cos(\sum_1^5 \Phi_n) = \cos(\gamma)$ . If  $\gamma$  changes then this term does also, and so the free energy changes. Thus, we may say that *non-locally isomorphic quasicrystals have different free energies*.

Note that for icosahedral quasicrystals there are six basis vectors, compared with five for the pentagonal case, and that these six are linearly independent over the integers. The effect of this linear independence is that for the icosahedral case modelled with these six fundamental density waves, there is no analog of  $\gamma$  (Note that we can obtain different LI classes if we include other density waves in our expansion.). There still are, of course, phonon and phason modes defined in exactly the same fashion as for the pentagonal case.

## 5 Matching Rules

The two rhombic unit cells out of which the Penrose tilings are constructed may, in the absence of stipulations to the contrary, be packed crystallographically. In order to guarantee that the Penrose tilings are non-periodic, a set of matching or bonding rules, restricting the ways in which

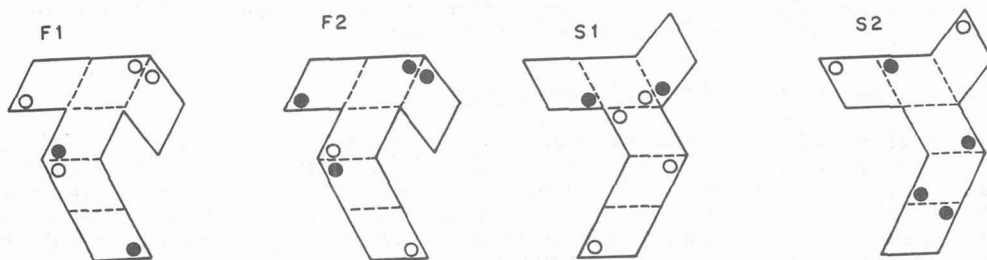


Figure 6: Rhombohedral unit cells, in an unfolded view, showing all of the faces. The faces have been decorated with solid and hollow circles. The matching rule is that the faces of adjacent rhombohedra have different types of circles, and that the circles overlay one another.

tiles may be laid one next to the other, are imposed<sup>[3]</sup> (One such manifestation, the demand for continuity of the Ammann line segments, was described in Section 1.). Indeed, matching rules may be thought of as choosing a specific LI class of packings from amongst all possible arrangements using the same unit cells.

In a physical system for which a quasicrystal unit cell packing serves as an underlying lattice, atoms will be placed in the unit cells, like cells containing the same atomic decoration. If this is the case, then we may imagine that the atomic interactions induces a matching rule: it may be energetically preferable for two unit cells to attach in some fashions but unfavorable to join in others. It should be noted that we do not claim that a physical system must grow in strict observance of these "rules" (in contrast to the case of the Penrose tilings where the matching rules must be obeyed absolutely). In this sense the rules merely serve as a guide for the system to indicate how to achieve energetically favorable configurations. When the unit cells are packed together to form an extended structure, we may expect that where there are "violations" of the bonding rules the atoms will relax so as to minimize the energy of the local cluster.

Matching rules also serve another important purpose, the identification of defects. We may readily identify the mismatches which occur in the growth of a structure (for example in a computer simulation) and assign energy costs to their formation. It is then of interest to see how quickly and in what fashion these defects anneal out under structural relaxation. We are currently involved in just such studies, which may bear on the growth and subsequent relaxation of icosahedral materials.

In Figure 6 we have depicted one set of matching rules discovered by us and independently by R. Ammann<sup>22</sup> which employs the rhombohedral unit cells mentioned in Section 3. The figure shows the rhombohedra in an "unfolded view", all of the faces are visible. If the rhombohedra were cut out of the paper along the solid lines, scored and folded along the dashed lines, then the edges would match up and could be taped to form the rhombohedral solids.

On the faces of the rhombohedra are drawn circles, some solid and some hollow. The matching rule is that the solid circle on one face of a given unit cell must match against a hollow circle on a face of a neighboring unit cell. One realization of this rule could be effected with the help of magnets, where the north pole of one magnet would be attracted by the south pole another.

Note that although only two *shapes* of unit cells are used, the prolate and the oblate rhombohedra, the matching rules distinguish between *four* cells, two of each shape. This is indicated in the figure by the labels  $F_1$ ,  $F_2$ ,  $S_1$ , and  $S_2$ , standing for "fat" (prolate) and "skinny" (oblate), respectively.

This set of matching rules is consistent with the LI class of quasicrystal packings obtained, for example, by using the projection technique beginning with a six dimensional hypercubic lattice. That is, given such a packing, we may consistently paint the solid and hollow circles in such a way that the matching rules are satisfied everywhere. It is our conjecture, although as yet unproven, that these matching rules force the packings to be in this LI class. It should be noted that inflation rules for this set of unit cells are very involved.

There is another set of unit cells, consisting of four zonohedra: a rhombic triacontahedron, a rhombic icosahedron, a rhombic dodecahedron, and the prolate rhombohedron (each of which



may be dissected into the above rhombohedral shapes), which has simple matching and inflation/deflation rules.[23] These quasicrystal packings are very much analogous to the Penrose tilings of the plane and so are said to belong to the Penrose LI class.

## 6 Physical Significance of Local Isomorphism

In general, as we have stated earlier, even for fixed orientational symmetry, quasiperiodicity, and unit cell shapes, there are infinitely many distinct LI classes (corresponding, for example, to shifts in the  $(\alpha_i, \beta_i)$  which are not of the form shown in Eqs. (2) and (3)). No such issue arises for the case of periodic crystals where there is a unique configuration of cells — a single LI class containing one element. Since locally isomorphic quasicrystals are geometrically indistinguishable, we may expect them to be physically indistinguishable as well. Indeed,

- Two quasicrystals have identical diffraction patterns (the same spot locations and intensities) if and only if they are locally isomorphic.[5]
- Quasicrystals in the same LI class have the same free energy (computed, say via Landau theory). By the same token, two quasicrystals in different LI classes have different free energies, unless there is some accidental degeneracy.
- Given this conjecture, if the ground state of a some physical system is a quasicrystal state, as determined by minimizing the Landau mean free energy, then it is degenerate and corresponds to a set of configurations in a *single LI class* (neglecting the possibility of accidental degeneracy). For example, configurations corresponding to the quasicrystal packings that obey the matching rules described in Section 5 have a different energy than configurations that don't obey the matching rules since, as we noted, they necessarily belong to different LI classes.
- The entropy of the ground state is determined by the number of energetically equivalent configurations. According to the arguments above, only configurations in the same LI class should be counted. Counting all possible rearrangements of the unit cells consistent with the quasiperiodicity and symmetry leads to a vast overestimate of the entropy.

In this paper we have sketched some of the details involved in the study of quasicrystals which do not arise for crystals. As samples improve in quality, these issues may take on greater relevance to experimental systems. In any event, they illustrate some of the richness inherent in quasicrystals.

## 7 Acknowledgements

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- [21] It should be noted that Equations (2) and (3) as written pertains to the icosahedral quasicrystal, while Equation (8) is written for the pentagonal case. For the icosahedral case, the phases may be parametrized by  $\Phi_n = \mathbf{G}_n \cdot \mathbf{u} - \mathbf{G}_{(n)} \cdot \mathbf{w}$ , with  $n$  going from 0 to 5, and  $\mathbf{G}_{(n)}$  being defined as in Equations (2) and (3).
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**COMMENTS AFTER D. LEVINE TALK :**

**N. RIVIER.**- Continuous transformations (tunneling modes) between two different, non locally isomorphic configurations are physically observable in glasses <sup>1</sup>.

The structure of a covalent glass can be modelled by a continuous random network (CRN = regular graph), made of 4-bonded tetrapods, with slight, random bending of the bonds. There appear rings with odd number of bonds, threaded through by uninterrupted lines ("disclinations" characterized by oddness).

Configurations are described by transporting the tetrapod about a ring (Burgers). They are labelled by classes of the permutation group  $S_4$  (permutations of the feet of the tetrapod) : even permutations for even rings, odd permutations for odd rings. There are 2 odd classes of  $S_4$ , hence two configurations per odd line, which are not locally isomorphic<sup>2</sup>.

Tunneling between these two configurations does occur, and has been observed experimentally, most directly by (acoustic) echo techniques<sup>1</sup>.

1. C.F. W.A. PHILLIPS, *Amorphous Solids*, Springer 1981
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M.V. JARIC.-

*Comments :*

I do not quite see how quenched phasons could explain distortions of the diffraction patterns observed experimentally. I would expect that any quenched phason displacements would be essentially random and zero in average. Obviously, such "self-averaging" would lead to no distortions and only to an effective thermal broadening in the form of  $1/q^2$  tails superimposed on the Bragg peaks. Also, since it is known that icosahedral quasicrystals also grow into icosahedral grains I cannot easily see what could produce the "orienting" of the quenched phason displacements which is necessary to obtain symmetry distortions of the diffraction patterns.