TWO-DIMENSIONAL RANDOM TILINGS OF LARGE CODIMENSION

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Random tilings of the plane by rhombi are projections into the plane of corrugated two-dimensional surfaces in a higher dimensional hypercubic crystal. We consider tilings of $2D$-fold symmetry projected from D-dimensional space. Thermodynamic properties depend on the relative numbers of tiles with different angles and orientations, and also on the boundary conditions imposed on the tiling. Relative tile numbers define the average slope of the corrugated two-dimensional surface and hence the average phason strain. We study tilings with large codimension and fixed boundaries inside a regular $2D$-sided polygon with p rhombi on each side. For $D \to \infty$ we show that the thermodynamic properties become independent of p. Furthermore, we argue that the boundary conditions become thermodynamically irrelevant in the large D limit. For p=1 we use exact enumeration for D up to 10, and "mean field theory" arguments, to propose an upper bound for the random tiling entropy of log(2)=0.693 per tile. The entropy for finite D increases monotonically and reaches a limit slightly below this bound.

1 Introduction

The discovery of quasicrystals [1] motivated widespread investigation of tiling models. It is presumed that favored atomic motifs form geometrical tiles. These tiles may be arranged quasiperiodically in space to describe the quasicrystal structure. The suggestion that random tilings exhibit quasiperiodicity created a subfield within the area of tiling theory [2,3]. It was shown, for at least one atomistic model quasicrystal [4], that quasicrystalline order emerges with random tiling, rather than Penrose-like, order. The best description for real quasicrystalline materials remains an open problem.

In addition to their role in the theory of quasicrystals, random tiling models appear in a number of other scientific contexts. Their combinatorial properties, for example their relationship to generalized partitions [5,6] make them interesting models for study within pure mathematics [7]. Some provide examples of exactly solvable models [8,9] of interest within statistical mechanics. We note, in this paper, a relationship with algorithms for sorting lists [10,11]. Random tiling

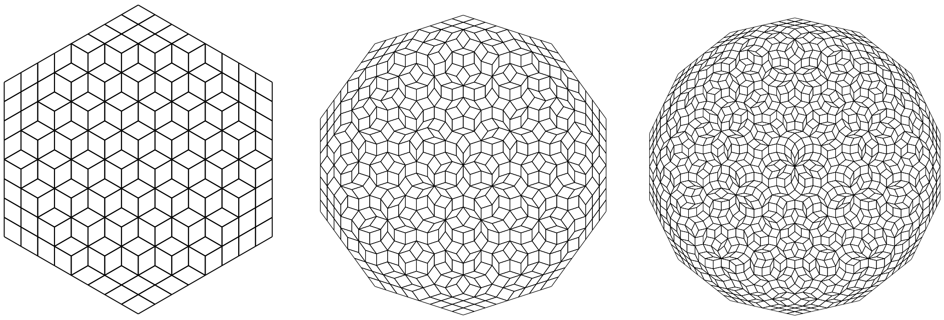

Figure 1: Example tilings of $2D$-gons of edge length $p = 8$ for $D = 3, 5$ and 7

models have also been proposed as models for elastic membranes [6,12].

The random tiling theory of quasicrystals focuses on two important properties: The tiling entropy contributes to the configurational entropy of the quasicrystal, reducing its free energy and enhancing thermodynamic stability against other competing phases [13]; Variation of the entropy with average phason strain defines the phason elastic constants. Techniques employed in theoretical studies include Monte Carlo computer simulation [14], numerical transfer matrix methods [15] and analytic exact solution [9]. For the models most relevant to quasicrystals (5 or 10-fold symmetry in two-dimensions and icosahedral symmetry in three-dimensions) only numerical analysis has proven successful.

The hope for an analytic approach to these complex problems motivates our study of random tiling models with high co-dimension. Tiling models are conveniently defined as projections from a higher D-dimensional lattice into a lower d-dimensional physical space. For example, 10-fold symmetric tilings may be projected from $D = 5$ into $d = 2$, and icosahedral tilings may be projected from $D = 6$ into $d = 3$. Figure 1 displays examples of tilings constructed as projections from D-dimensional simple cubic lattices into $d = 2$-dimensional physical space.

We anticipate [3] the limit $D \to \infty$ may prove easier to analyze than specific finite values of D. We argue that a conventional thermodynamic limit exists for tilings in the limit $D \to \infty$, while the entropy depends on boundary conditions for finite D tilings. We suggest the entropy density is spatially homogeneous, independent of tiling size and boundary conditions. Based on this analysis, we demonstrate that the entropy per tile remains finite as $D \to \infty$, and we derive an upper bound of $\log 2 = 0.693$ on the entropy of $D \to 2$ tilings. This paper presents only brief discussions of our main results. Further results and details may be found in a forthcoming publication [11].

2 Model

We define our $D \to 2$ tilings as projections from a D-dimensional simple cubic lattice into a $d = 2$-dimensional plane. The plane is selected, and the lattice scaled, so that the basis vectors of the cubic lattice project into unit vectors $\mathbf{e}_i$ belonging to a symmetric star. Faces of the simple cubic lattice project into rhombi with unit edge length whose internal angles are multiples of π/D. The tiles may be arranged in patterns with (exact or statistical) $2D$-fold rotational symmetry.

Figure 1 shows examples of such tilings. In this figure, the tilings are constrained to fill regular $2D$-gons with edge length $p = 8$. The value of p equals the number of de Bruijn[16] lines of each orientation running through the tiling. A de Bruijn line is the union of line segments joining parallel edges of adjacent rhombi. The orientation of the de Bruijn line refers to the orientation of these parallel edges. A de Bruijn line cannot cross another de Bruijn line of the same orientation. More general convex $2D$-gons may be filled by varying independently the numbers p_i of de Bruijn lines associated with tile edges of orientation $\mathbf{e}_i$. In the context of de Bruijn's grid construction, the constraint of filling a $2D$-gon amounts to demanding a full dualization of the de Bruijn grid in which all non-parallel lines eventually cross. These tilings are equivalent to generalized partitions[5,6].

Define the rhombus R_{ij} as a rhombus with edges parallel to $\mathbf{e}_i$ and $\mathbf{e}_j$. The rhombus defines the crossing of a de Bruijn line of family i with one of family j. In the general case with arbitrary p_i, the number of rhombi R_{ij} is the product $p_i p_j$. For simplicity we will focus on the case of boundaries which are regular $2D$-gons with all edges of length p. The total number of rhombi in this case equals

$$N_R(p, D) = p^2 \frac{D(D-1)}{2}. \tag{1}$$

Denoting the number of fixed boundary tilings $B_D(p)$, we define the entropy per tile

$$\sigma_{fixed}(p, D) \equiv \frac{\log B_D(p)}{N_R(p, D)}. \tag{2}$$

Generalizing the boundary condition, we may consider free-boundary tilings in which all non-overlapping, simply connected, arrangements of tiles are allowed. We denote the free boundary entropy $\sigma_{free}(p, D)$. Periodic and free boundary conditions give identical results in the limit of infinite area[17], and this value is independent of the sample shape.

An interesting fact about fixed boundary tilings, which we exploit in this paper, is that they are in one-to-one correspondence with equivalence classes

Table 1: Exact data for $p = 1$ tilings for $D = 1, 2, \cdots, 10$

D	1	2	3	4	5
B_D	1	1	2	8	62
$\sigma_{fixed}(D)$		0	0.231	0.347	0.413
B_{D+1}/B_D	1	2	4	7.75	14.65
D	6	7	8	9	10
B_D	908	24,698	1,232,944	112,018,190	18,410,581,880
$\sigma_{fixed}(D)$	0.454	0.482	0.501	0.515	0.525
B_{D+1}/B_D	27.20	49.92	90.85	164.35	

of sorting algorithms [10,11]. Tilings of the $2D$-gon with edge lengths $p_i = 1$ define networks for the sorting of D items. The general case with arbitrary p_i relates to the merging of D pre-sorted lists, each of length p_i. We exploit this relationship to obtain data on the numbers of tilings $B_D(p)$ for small values of D in the important special case with all $p_i = 1$ (see table 1). When $p = 1$ we occasionally drop it as an explicit argument. From the work of Knuth [10] we extract bounds on the entropy of the form

$$\frac{1}{3}\log 2 \leq \lim_{D \to \infty} \sigma_{fixed}(D) \leq 2\log 2. \tag{3}$$

3 Thermodynamic limit

Tiling models generally lack a proper thermodynamic limit. For example, Elser [18] showed that the entropy density of tilings confined within a hexagon is always lower than the value obtained with periodic boundary conditions [8]. Similar influence of the fixed boundary conditions is expected for models projected from higher values of D. Conventional thermodynamics [19] assumes that intensive thermodynamic quantities such as the entropy density exist independent of system boundary conditions and shape. It seems that these tiling models enjoy a conventional thermodynamic limit except when confined within $2D$-gons.

The source of the difficulty is evident from inspection of figure 1. Along the perimeters of the tilings we see nearly crystalline domains. Viewing the tiling as a membrane embedded in D-dimensional hyperspace [6], the tiling boundary serves as a frame over which the membrane is stretched. On average the frame lies parallel to physical space, but edges of the frame are inclined, forcing the membrane away from its preferred orientation near the boundary. In quasicrystalline terms, the fixed boundary condition forces large phason strains. Phason strains lower the tiling entropy, explaining the fact that fixed boundary entropies lie below the free boundary value. Hence

$$\sigma_{fixed}(p, D) \leq \sigma_{free}(p, D) \tag{4}$$

holds for all p and D. Indeed, these fixed boundary models provide an excellent way to study random tilings in the presence of strong, spatially varying, phason strain gradients.

Inspection of figure 1 suggests that the influence of the boundary may vanish as D increases. This may be demonstrated from the observation that a fraction $\alpha < 1$ of all the tiles in a fixed boundary tiling lie in regions of the tiling in which at least $\beta\ D$ de Bruijn line families cross, with β a finite valued function of α. As $D \to \infty$, the entropy within this fraction of the tiles approaches the free boundary entropy. Since these tiles comprise a subset of the fixed boundary tiling, we obtain the inequality

$$\alpha \lim_{D \to \infty} \sigma_{free}(p, D) < \lim_{D \to \infty} \sigma_{fixed}(p, D) \tag{5}$$

valid for any $\alpha < 1$. Taking the limit of equation (5) as $\alpha \to 1$, and comparing with equation (4) we observe[11]

$$\lim_{D\to\infty} \sigma_{fixed}(p, D) = \lim_{D\to\infty} \sigma_{free}(p, D) \tag{6}$$

implying the existence of a conventional thermodynamic limit.

Finally, we point out that the entropy density $\sigma_{free}(p, D)$ becomes independent of p in the limit $D \to \infty$. To see this, consider any fixed value of p in the limit $D \to \infty$. De Bruijn lines effectively repel each other, because of the non-crossing condition, so they tend to spread out with roughly uniform spacing. The diameter of the tiling comprises pD line segments and must accommodate p de Bruijn lines of each family. The mean distance between lines therefore grows as D. Assuming random walk statistics of de Bruijn line meandering, the interval along a de Bruijn line between successive contacts with a neighbor in the same family grows proportionally to D^2. The total number of contacts between de Bruijn lines within a given family varies as p^2/D. Among the set of all D de Bruijn line families, we expect p^2 such contacts. Each contact results in a loss of total entropy of order $\log 2$. To see the impact on entropy density, compare the number of contacts p^2 with equation (1) for the total number of tiles. The loss of entropy density due to de Bruijn line contact falls off as $1/D^2$, regardless of the value of p. In the limit of large D,

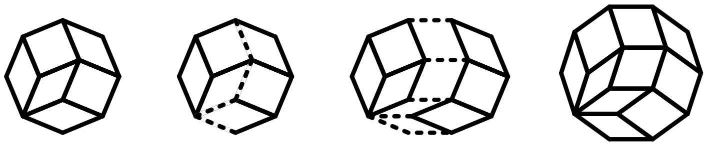

Figure 2: Bootstrap method for constructing a $D+1$ tiling from a D tiling.

the entire tiling becomes locally equivalent to a $p=1$ tiling, with the entropy density determined entirely by the number of distinct de Bruijn line families, and the entropy density loses any dependence on p. We exploit this fact by considering only $p=1$ tilings in the next section.

4 Upper bound

Figure 2 illustrates a method[5] to construct a fixed boundary tiling of dimension $D+1$ from one of dimension D. Starting from any tiling of dimension D, choose any path of length D along tile edges from the top of the tiling to the bottom. Cut the tiling along this path, separate the two parts by length 1, and draw new bonds connecting previously identical vertices. Finally, adjust all edge orientations to match the set of symmetry $D+1$.

This method of construction shows we can count the number of tilings projected from dimension $D+1$, using only information about the tilings projected from dimension D. Tilings at level $D+1$ are in one-to-one correspondence with {path,tiling} sets at level D. We relate the number of $D+1$ tilings to the mean number of paths on D tilings,

$$B_{D+1} = P_D B_D, \tag{7}$$

where the mean path count

$$P_D \equiv \frac{1}{B_D} \sum_{\tau=1}^{B_D} P_D(\tau) \tag{8}$$

and $P_D(\tau)$ is the number of top-to-bottom paths on the D tiling labeled τ.

Estimation of P_D is aided by our thermodynamic hypothesis. For large D, we suppose that among the B_D distinct tilings, the majority are statistically similar to each other, while there are a minority of exceptional cases[19]. The distribution of properties, such as the individual values of $P_D(\tau)$, should be sharply peaked near the mean value. In the limit $D \to \infty$ the distribution should approach a δ-function. This expectation is supported by numerical simulations [11]. It suffices, then, to calculate only one "typical" value of $P_D(i)$ to estimate the mean value.

To calculate a typical value of $P_D(\tau)$, consider the problem of constructing top-to-bottom paths on a typical tiling. Most of these paths travel through the bulk of the tiling, far from any boundary. At each step, the path may follow one or more routes. The only requirement is that the path segment leading out of a vertex must contain a downwards component. We estimate the number of paths as the product over vertices v of the number of choices $N_c(v)$ to be made at each step

$$P_D \approx \prod_{v=1}^{D} N_c(v). \tag{9}$$

Evaluation of equation (9) requires the distribution of values $N_c(v)$ along paths.

Because we do not know the distribution of values of $N_c(v)$, we settle for an estimate that yields an upper bound to P_D, and hence to $\sigma(D)$. Note that the product in equation (9) is the D^{th} power of the geometric mean of $N_c(v)$. The geometric mean of any set of positive numbers is bounded above by the arithmetic mean, reaching this bound only when all values are equal. The arithmetic mean $\bar{N}_c = \bar{Z}/2$, with $\bar{Z}$ the mean coordination number, because on average half the tile edges at each vertex have a vertical component in the southerly direction. From Euler's theorem applied to rhombus tilings with a boundary, we know $\bar{Z} \leq 4$. We deduce the upper bound $P_D \leq 2^D$ for typical tilings. This explains why the ratios B_{D+1}/B_D in table 1 increase by slightly less than a factor of 2 between successive values of D. Knuth [10] conjectures a related bound $P_D(\tau)$ expected to hold for all tilings τ. Iterating equation (7) it follows that $B_D \leq 2^{N_R(d)}$ and finally,

$$\sigma(D) = \frac{\log B_D}{N_R(D)} \leq \log 2. \tag{10}$$

From numerical path enumeration studies of generic higher codimension tilings we believe the true $D \to \infty$ limit lies about 15% below our bound (10).

In conclusion, we have established the existence of a thermodynamic limit for random tilings in the limit $D \to \infty$, and have proposed an upper bound of $\log 2$ on the entropy per tile. Topics for future investigation include variation of $\sigma_{free}(D)$ with D, and analysis of phason elasticity. Also of interest is the extension of our current theory to random tilings of three-dimensional space by rhombahedra.

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