Bethe Ansatz Solution of the Square-Triangle Random Tiling Model

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(Received 22 September 1992)

Random tiling models cover the plane with a set of rigid tiles without gaps between tiles and without overlap. This paper considers tilings of the plane by squares and equilateral triangles which display twelvefold rotational symmetry and quasi-long-range quasiperiodic translational order. Tiling configurations may be described as networks of interacting domain walls, for which the Bethe ansatz provides the exact (formal) partition function. Numerical evaluation yields the entropy and phason elastic constants with high accuracy.

PACS numbers: 61.43.Bn, 05.20.−y, 64.70.Dv, 64.70.Rh

Random tiling models cover the plane with a set of rigid tiles without gaps between tiles or overlap. Many problems of two-dimensional statistical mechanics correspond to such coverings of the plane by sets of tiles. For example, the ground state configurations of the triangular lattice antiferromagnetic Ising model tile the plane with the 60° rhombi formed by removing all frustrated bonds from the triangular lattice [1]. The famous ground state degeneracy [2] of this model thus counts the number of distinct coverings of the plane by 60° rhombi. Kagomé lattice antiferromagnets [3] provide another example of a random tiling model. The discovery of quasicrystals [4–6] introduced many new tiling models displaying noncrystallographic rotational symmetries and quasiperiodic translational order [7,8]. Thermodynamic stability of quasicrystalline alloys may result in part [9] from the entropy associated with random rearrangements of the tiles [8]. Entropy and fluctuations for many such "random tiling models" have been studied by means of transfer matrix [10–12] and Monte Carlo [13,14] calculations. I show now that at least one such model may be solved exactly in two dimensions.

Consider a set of squares and equilateral triangles with unit edge lengths. Figure 1 illustrates tilings of the plane at three different concentrations of the two tile types. Define the area fractions α_s and $\alpha_t = 1 - \alpha_s$ as the fractions of total tiling area occupied, respectively, by squares and triangles. As $\alpha_s \to 0$ [Fig. 1(a)] the tiling becomes a triangular lattice with an incommensurate hexagonal domain wall network. The tiling entropy is simply the domain wall breathing entropy [15]. In fact, Collins [16] introduced this tiling model as a model for melting of two-dimensional close-packed crystals.

When the area fractions $\alpha_s = \alpha_t = \frac{1}{2}$ [Fig. 1(b)] the tiling may exhibit twelvefold rotational symmetry. Indeed, a binary alloy of two-dimensional Lennard-Jones atoms, whose equilibrium state is a twelvefold quasicrystal, is well approximated as a random tiling by squares and triangles [17]. Furthermore, high resolution lattice images of twelvefold symmetric quasicrystals in NiCr and NiV alloys [18] reveal planar networks [19] consisting of atoms at the vertices of tilings containing primarily squares and triangles. Note that equality of the square and triangle area fractions implies the number of squares divided by the number of triangles takes the irrational value $\sqrt{3}/4$.

In the limit $\alpha_t \to 0$ [Fig. 1(c)] the tiling becomes a

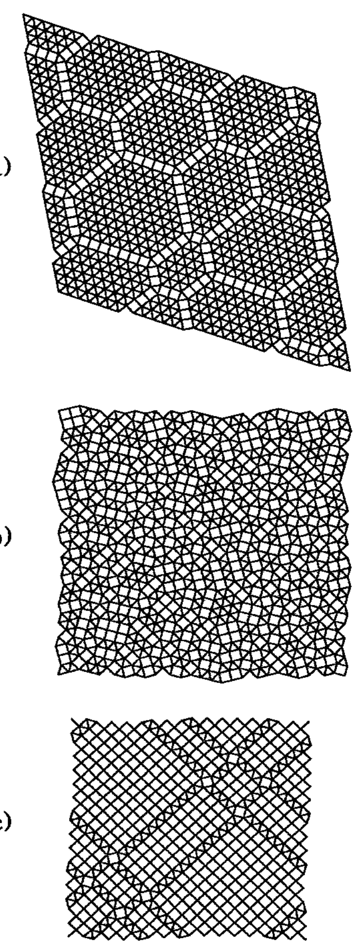

FIG. 1. (a)–(c) Square triangle tilings at three different concentrations. Lattice size is $L = M = 30$ in all three cases, and the orientations are chosen so that tile edges lie at odd multiples of 15° with respect to the horizontal. (b) The outcome of a Monte Carlo simulation by Oxborrow.

square lattice with tile edges rotated by 45° from the horizontal with a small density of domain walls. The domain walls fall into two families, one running upwards to the right, the other to the left. Geometrical constraints of tiling the plane prevent domain walls from terminating in the bulk. Domain walls of a given family are forbidden to cross one another, while domain walls of opposite families may cross in two distinct ways. These domain walls consist entirely of triangles [20], except where two domain walls cross and one finds a square rotated by $\pm 15°$ from the horizontal. I emphasize the properties of these domain walls because they make the model solvable. It is worth noting that analogous domain wall constructions exist in all the random tiling models examined so far [8,21].

Oxborrow and Henley [14] show how to set up a transfer matrix representing the evolution of domain wall positions as the tiling extends in the vertical direction. Decompose the tiling into layers bounded by $\pm 15°$ edges locating the two domain wall types, and "double 0's" extending horizontally across squares [Fig. 2(a)]. Each layer edge is thus described by a sequence of n_+ + walls, n_- − walls, and n_0 0's. Between the two edges of a layer the + walls step one unit to the left, while the − walls step one unit to the right. When two walls cross, either the left moving + wall stands nearly still while the right moving − jumps over it (thereby creating a $+15°$ square), or vice versa (creating a $-15°$ square). In this manner a correspondence is made between square-triangle tilings and an ensemble of +'s, −'s, and 0's on a square lattice [Fig. 2(b)]. I impose periodic boundary conditions connecting the end points of each layer, and also connecting the bottom and top layers (see Fig. 1).

For a tiling of fixed area there are three independent thermodynamic degrees of freedom (note that I set $k_BT=1$ in the following). To see this, note that the squares come in three orientations, and the triangles in four orientations, yielding seven potentially distinct tile densities. But the constraint of filling the given area removes one variable. One can show, further, that the triangles with $+15°$ edges always occur in pairs, and likewise the triangles with $-15°$ edges, removing two more variables. Finally, consider the squares with $\pm 15°$ edges. Denote the number of these squares in a given layer of the tiling by $S_\pm$. These squares occur only at crossings of domain walls, so their total density is a function of the domain wall (and hence triangle) densities, removing a fourth variable.

There remain three independent thermodynamic parameters, the numbers of + and − domain walls, and the relative numbers of $\pm 15°$ squares. While n_+ and n_- are conserved by the transfer matrix, $\Delta \equiv S_+ - S_-$ is not. I introduce a conjugate field ϕ to control the average value of Δ. Each $\pm 15°$ square in a tiling carries a weight factor $\exp(\pm\phi)$. The transfer matrix element of T between two edge configurations bounding a layer equals the weight factor for the layer $\exp(\phi\Delta)$. Since ϕ breaks reflection symmetry, it must vanish for the quasicrystalline state shown in Fig. 1(b). The partition function of this lattice model, on a lattice of horizontal length $L=n_0+n_++n_-$ and vertical height M, is the trace of T^M. In the thermodynamic limit this trace equals Λ^M, with Λ the largest transfer matrix eigenvalue. The free energy per layer

$$F(n_+,n_-,\phi) \equiv -\log\Lambda = -S - \phi\Delta\,, \tag{1}$$

where S is the entropy per layer.

Eigenvectors of T follow the usual [22] Bethe ansatz superposition of plane waves of the form $A(\mathbf{k})\exp i\mathbf{k}\cdot\mathbf{z}$. The elements of $\mathbf{k}$ are + wall wave numbers and − wall wave numbers (denoted p_i and q_k, respectively). The elements of $\mathbf{z}$ are + and − wall positions (denoted x_i and y_k, respectively) arranged in increasing order ($z_1 < z_2 < \cdots$). The sequence of x and y in $\mathbf{z}$ define a sector of configuration space. Within a sector the sequence of x and y in $\mathbf{z}$ must match the sequence of p and q in $\mathbf{k}$. Thus the coefficients $A(\mathbf{k})$ are independent of domain wall positions within a sector, but may vary from one sector to another. The ordering of the p_i and q_k among themselves reflects permutations of wave numbers among identical walls, and the coefficients $A(\mathbf{k})$ depend on the permutation.

Within a sector the transfer matrix shifts all + walls to the left, and all − walls to the right, so the transfer matrix eigenvalue must be

$$\Lambda = \frac{\prod_{i=1}^{n_+} e^{ip_i}}{\prod_{k=1}^{n_-} e^{iq_k}}\,. \tag{2}$$

At sector boundaries + and − walls cross, creating $\pm 15°$ squares. Consider two sectors related by the crossing of the + wall at x_i and the − wall at y_k, and the amplitudes of a term in the eigenvector containing $\exp(ip_ix_i+iq_ky_k)$ in these two sectors. The ratio of the amplitude $A(\ldots,p_i,q_k,\ldots)$ after crossing divided by the amplitude $A(\ldots,q_k,p_i,\ldots)$ before crossing is

$$G[p_i,q_k] \equiv A(\ldots,p_i,q_k,\ldots)/A(\ldots,q_k,p_i,\ldots) = e^{\phi-i(p_i+q_k)} + e^{-\phi+i(p_i+q_k)}\,. \tag{3}$$

The presence of two terms reflects the fact that the −

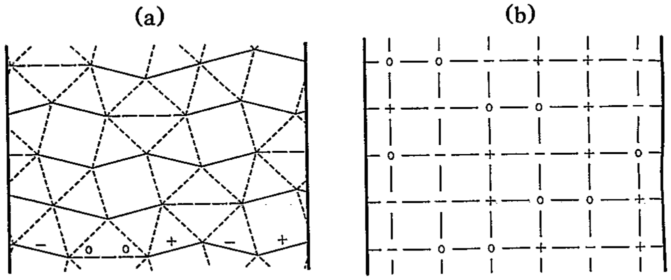

FIG. 2. (a) Layer decomposition of a tiling. (b) Associated lattice model. This figure was provided by the courtesy of Oxborrow and Henley [14].

may jump over the + (first term) or vice versa (second term). When two like walls are neighbors, say + walls at $x_j = x_i + 1$, a wall of the opposite type may jump over both simultaneously. To maintain consistency with the above rule (3), the amplitude $A(\ldots, p_i, p_j, \ldots)$ of a term containing $\exp(ip_i x_i + ip_j x_j)$ must be multiplied by

$$H[p_j, p_i] \equiv A(\ldots p_j, p_i, \ldots)/A(\ldots, p_i, p_j, \ldots) = -e^{i(p_i - p_j)} \quad (4)$$

to produce the amplitude $A(\ldots, p_j, p_i, \ldots)$ of the corresponding term containing $\exp(ip_j x_i + ip_i x_j)$, with a similar factor for − walls.

Now transfer momentum p_i or q_k across all walls of a given type. H factors accumulate from swapping momenta among neighboring like walls, while sector boundaries, which must be crossed in general in order to make contact between a given pair of like walls, contribute G factors. Using periodic boundary conditions to return the momentum to its initial wall, we find that plane wave amplitudes may be chosen consistently only if the wave vectors obey

$$e^{ip_i L} = \prod_{j \neq i=1}^{n_+} H[p_i, p_j] \prod_{l=1}^{n_-} G[p_i, q_l],$$
$$e^{-q_k L} = \prod_{l \neq k=1}^{n_-} H[q_l, q_k] \prod_{j=1}^{n_+} G[p_j, q_k]. \quad (5)$$

Values of the wave numbers p_i and q_k which solve the Bethe ansatz equations (5), and correspond to the equilibrium state with a given α_t and ϕ, lie close to (and approach in the thermodynamic limit) a pair of curves in the complex plane. So far I have examined in detail the case $\alpha_t \leq \frac{1}{2}$, with $\phi = 0$. I find $\{p_i\}$ approximates a smooth curve in the lower half plane, with reflection symmetry in the imaginary axis, while $\{q_k\}$ lies in the upper half plane and also has reflection symmetry in the imaginary axis. When $n_+ = n_-$ the two curves are reflections of each other in the real axis. This form of the ground state solutions indeed has been checked by explicit construction of transfer matrices for a variety of special cases and finite size systems. In the limit $\alpha_t \to 1/2$ with $n_+ = n_-$, it appears that the curves develop logarithmic singularities and terminate on the real axis at $\pm \pi/4$.

By solving these equations numerically in the limit $\alpha_t \to \frac{1}{2}$, I extract the entropy density [10,14] $\sigma = S/A$ and also the phason elastic constants [14] K_μ and K_ξ. These are the two principal curvatures of the entropy density

$$\sigma = \sigma_0 - \tfrac{1}{2} K_\mu I_\mu - \tfrac{1}{2} K_\xi I_\xi + \cdots \quad (6)$$

with respect to characteristic symmetry breaking shifts in tile densities known as "phason strains" [6,8]. Oxborrow and Henley [14] estimate $\sigma_0 = 0.131\,37 \pm 0.000\,44$, $K_\mu = 0.4602 \pm 0.0024$ and $K_\xi = 1.09 \pm 0.24$, while Kawamura [10] estimates $\sigma_0 = 0.128 \pm 0.001$. Measure the deviation from ideal tile densities by

$$\delta_\pm = (n_+ - n_-)/2, \quad (7)$$

$$\delta_0 = n_0 - \frac{\sqrt{3} - 1}{2}(n_+ + n_-), \quad (8)$$

in addition to the variable Δ introduced above. Then the two quadratic invariants in phason strain are [14]

$$I_\mu = \tfrac{1}{12}[\Delta^2 - 4(\sqrt{3}+1)\Delta\delta_\pm + 8(\sqrt{3}+2)\delta_\pm^2], \quad (9)$$

$$I_\xi = \tfrac{1}{12}[\delta_0^2 + (\sqrt{3}+1)\Delta\delta_\pm - 2(\sqrt{3}+2)\delta_\pm^2]. \quad (10)$$

Since there are only two principal curvatures of the entropy, I need only two independent variables and choose to eliminate Δ in favor of $\delta_\pm$ and δ_0. Varying Δ to maximize the entropy, with fixed δ_0 and $\delta_\pm$ and $\phi = 0$, yields

$$\sigma(\delta_0, \delta_\pm) = \sigma_0 - \frac{K_\xi}{24}(\delta_0/n)^2 - \frac{2+\sqrt{3}}{48}\frac{K_\xi(4K_\mu - K_\xi)}{K_\mu}(\delta_\pm/n)^2 \quad (11)$$

with $n = (n_+ + n_-)/2$. Here I keep only terms up to second order in δ_0 and $\delta_\pm$. Table I displays numerical data for finite size systems. Fitting these data to power series in the variable $1/n$ yields $\sigma_0 = 0.129\,341\,555\,166(6)$, $K_\mu = 0.460\,458\,546\,66(2)$, and $K_\xi = 1.430\,083\,830\,79(3)$. To obtain the entropy per vertex, divide σ_0 by the density of vertices, $1/2 + 1/\sqrt{3}$, yielding $\sigma = 0.120\,055\,249\,315(6) k_B$ per tile vertex. Hydrodynamic stability [9,14] of the twelvefold symmetric state requires positivity of the two principal curvatures. The numerical results found above satisfy this condition since $4K_\mu > K_\xi > 0$. Entropy therefore selects the quasicrystalline state with noncrystallographic rotational symmetry and quasiperiodic translational order.

Finally, consider the origin of the kink in the entropy as a function of α_t. The entropy has a smooth quadratic

TABLE I. Variation of the entropy density $\sigma(\delta_0, \delta_\pm)$. The total number of domain walls $n_+ + n_- = 2n$.

n	$\sigma(0,0)$	$n^2[\sigma(1,0) - \sigma(0,0)]$	$n^2[\sigma(0,1) - \sigma(0,0)]$
3	0.146 136 555 164 779	0.030 221 215 231 495	0.232 986 457 429 866
11	0.130 761 425 913 366	0.056 368 598 348 796	0.099 884 069 719 622
41	0.129 445 257 373 655	0.059 341 476 693 508	0.099 461 139 122 698
153	0.129 349 010 329 241	0.059 569 125 177 518	0.099 430 919 968 124
571	0.129 342 090 477 373	0.059 585 554 941 999	0.099 428 751 023 926
∞	0.129 341 555 166(6)	0.059 586 826 283(1)	0.099 428 583 256(3)

maximum as a function of rotational symmetry breaking densities δ_0 and $\delta_\pm$. But the rotationally invariant area fraction varies as

$$\alpha_t = \frac{1}{2} - \frac{1}{24}(\delta_0/n)^2 + \frac{2+\sqrt{3}}{12}(\delta_\pm/n)^2 - \frac{3+2\sqrt{3}}{36}(\delta_0\delta_\pm^2/n^3) + \cdots . \quad (12)$$

At fixed α_t, δ_0 and $\delta_\pm$ vary to maximize the entropy subject to the constraint Eq. (12) to find

$$\sigma = \begin{cases} \sigma_0 - K_\xi(1/2-\alpha_t), & \alpha_t < 1/2, \\ \sigma_0 - \dfrac{K_\xi(4K_\mu - K_\xi)}{4K_\mu}(\alpha_t - 1/2), & \alpha_t > 1/2. \end{cases} \quad (13)$$

Following Kawamura [10], we denote the field conjugate to a rotationally invariant area fraction as a "pressure." At a given pressure, the triangle area fraction takes a value such that the derivative of free energy with respect to area fraction matches the pressure. Such a kink in the entropy density as a function of tile area fractions thus provides a mechanism for locking on the quasicrystal state over a range of pressures [12,23,24].

This paper applies the Bethe ansatz to solve a random tiling model. Such models describe a variety of interesting physical systems [1–3]. The square-triangle tilings studied here model twelvefold quasicrystals [18], a two-dimensional Lennard-Jones alloy [17], and possibly two-dimensional melting [16,20]. This is also the only exactly solved model displaying a phase transition from the triangular lattice to the hexagonal incommensurate phase [15] illustrated in Fig. 1(a). As an initial application of this exact solution, I present highly accurate values for the quasicrystal entropy and elastic constants, as well as a mechanism for locking on this state.

I wish to acknowledge many useful discussions with Chris Henley and Mark Oxborrow. I wish to thank M. Oxborrow further for help with the figures, and Curtis Doty for discussions on the derivation of the Bethe ansatz equations and comments on this manuscript. This work was supported in part by NSF Grant No. DMR-9221596 and by a grant from the Sloan Foundation. Partial support at Cornell was also provided by DOE Grant No. DE-FG02-89ER-45405.

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