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DOI

[10.1103/PhysRevLett.76.2918](https://doi.org/10.1103/PhysRevLett.76.2918)

Publication date

1996

Published in

Physical Review Letters

[Link to publication](#)

Citation for published version (APA):

Nienhuis, B., & de Gier, J. C. (1996). Exact Solution of an Octagonal Random Tiling Model. *Physical Review Letters*, 76, 2918-2921. <https://doi.org/10.1103/PhysRevLett.76.2918>

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Exact Solution of an Octagonal Random Tiling Model

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(Received 16 November 1995)

We consider the two-dimensional random tiling model introduced by Cockayne, i.e., the ensemble of all possible coverings of the plane without gaps or overlaps with squares and various hexagons. At the appropriate relative densities the correlations have eightfold rotational symmetry. We reformulate the model in terms of a random tiling ensemble with identical rectangles and isosceles triangles. The partition function of this model can be calculated by diagonalizing a transfer matrix using the Bethe Ansatz (BA). The BA equations can be solved providing *exact* values of the entropy and elastic constants.

PACS numbers: 61.44.Br, 05.20.-y, 64.70.Rh

Since the discovery of quasicrystals, materials with noncrystallographic rotational symmetry and quasiperiodic translational order have been modeled by tilings. A tiling model consists of a set of elementary building blocks, tiles, that cover space without gaps or overlaps. One of the main questions concerning quasicrystalline alloys is their thermodynamic stability. It has been argued by several authors [1,2] that this may result partly from entropy associated with local random rearrangements of the tiles. One is then naturally led to study ensembles of “random tilings” [2].

It has been known for some time [3,4] that in two dimensions the square-triangle random tiling (RT) model, which has a twelvefold rotational symmetry, can be solved, i.e., its entropy and phason elastic constants can be calculated exactly. In this Letter we give the results of such a calculation for an eightfold symmetric RT model.

The model under consideration consists of squares and hexagons of arbitrary size, and was first introduced by Cockayne [5]. The hexagons are built out of rectangles with sides $1 : \sqrt{2}$ and a pair of isosceles and rectangular triangles. The squares can be viewed as two triangles. The model is therefore equivalent to a triangle-rectangle random tiling with an extra Boltzmann weight such that the two ways two triangles form a square are counted as one, i.e.,

$$\begin{array}{c} \diamond \\ \hline \diamond \end{array} + \begin{array}{c} \diamond \\ \hline \diamond \end{array} = \begin{array}{c} \diamond \\ \hline \diamond \end{array} .$$

There is a repulsive potential of $kT \log 2$ for each pair of triangles adjacent by their long edge. Since the configuration of vertices does not depend on which of the two diagonals is drawn in a square, the partition sum is precisely the sum of all vertex configurations, rather than of all tilings.

It is interesting to note that the perfect quasicrystalline square-hexagon tiling generated by an inflation rule [5] is in one-to-one correspondence with the binary octagonal tiling of squares and rhombi. Although the random tiling ensemble of the latter set of tiles has been studied [6],

no exact solution in the quasicrystalline phase has been found yet.

As in the square triangle tiling, we can set up a transfer matrix. This is done by decomposing the tiling into layers. Different layers are bounded by the short horizontal edges, the horizontal diagonals of the squares, and the almost horizontal diagonals of the $\pm \frac{\pi}{4}$ tilted rectangles. In addition, the layer edges cut the triangles and rectangles with a vertical long edge in half. In this way the tiles are deformed in such a way that the vertices of the tiling form a subset of those of the square lattice,

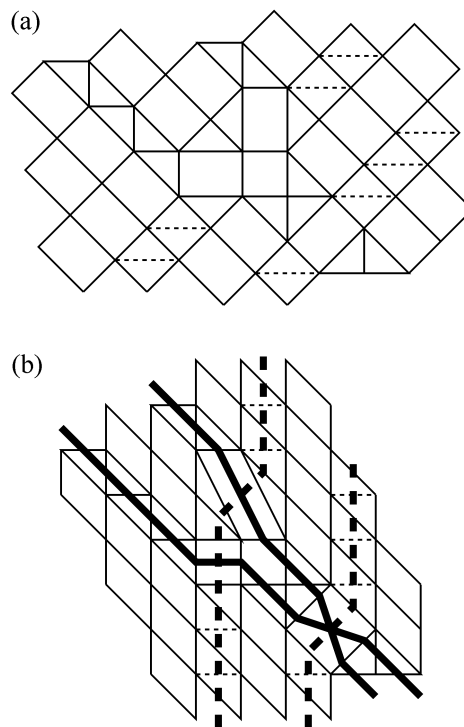


FIG. 1. (a) Patch of the tiling model. (b) Corresponding patch on the lattice. Bold solid lines are domain walls of horizontal short edges referred to as *s* walls in the text. Bold dashed lines represent the *l* walls of horizontal long edges.

see Fig. 1(b). The horizontal diagonals of the squares are denoted by the dashed lines in Fig. 1(a). A matrix element T_{ij} of the transfer matrix \mathbf{T} is 0 if layer j cannot be followed by layer i . Otherwise, it is given by the statistical weight of the layer i . In the following we will denote the tilted rectangles by R_{\pm} and the rectangles with the short and long horizontal edges by R_s and R_l , respectively.

Because different tiles of the original tiling are mapped onto the same shapes on the square lattice, we have to decorate the new configurations. This is done with bold dashed and solid lines, see Fig. 1(b). Thus it is clear that the horizontal short and long edges of the original tiling form domain walls, which we denote by type s and l , respectively. Between two layer edges on the square lattice, the s walls step one unit to the left and the l walls do not move. Two walls may cross in one of two ways: (i) The s wall may jump over the l wall moving two places to the left and thereby creating a rectangle R_l . (ii) Over two layers, the walls may exchange places creating a rectangle R_s . In the latter case the crossing therefore is completed after application of the transfer matrix twice. It may also happen that two walls of type s and one of type l cross simultaneously over two layers. The l wall and the s wall nearest to it then exchange place, while the second s wall jumps over both these walls moving three places to the left, creating a rectangle R_- .

We can express the tile densities in terms of the domain wall densities. We shall denote the horizontal size of the tiling by L and the corresponding system size of the lattice model by N . Let $\Delta_{ls} = R_l - R_s = 0$, i.e., both types of collisions of two domain walls occur with the same frequency, and let n_s and n_l be the number of s and l walls. Apply the transfer matrix $p = 2N - n_s$ times on some initial configuration of domain walls at $t = 0$ on the lattice, and suppose that both types of collisions occur for every pair of s and l walls. The final state at $t = 2N - n_s$ will then be the same configuration of domain walls as the initial one shifted by n_l . The total number of rectangles and triangles per layer can then be calculated to be

$$\begin{aligned} n_{\text{rect}} &= N - n_s - n_l + 2n_s n_l / p, \\ n_{\text{tri}} &= 2(n_s + n_l) - 6n_s n_l / p. \end{aligned} \quad (1)$$

The tile densities that belong to the quasicrystalline phase are $n_{\text{rect}}/N = 6 - 4\sqrt{2}$, $n_{\text{tri}}/N = 12\sqrt{2} - 16$, corresponding to an area fraction of triangles $\alpha_t = 1/2$.

As a function of the domain wall densities, the model displays two incommensurate phases. A fourfold symmetric phase is formed in the high density region, $\alpha_t > 1/2$, where the triangles form octagonal and square cells bounded by domain walls consisting of rectangles. There is a twofold symmetric phase in the low density region where the rectangles form rectangular cells bounded by domain walls consisting of triangles.

Like the square-triangle tiling, this tiling has the irrational property [7] which implies that, according to the random tiling hypotheses, the entropy density $\sigma_a = S/A$ has the following form:

$$\sigma_a = \sigma_{a,0} - \frac{1}{2}K_{\mu}(\text{Tr}\mathbf{E})^2 + \frac{1}{2}K_{\xi} \det\mathbf{E} + \mathcal{O}(\mathbf{E}^3), \quad (2)$$

where \mathbf{E} is the phason strain tensor. The conditions on the elastic constants for $\mathbf{E} = 0$ to be a local maximum are

$$K_{\mu} > 0, \quad K_{\xi} > 0, \quad 4K_{\mu} - K_{\xi} > 0. \quad (3)$$

We denote the deviations of the ideal tile densities by

$$\delta_{ls} = n_l \sqrt{2} - n_s, \quad (4)$$

$$\Delta_{\pm} = N - n_l - n_s. \quad (5)$$

The quadratic forms in (2) can be expressed in these:

$$\begin{aligned} (\text{Tr}\mathbf{E})^2 &= \frac{1}{L^2} [2\delta_{ls} - \Delta_{\pm}(2 - \sqrt{2}) - \Delta_{ls}(1 + \sqrt{2})]^2, \\ \det\mathbf{E} &= \frac{1}{L^2} \{ \delta_{ls}^2 - (2 - \sqrt{2})\Delta_{\pm}\delta_{ls} - 2\Delta_{\pm}^2\sqrt{2} \\ &\quad - (1 + \sqrt{2})\Delta_{ls}[\delta_{ls} - (1 - 1/\sqrt{2})\Delta_{\pm}] \}. \end{aligned} \quad (6)$$

The quantities n_s and n_l are conserved by the action of the transfer matrix \mathbf{T} . To control the average value of Δ_{ls} , the tiles R_s and R_l are given a weight $\exp(-\phi)$ and $\exp(\phi)$, respectively. Furthermore, as the tiles R_s and R_+ in the lattice representation have an area that is twice that of the other two transformed rectangles, we have to introduce a chemical potential for them to compensate for this asymmetry. The tiles R_s and R_+ therefore get an extra weight $\exp(\eta)$.

The free energy per layer of the lattice model is given by the logarithm of the largest eigenvalue of \mathbf{T} :

$$\begin{aligned} F(n_s, n_l, \phi) &= -\log\Lambda \\ &= -S - \phi\Delta_{ls} - \eta(n_{R_s} + n_{R_+}). \end{aligned} \quad (7)$$

We denote the horizontal coordinate of the i th s wall by ξ_i and of the k th l wall by z_k . The vertical coordinate is denoted by t . Let l_i be the total number of l walls to the left of the i th s wall, then the quantity $\xi_i + t + l_i \bmod 2$ is conserved for every s wall. This means that the s walls lie on a sublattice structure and split up into two kinds: odd and even ones. Denote their coordinates by x_i and y_j , respectively.

The eigenvectors of \mathbf{T} as a function of the coordinates x , y , and z of the domain walls are of the Bethe Ansatz form. If all the domain walls are separated, the Ansatz is

$$\sum_{\pi, \mu, \rho} A(\Gamma) \prod_{i=1}^{n_{s,o}} u_{\pi_i}^{x_i} \prod_{j=1}^{n_{s,e}} v_{\mu_j}^{y_j} \prod_{k=1}^{n_l} w_{\rho_k}^{z_k}. \quad (8)$$

The form of the eigenvector for configurations where domain walls cross can be found by application of \mathbf{T} on (8). Here, $w_k = \exp(iq_k)$, $u_i = \exp(ip_{o,i})$, and $v_j = \exp(ip_{e,j})$ are the exponentiated momenta; and ρ , π , and μ are the permutations of these belonging to the l and odd

and even s walls, respectively. The amplitudes A depend on the permutations ρ , π , and μ and on the configuration of the various domain walls. These together are coded in a vector Γ in the following way. Let \mathbf{r} be the vector of coordinates x_i , y_j , and z_k of all domain walls, ordered so that $r_m < r_{m+1}$. The entries of Γ are the elements of the permutations π , μ , and ρ . The order of succession in Γ of elements taken from π , μ , and ρ matches that of the elements of x , y , and z , respectively, in \mathbf{r} . So, for example, in the case of an odd s wall at x_1 and an l wall at z_1 we would have either $x_1 < z_1$ or $x_1 > z_1$. In the first case we write $\mathbf{r} = (x_1, z_1)$ with $\Gamma = (\pi_1, \rho_1)$, while in the second case $\mathbf{r} = (z_1, x_1)$ and $\Gamma = (\rho_1, \pi_1)$.

When the different domain walls are separated, the transfer matrix shifts all s walls to the left and leaves all l walls at rest, so the eigenvalue of \mathbf{T} must be

$$\Lambda = \prod_{i=1}^{n_{s,o}} u_i \prod_{j=1}^{n_{s,e}} v_j. \quad (9)$$

Inspecting the eigenvalue equations for the case that an s - and an l -domain wall collide, one sees that the amplitudes A before and after the collision must satisfy the following relation for (8) to be an eigenvector of \mathbf{T} :

$$\frac{A(\dots \pi_i, \rho_k \dots)}{A(\dots \rho_k, \pi_i \dots)} = (e^\phi u_{\pi_i} + e^{\eta-\phi} u_{\pi_i}^{-1} w_{\rho_k}^{-1}). \quad (10)$$

A same relation holds for the amplitudes with π_i replaced by μ_j and u replaced by v . From configurations involving three domain walls one deduces that interchanging domain walls of the same kind in the amplitude gives a factor -1 , and that interchanging an odd and an even s wall leaves the amplitude unchanged. The eigenvalue equations therefore do not mix the momenta of the even and odd s walls. It turns out that all relations among amplitudes involving more than two domain walls factorize into the ones already mentioned. These relations therefore suffice to make (8) an eigenvector of \mathbf{T} . Imposing periodic boundary conditions and eliminating the amplitudes A from the eigenvalue equations, one gets the following equations for the momenta:

$$\begin{aligned} u_i^L &= (-1)^{n_{s,o}-1} \prod_{k=1}^{n_l} (e^\phi u_i + e^{\eta-\phi} u_i^{-1} w_k^{-1}), \\ v_j^L &= (-1)^{n_{s,e}-1} \prod_{k=1}^{n_l} (e^\phi v_j + e^{\eta-\phi} v_j^{-1} w_k^{-1}), \\ w_k^{-L} &= (-1)^{n_l-1} \prod_{i=1}^{n_{s,o}} (e^\phi u_i + e^{\eta-\phi} u_i^{-1} w_k^{-1}) \\ &\quad \times \prod_{j=1}^{n_{s,e}} (e^\phi v_j + e^{\eta-\phi} v_j^{-1} w_k^{-1}). \end{aligned} \quad (11)$$

These are the so-called Bethe Ansatz equations (BAE). Like the BAE for the square-triangle tiling, these equations can be solved along a line in the thermodynamic limit for the largest eigenvalue. The details of this calcu-

lation, which resembles the one by Kalugin for the square-triangle tiling [4], will be published elsewhere. Here we give only the results.

The entropy can be calculated exactly in the entire regime $\alpha_t \geq 1/2$, $\Delta_\pm = \Delta_{ls} = 0$. In this region the three curves formed by the solutions of the BAE have the same limit point. After a change of variables, this limit point can be written in the notation of Kalugin as $b = i|b|e^{i\gamma}$. The tile densities and the area fraction can be expressed in γ :

$$n_l/N = 1 - n_s/N = \frac{1 - \sqrt{2} \sin \gamma/2}{1 + \sqrt{2} \cos \gamma/2}, \quad (12)$$

$$\alpha_t = (\sqrt{2} + 1) \frac{\sqrt{2} - \cos \gamma/2}{1 + \cos \gamma/2}. \quad (13)$$

The entropy per area of the square-hexagon random tiling in the regime $1/2 \leq \alpha_t \leq 1$ in terms of γ is

$$\begin{aligned} \sigma_a &= \frac{2 + \sqrt{2}}{4 \cos^2 \gamma/4} [\log(4/\cos \gamma) \\ &\quad + \cos(\pi/4 + \gamma/2) \log \tan(\pi/8 + \gamma/4) \\ &\quad + \cos(\pi/4 - \gamma/2) \log \tan(\pi/8 - \gamma/4)]. \end{aligned} \quad (14)$$

The entropy has its maximum at $\gamma = 0$. Expanding σ_a up to second order in γ results in

$$\begin{aligned} \sigma_a &= \sigma_{a,0} - \gamma^2 \frac{1 + \sqrt{2}}{32\sqrt{2}} \\ &\quad \times [4 - \log 4 - \sqrt{2} \log(1 + \sqrt{2})], \end{aligned} \quad (15)$$

where the residual entropy at $\gamma = 0$ is given by

$$\begin{aligned} \sigma_{a,0} &= \frac{1 + \sqrt{2}}{2\sqrt{2}} [\log 4 - \sqrt{2} \log(1 + \sqrt{2})] \\ &\approx 0.1193642186 \dots \end{aligned} \quad (16)$$

As in the square triangle tiling, the entropy is a convex function of the area fraction α_t , see Fig. 2.

In the twofold phase ($\alpha_t < 1/2$) this exact calculation fails because the solution curves do not have the same limit point. Nevertheless, it is possible to calculate the

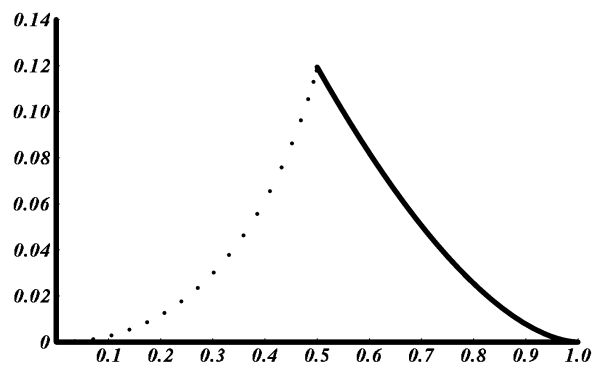


FIG. 2. σ_a as a function of α_t . The solid line corresponds to the exact solution (14). The dots are numerical results for $N = 198$.

lowest order correction to the entropy. With $\epsilon = \Delta_{\pm}/N$ this is given by

$$\sigma_a = \sigma_{a,0} - \epsilon\gamma \frac{1}{16\sqrt{2}} [4 - \log 4 - \sqrt{2} \log(1 + \sqrt{2})] - \epsilon^2 \frac{1 + \sqrt{2}}{8} [\log 4 + \sqrt{2} \log(1 + \sqrt{2})]. \quad (17)$$

This expression gives the exact slope of the numerical curve shown in Fig. 2 for $\alpha_t \uparrow 1/2$:

$$\left. \frac{d\sigma_a}{d\alpha_t} \right|_{\alpha_t \uparrow 1/2} = \frac{\sqrt{2} - 1}{\sqrt{2}} [\log 4 + \sqrt{2} \log(1 + \sqrt{2})]. \quad (18)$$

Expanding Eq. (12) up to first order in γ and using (2)–(6), it is straightforward to find the elastic constants K_{μ} and K_{ξ} from (15) and (17). Their numerical values are

$$K_{\mu} = 0.2842712\dots, \quad K_{\xi} = 0.7366252\dots \quad (19)$$

Since the two elastic constants fulfill the relations (3), the quasiperiodic eightfold symmetric state is entropically stable.

In this paper we successfully apply the Bethe *Ansatz* to an octagonal random tiling model. The BAE (11) are solved to find *exact* values of the entropy and elastic constants. The model shows qualitatively the same

behavior as the square-triangle tiling. It is not yet clear how generic the solvability of these two tilings is, but we have discovered that a tenfold symmetric tiling of rectangles and triangles does admit a Bethe *Ansatz*. It appears, however, from numerical calculations that their solutions do not allow for an exact solution using the method of Kalugin which is employed in this paper.

We thank Chris Henley and Mike Widom for providing us with some useful information. This work was supported by FOM, part of NWO, Institute for Dutch Scientific Research.

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