Binary tiling quasicrystals and matching rules

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A general theory on the transfer of perfect matching rules for a quasiperiodic tiling to perfect matching rules for an atomic decoration of the tiling is presented. General conditions on the possibility of such a transfer are discussed, and an upper bound on the range of the matching rules for the atomic structure is derived. This range is identical to the range of interactions needed to stabilize such a quasiperiodic ground state. The main tool in this analysis is the concept of mutual local derivability. The general principles are then applied to two examples of binary tiling quasicrystals. The first one, based on the Tübingen triangle tiling, needs matching rules of a rather long range, whereas the second example, which is a decoration of the Penrose rhombus tiling, has matching rules of reasonable range. Finally, the concepts put forward in this paper are set into a broader context, and we compare them with other theories for the propagation of quasiperiodic order.

I. INTRODUCTION

Since the experimental discovery of quasicrystals in 1984, a vast number of further quasicrystalline structures have been found, among them several thermodynamically stable ones, some of which are extremely perfect and well ordered. It is still somewhat mysterious, however, how the laws of nature can select these well-ordered, albeit nonperiodic structures and favor them against other, periodic, or nonperiodic, but less well-ordered structures. There are several mechanisms which help in the formation of quasicrystals, notably contributions from the electronic energy (Hume-Rothery mechanism) and from the high entropy of these nonperiodic structures at higher temperatures. We believe, however, that the high perfection found in many of the thermodynamically stable quasicrystals can only be explained if there is a fairly local *energetic* mechanism present as well, which selects the local neighborhoods that may occur in the structure. We therefore propose to study local, finite range interactions having a quasiperiodic ground state. With such interactions, the global quasiperiodic order of quasicrystals is enforced by their local order.

In a slight idealization, perfect quasicrystals can be described as certain atomic decorations of quasiperiodic tilings. Many such quasiperiodic tilings are known to allow for perfect matching rules,[1–11] which means that they can uniquely be recognized by inspection of local configurations only. One could therefore also call them perfect local matching rules, but because we shall not talk about matching rules other than local ones, we drop the attribute "local" from now on. It is important to notice, though, that, in order to formulate these matching rules, it is often necessary to introduce arrows and flags and other rather unnatural decorations of the tiles that must match,[3,6,7] and it is hard to see how atomic interactions could mimic those decorations. Even worse, these decorations sometimes require additional, nonlocal information that is not contained in the bare, undecorated tilings.

It is the purpose of this paper to investigate under what circumstances perfect global order in quasicrystals can be obtained by requiring *local order* only, and we shall do this not only for quasiperiodic tilings, but rather for the atomic structures themselves. The latter are local decorations of quasiperiodic tilings, and the order is defined by specifying which local neighborhoods an atom in the structure may have. Our main technical tool will be the concept of *mutual local derivability*,[12] which had been developed to classify tilings, but which also proves very useful to transfer perfect matching rules between different tilings,[8] or between a tiling and an atomic decoration of the tiling,[8] providing a purely local characterization of the atomic structure so obtained. Local derivability, moreover, provides us with an upper bound on the range of the interactions needed to produce a perfect quasicrystal.

Our paper is organized as follows. In Secs. II and III, the concepts of local derivability and of perfect matching rules for tilings and atomic structures are reviewed. We then explain in Sec. IV how matching rules can be transferred between tilings that are locally derivable from each other, and how the same mechanism can be used to transfer matching rules for a tiling to an atomic decoration of the tiling. We also discuss how local derivation can be used to relate different matching rules for the same tiling. In particular, the question of the necessity of decoration of the tiles is addressed, and how decoration may have an influence on the range of the matching rules. These ideas will then be applied to two examples, both from the

class of binary tilings. Binary tilings, shortly reviewed in Sec. V, allow for a very simple and natural atomic decoration with two kinds of atoms. The first example, presented in Sec. VI, is of a very simple structure, but has only matching rules of a rather long range. In Sec. VII, a second binary tiling example is presented, which has a somewhat more complicated structure, but allows for matching rules of considerably shorter range. In Sec. VIII, we put our results into a broader context, and discuss how they apply to realistic quasicrystal models.

II. THE CONCEPT OF MUTUAL LOCAL DERIVABILITY

The concept of local derivability had been introduced to bring some order into the formidable zoo of quasiperiodic tilings.[12] When classifying quasiperiodic tilings one faces a situation somewhat similar to that with ordinary periodic crystals, where the choice of a unit cell is rather ambiguous. In fact, there are infinitely many ways to choose a unit cell, although one might reduce this ambiguity by choosing a symmetric unit cell, such as the Wigner-Seitz (or Voronoi) cell. From a fundamental point of view, however, there is no preferred choice: tilings by unit cells, with just different choices of a unit cell for the very same structure, should be considered equivalent in most contexts. With quasiperiodic tilings, the situation is similar, but somewhat more complicated, since quasiperiodic tilings are typically built from two or more types of tiles. Again, the choice of these tiles is not unique, and, furthermore, there is nothing like a preserved fundamental volume. As an example, one may consider the Penrose tilings, of which there exist several variants,[2] such as the Penrose kite and dart tilings, Penrose rhombus tilings, and Penrose tilings by Robinson triangles. All these variants, although looking quite different from each other, are equivalent and have the same basic structure: they can be locally derived from each other.

Let us now give a more formal definition of local derivability. We shall formulate the definition for tilings, but, in fact, the same definition can be used also for more general discrete structures, constructed from translations of a finite number of (bounded) objects. In the case of a tiling, these objects are the tiles, but later on we shall consider also discrete structures whose constituent objects are atoms, and one might think of still other kinds of objects forming discrete structures to which it makes sense to apply the concept of local derivability. The only requirement we shall impose on these discrete structures is that they are locally finite. This means that for any $d > 0$ (and up to translations) the number of different configurations of diameter d occurring in the structure is finite, where configurations are supposed to consist of entire objects.

Let $B_{R,q}$ denote the ball of radius R around q. The restriction of a tiling to this ball is defined to consist of all (entire) tiles which touch the ball. Suppose now that two tilings, $\mathcal{T}_1$ and $\mathcal{T}_2$, are given. If there exists a superposition of the two tilings, possibly after rescaling and/or rotating one of them, such that for any ball $B_{R,q}$ tiling $\mathcal{T}_1$ restricted to this ball is uniquely determined by tiling $\mathcal{T}_2$ restricted to the larger ball $B_{R_{21}+R,q}$, with a value of R_{21} which is uniform in R and q, then tiling $\mathcal{T}_1$ is said to be locally derivable from tiling $\mathcal{T}_2$. R_{21} is called the *derivability radius* (for the direction $2 \rightarrow 1$). We remark that it is even sufficient to require this relationship between local neighborhoods for $R = 0$, from which the corresponding relations for general R follow immediately. If, for the same superposition, tiling $\mathcal{T}_2$ is also locally derivable from tiling $\mathcal{T}_1$, with a derivability radius R_{12} which may be different from R_{21}, we say that the two tilings are *mutually locally derivable*, or *locally derivable from each other*. In other words, if two tilings are mutually locally derivable, then there exists a unique, local correspondence between local neighborhoods in the two tilings. If this correspondence between local neighborhoods moreover preserves the symmetry of these neighborhoods, then the local derivability is called *symmetric*. In the following, we shall drop the term symmetric, implying that we always mean symmetric local derivability. It may happen that local derivability exists only in one direction, but not in the other. In this case, two situations have to be distinguished: there may be real loss of information in the derivation in one direction, so that it cannot be inverted, or there may be no loss of information, but loss of local information, so that the information is still present, but can not be accessed in a local way. In this latter case we may say that one of the two derivability radii is infinite.

Mutual local derivability is an equivalence relation between tilings [or, more generally, between local isomorphism (LI) classes of tilings; see below]. It has been widely used to classify tilings into groups of equivalent ones. We have already mentioned the different variants of Penrose tilings, which are all mutually locally derivable.[2] Other examples include a class of dodecagonal tilings[13,8] containing very many, astonishingly different-looking variants, which nevertheless are all equivalent to each other. Similarly, such classes can be built from octagonal tilings[8] and from decagonal tilings,[12,8] as well as from icosahedral tilings.[14,15]

An interesting application of local derivability concerns the question of decoration with arrows and other markers of certain tilings. For example, it can be shown that the well-known decoration with arrows of the Penrose rhombus tilings does not introduce any new local information: the decorated and the undecorated Penrose rhombus tilings are locally derivable from each other. There are other decagonal tilings whose decoration is redundant in the same sense: it can be recovered from the undecorated tiling in a local way.[8] For many octagonal and dodecagonal tilings, the situation is different: their decorations, needed for formulating the matching rules (see below), cannot be locally recovered from the undecorated tiling, and are thus not redundant.[7] Nevertheless, in the octagonal and dodecagonal cases also it is possible to construct simple, undecorated tilings containing all the local information of the aforementioned decorated ones already in their vertex set.[8] But even if the decoration can be locally derived from the undecorated tiling, the

derivability radius may be rather large,[8] so that the decoration may code local information that was dispersed over much larger regions in the undecorated tiling. We shall return to these questions when we discuss perfect matching rules.

III. MATCHING RULES FOR TILINGS AND ATOMIC STRUCTURES

Perfect matching rules for quasiperiodic tilings are constraints on the local neighborhoods allowed in a tiling, which, when satisfied everywhere in a given infinite tiling, ensure that the tiling is perfectly quasiperiodic and belongs to a unique LI class (to be defined below). These matching rules should not be confused with growth rules, which would allow one to successively grow a tiling by adding tiles according to the rules. Local growth rules usually do not exist without leading to potential contradictions. The matching rules considered in this paper only allow one to check whether an infinite tiling, after it has been built, is a perfectly quasiperiodic one.

First we give some formal definitions. We shall essentially use the formulation of Levitov,[5] which appears to be best suited for our purposes. The set of all tiles in a tiling which overlap with a ball $B_{R,q}$ is called an *R-map* of the tiling. Note that for any given $R \geq 0$, only finitely many different R-maps can occur in the tiling (we assume here that there are only finitely many prototiles). All R-maps together constitute the *R-atlas* of the tiling. Two tilings for which the R-atlases agree for all $R \geq 0$ are called *locally isomorphic*. This means that any finite subset of one tiling occurs also in the other tiling, and vice versa. The set of all tilings which are locally isomorphic to a given one is called its *local isomorphism class*, or *LI class* for short. Particularly interesting LI classes of tilings are those for which it is not necessary to specify all the R-atlases, but only R-atlases up to some given, finite R_{mr}. It can then be checked by local inspection of all R_{mr}-neighborhoods whether a given tiling belongs to such a LI class. Tilings with this property are said to be *locally characterizable*. The corresponding matching rules, or the local characterization, consist of the R_{mr}-atlas of the LI class, and R_{mr} is called the range or radius of the matching rules.

It should be emphasized that the kind of matching rules described above, which enforce tilings from a single LI class, are the strongest matching rules possible. Such matching rules have been called *perfect matching rules* by Ingersent,[11] extending an earlier hierarchy of matching rules given by Levitov.[5] We also note that the concept of perfect matching rules does not only apply to quasiperiodic tilings. It is, in fact, a very general concept: perfect matching rules just are required to enforce tilings from a single LI class, which may be a LI class of any kind of tilings. In this paper, however, we shall restrict ourselves to quasiperiodic tilings, and we shall consider only perfect matching rules, which are the only ones which can be transferred to other tilings by means of local derivation (see next section). The proof that an R-atlas completely specifies a unique local isomorphism class is usually done by making use of the self-similarity present in many quasiperiodic tilings.[1–3,7,8]

We remark that from the definition of LI classes it follows that, if two tilings from different LI classes are locally derivable from each other, then the local derivability can readily be extended to the whole LI classes of the two tilings, providing a bijection between the two LI classes. This bijection assigns to each tiling in one LI class a unique partner tiling in the other LI class, such that the two tilings are locally derivable from each other. Local derivability therefore not only is an equivalence relation between tilings, but, in fact, an equivalence relation between LI classes of tilings.

All the concepts introduced above, such as the formulation of matching rules in terms of a finite R-atlas completely characterizing a LI class of tilings, can easily be extended to more general discrete structures. In fact, these concepts apply to any locally finite discrete structure, consisting of finitely many types of bounded objects. In particular, for the constituent objects of the discrete structure, which play the roles of the tiles, we can take atoms, thereby obtaining a very natural characterization of an atomic structure in terms of an R-atlas of local neighborhoods of atoms. It then makes perfect sense to ask whether a finite R-atlas already fixes the local isomorphism class of an atomic structure, and what the minimal radius of such an atlas is.

IV. MUTUAL LOCAL DERIVABILITY AND MATCHING RULES

Local derivability can now be used to transfer perfect matching rules for one tiling to other tilings in the same local derivability class.[8] Suppose two tilings, $\mathcal{T}_1$ and $\mathcal{T}_2$, are given, which are locally derivable from each other, with derivability radii R_{12} and R_{21}, and assume that tiling $\mathcal{T}_2$ allows for perfect matching rules with radius R_2. The idea then is to pull this local characterization back to $\mathcal{T}_1$. Recall that any $(R_{12}+R')$-map of $\mathcal{T}_1$ uniquely determines the corresponding R'-map of $\mathcal{T}_2$ centered at the same point. If we choose $R' > R_2$, then every tiling $\mathcal{T}$ containing only $(R_{12} + R')$-maps from $\mathcal{T}_1$ can locally be transformed into a tiling in which only R_2-maps from $\mathcal{T}_2$ occur, and which therefore, since the LI class of $\mathcal{T}_2$ is completely characterized by its R_2-atlas, must be locally isomorphic to $\mathcal{T}_2$. This is, however, not yet sufficient, in general, to ensure the tiling $\mathcal{T}$ to be in the same LI class as $\mathcal{T}_1$. In fact, the derivation from $\mathcal{T}$ to $\mathcal{T}_2$ might not be one to one, or its inverse might not be local, so that we might have lost information or local information during the process. In order to avoid this we really need local derivability in *both* directions, and we have to require that R' is not only larger than R_2, but also strictly larger than R_{21}, the derivability radius in the inverse direction. If we do so, every $(R_{12} + R')$-map from $\mathcal{T}_1$ gives rise to a unique R'-map from $\mathcal{T}_2$, which in turn maps back into a unique R-map from $\mathcal{T}_1$ of some positive radius, which, due to the uniqueness of all the processes, is a submap of the one we started with. In other words, we need that $\mathcal{T}$ is uniquely mapped to $\mathcal{T}_2$, which in turn uniquely maps

back to $\mathcal{T}$. A more detailed analysis (which we shall skip here) reveals that under some circumstances one has to increase R' still further, so that we arrive at the following final result: there exists a finite radius $R_1 = R_{12} + R'$ such that the R_1-atlas of $\mathcal{T}_1$ completely determines its LI class, and we have an upper bound on the matching rule radius R_1 of $\mathcal{T}_1$:

$$R_1 \leq \max(R_2, R_{21}, d_2) + R_{12}, \tag{1}$$

where d_2 is the maximal diameter of the tiles in $\mathcal{T}_2$. A local characterization of a tiling can therefore be transferred to all members of its local derivability class, and for each case an upper bound for the matching rules can be obtained. This bound need not be optimal, however, which can already be seen from the fact that the upper bound (1) always increases under local derivation.

Local derivation has been used in several cases to transfer matching rules between tilings,[8] or to prove the equivalence of known matching rules for different tilings.[14,15] In particular, simple octagonal and dodecagonal tilings have been constructed[8] which are completely locally characterized by their vertex set alone. These tilings are in the same local derivability class as the decorated tilings constructed earlier,[3,6,7] the decorations of which are nonlocal and thus not redundant. Local derivation may also be used to relate matching rules for the same tiling, but using different decorations, or matching rules with and without decoration of the tiles.[8] As an example, we may consider again the Penrose rhombus tiling, the matching rules of which are usually formulated in terms of arrows on the tile edges that must match.[1] As explained in Sec. II, this arrow decoration is redundant: it can be locally recovered from the undecorated tiling, and therefore the undecorated Penrose rhombus tiling is locally characterizable as well. To locally characterize the undecorated Penrose tiling, it is sufficient to require that only the seven vertex neighborhoods of the Penrose tiling occur, and to give some further constraints on the environment of two of these vertex neighborhoods, which are labeled K and $S4$ by de Bruijn.[1] More precisely, if a vertex is of type K, its nearest-neighbor vetices which are located between two thick rhombs must be of type D, and if a vertex is of type $S4$, its nearest-neighbor vertices between two thick rhombs must be of type J. These vertex types are forced in the Penrose tiling. Other constraints are not needed. It is then easy to check that any rhombus tiling satisfying the above constraints can always consistently be arrowed, and thus is a genuine Penrose tiling.

Although local derivability gives only an upper bound on the new matching rule radius, this bound gives a hint that the range of matching rules may greatly vary between different decoration schemes. For instance, a decoration may code in a very local way information that was dispersed over rather large regions, so that with the decoration the range of the matching rules may be fairly small. Although the decoration may be redundant, in the sense that the decorated and the undecorated tiling are locally derivable from each other, a high price might have to be paid in terms of a much longer range of the matching rules if one wanted to do without decoration. The range of the matching rules therefore sensitively depends on the decoration scheme, which must be kept in mind when talking about the range of matching rules.

As explained in Sec. II, the definition of local derivability applies not only to tilings, but also to more general discrete structures. One just has to replace the tiles by the constituent objects of these structures. In particular, an atomic decoration of a tiling may be considered whose constituent objects are atoms, comprising their positions and the assignment of a chemical species for each atom. Therefore the tools described in this section can equally well be used to transfer a local characterization of a tiling to an atomic decoration of the tiling, provided the two are locally derivable from each other.

V. BINARY TILING QUASICRYSTALS

Binary tilings[16,17] are tilings by the two Penrose rhombs, but subject to certain conditions on the vertex neighborhoods that may occur. These conditions are chosen in such a way that binary tilings allow for a very simple and natural decoration with atoms of two different sizes. More specifically, small atoms are placed on acute corners of thick rhombs and on obtuse corners of thin rhombs, and big atoms are placed on all the remaining corners (Fig. 1). The matching condition then is that at any given vertex only rhomb corners decorated with the same atom type meet. For what follows, we note that any binary tiling and its vertex set, divided into positions of big and small atoms, are trivially locally derivable from each other. This derivability is so local that in the following we shall not always distinguish between the binary tiling and its atomic decoration.

The matching conditions just described are not very restrictive. There is an enormous number of tilings allowed by them, among them quasiperiodic, periodic, and completely disordered ones. If the interactions between the two types of atoms are sufficiently short range, so that only nearest neighbors interact, it can be shown[17] that atomic structures based on any binary tiling are all exactly degenerate. For this reason, binary tilings have been used as a very attractive example of random tilings,[18,19] in which the random tiling hypothesis is backed by the underlying atomic decoration.

In this paper, we show that appropriately chosen interactions of somewhat longer range can select much more restrictive classes of binary tilings. It is, in fact, possible to find finite range interactions for the two types of

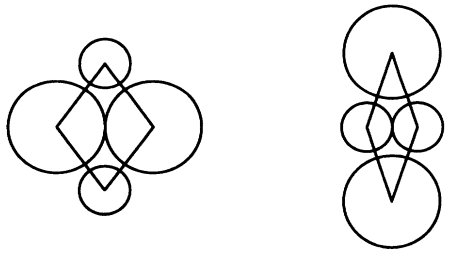

FIG. 1. Decoration scheme for the two binary tiling rhombs.

atoms which enforce a quasiperiodic ground state within a single LI class, i.e., one can find quasiperiodic binary tilings with perfect matching rules.

Before we present examples of binary tilings with matching rules we remark that binary tilings have successfully been used by Burkov[20] to model thermodynamically stable decagonal Al-Cu-Co quasicrystals. In Burkov's model, fairly big, partially interpenetrating clusters of atoms are placed on the vertices of a binary tiling. Since decagonal Al-Cu-Co quasicrystals are very perfect it seems unlikely that they can be explained by an underlying random binary tiling. On the other hand, the range of the matching rules we shall present is, taking into account the size of Burkov's clusters, not so short either that this would present a reasonable range of interatomic interactions. More recently, Burkov has presented a refined model,[21] which directly decorates the Tübingen triangle tiling,[22] with a decoration that enforces the matching rules of that tiling.

VI. MATCHING RULES FOR A BINARY TILING BASED ON THE TÜBINGEN TRIANGLE TILING

The decagonal Tübingen triangle tiling,[22] or simply triangle tiling, which is naturally obtained by dualization from the A_4 root lattice, gives rise to a binary tiling in a very simple way. Because of the simplicity of its atomic surfaces, we shall call it here the standard binary tiling. The vertex set of the triangle tiling, whose atomic surface is a regular decagon (Fig. 2), is identical to the set of big atom positions in the binary tiling. The positions of the small atoms are then easily obtained as the circumcenters of the large triangles. These small atoms give rise to two further atomic surfaces, two pentagonal stars (Fig. 2), which are located at positions of D_5 site symmetry, and which form together one orbit under the decagonal point group. Compared to the Penrose tiling, the decagon occupies the lattice nodes which are left empty in the Penrose tiling, whereas the pentagonal stars occupy the positions of the small pentagons of the Penrose tiling. While the standard binary tiling can be easily obtained from the triangle tiling, in the way just described, as a very local decoration of the triangle tiling, the derivation of the triangle tiling from the binary tiling is much more difficult and less local, although possible. We first observe that by connecting neighboring big atoms we can derive a tiling made by triangles, trapezoids, and pentagons. In order to recover the triangle tiling, the latter two tiles have to be split into big and small triangles, which can be done in several ways. The right choice can be determined by inspecting a rather large, but uniformly bounded region around the tile to be split.

Binary tilings based on the triangle tiling are interesting because the triangle tiling allows for perfect matching rules. Such matching rules have been described for a version of the tiling where tiles are decorated with arrows,[8] in which case it is enough to specify the allowed vertex neighborhoods in order to enforce quasiperiodicity. Since the arrows are locally derivable from the undecorated tiling,[8] matching rules exist also for the undecorated tiling. Their range is somewhat larger in that case, since one has to look at the second shell of tiles to determine the arrows from the undecorated triangle tiling. When one passes on to the binary tiling, however, even more local information is lost, so that rather large regions have to be inspected in order to recover the triangle tiling from the binary tiling.

The bound on the range of the matching rules so obtained is thus rather large, and it is, unfortunately, a nearly optimal bound. This can be seen by using an argument due to Levitov.[23] We have to look at the phason flips that occur when physical space cutting the atomic surfaces is moved in perpendicular space. When physical space is moved so that it leaves an atomic surface, then it enters at the same time another atomic surface, so that the atom belonging to that surface does not disappear, but just jumps to a nearby place. This is due to the closedness condition[24] satisfied by many quasiperiodic tilings, among them the triangle tiling. Since the

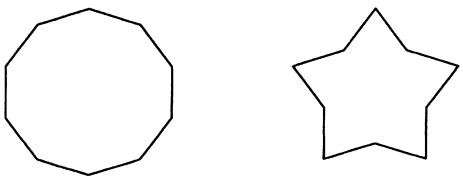

FIG. 2. Atomic surfaces for the standard binary tiling. The decagon is for the big atoms, the pentagonal star for the small atoms. The pentagonal star occurs at two positions, in two different orientations.

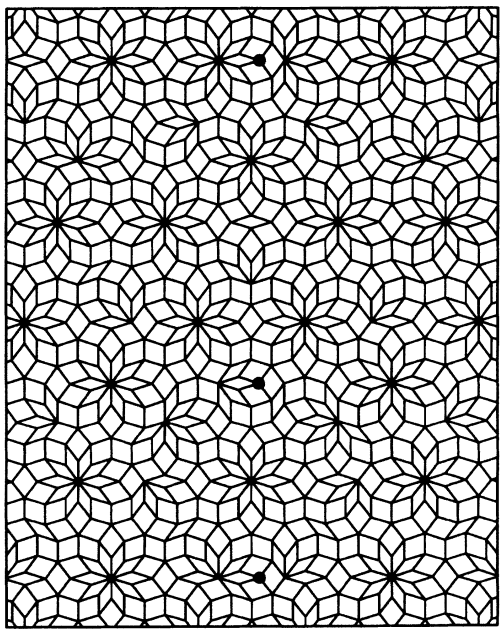

FIG. 3. Standard binary tiling. The large atoms which must jump simultaneously in a phason flip are marked. In such a flip, the interiors of octagons made of three thick and three thin rhombs are rearranged.

boundaries of the atomic surfaces are straight and parallel to rational directions of the decagonal module in perpendicular space, there is not only one atom that jumps on that occasion, but a whole row of atoms, a one-dimensional quasicrystal in fact. Such rows are usually called "worms." In the case of the Penrose tiling, such a worm is formed by a continuous row of tiles. In general, the density of this one-dimensional quasicrystal of atoms which jump simultaneously is determined by the length of the boundary of the atomic surface which is crossed. In the case under consideration, the row of large atoms which jump simultaneously is rather sparse. In Fig. 3, a large piece of a standard binary tiling is shown, where the big atoms which are about to jump are marked. Note that big and small atoms are tightly coupled: with each big atom, two small ones jump as well. These three atoms are in the interior of octagons made of three thick and three thin rhombs. As can be seen from Fig. 3, there are large distances between such groups of atoms, and their jumps must be correlated. In order that the matching rules can enforce this, their range must be at least half of the largest distance between two such groups of atoms. This defines a lower bound on the range of the matching rules, which in the present case is about equal to the upper bound obtained from local derivability, so that the true range of the matching rules is fairly well known.

VII. MATCHING RULES FOR A BINARY TILING BASED ON THE PENROSE TILING

Since the matching rule radius for the standard binary tiling presented in the last section is rather large, we have to look for other such structures, having shorter range matching rules. Good candidates appear to be binary tilings which are decorations of the Penrose tiling, because the Penrose tiling itself has extremely short range matching rules. As mentioned earlier, Penrose tilings are completely specified by local patches which go only marginally beyond vertex neighborhoods. Several kinds of binary tiling decorations of Penrose tilings have appeared in the literature.[16,17] In one of these decoration schemes,[16] the Penrose vertices are taken as positions of big atoms, and one more big atom is placed on the long diagonal of each thick Penrose rhomb, dividing it in the ratio τ:1. The positions of the small atoms are then fixed (Fig. 4). For each thick rhomb there are thus two possible choices for the position of the additional big atom in the interior, but for different rhombs these choices are not independent of each other: in two adjacent rhombs sharing an acute corner, not both additional atoms may be near that corner. Once a choice has been made for the big atoms, the positions of all the small atoms are completely determined.

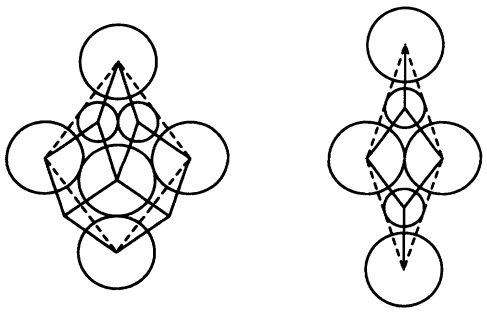

FIG. 4. The decoration of Penrose tiling rhombs with big and small atoms.

In this paper we are interested in a decoration which is as local as possible. We therefore base our choice of the positions of the additional big atoms on the vertex neighborhoods to which a thick rhomb belongs. The simplest choice appears to be the one depicted in Fig. 5. There are four vertices shown in Fig. 5, together with their as-

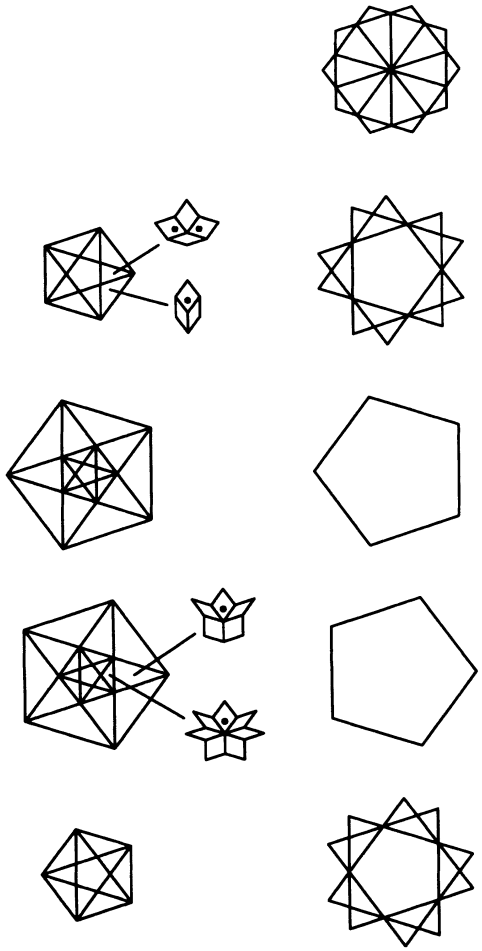

FIG. 5. On the left side, the acceptance domains of the Penrose tiling are shown, with their subdivision according to the vertex type. The four vertex types which are decorated with further big atoms are shown, together with the corresponding subwindows (vertices are not necessarily in the right orientation). The new, enlarged acceptance domains for the big atoms are shown on the right. The two triangles indicated in the big Penrose pentagon together form a spike, ten of which form the stellated decagon occurring at the position left empty in the Penrose tiling. The big Penrose pentagons remain as they are, whereas to every face of the small Penrose pentagons a crown is added. This crown is formed by triangles from the small Penrose pentagon. Note that two copies of the smaller one of these triangles are added, since the corresponding vertex is decorated with two additional atoms.

sociated subwindows of the Penrose tiling. Some of the thick rhombs in these vertex neighborhoods are marked by an additional big atom. The rule is that whenever a thick rhomb occurs in a vertex neighborhood in a position marked by an additional atom, then a big atom is added at the marked position. No atoms are added for vertex types not shown, or for rhombs not marked — these rhombs get their additional atom from a different vertex. Since every rhomb belongs to four vertex neighborhoods, this rule has to be checked for consistency: we have to make sure that every thick rhomb is decorated with exactly one atom, no more and no less. For the rule shown in Fig. 5, this is easy to check.

A binary tiling obtained according to this rule, with and without the original Penrose tiling superimposed, is shown in Figs. 6 and 7, respectively. We observe that the number of vertex types occurring in this tiling is six, three for small atoms and three for big atoms. There are thus fewer vertex types than in the standard binary tiling, where there were seven. The smaller number of local neighborhoods makes the tiling appear more homogeneous.

Since this Penrose binary tiling is locally derived from the Penrose tiling, its atomic surfaces can also be derived from those of the Penrose tiling. This is shown in Fig. 5. We see that, compared to the standard binary tiling, the single decagon for the big atom positions has been differentiated into 5 different atomic surfaces. The two pentagonal stars for the small atoms will split into ten different atomic surfaces, which are all congruent, but occur in ten different orientations, forming one orbit under the decagonal point group. This implies that the Penrose binary tiling can be viewed as a superstructure of the standard binary tiling. By additional ordering, its translation symmetry (in higher dimensional space) has

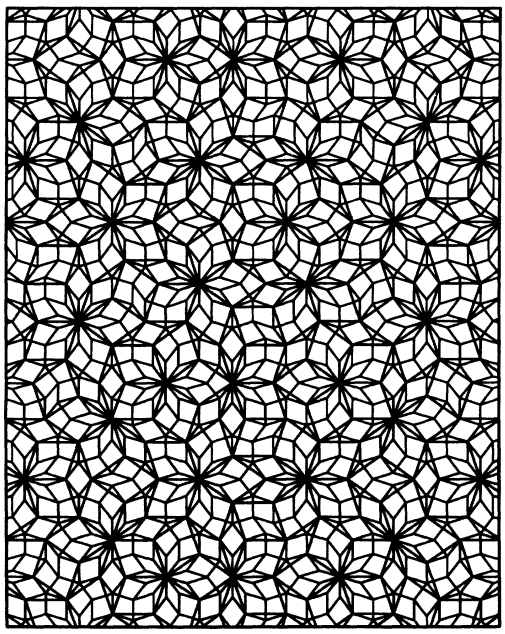

FIG. 6. Penrose binary tiling, with the underlying Penrose tiling superimposed.

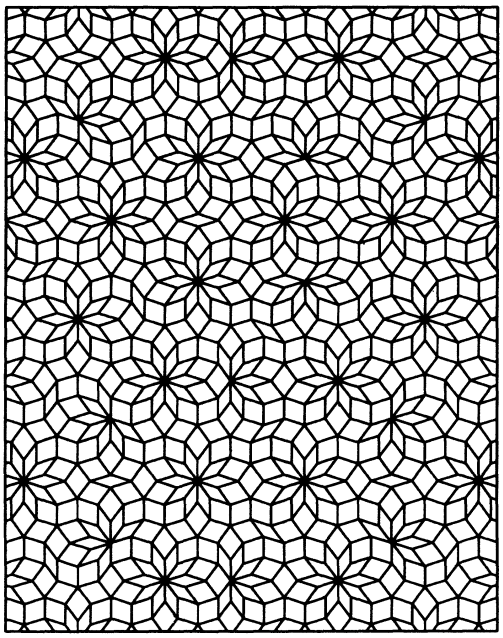

FIG. 7. Penrose binary tiling.

been broken to a sublattice of index five. It should be noted that the new atomic surfaces (Fig. 5) are heavily stellated and have long boundaries.

Let us also remark that the tiling derived by Lançon and Billard[16,17] is very similar to the Penrose binary tiling presented here. Lançon and Billard have added the additional big atom in the thick Penrose rhombs near the corner which is farthest from the diagonal of the rhombic icosahedron which serves as acceptance domain for the Penrose tiling in five dimensions. In their decoration scheme, the decagonal atomic surface is, in contrast to ours, not stellated. Instead, the stellation triangles fill some of the wedges in the other atomic surfaces for the large atoms. The atomic surfaces for the small atoms change accordingly. We have chosen a different decoration scheme because the locality of that of Lançon and Billard[16] was not immediately evident. Judging from the atomic surfaces, however, we conclude that their decoration is also local, although possibly with a larger derivability radius, and the resulting tiling definitely looks somewhat more complicated.

In order to make sure that our Penrose binary tiling possesses perfect matching rules, and to determine the radius of these matching rules, we have to be able to recover the Penrose tiling used for its construction in a local way. We do this in two steps. We first observe that the vertices where ten or seven thin rhombs meet form the vertices of a big Penrose tiling (Fig. 8). This is not the Penrose tiling we started with, but its second inflation. Since inflation and deflation are local processes for the Penrose tiling, we can then recover the original Penrose tiling in a local way, so that we have proved the existence of perfect matching rules. In order to determine the range of these matching rules it is easier, however, to directly consider the binary tiling as a decoration of the inflated Penrose tiling. This decoration

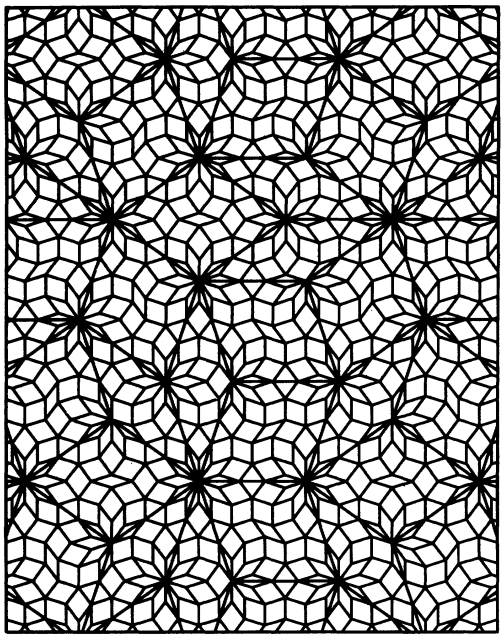

FIG. 8. Penrose binary tiling, with the doubly inflated Penrose tiling superimposed.

had earlier been considered[25] in a different context. The matching rule radius R_{mr} then basically is determined by the requirement that the inspection of R_{mr}-patches allows to check whether the binary tiling can be composed to a unique tiling of big Penrose rhombs, and that these Penrose rhombs form a Penrose tiling. To reconstruct a tiling of big Penrose rhombs, we need R_{mr} to be at least the edge length of the Penrose tiles, and to make sure that the big rhombs so constructed actually form a Penrose tiling, R_{mr} needs to be just marginally bigger. The reason is that the additional constraints on neighboring vertex types for the Penrose tiling can be checked very locally in the binary tiling. In the case of a Penrose vertex of type K, the neighboring Penrose vertices whose vertex type is constrained must be touched by exactly 7 binary thin rhombs, whereas in the case of a Penrose vertex of type $S4$, the corresponding neighboring vertices must be touched by 10 binary thin rhombs. This leads to a matching rule radius slightly bigger than the edge length of the big Penrose rhombs, which is considerably shorter than the matching rule radius of the standard binary tiling. We note that the above reasonning leads to a smaller matching rule radius than a naive application of the bound (1).

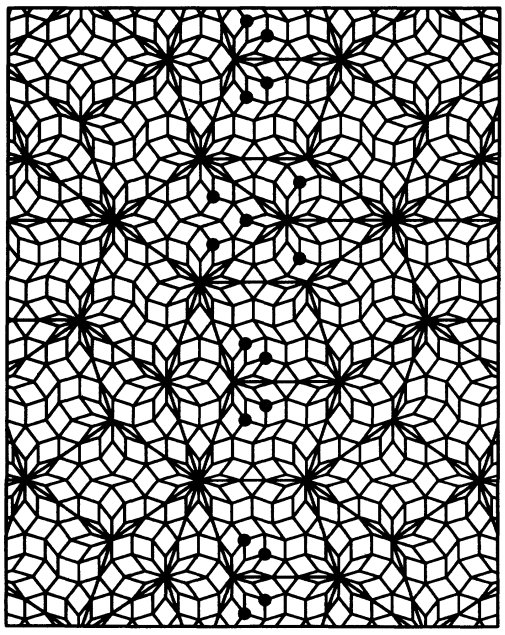

FIG. 9. Penrose binary tiling, with marks on big atoms jumping simultaneously.

As for the standard binary tiling, we can derive a lower bound on the matching rule radius for the Penrose binary tiling. In Fig. 9 we have marked the big atoms which have to flip simultaneously, because physical space leaves their respective atomic surfaces simultaneously when it is moved. We see that the longest distance ℓ between two such atoms is nearly twice the matching rule radius derived above. A closer analysis shows that the lower bound ℓ on twice the matching rule radius is not yet enough to ensure quasiperiodicity, since flipping only one-half of the "worm" does not lead to a configuration whose incorrectness could be detected in patches of diameter ℓ, so that ℓ has to be increased slightly, which leads again to the upper bound derived above.

VIII. DISCUSSION AND CONCLUSION

We have presented a general theory on how and under what conditions perfect matching rules for a quasiperiodic tiling can be transferred to an atomic decoration of the tiling, and an upper bound for the range of these matching rules has been derived. The general principles have then been illustrated with two examples from the class of binary tiling structures. Binary tilings seemed particularly interesting for this purpose because they have so far always been considered as the ideal example for a random tiling system.[18,19] Our work shows that, if the interactions are allowed to have a sufficiently long, yet still finite range, they can in principle be chosen in such a way that they can stabilize a quasiperiodic ground state at zero temperature — though it might not be easy to realize such interactions explicitly.

For our first example, the standard binary tiling, the range needed for the interactions is certainly unrealistically big, whereas for the second example it is perhaps rather big, but still within reasonable limits. Nevertheless, the list of patches that have to be energetically favored against all other configurations even in this case grows rather long, so that fairly complicated and finely tuned interactions will be needed. Some of these interactions might also involve several atoms at a time, i.e., they might not be pure two-body interactions. It should be kept in mind, however, that our examples, which are two dimensional and thus only a caricature of real quasicrystals, are not meant to be realistic models. They are rather meant for the laboratory of the theoretician, to il-

lustrate how the general principles work. On the other hand, it is well known that in complicated intermetallic compounds, such as quasicrystals, interactions *are* complicated. For instance, interatomic potentials have a rather long range and typically show oscillatory behavior (Friedel oscillations), and the electronic contribution to the energy, which is of a rather nonlocal nature, is believed to be of vital importance for these structure, so that our picture with complicated and relatively long range interactions appears not too unreasonable.

A closer analysis of the standard binary tiling shows that most of the structure is determined by much shorter range matching rules. There are only very few, infrequent local configurations whose correctness can be checked only by inspection of a neighborhood with the true matching rule radius. This means that by imposing much shorter range matching rules one could enforce a structure which is perhaps not perfectly quasiperiodic (and certainly not restricted to a single LI class anymore), but which has a very low density of defects and thus could hardly be distinguished from a perfectly quasiperiodic state. By construction, such a structure would look perfect on all scales up to the radius of the matching rules used. For the Penrose binary tiling somewhat shorter range matching rules still might lead to a tiling of big Penrose rhombs. This tiling, however, would not be a Penrose tiling anymore, but rather some random tiling. Since the Penrose tiles are large, the randomness on the length scale of the binary tiling would still be rather small and not so easy to detect.

This leads us to a picture of a hierarchy of matching rules: for each radius R there are matching rules $\mathcal{M}_R$ which enforce that all clusters of radius up to R are among those which occur in the perfectly quasiperiodic tiling. With increasing R, the matching rules M_R become more and more restrictive, enforcing structures which approximate the ideal, quasiperiodic structure better and better, until, at some critical radius — the radius of perfect matching rules — they finally enforce the perfect structure. In order to obtain a structure that is practically indistinguishable from the perfect structure one possibly need not go that far, however. Such a hierarchy of matching rules would interpolate between a pure random tiling picture and a perfect matching rule picture. The degree of perfection of the structure that is obtained could be tuned to a large extent by the range of the matching rules that are imposed. On the other hand, such concepts could also be used to estimate the deviation of a given, defective structure from the ideal, quasiperiodic one.[26] The smaller the scale at which a defect can be detected, the higher is the importance of this defect, and the bigger is the violation of the perfect matching rules. Such a classification of defects makes sense in particular for structures which are nearly perfect.

Another important question is how structures must look if they should have short range matching rules. There are some necessary requirements in order that a structure allows for finite range matching rules at all,[5,27] but in addition to the mere existence of matching rules these moreover should be of short range, so that interactions enforcing them need not be too complicated. If we go through the many examples of quasiperiodic tilings for which matching rules are known, we see that many of them, in particular those with simple rules, have several atomic surfaces,[1,8,6,10,9] and for some the atomic surfaces are stellated. The latter is the case for Danzer's tiling,[10] which has particularly simple and short range rules, and the Penrose binary tiling presented in this paper, which, moreover, is a superstructure of a similar, but simpler tiling. It thus appears that short range matching rules, which means a simple structure in physical space, call for more complicated atomic surfaces, i.e., a more refined ordering of the structure. The empirical fact that atomic surfaces with long boundaries and with boundaries in many directions help make short range matching rules possible can be understood intuitively. It is again Levitov's argument[23] which comes into play: the longer the boundaries of the atomic surfaces, the more atoms must jump simultaneously in a phason flip. If the maximal distance between correlated phason flips is small, then mistakes in the correlation of these flips can be detected at small scales, which is necessary for short range matching rules to exist. Unfortunately, such complicated atomic surfaces are very difficult to determine experimentally,[28] so that it might prove impossible to confirm them in experiment. This then would leave us in the uncomfortable situation that we cannot decide whether the atomic surfaces are sufficiently complicated to support matching rules of reasonably short range, or whether we need to find another explanation for the perfectness of quasicrystals.

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