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An alternative view on quasicrystalline random tilings

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Abstract. We apply a framework for the description of random tilings without height representation, which was proposed recently, to the special case of quasicrystalline random tilings. Two important examples are discussed, thereby demonstrating the consistency of this alternative description with the conventional one. We also clarify the latter by deriving a group theoretic criterion for the validity of the first random tiling hypothesis.

1. Introduction

The systematic study of random tilings arose from the insight that they may serve as models for entropically stabilized quasicrystals [2, 3]. As such, they are an important and interesting alternative to the perfect tilings based upon the projection method. Although random tilings have been used intensively to study transport properties and dynamical properties of real quasicrystals, not much effort has been expended on deducing random tiling properties from general grounds [6, 7]. We mention the two random tiling hypotheses stated by Henley in 1991, which serve as a starting point to infer diffraction properties, using ideas of the Landau theory of phase transitions. Recently, a more general approach was investigated [8, 16, 17], mainly for two reasons. On the one hand, the concept of entropic stabilization applies also to crystalline solids which therefore should be included in a more general description. On the other hand, the quasicrystalline random tilings share a special feature which stems from the fact that these tilings are derived from the perfect ones: they have a height representation—each tiling can be embedded as a surface in a higher-dimensional space. Since tiling surfaces with equal (mean) density of prototiles have equal (mean) slope, the slope parameters can be used to describe the random tiling ensemble. This is the so-called *phason strain* parametrization which governs the conventional description.

This description has a number of shortcomings: first of all, it only allows the description of those random tilings which do allow a height representation—being the vanishing (though interesting) minority of all possible tilings. Second, symmetry analysis in this framework is constrained to *geometric* symmetries, whereas there may be other relevant symmetries of the tiling ensemble. An example are colour symmetries modelling chemical disorder, which has been shown to play an important role for real quasicrystals [9, 10]. Third, it was expected that a more general analysis could also clarify the origin of the random tiling hypotheses mentioned above.

This was the viewpoint which led to the random tiling description proposed in [16]. There, the grand-canonical tiling ensemble was considered where prototiles are energetically degenerate, and the chemical potentials of the different prototiles or their (mean) densities are

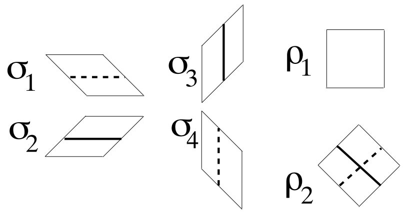

Figure 1. Prototiles of the Ammann–Beenker random tiling.

the only macroscopic parameters. It was explained how to perform a symmetry analysis in this framework. This led to a proof of a generalization of the first random tiling hypothesis which asserts that the point of maximum entropy is a point of maximum symmetry. In addition, the range of validity of the second hypothesis could be analysed using the grand-canonical setup, and an exactly solved (crystallographic) counterexample could be given. A rigorous treatment of diffraction is also possible using this setup [1].

The examples presented so far have been taken only from the crystallographic case. It remains to apply the proposed description scheme to quasicrystallographic random tilings and to show the consistency of the two approaches. That is the aim of this paper. Sections 2 and 3 are devoted to the description of two important examples of quasicrystallographic random tilings: the Ammann–Beenker tiling [14] and the square-triangle tiling [11, 12, 15, 18]. We perform a symmetry analysis along the lines of [16] and compare the approach with the conventional one, thereby showing the consistency of the two approaches. In the appendix, we briefly review and clarify the conventional description. We analyse the connection between maximal symmetry and vanishing phason strain and derive a group theoretic criterion. If the criterion is valid—which is the case in all examples we met—the first random tiling hypothesis is fulfilled in its original formulation: the point of maximum entropy is a point of maximum symmetry [16], and maximum symmetry in turn implies vanishing phason strain. A comparison of the two approaches concludes the paper.

2. The Ammann–Beenker random tiling

The prototiles of the Ammann–Beenker random tiling are two squares and four 45°-rhombi as shown in figure 1. There is no further matching rule apart from the face-to-face tiling condition, which imposes the relation $\sum \rho_i + \sum \sigma_i = 1$ on the prototile densities. Tilings can alternatively be viewed as world lines of particles of two different kinds, as is indicated by the decoration. It was shown in [14] that there is a nonlinear constraint among the different prototile densities which reduces the number of independent variables to four. This constraint was obtained using the height representation of this model, which is given below. It should be noted that it can be independently derived relating the tile description to the line interpretation. This method was introduced in [5]. The constraint reads

$$\rho_1\rho_2 = 2(\sigma_1\sigma_3 + \sigma_2\sigma_4). \tag{1}$$

The derivation imposes periodic boundary conditions. It is highly plausible that the constraint also holds (asymptotically) in the case of free boundary conditions, though there is no proof of this assumption. Complementarily, the line representation suggests four independent parameters since it is possible to fix the densities of different lines as well as their mean direction independently. Moreover, care has to be taken in choosing a set of independent parameters: the four rhombi densities, for example, allow the determination of the square densities only up to a permutation, due to the nonlinear constraint. This subtlety does not arise if, for example, three rhombi densities and one square density are chosen. The quadratic invariants given below are insensitive to this because only absolute values of square density differences occur.

At the point of maximum symmetry, the four rhombi densities and the two square densities have the same value. The nonlinear constraint fixes them to

$$\rho_i = \tfrac{1}{4} \qquad \sigma_i = \tfrac{1}{8}. \tag{2}$$

This is the point where the squares and the rhombi each occupy half of the tiled area. We determine the second-order expansion of the entropy density according to $\mathcal{D}_8$-symmetry. We introduce reduced prototile densities

$$r_i = \rho_i - \tfrac{1}{4} \qquad s_i = \sigma_i - \tfrac{1}{8} \tag{3}$$

such that the point of maximum symmetry is the origin. The vector space relevant for the symmetry analysis is obtained through *linearization* of the constraints. It is four-dimensional and determined by

$$r_1 + r_2 = 0 \qquad s_1 + s_2 + s_3 + s_4 = 0. \tag{4}$$

The analysis of the symmetries in the vector space of the independent, reduced prototile densities leads to a second-order entropy expansion of the form

$$s(r, s) = s_0 - \tfrac{1}{2} \sum_i \lambda_i I^{(i)}(r, s) + \cdots. \tag{5}$$

There are three (positive) elastic constants λ_i with invariants

$$\begin{aligned} I^{(1)}(r, s) &= 2r_1^2 \\ I^{(2)}(r, s) &= (s_1 + s_3)^2 \\ I^{(3)}(r, s) &= \tfrac{1}{2}(s_1 - s_3)^2 + \tfrac{1}{2}(s_1 + 2s_2 + s_3)^2. \end{aligned} \tag{6}$$

The elastic constants are obtained as expansion coefficients of the Hessian of the entropy in terms of projectors onto the irreducible subspaces of the symmetry group [16]. We now derive the relation to the elastic constants defined from the height representation approach. This is done by expressing expansion (5) in terms of the slope parameters of the height representation. The positions of tiling vertices belong, viewed as complex numbers, to the module $\mathbb{Z}[\xi]$ with $\xi = e^{2\pi \mathrm{i}/8}$. We characterize the height function algebraically. To this end, we recall some facts concerning the associated cyclotomic field [13]. ξ is a root of the eighth cyclotomic polynomial $P_8(x) = x^4 + 1$. The other roots are ξ^3, $\xi^5 = -\xi$ and $\xi^7 = \bar{\xi}$. The automorphism group on this set of primitive roots of unity is the Galois group $\mathcal{G} \simeq \mathcal{C}_2 \times \mathcal{C}_2$. The automorphisms can be uniquely extended to automorphisms of the corresponding module. The usual height function h on the set of possible vertex positions is defined by

$$h(\alpha) = \sigma(\alpha) \tag{7}$$

with $\alpha \in \mathbb{Z}[\xi]$, $\mathcal{G} \ni \sigma : \xi \mapsto \xi^5$. The set of all embedded vertex positions constitutes the four-dimensional primitive hypercubic lattice $\mathbb{Z}^4$, and each tiling corresponds to a two-dimensional surface. This is the geometric origin of the height representation. It is possible to define a height function on the prototiles by linear extrapolation of the height function on the corresponding vertices. The new macroscopic parameters to describe the tiling ensemble are the components of the *phason strain tensor*

$$E = \begin{pmatrix} E_{1,1} & E_{1,2} \\ E_{2,1} & E_{2,2} \end{pmatrix}$$

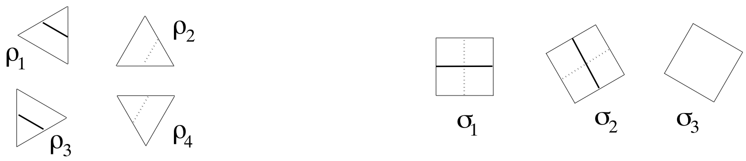

Figure 2. Prototiles of the square–triangle random tiling.

in Cartesian coordinates. The phason strain is defined as the (mean) slope of the height function. This leads to the relations

$$\begin{aligned} E_{1,1} &= \rho_1 - \rho_2 + (\sigma_1 + \sigma_2) - (\sigma_3 + \sigma_4) \\ E_{2,2} &= \rho_1 - \rho_2 - (\sigma_1 + \sigma_2) + (\sigma_3 + \sigma_4) \\ E_{1,2} &= 2(\sigma_4 - \sigma_3) \\ E_{2,1} &= 2(\sigma_1 - \sigma_2). \end{aligned} \tag{8}$$

We observe $E = 0$ at the point of maximal symmetry, which already follows from group theoretical considerations given in the appendix. In order to write the entropy expansion (5) in terms of the phason strain, the relation between phason strain and independent tile densities has to be invertible at the point of maximum symmetry. This is not the case if the four rhombi are taken as parameters. If three rhombi densities and one square density are taken instead, relation (8) is invertible in the whole phase space. This leads to an expansion

$$\begin{aligned} s(E) = s_0 &- \tfrac{1}{2}K_1(E_{1,1} + E_{2,2})^2 - \tfrac{1}{2}K_2(E_{1,2} - E_{2,1})^2 \\ &- \tfrac{1}{2}K_3((E_{1,1} - E_{2,2})^2 + (E_{1,2} + E_{2,1})^2) + \cdots \end{aligned} \tag{9}$$

which is the form appearing in the literature [14]. We find

$$\lambda_1 = 8K_1 > 0 \qquad \lambda_2 = 16K_2 > 0 \qquad \lambda_3 = 16K_3 > 0. \tag{10}$$

3. The square–triangle random tiling

The prototiles of this tiling are three squares and four equilateral triangles as shown in figure 2. We treat the model similarly to the example above, stressing important differences. The only matching rule is the face-to-face tiling condition, imposing the relation $\sum \rho_i + \sum \sigma_i = 1$ on the prototile densities. Triangles always occur in pairs, which is evident from the line decoration indicated in figure 2. This implies the relations $\rho_1 = \rho_3$ and $\rho_2 = \rho_4$ between the prototile densities. The nonlinear constraint [4]

$$16\rho_1\rho_2 = 3(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) \tag{11}$$

reduces the number of independent variables to three. This constraint, derived under the assumption of periodic boundary conditions, is believed to hold asymptotically in the case of free boundary conditions as well. This is supported by the observation that the line representation allows three independent parameters: the densities of the lines of different type and the frequency of one type of crossing. A set of independent parameters is given by two square densities and one triangle density. In order to derive the entropy expansion, we introduce reduced prototile densities

$$r_i = \rho_i - \tfrac{1}{8} \qquad s_i = \sigma_i - \tfrac{1}{6}. \tag{12}$$

Symmetry analysis with respect to the group $\mathcal{D}_{12}$ is done in the three-dimensional vector space given by the relations

$$r_1 + r_2 = 0 \qquad s_1 + s_2 + s_3 = 0. \tag{13}$$

Expansion (5) yields two elastic constants λ_i with invariants

$$\begin{aligned} I^{(r)}(r,s) &= 2r_1^2 \\ I^{(s)}(r,s) &= 2(s_1^2 + s_1 s_2 + s_2^2). \end{aligned} \tag{14}$$

Tiling vertices can be regarded as elements of the module $\mathbb{Z}[\xi]$ with $\xi = e^{2\pi i/12}$. The usual height function is defined using the transformation $\sigma : \xi \mapsto \xi^7$, which is a Galois automorphism on the set of primitive roots of unity of the 12th cyclotomic polynomial $P_{12}(x) = x^4 - x^2 + 1$ [13]. The coefficients of the phason strain tensor are

$$\begin{aligned} E_{1,1} &= \sigma_1 - \tfrac{1}{2}(\sigma_2 + \sigma_3) + (\rho_1 + \rho_3) - (\rho_2 + \rho_4) \\ E_{2,2} &= -\sigma_1 + \tfrac{1}{2}(\sigma_2 + \sigma_3) + (\rho_1 + \rho_3) - (\rho_2 + \rho_4) \\ E_{1,2} &= E_{2,1} = \tfrac{\sqrt{3}}{2}(\sigma_3 - \sigma_2). \end{aligned} \tag{15}$$

Since the model has three degrees of freedom, we expect a special property of the height function, reducing the number of independent slope parameters. This is the *irrotationality* property $\mathrm{Re}\,(\oint h(z)\,\mathrm{d}\bar{z}) = 0$ [15]. As a consequence, the off-diagonal elements of the phason strain tensor are equal. With the choice of independent parameters as above, (15) is invertible†. We arrive at the common expansion [15]

$$s(E) = s_0 - \tfrac{1}{2}K_\mu(\mathrm{tr}(E))^2 + \tfrac{1}{2}K_\xi \det(E) + \cdots. \tag{16}$$

The relation between the elastic constants is

$$\lambda_s = \tfrac{3}{2}K_\xi > 0 \qquad \lambda_r = 8(4K_\mu - K_\xi) > 0. \tag{17}$$

4. Conclusion

We have performed a symmetry analysis of well known planar quasicrystalline random tilings using the prototile density approach. We were able to show the consistency to the conventional approach via the height representation of these models. For the square–triangle tiling, the approach illuminated the irrotationality property whose appearance was rather unexpected before. Whereas it seems to be natural to describe random tilings using the prototile densities as macroscopic parameters, the approach is commonly hard to follow because it requires the knowledge of all (possibly nonlinear) constraints in order not to overestimate the number of elastic constants. The height representation, in turn, has the disadvantage that it is not obvious whether the slope parameters are independent and whether they constitute a sufficient set to describe all degrees of freedom of the ensemble. Furthermore, to describe other than geometric symmetries, one has to derive the relation between phason strain and the prototile densities explicitly. Therefore, the two approaches are in fact complementary in deriving properties of random tilings. The exactly solved eightfold random tiling, for example, must possess a constraint additional to the ones derived in [5], since the height representation and the density description yield different numbers of elastic constants otherwise, as can be shown. Research in this direction is in progress.

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† If the square densities are taken instead, (15) is not invertible in the phase with $\mathcal{C}_4$-symmetry.

Appendix: Symmetry and phason strain

We briefly deal with the symmetry analysis of random tilings which permit a height representation, in the framework of our viewpoint expressed elsewhere [16]. In particular, this will lead to a criterion for the validity of the first random tiling hypothesis [7] which states that the point of maximum entropy occurs at vanishing phason strain.

Let a random tiling ensemble of the $d_{||}$-dimensional vector space $V_{||}$ be given. A height representation assigns to each tiling a $d_{||}$-dimensional surface in a higher-dimensional vector space $V = V_{\|} \oplus V_{\perp}$ with the property that surfaces of tilings with equal prototile (mean) density have the same (mean) slope in V. In this situation, the (mean) surface slope can be used to parametrize the grand-canonical tiling ensemble. We discuss the influence of geometric symmetries on this description. The (mean) tiling slope can be represented by a linear map $E : V_{\|} \to V_{\perp}$, usually called *phason strain*. Symmetries are bijections on the (mean) prototile densities which leave the entropy density invariant. Let $D_{\|}$ denote the representation of the geometric symmetries in the physical space $V_{\|}$. The height representation induces a representation $D_{\perp}$ of the geometric symmetries in the internal space $V_{\perp}$. The phason strain tensor transforms under geometric symmetries according to

$$\tilde{E} = D_{\perp} E D_{||}^{-1}. \qquad (18)$$

We now focus on the point of maximum symmetry. E is invariant at this point, since this is by definition true of the (mean) prototile densities, which determine E uniquely. If the representations $D_{||}$ and $D_{\perp}$ are irreducible and not equivalent, Schur's lemma yields $E = 0$. In the general case we have

- The phason strain tensor vanishes at maximal symmetry if no irrep in internal space is equivalent to an irrep in physical space.

If this criterion is fulfilled, the first random tiling hypothesis in the formulation of Henley is satisfied since the point of maximum entropy is always a point of maximum symmetry, as shown in [16]. On the other hand, the criterion is fulfilled in all situations we met due to the special construction of the height function.

Symmetry analysis may alternatively be performed in the tensor product $V_{\|} \otimes V_{\perp}$, which is most advantageous when discussing the influence of symmetries on the entropy density. In this case, E is regarded as a vector with components of the matrix $E : V_{\|} \to V_{\perp}$. The geometric symmetries are represented via

$$\tilde{E} = D \cdot E = ((D_{\|}^{-1})^t \otimes D_{\perp}) \cdot E. \qquad (19)$$

Since the point of maximum symmetry is by definition a fixed point, we conclude:

- The phason strain at the point of maximum symmetry consists of components in direction to the trivial one-dimensional irreps of the representation in $V_{\|} \otimes V_{\perp}$.
- In particular, the phason strain vanishes at maximal symmetry, if the representation in $V_{\|} \otimes V_{\perp}$ does not contain trivial parts.

This criterion is equivalent to the statement given above, as follows from a closer look at the Clebsch–Gordan decomposition of the product representation. The second-order expansion of the entropy density is obtained by expanding the Hessian of the entropy in terms of projectors onto the irreducible subspaces of the symmetry group [16, 17].

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