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# The arctic octahedron phenomenon in three-dimensional codimension-one rhombohedral tilings

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**Abstract**

We calculate the configurational entropy of codimension-one three-dimensional random rhombus tilings. We use three-dimensional integer partitions to represent these tilings. We apply transition matrix Monte Carlo simulations to evaluate their entropy with high precision. We explore free- as well as fixed-boundary conditions and our numerical results suggest that the ratio of free- and fixed-boundary entropies is $\sigma_{\text{free}}/\sigma_{\text{fixed}} = 3/2$, and can be interpreted as the ratio of the volumes of two simple, nested, polyhedra. This ratio confirms a conjecture by Linde et al. concerning the 'arctic octahedron phenomenon' in three-dimensional codimension-one random tilings.


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## 1. Introduction

After the discovery of quasicrystals in 1984 [1], quasiperiodic and random rhombus tilings [2,3] have been extensively studied as models of quasicrystal structure. When tiles are appropriately decorated with atoms, random tilings become excellent candidates for modeling real quasicrystalline materials [4]. Therefore the statistical mechanics of random tilings is of fundamental interest for quasicrystal science. The relation between random tilings and integer partitions provides an important tool for the calculation of random tilings entropy [5–9]. Integer partitions are arrays of integers, together with suitable inequalities between these integers. One-to-one correspondences can be established between integer partitions and tilings of rhombi filling specified polyhedra. However, such strictly controlled 'fixed' boundary conditions inflict a non-trivial macroscopic effect on random tilings [5], even in the large-size limit, lowering the entropy per tile below the entropy with free or periodic boundary conditions. This effect a priori makes difficult a calculation of free-boundary entropies via the partition method. This boundary sensitivity is well described, for the simple case of hexagonal tilings [10,11], in terms of the spectacular 'arctic circle phenomenon': the constraint imposed by the boundary effectively freezes macroscopic regions near the boundary, where the tiling is periodic and has a vanishing entropy density. Outside these 'frozen' regions the entropy density is finite and we call the tiling 'unfrozen'. The boundary of the unfrozen region is a perfect circle inscribed in the hexagonal boundary. The entropy density varies smoothly within the unfrozen region, reaching a maximum equal to the free boundary entropy density at the center.

It was therefore tempting to analyze the 3d case. Since no exact solution is known for the free boundary case, one has to rely on numerical simulations. It has recently been conjectured by Linde et al. [12] that in dimensions higher than 2, the corresponding arctic region should be a polyhedron itself at the large size limit. It was further conjectured [13] that in this case the entropy density should be spatially uniform and maximal in the unfrozen region. These conjectures renew the

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interest for the partition method since the relation between both entropies becomes amazingly simple in this case. Note that, except for an early Ansatz [6] and some exact numerical results for small tilings [8], almost nothing is known about the entropy of codimension-one tilings of dimension $d > 2$.

The present paper proposes a numerical investigation of codimension-one three-dimensional tilings. A powerful transition matrix Monte Carlo algorithm enables us to achieve accurate estimates of both fixed- and free-boundary entropies. The latter is calculated via a modified partition method, which produces tilings with fixed boundaries that do not impose any strain to the tilings, thus generalizing a former two-dimensional approach [11]. Comparing both entropies, we support the above conjecture with good confidence. This paper is a shortened version of a more detailed one [14].

## 2. Partitions and tilings

Solid partitions are defined inside a three-dimensional array of sides $k_1 \times k_2 \times k_3$. Fix an integer $p > 0$, called the *height* of the partition problem. Put non-negative integers $n_{ijk}$ in the array, no larger than $p$, with the constraint that these integers decrease in each of the three directions of space. Four-dimensional hypercubes are stacked above the three-dimensional partition array, with the heights of the stacks equal to the corresponding parts. Then project into three dimensions along the (1,1,1,1) direction of the hypercubic lattice. The so-obtained tilings fill a polyhedron, a 'rhombic dodecahedron' (RD) of integral sides $k_1$, $k_2$, $k_3$ and $p$ (see the outer frame in Fig. 1). The total number of tiles is $N_t = k_1k_2k_3 + k_1k_2p + k_1k_3p + k_2k_3p$. We call tilings with rhombic dodecahedron boundaries 'RDB-tilings' and denote their configurational entropy per tile by $\sigma_{\text{fixed}}$.

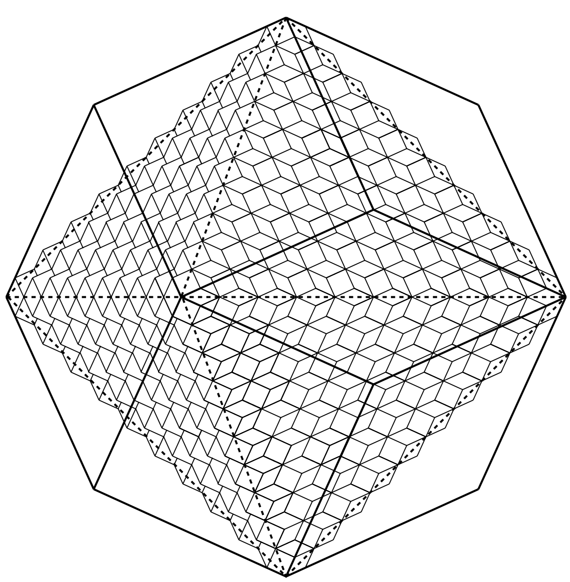

Fig. 1. The puckered octahedral boundary conditions nested inside the outer rhombic dodecahedron (RD).

Polyhedral boundary conditions, such as in the RDB tilings, have macroscopic effects on random tilings. In the 'thermodynamic limit' of large system size, the statistical ensemble is dominated by tilings which are fully random only inside a finite fraction of the full volume and are frozen in macroscopic domains. By frozen, we mean they exhibit simple periodic tilings in these domains with a vanishing contribution to the entropy. Therefore such boundary conditions are not very physical. Consequently, it is desirable to relate fixed boundary condition entropies to the more physical free boundary ones. To exploit the calculational advantages of a partition representation, while achieving the physical free-boundary entropy in the thermodynamic limit, we adapt the partition method so that the corresponding tilings exhibit no frozen regions. The new boundary, even though fixed, has no macroscopic effect on tiling entropy in the thermodynamic limit. The tilings become homogeneous, displaying the free-boundary entropy density throughout. The idea is to consider tilings (we focus on 'diagonal' tilings with $k_1 = k_2 = k_3 = p$) that fill a regular octahedron O instead of the rhombic dodecahedron RD. Eight vertices of the RD must be truncated to produce the O. We call tilings with octahedron boundaries OB-tilings. Such an octahedron is displayed in Fig. 1. It is inscribed in an RD and has puckered boundaries instead of flat ones. Despite this puckering, the boundaries are effectively flat in the thermodynamic limit. These OB-tilings are easily shown to have free boundary entropy. In terms of solid partitions, they are obtained by changing the boundary constraints [14]. The partition array is no longer a cube, but two opposite pyramidal corners have been truncated, leaving a slab of $D_{3d}$ symmetry. This slab contains $N_p = p^3 - (p-1)p(p+1)/3$ parts. For an original partition cube of sides $k_1 = k_2 = k_3 = p$, the full RD contains $N_t = 4p^3$ tiles. The O contains only $N_t = 4p^3 - 4(p-1)p(p+1)/3$ tiles.

In three dimensions, Linde et al. have recently explored numerically the typical shape of a RDB-tiling [12] and have been led to conjecture that the boundary of the frozen region is a regular octahedron, inscribed in RD like in Fig. 1. More precisely, the unfrozen region is not exactly an octahedron but tends to such a shape at the large size limit. This conjecture has a crucial consequence [13,14]: the statistical ensemble of RDB-tilings is dominated by tilings periodic outside O and random inside O, equivalently OB-tilings like in the previous section completed by eight periodically tiled pyramids to fill RD. Taking into account the tiles in the frozen regions to calculate an entropy per tile, one finally gets $\sigma_{\text{fixed}} = (N_{\text{O}}/N_{\text{RD}})\sigma_{\text{free}} = 2\sigma_{\text{free}}/3$, since the ratio of the numbers of tiles in RD and O is 3/2.

## 3. Monte carlo simulations

In this section, we calculate the above ratio via Monte Carlo simulations. We develop a variant of the transition matrix method [15] that couples a conventional Metropolis simulation with a novel data collection scheme to construct a numerical approximation of the *transition matrix:* For any legal partition $P = \{n_{ijk}\}$, we define its 'energy' as its total height, $E(P) = \sum_{i,j,k} n_{ijk}$. Single vertex flips increases or decreases by one unit a single variable $n_{ijk}$, resulting in an energy change $\Delta E = \pm 1$. For the boundary conditions employed here, the ground state (resp. the maximum energy state) is unique and we denote its energy as $E_{\min}$ (resp. $E_{\max}$). Our aim is to calculate $W(E)$, the total number of partitions with energy $E$, and to sum up on all energies to get the total number of partitions $Z = \sum_E W(E)$ (see Ref. [14]). Detailed balance requires that the total number of forward transitions from energy $E$ to energy $E+1$ must equal the total number of backwards transitions, hence $\omega_+(E)W(E) = \omega_-(E+1)W(E+1)$ where $\omega_+(E)$ and $\omega_-(E)$ are respectively the average numbers of backward and forward transitions per tiling of the energy level $E$. It is useful to rearrange the detailed balance equation to find $W(E+1) = W(E)\omega_+(E)/\omega_-(E+1)$. If the transitions $\omega_+$ and $\omega_-$ are estimated numerically, we can iteratively extract the full density of states $W(E)$ using the uniqueness of the ground state, $W(E_{\min}) = 1$. Finally, the total entropy is $S = \ln Z$, and the entropy density is $\sigma = S/N_t$.

To ensure that all energy levels are (almost) uniformly visited, we perform sweeps over temperature (for both negative and positive temperatures). Fig. 2 shows a plot of the number of partitions sampled as a function of $E$ during the longest runs for the $p = 4$ case, the number of hits exceeds $10^6$ uniformly for each energy $0 \leqslant E \leqslant 256$. The density of states $W(E)$ shown in Fig. 2 (center), is nearly a Gaussian. It reaches a peak value of $1.7 \times 10^{15}$ states at energy $E = 128$, and has a width of $\Delta E = 40$. As the system size grows this width grows more slowly than the number of tiles, so the density of states asymptotically approaches a delta function. The microcanonical entropy $S(E) = \log W(E)$ is plotted in the lower panel of Fig. 2.

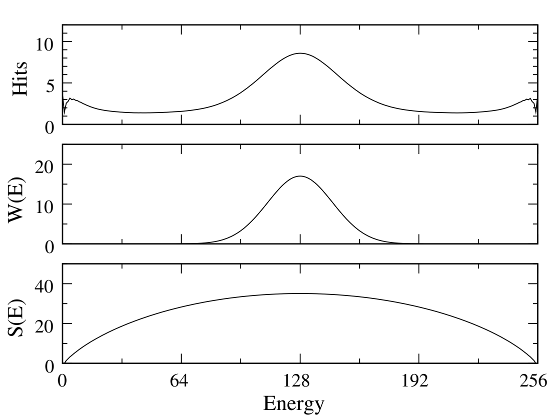


Fig. 2. Numerical data for $p = 4$ fixed boundary conditions. From top to bottom: number of sampled configurations; density of states; entropy.

Table 1
Finite-size entropies in function of $p$

| $p$ | $\sigma_{\text{free}}$ | $\sigma_{\text{fixed}}$ | $\sigma_{\text{free}}/\sigma_{\text{fixed}}$ |
|---|---|---|---|
| 1 | 0.1732868 | 0.1732868 | 1.000 |
| 2 | 0.1732868 | 0.1601239 | 1.080 |
| 3 | 0.17947(2) | 0.1545769 | 1.161 |
| 4 | 0.18455(6) | 0.1517949 | 1.216 |
| 5 | 0.18829(3) | 0.15017(2) | 1.254 |
| 6 | 0.19108(4) | 0.14918(6) | 1.281 |
| 7 | 0.19320(4) | 0.14848(1) | 1.301 |
| 8 | 0.19486(2) | 0.14780(1) | 1.318 |
| 9 | 0.19618(1) | 0.14762(2) | 1.329 |
| 10 | 0.19727(4) | 0.14735(5) | 1.339 |
| $\infty$ | 0.214(2) | 0.145(3) | 1.48(3) |

Values in parentheses are uncertainties in final digit. Values without uncertainties are exact.

In Table 1 are displayed our data for the system sizes studied. For both fixed and free boundary tilings, the data fit quite well to

$$\sigma_{\text{fixed}}(p) \simeq 0.145 - 0.0049\frac{\log(p)}{p} + \frac{0.034}{p}, \quad (1)$$

$$\sigma_{\text{free}}(p) \simeq 0.214 - 0.052\frac{\log(p)}{p} - \frac{0.046}{p}, \quad (2)$$

from which we conclude that $\sigma_{\text{fixed}} = 0.145(3)$ and $\sigma_{\text{free}} = 0.214(2)$. The presence and consequences of logarithmic corrections are discussed in Ref. [14]. The limiting ratio fits to $\sigma_{\text{free}}/\sigma_{\text{fixed}} = 1.48(3)$.

## 4. Conclusion

Returning to the arctic octahedron conjecture, we recall that a ratio $\sigma_{\text{free}}/\sigma_{\text{fixed}} = 3/2$ was expected. This fits our numerical results and supports the previous conjectures. This result emphasizes the important dimensional dependence of the spatial transition between the frozen and unfrozen regions. In 2d, the transition is continuous, since the entropy density is 0 by the arctic circle and then continuously varies to reach its maximum value near the center of the hexagon, with a non-zero gradient everywhere except near the center. By contrast, the situation seems to be radically different in 3d, where the entropy density is constant in the arctic octahedron O, with a vanishing gradient everywhere and a discontinuous transition at the boundary of O. This result (as well as its possible generalization to higher dimensions) is a strong support of the partition method, of which it was formerly believed that it could not easily provide relevant results about free boundary entropies. Indeed, provided the arctic region is polyhedral with a strain-free boundary, the ratio of both entropies is simply the ratio of the volumes of polytopes.

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