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Phase Defects and Order Parameter Space for Penrose Tilings

T.Sh. Misirpashaev(*)

Landau Institute for Theoretical Physics, 2 Kosygin St-t Moscow 117334, Russia

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Abstract. — A new invariant classifying phase defects of Penrose tilings is constructed. This invariant takes values in the group closely related to the fundamental group of a certain topological space, which is the image of the tiling itself under identifications dictated by matching rules. This space plays the role of the order parameter space for pentagonal quasicrystals. The invariant enables us to discriminate between mismatches of different directions.

1. Introduction

It is known that studying any regular ordered medium one cannot avoid the question of its structural defects. Defects are inevitably created under the most careful fabricating techniques, often being necessary to explain the most fundamental properties of materials (e.g., plasticity is explained with the aid of dislocations). Sometimes, they facilitate the growth of new phases. Finally, they give rise to the most striking properties of ordered matter (such as phenomena connected with the existence of vortices in liquid phases of He and superconductors).

Among all possible violations of a perfect structure those whose stability is dictated by some topological reasons are of the main interest. The topological theory of defects is especially well elaborated for media with broken continuous symmetry [1–3]. In this case the state of the medium at each point is characterized by a value of the order parameter that belongs to the relevant order parameter space P (also called the manifold of degenerate states). The problem of finding topological defects in a physical volume V then reduces to a homotopy classification of continuous mappings from V \ D to P where D is a point for pointlike defects, a line for linear defects, etc. For contractible volumes V the mappings are classified by elements of the appropriate homotopy group \( \pi_k(P) \) or by conjugation classes if \( k = 1 \), and \( \pi_1(P) \) is non-commutative. In particular, pointlike defects of a 2-dimensional matter are classified by conjugation classes in \( \pi_1(P) \).

One can also try to use a similar approach for ordered media that are essentially discrete, namely crystals and quasicrystals. Consider, for example, a flat 2-periodic lattice. Taking the quotient space of the plane by the group of translations of the lattice one obtains a torus. Elements of the fundamental group of the torus \( \pi_1(T^2) = \mathbb{Z}^2 \) consistently classify complete

(*) e-mail: missir@landau.ac.ru.

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dislocations of the lattice in terms of components of the Burgers vector. That is why one sometimes says that the torus is the relevant order parameter space, though important partial dislocations are not included, neither can complicated rearrangements of atomic planes observed in experiments be described in these terms. Even more serious difficulties arise in the case of quasicrystals [4, 5], in which apart from dislocations a variety of defects of matching rules called mismatches becomes possible. An attempt to build the general approach to the latter based on the homotopy theory was done in [4, 5]. Hereafter we present a concrete treatment specific for the case of a pentagonal quasicrystal. We disregard the atomic decoration of unit cells, studying only their packing arrangements, i.e., quasiperiodic tilings. Associated with ideal pentagonal quasicrystals are Penrose tilings of the plane [6], formed by two types of rhombi. In general, tilings corresponding to non-ideal quasicrystals may contain distorted rhombi, overlaps, and non-covered regions, characteristic for elastic (or phonon) defects [7]. Another class of defects (phase defects) arises because of non-trivial matching rules of Penrose tilings. Phase defects on which we focus our attention in this paper do not invoke any distortion of the tiling. From now on the word “tiling” will everywhere mean a tiling of a whole plane or its finite part by thick and thin rhombi of the Penrose tiling.

2. Mismatches of Penrose Tilings

It follows from the algebraic theory of Penrose tilings [6] that for an infinite tiling of a whole plane the two following statements are equivalent.

1) The tiling belongs to the local isomorphism class of Penrose tiling, which is the class \( \gamma = 0 \) in terms of references [6, 8].

2) A decoration of all edges of the tiling with simple and double arrows exists such that each thick and thin rhombi are decorated as shown in Figure 1.

One can, therefore, define an ideal tiling as a decorated tiling with matching arrows. While studying structural defects one always assumes that violations of the structure are not too drastic, i.e. that the ideal structure persists almost everywhere except for separate and localized defective regions. We thus restrict ourselves to the case of tilings that can be decorated with arrows in such a way that matching rules are satisfied almost everywhere except for small isolated clusters of mismatches. A primitive defect in this approach is a single isolated mismatch, that is an isolated edge that cannot be consistently decorated (Fig. 2). In many practically interesting cases only this kind of defects appears. In particular, there is a suitable way of obtaining defective tilings, which consists in applying the cut-and-projection method [9], the band or/and the multidimensional integer lattice being deformed. (Only deformations with no net displacement along the direction \((1, 1, 1, 1)\) should be considered in order for the tiling to stay in the same local isomorphism class.) One can show [10–12] that the only defects arising for small curvature deformations of the band are isolated mismatches. In particular, this is the case of approximants [13] that can be considered as defective quasicrystals with one mismatch per approximant unit cell [10]. Isolated mismatches are also the only defects which appear
outside the core of a dislocation, with a density decreasing as $1/r$.

Note that each isolated mismatch is situated on an edge connecting two vertices prohibited for Penrose tiling. (By vertex we mean the configuration of rhombi sharing the vertex point.) Disregarding the arrow decoration there are 7 different permitted vertices [6]. Isolated prohibited vertices are possible but they are not primary defects, as they come along with non-isolated mismatches and appear only for large curvature deformations of the band. We also note that each isolated mismatch is localized on such an edge that two adjacent rhombi demand different orientations of two simple arrows (not two double arrows or one simple and one double arrow). This fact which can be verified directly will be given below a topological explanation.

Isolated mismatches can be created in pairs with the aid of a simple rearrangement of a previously ideal region of a tiling and can be moved by limited distances along "worms". This primary dynamics of primary defects probably plays an important role in the quasicrystal kinetics [10].

3. Topological Invariants for Mismatches

To show that a given defect is stable one should attribute a topological charge to it. To this end one can encircle the defect by a sufficiently large loop passing entirely through non-deformed regions. In order to be sure that the defect cannot dissipate involving only changes in the very vicinity of its core one should be able to detect its presence knowing only the local arrangement in the vicinity of the loop. This is done by assigning an element of a certain classifying group $G$ to each such loop so that elements assigned to homotopic loops are in the same conjugation class. Dissipation of such a defect, then, would involve rearrangements on a whole line joining the defect with another defect or with a boundary. The energy cost of such rearrangements guarantees the relative stability of the defect. In the case of tilings it is natural to consider loops which are broken lines, segments being the edges of the tiling. Such loops will be called tiling loops. Choosing a tiling loop that belongs to perfect regions, one can use arrows to construct invariants.

The simplest possibility [14] is to orient the loop and take the algebraic sum of all edges belonging to it, orientation of each edge being given by its arrow. An edge contributes $+1$ to the invariant if it is oriented along the loop and $-1$ otherwise. This commutative invariant

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**Fig. 2.** A piece of a tiling containing a single isolated mismatch. Bolded edge should carry a simple arrow but orientations of this arrow dictated by two adjacent tiles are contradictory.
Fig. 3. — A group generator $a, b, c, d, e$ $(A, B, C, D, E)$ is attributed to each edge in the corresponding direction, carrying simple (double) arrow. There are 10 different relations of "commutativity" of tiles. All 10 rhombi giving different relations are present in this figure, they form a decagon occurring in Penrose tilings. Instead of this decagon any other configuration of the same 10 rhombi could have been chosen. Vertices of type 1 are bolded.

$\sigma$ takes values in the group of integers $Z$ and assures the topological nature of mismatches that have $\sigma = \pm 2$, while it does not enable us to distinguish between mismatches of different directions. Nothing new is achieved if one counts separately simple and double arrows, which gives an invariant with values in a commutative group $Z^2$. Principally new invariants can be constructed with values in non-commutative groups.

To define the most general invariant we introduce $10 = 5 \times 2$ group generators $a, b, c, d, e, A, B, C, D, E$ corresponding to 5 possible orientations of an edge carrying a double or a single arrow. In order for invariant to be independent of the loop all rhombi of the tiling must be "commutative", which gives 10 relations

$$
\begin{align*}
ab^{-1} &= BA^{-1}, & ad^{-1} &= D^{-1}A, \\
bc^{-1} &= CB^{-1}, & db^{-1} &= B^{-1}D, \\
\text{cd}^{-1} &= DC^{-1}, & be^{-1} &= E^{-1}B, \\
d\text{e}^{-1} &= ED^{-1}, & ec^{-1} &= C^{-1}E, \\
\text{ea}^{-1} &= AE^{-1}, & ca^{-1} &= A^{-1}C
\end{align*}
$$

(Fig. 3). We have thus defined a non-commutative group $G$ of values of the invariant. To each defect of a tiling a certain conjugation class of $G$ corresponds [1].

Let $\gamma$ be an oriented tiling loop passing through ideal regions of the tiling. The element $g(\gamma)$ of $G$ attributed to $\gamma$ is defined as a formal product of generators attributed to segments of the loop in their sequence, the generator being replaced by its inverse if its orientation given by the arrow on the corresponding edge differs from the orientation of the loop (Fig. 4). This element is determined up to a conjugation because loops have no fixed origin. Obviously, absence of defects inside the loop entails that the invariant $g(\gamma) = 1$. We do not know whether the inverse is true, that is if this invariant is fine enough to detect any phase defect and distinguish between any pair of different defects. On the other hand, the group $G$ already looks quite complicated and the invariant hard to calculate. Some information can be obtained, however, by studying quotient groups of $G$. Let $F$ be a normal subgroup of $G$ and $H = G/F$ — the corresponding quotient group. Then to get an invariant with values in $H$ it is sufficient to replace the class of conjugation in $G$ of the element $g(\gamma)$ by the class of conjugation in $H$ of its coset $g(\gamma)F$. One thus obtains a "reduced" version of the invariant in which some information is lost but which may occur easier to treat. The simplest way of constructing quotient groups is to introduce additional relations. Each group, for example, can be "commuted" by adding to the defining relations those of commutativity of each pair of generators. One can see that commuting the
Fig. 4. — Definition of the general invariant. Take an arbitrary tiling loop that does not contain any mismatch. Choose arbitrarily an initial vertex and fix an orientation. Then the corresponding invariant is the conjugation class in G of a product of generators attributed to edges in their sequence, orientation being taken into account. E.g., the element attributed to the bolded loop oriented counterclockwise with the initial point Q equals $ae^{-1}Dbe^{-1}C^{-1}bd^{-1}Cae^{-1}Dbe^{-1}C^{-1}bd^{-1}C$, which is in the same class with $A^2$.

Group G one obtains $Z^2$ and the corresponding reduced invariant coincides with that introduced above. Putting further $a = A$ one obtains the invariant $\sigma$.

We will apply this scheme to construct 5 simple invariants that enable to distinguish isolated mismatches of different directions. It was mentioned above that isolated mismatches are always mismatches of simple arrows. Take the defective edge itself, passed from one end to another and back, as a loop defining the invariant. One thus obtains the following elements $A^{\pm 2}$, $B^{\pm 2}$, $C^{\pm 2}$, $D^{\pm 2}$, $E^{\pm 2}$ of the group G corresponding to isolated mismatches in 5 different directions. To get the invariants we impose additional relations

$$a = A, \quad b = B, \quad c = C, \quad d = D, \quad e = E$$

and one of the five following sets of relations (3a-e)

$$E = B = E^{-1} = B^{-1}, \quad C = D = 1$$

$$A = C = A^{-1} = C^{-1}, \quad D = E = 1$$

$$B = D = B^{-1} = D^{-1}, \quad E = A = 1$$

$$C = E = C^{-1} = E^{-1}, \quad A = B = 1$$

$$D = A = D^{-1} = A^{-1}, \quad B = C = 1$$

Consider, e.g., the resulting group $G_A$ defined by (1), (2) and (3a). It is engendered by two independent generators $A, B$ with relations

$$B^2 = 1, \quad BAB = A^{-1}$$

This group is isomorphic to the semidirect product of $Z_2$ and $Z$ and can be realized as the group of symmetries of the set $\{x \in Z\}$ of integer points on a line, $B : x \mapsto -x, \quad A : x \mapsto x + 1$. It follows that the order of $A$ is infinite and, in particular, $A^2 \neq 1$. Consequently, the invariant
in \( G_A \) assigned to a mismatch \( A^{\pm 2} \) is non-trivial, whereas invariants attributed to \( B^{\pm 2}, C^{\pm 2}, D^{\pm 2}, E^{\pm 2} \) are trivial. Repeating this consideration with groups \( G_B \),..., \( G_E \) defined by (1), (2) and (3b),..., (3e) one proves that all mismatches in different directions are different (and cannot annihilate).

An important property of Penrose tilings is the possibility of inflation and deflation transformations of ideal infinite tilings [6]. To deflate a tiling one cuts tiles into smaller pieces and then applies a scale transformation restoring the initial size of tiles, which is also possible for finite and even defective tilings. A finite tiling with a single mismatch becomes after deflation another tiling with a single mismatch in the same direction. Consequently, the deflation diminishes the density of defects by the factor \( \tau^2 \). In the algebraic language, deflation determines an endomorphism \( a \mapsto \tilde{a}, b \mapsto \tilde{b} \) of the group \( G \), where

\[
\tilde{a} = e^{-1}B^{-1}, \quad \tilde{A} = d^{-1}A^{-1}c, \\
\tilde{b} = a^{-1}C^{-1}, \quad \tilde{B} = e^{-1}B^{-1}d, \\
\tilde{c} = b^{-1}D^{-1}, \quad \tilde{C} = a^{-1}C^{-1}e, \\
\tilde{d} = c^{-1}E^{-1}, \quad \tilde{D} = b^{-1}D^{-1}a, \\
\tilde{e} = d^{-1}A^{-1}, \quad \tilde{E} = c^{-1}E^{-1}b.
\]

(4)

Geometrically, \( \tilde{a}, \tilde{b}, \ldots \) are generators attributed to old edges and arrows, while \( a, b, \ldots \) — generators on new edges and arrows (Fig. 5). One can see that this endomorphism conserves the invariants with values in groups \( G_{A}, \ldots, G_{E} \), which is in agreement with the statement that deflation does not change isolated mismatches.

4. Order Parameter Space

We are now going to give some geometrical interpretation of the invariant introduced above in a purely algebraic way. We will appeal to the general theory of cellular complexes [15]. For our purposes the following intuitive description of what a cellular complex \( C \) is will be sufficient. It is built inductively from cells of increasing dimensionality. First, take several points, which are 0-dimensional disks (0-cells). They form the 0-skeleton \( \text{sk}_0 \) of the complex \( C \) being built. Then take several segments, 1-dimensional disks (1-cells), and somehow attach their ends to 0-cells chosen in the previous step. This gives us the 1-skeleton \( \text{sk}_1 \) of the complex. After that take several 2-dimensional disks (2-cells), and attach their boundary circumferences to the
1-skeleton. Actually, at this stage a restriction for possible attachments arises, this restriction will be described below. We thus get the 2-skeleton sk\textsubscript{2} \textit{C}. Continuing this procedure up to cells of the highest dimensionality \( n \) (or infinitely for infinite-dimensional complexes) we get the whole cellular \( n \)-complex. The topology of the resulting space depends upon the quantities of cells of each dimension \( k \leq n \) and upon the mappings we have used to attach boundaries of \( \mathbb{P} \)-cells to \((k-1)\)-skeleta. The above-mentioned restriction for possible attachments is the following. An attachment of any new \( k \)-cell is some mapping \( F \) from its boundary \( \partial D^k = S^{k-1} \) to \( sk_{k-1} \textit{C} \) (called attaching mapping). Consider the image of this mapping \( F(\partial D^k) \) in \( sk_{k-1} \textit{C} \). Let \( D^l \) be any \( l \)-cell in \( sk_{k-1} \textit{C} \), \( l \leq k - 1 \). We demand that either \( D^l \setminus \partial D^l \) is entirely inside the image \( F(\partial D^k) \) or has empty intersection with the image.

Consider Figure 3 as a cellular 2-complex assuming that edges marked by the same letters are identified along arrows. One can easily see that there remain 2 non-identical vertices (0-cells), 10 non-identical edges (1-cells), and 10 non-identical rhombi (2-cells). Denote \( \textit{P} \) the resulting topological space. Instead of the decagon in Figure 3 one could have considered the entire decorated Penrose tiling as a complex and then identify tiles of the same orientation along arrows. The resulting complex would be the same. We stress the fact that vertices of Penrose tilings fall into two types:

1) vertices in which at least one edge with a double arrow ends;
2) all other vertices, i.e. vertices in which edges carrying simple arrows can start and end while edges with double arrows can only start.

Edges with simple arrows connect vertices of type 2 and edges with double arrows go from type 2 to type 1 vertices. All the vertices of the same type are identified in \( \textit{P} \). Suppose that there is an isolated mismatch in the tiling. The presence of a single mismatch does not break the division of vertices into two types, therefore this is a mismatch of a simple arrow as was stated in Section 2.

The way we have defined the group \( \textit{G} \) almost coincides with the standard algorithm for a cellular calculation of \( \pi_1 \) [15]. This algorithm is based on the theorem which states that \( \pi_1(\textit{C}) = \pi_1(\textit{sk}_2 \textit{C}) \) for any cellular complex \( \textit{C} \), permitting to reduce the question to that for 2-complexes. We assume that \( \textit{C} \) is connected and the fixed point \( O \) in \( \textit{C} \) with respect to which we define \( \pi_1(\textit{C}) \) coincides with one of 0-cells. The fundamental group is found in terms of generators and relations in three steps.

1) For each 1-cell \( i \) choose an orientation and attribute a formal generator \( \alpha_i \).
2) For each 2-cell consider the corresponding attaching mapping \( S^1 \to \textit{sk}_1 \textit{C} \), decompose its image into the sequence of oriented 1-cells \( i_1 i_2 \ldots i_n \) (taking into account that some of 1-cells may enter more than once if the image contains multiple points), and add the relation \( \alpha_1 \alpha_2 \ldots \alpha_n = 1 \). Note that the restriction on possible attachments is important here.
3) For any 0-cell different from the fixed point \( O \) choose a path connecting it with \( O \) and consisting of oriented 1-cells \( j_1, j_2, \ldots, j_p \), and add the relation \( \alpha_{j_1} \alpha_{j_2} \ldots \alpha_{j_p} = 1 \).

The only distinction between groups \( \pi_1(\textit{P}) \) and \( \textit{G} \) arises on the third step of calculation of \( \pi_1(\textit{P}) \) from the fact that the cellular complex defining \( \textit{P} \) has 2 different 0-cells. It follows that in order to calculate \( \pi_1(\textit{P}) \) one has to contract one of the edges joining vertices of different types, e.g., just join the relation \( a = 1 \) to the relations (1).

Note that we have obtained the space \( \textit{P} \) from the Penrose tiling nearly in the same way as that we followed to get a torus from a periodic lattice, namely by some identifications of equivalent areas. This analogy together with an intimate connection between \( \pi_1(\textit{P}) \) and the group \( \textit{G} \) classifying defects suggests to call \( \textit{P} \) the order parameter space for pentagonal quasicrystals. The essential difference between periodic and quasiperiodic cases consists in the fact that the torus is the quotient space of a plane under the action of the group of translations \( \mathbb{Z}^2 \), while \( \textit{P} \) and the group \( \textit{G} \) do not admit such an interpretation. This means that we are
dealing with some generalization of the standard situation in which a discrete group acts on a homogeneous space. In the standard case the space is partitioned into disjoint fundamental regions, so that each of them contains no equivalent points, and any two can be identified by the action of some element of the discrete group. We see no straightforward analogy for the quasiperiodic case. A related complication is that our quotient space P is self-intersecting singular surface. Indeed, a simple inspection shows (see Fig. 3) that each edge of P is shared by 4 faces, instead of 2 as it should be for regular surfaces. Unfortunately, we do not possess any general theory of quasiperiodic group actions, and do not know whether such a theory exists.

Note that our candidate P for the order parameter space in the case of pentagonal symmetry does not coincide with rhombic icosahedron with identified opposite faces (RI), proposed in references [4, 5]. As a matter of fact, \( \pi_1(\text{RI}) = \mathbb{Z}^5 \) is commutative, while we believe that mismatches should be described by non-commutative invariants. The advantage of the approach adopted in [4, 5] consists in its generality, the drawback being the absence of clear connection with concrete phase defects. Our treatment has been empirical, since we have started from Penrose matching rules which are themselves empirical, but has permitted us to analyze mismatches. The problem consists in finding a geometrical derivation of Penrose matching rule. We believe that the notion of the order parameter space P will be helpful to achieve such a derivation.

5. Conclusions

We have constructed a new geometrical invariant for mismatches of Penrose tilings. The invariant takes values in a non-commutative group G which plays the role of the fundamental group of the order parameter space introduced for ordinary crystals and continuous media with broken symmetry. This group is closely related to the fundamental group of a certain space, which may be considered, therefore, as the relevant order parameter space. To any quotient group of G a reduced version of the invariant corresponds. We have shown using these simpler invariants that mismatches of different directions are topologically different. We do not know if this invariant permits a complete description of all phase defects of Penrose tilings. The relation with another approach to the topological defects, based on homology classes [16], also remains to be elucidated.

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