

Triangular Trimers on the Triangular Lattice: An Exact Solution

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A model, consisting of triangular trimers on the triangular lattice is presented. In analogy to the dimer problem, these particles cover the lattice completely without overlap. The model has a honeycomb structure of hexagonal cells separated by rigid domain walls. The transfer matrix can be diagonalized by a Bethe Ansatz with two types of particles. This leads to an exact expression for the entropy on a two-dimensional subset of the parameter space.

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In the course of years many exactly solvable lattice models have been found. Relatively few of them admit a natural interpretation as a lattice gas. The Ising model [1], proposed in 1920 by Lenz [2] as a model of a ferromagnet, can be interpreted as a lattice gas with hard-core repulsion and short-range attraction. The (zero-field, square-lattice) Ising model was solved in 1944 by Onsager [3]. It exhibits gas-liquid coexistence below a critical temperature and a single fluid phase above.

Another lattice gas is the hard hexagon model [4], solved in 1980 by Baxter [5]. It has a continuous fluid-solid transition. At high density (solid) the particles select one of three sublattices; at low density (fluid) these sublattices are evenly occupied.

As a final example we mention the dimer problem. It was solved for planar lattices in 1961, independently by Kasteleyn [6] and by Temperley and Fisher [7]. A dimer is a particle that occupies two adjacent lattice sites. As in the Ising and the hard hexagon model two particles cannot occupy the same lattice site. In contrast to these models it is also required that all sites are occupied. The configurations are coverings of a lattice with dimers, without empty sites or overlap. The dimer problem is reviewed in Ref. [8]. We discuss the dimer model on the honeycomb lattice in some detail, because it has illustrative similarities to a new model we shall introduce below.

A configuration of the honeycomb-lattice dimer model can be viewed as a number of domains consisting of vertical dimers, separated by zigzagging domain walls made up of dimers of the other two orientations. This is illustrated in Fig. 1. The domain walls run from the bottom to the top of the lattice, so that any horizontal line through the system meets all domain walls once. Hence the number of domain walls is the same in each horizontal slice; in other words, it is a conserved quantity.

Consider the entropy for fixed density ρ of domain-wall dimers. From the exact solution of the model it can be calculated that for low ρ the entropy per dimer is given by

$$S \approx (\log 2)\rho - \frac{\pi^2}{24} \rho^3.$$

The linear term reflects the zigzag freedom of the domain walls; each domain-wall dimer contributes $\log 2$ to the entropy. The cubic term is due to the (repulsive) interaction between the domain walls: when two domain walls meet, some of the zigzag freedom is lost [9,10].

Now give chemical potentials μ to the dimers in the domain walls and 0 to the vertical dimers. For $\mu \leq -\log 2$ the free energy $F = -\mu\rho - S(\rho)$ is an increasing function of ρ for small ρ , so no domain walls will be present. For $\mu \geq -\log 2$ the free energy has a minimum at some small positive value of ρ . At $\mu = -\log 2$ there is a transition between a frozen phase consisting of vertical dimers only and a disordered phase where dimers of all three orientations are present.

Inspired by the dimer model we consider the coverings of the triangular lattice by triangular trimers. A trimer is a particle that occupies three lattice sites. As in the dimer problem we require that there are no empty sites and that there is no overlap. Figure 2 shows a typical configuration. In this Letter we present our main results on this model. We intend to publish a more detailed account later [11].

The model admits very regular configurations where the trimers occupy a sublattice of the triangular faces. There are six such sublattices, which we number $0, 1, \dots, 5$ as indicated in Fig. 2. Note that the up and down

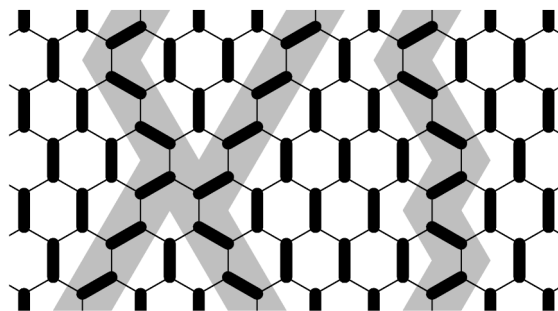


FIG. 1. The dimer model on the honeycomb lattice. Domains of vertical dimers are separated by domain walls consisting of dimers of the other two orientations. To guide the eye the domain walls are shaded.

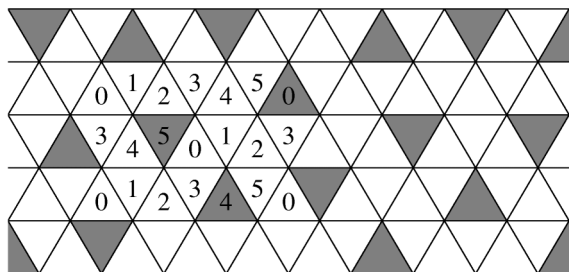


FIG. 2. A typical configuration of the trimer model. Each lattice site belongs to precisely one trimer. We divide the lattice faces into six sublattices, numbered $0, 1, \dots, 5$. Filling one sublattice completely and leaving the other five empty give a very regular configuration of the model.

triangles make up the even-numbered and odd-numbered sublattices, respectively.

Consider configurations where trimers on sublattice 0 predominate. They cover hexagonal domains of trimers on this sublattice, separated by straight domain walls that form an irregular honeycomb network. There are three types of domain walls, of different orientations. The domain walls which run from lower right to upper left will be termed L ; they are made up of trimers on sublattice 5. Those running from lower left to upper right will be called R ; they consist of trimers on sublattice 1. The vertical domain walls are made up of trimers on sublattice 3. When domain walls of the three different types meet in a Y shape, but not an upside-down-Y shape, a trimer on sublattice 2 or 4 occurs. This is illustrated in Fig. 3.

For the time being we require that the model be isotropic, in the sense that there are equal amounts of the

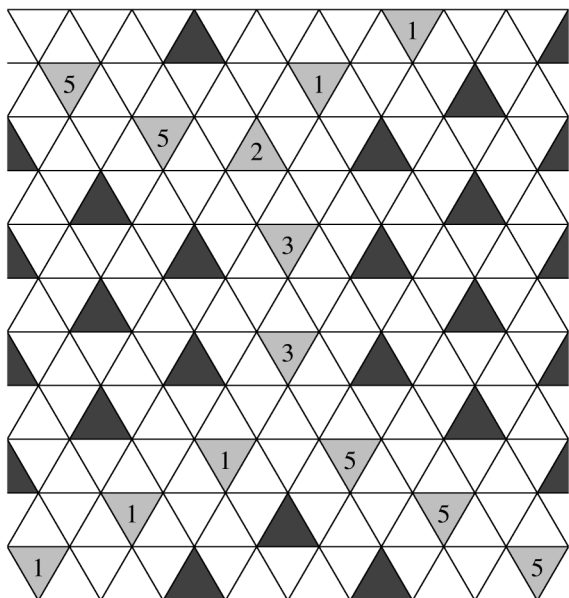


FIG. 3. The trimer model has three types of domain walls, corresponding to the three odd-numbered sublattices. The trimers on sublattice 0 are shaded dark grey; the trimers on the other sublattices are shaded light grey, and their sublattice number is given.

three types of domain walls. Let ρ denote the density of domain-wall trimers. The domain walls are rigid, so they have no zigzag freedom contributing to the entropy. Therefore the low-density expansion of the entropy contains no term linear in ρ . There is, however, freedom in the sizes of the domains [12]. For example, it is possible to enlarge a single domain while simultaneously shrinking its six neighbors. The contribution to the entropy per domain depends on the linear dimensions of the domains, and is roughly proportional to $-\log\rho$. The number of domains is approximately proportional to ρ^2 . Hence the “breathing” entropy is given for low ρ by

$$S \approx -K\rho^2 \log\rho, \quad (1)$$

where K is some (positive) proportionality constant.

If a chemical potential μ is given to the domain-wall trimers, the free energy for low ρ is

$$F \approx -\mu\rho + K\rho^2 \log\rho.$$

This is an increasing function of ρ for $\mu < 0$ and a decreasing function for $\mu \geq 0$. Hence the free energy takes its minimum either at $\rho = 0$ or at a large value of ρ , for which the approximation (1) is not valid. For small μ there are no domain walls, but, when μ passes some threshold, ρ jumps to a positive value. Thus the phase transition is different from that in the honeycomb-lattice dimer model, where the domain-wall density increases continuously at the phase transition.

Now we return to the model without the isotropy requirement. Let N denote the total number of trimers, N_i the number of trimers on sublattice i , and ρ_i the partial density N_i/N . These six sublattice densities obviously satisfy

$$\rho_0 + \rho_1 + \rho_2 + \rho_3 + \rho_4 + \rho_5 = 1. \quad (2)$$

It can be shown that, when toroidal boundary conditions are imposed, they also satisfy

$$\rho_0\rho_2 + \rho_2\rho_4 + \rho_4\rho_0 = \rho_1\rho_3 + \rho_3\rho_5 + \rho_5\rho_1. \quad (3)$$

When the total density of down trimers $\rho_{\nabla} = \rho_1 + \rho_3 + \rho_5$ is small, it follows easily from (2) and (3) that one of ρ_0, ρ_2 and ρ_4 , say ρ_0 , is larger than the other two. If there is no further symmetry breaking, one has $\rho_0 > \rho_1 = \rho_3 = \rho_5 > \rho_2 = \rho_4$. By the same token, when ρ_{∇} is close to 1, the symmetry between the down sublattices is broken. Therefore, when ρ_{∇} is increased from 0 to 1, at least one phase transition is expected.

Besides (2) and (3), we have found no more constraints on the sublattice densities. Therefore of the six sublattice densities, four are independent. We would like to know the entropy (per trimer) as a function of these four parameters. We have been able to compute it for a two-dimensional

subset of the four-dimensional parameter space. The calculation is rather lengthy, so here we only give an outline of the method, and a description of the final result.

View each vertical domain wall as a combination of one L domain wall and one R domain wall. Then the L and R domain walls run without interruption from the bottom to the top of the lattice. Therefore the number of L domain walls and the number of R domain walls are constant throughout the system. This is analogous to the situation described above for the dimer model on the honeycomb lattice, except that there are now two conserved quantities, n_L and n_R , instead of a single one. We introduce the densities $\rho_L = n_L/L$ and $\rho_R = n_R/L$, where $3L$ is the number of sites in a horizontal row of the lattice. They can be expressed in terms of the sublattice densities,

$$\begin{aligned} \rho_L &= 1 - \rho_0 - \rho_1 + \rho_3 + \rho_4, \\ \rho_R &= 1 - \rho_0 + \rho_2 + \rho_3 - \rho_5. \end{aligned}$$

It is suggestive to interpret the vertical lattice direction as “time” and the horizontal direction as “space.” The domain walls are then viewed as world lines of two types of particles, L and R . In a vertical domain wall, one L and one R particle form a “bound state.”

The model can be formulated in terms of a transfer matrix, which describes the time evolution of the system of L particles and R particles in one space dimension. Solving the model boils down to determining the largest eigenvalue of this operator, or more precisely, its maximum over all particle numbers n_L and n_R . We have achieved this by using coordinate Bethe Ansatz; the solution is similar to that of the square-triangle random tiling model, due to Widom [13] and Kalugin [14]. A model can be solved in this way only if, in some sense, the many-particle interactions factorize into two-particle interactions. It turns out that for the present model this is indeed the case. It is noteworthy that the L particles among each other are free fermions, as are the R particles, but that the interaction between an L and R particle is nontrivial.

The Bethe Ansatz allows for numerical computations for the system on an infinitely long cylinder of finite circumference. These computations can be done to arbitrary precision, and effectively for the full four-dimensional parameter space of the model. In the thermodynamic limit the Bethe Ansatz gives rise to a set of two coupled integral equations. The physical quantities we are interested in, such as the sublattice densities ρ_i and the entropy, can be expressed in terms of the functions satisfying these equations. These can be solved analytically in a special case [14]. Thus we have obtained an exact expression for the entropy of a two-dimensional family of sublattice densities. It will be seen below that this family is given by $\rho_1 = \rho_3 = \rho_5$ (or $\rho_0 = \rho_2 = \rho_4$).

This solution is parametrized by a complex number \hat{b} with $\text{Im}\hat{b} > 0$. Write

$$\hat{b} = b_L - b_L^{-1} = b_R - b_R^{-1} \tag{4}$$

with $\text{Re}b_L \geq 0$ and $\text{Re}b_R \leq 0$. It follows that $\text{Im}b_L > 0$, $\text{Im}b_R > 0$, and $b_L b_R = -1$. Take contours C_L and D_L running from b_L^* to b_L , and C_R and D_R running from b_R to b_R^* . The arrangement of these four curves must be as shown in Fig. 4, but their precise shape is immaterial. Other solutions, corresponding to contour configurations different from that in Fig. 4, result from symmetry operations permuting the six sublattices. Define the complex function

$$t(z) = \left(\frac{z - z^{-1} - \hat{b}}{z - z^{-1} - \hat{b}^*} \right)^{1/6}.$$

Fix a branch $t_L(z)$ with branch cuts C_R and D_L by $t_L(0) = \exp(\pi i/3)$, and a branch $t_R(z)$ with branch cuts C_L and D_R by $t_R(0) = \exp(-\pi i/3)$. The domain-wall density ρ_L is given by

$$\rho_L = \frac{1}{2\pi i} \int_{C_L} \frac{t_L(z) + t_L(z)^{-1}}{z} dz,$$

and ρ_R is given by the same equation with all subscripts L changed to R . The sublattice densities are

$$\begin{aligned} \rho_0 &= 1 - \frac{1}{2}(\rho_L + \rho_R) + \frac{1}{6}(\rho_L^2 - \rho_L \rho_R + \rho_R^2), \\ \rho_2 &= \frac{1}{2}(\rho_R - \rho_L) + \frac{1}{6}(\rho_L^2 - \rho_L \rho_R + \rho_R^2), \\ \rho_4 &= \frac{1}{2}(\rho_L - \rho_R) + \frac{1}{6}(\rho_L^2 - \rho_L \rho_R + \rho_R^2), \\ \rho_i &= \frac{1}{6}(\rho_L + \rho_R) - \frac{1}{6}(\rho_L^2 - \rho_L \rho_R + \rho_R^2) \quad \text{for odd } i. \end{aligned} \tag{5}$$

Define auxiliary integrals ϕ_L and Σ_L by

$$\begin{aligned} \phi_L &= \frac{1}{2} \text{Re} \int_{b_L}^{-b_L^{-1}} \frac{t_L(z) + t_L(z)^{-1}}{z} dz, \\ \Sigma_L &= \frac{1}{4} \text{Re} \int_0^\infty \frac{t_L(z) + t_L(z)^{-1} - 1}{z} dz. \end{aligned}$$

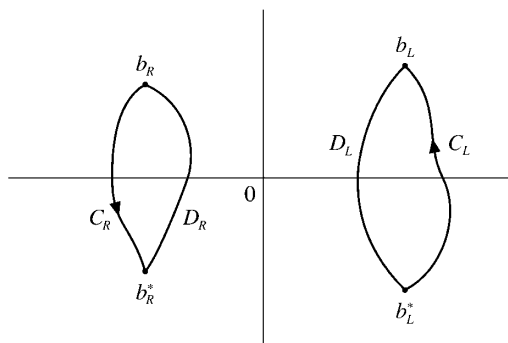


FIG. 4. The exact expression for the entropy is formulated in terms of contour integrals. The curves C_L and D_L in the right half plane are deformations of the line segment joining b_L and b_L^* , and C_L lies to the right of D_L . No orientation of D_L needs to be specified because it does not occur as an integration contour but only as a branch cut. Analogous remarks apply to C_R and D_R .

The real parts of these integrals do not depend on the choice of the integration contours, which must not meet the branch cuts C_R and D_L . The auxiliary integrals ϕ_R and Σ_R are defined analogously. The entropy per trimer is given by

$$S = \Sigma_L + \Sigma_R + \frac{1}{6}(2\rho_R - \rho_L)\phi_L + \frac{1}{6}(2\rho_L - \rho_R)\phi_R.$$

We started out with the model parametrized by the six sublattice densities satisfying the constraints (2) and (3). The exact solution described above has two parameters, so it covers a two-dimensional set of sublattice densities. The solution is, however, parametrized by a complex number \hat{b} , and not in terms of these densities. It follows from (5) that $\rho_1 = \rho_3 = \rho_5$ for the exact solution. The space of sublattice densities satisfying this constraint as well as (2) and (3) is two dimensional.

When \hat{b} tends to a point on the real axis the domain-wall densities ρ_L and ρ_R tend to zero. From the exact solution it can be calculated that in this limit $\rho_L = \rho_V + O(\rho_V^2)$ and $\rho_R = \rho_V + O(\rho_V^2)$, and

$$S = -\frac{1}{3}\rho_V^2 \log \rho_V + O(\rho_V^2).$$

This confirms the validity of (1) for the trimer model and explicitly gives the coefficient K , which is independent of the relative densities of the sublattice-2 and the sublattice-4 trimers. At $\hat{b} = 2i$ the system is in a symmetric phase with all sublattice densities equal to $1/6$; its entropy is $S_{\text{sym}} = \log(3\sqrt{3}/4)$. When \hat{b} is taken between 0 and $2i$ on the imaginary axis, b_L and b_R lie on the unit circle. Then $\rho_L = \rho_R$, so the sublattice densities satisfy $\rho_2 = \rho_4$. For small $\rho_V \leq 1/2$ this equation together with $\rho_1 = \rho_3 = \rho_5$, describes the most symmetric case for the sublattice densities. Based on numerical Bethe Ansatz calculations we believe that, for a given $\rho_V \leq 1/2$ the system takes its maximum entropy at these sublattice densities. Figure 5 shows the entropy S as a function of ρ_V . The entropy for $\rho_V \geq 1/2$ was obtained from that for $\rho_V \leq 1/2$ using the symmetry between the up and the down trimers.

The entropy S is a convex function of ρ_V for $0 \leq \rho_V \leq 1/2$. A system with ρ_V in this interval is thermodynamically unstable. It would separate into a phase with $\rho_V = 0$ and a phase with $\rho_V = 1/2$, except for the fact that the model does not admit an interface between these two phases. Similarly a system with $1/2 \leq \rho_V \leq 1$ would demix into phases with $\rho_V = 1/2$ and $\rho_V = 1$.

The transition between these phases can also be controlled by assigning a chemical potential μ to the down

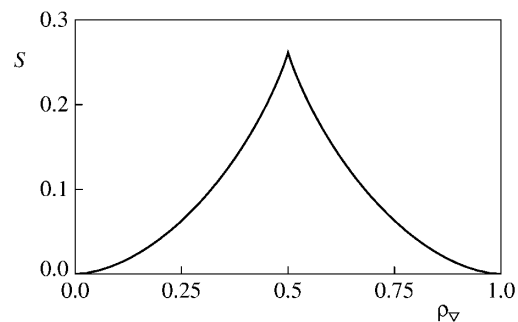


FIG. 5. The entropy per trimer versus the density ρ_V of down trimers in the special case of $\rho_1 = \rho_3 = \rho_5$ and $\rho_2 = \rho_4$ for $\rho_V \leq 1/2$, and similarly for $\rho_V \geq 1/2$.

trimers instead of imposing their density ρ_V . From Fig. 5 it is seen that for $\mu \leq -2S_{\text{sym}}$ the free energy $F = -\mu\rho_V - S(\rho_V)$ takes its minimum at $\rho_V = 0$, so all trimers are on one of the up sublattices. For $-2S_{\text{sym}} \leq \mu \leq 2S_{\text{sym}}$ the minimum of F is at $\rho_V = 1/2$, so all sublattices are equally occupied. For $\mu \geq 2S_{\text{sym}}$ the minimum of F is at $\rho_V = 1$, so the system is again in a frozen phase.

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- [1] E. Ising, *Z. Phys.* **31**, 253 (1925).
 - [2] W. Lenz, *Phys. Z.* **21**, 613 (1920).
 - [3] L. Onsager, *Phys. Rev.* **65**, 117 (1944).
 - [4] D.M. Burley, *Proc. Phys. Soc.* **75**, 262 (1960).
 - [5] R.J. Baxter, *J. Phys. A* **13**, L61 (1980).
 - [6] P.W. Kasteleyn, *Physica (Utrecht)* **27**, 1209 (1961).
 - [7] H.N.V. Temperley and M.E. Fisher, *Philos. Mag.* **6**, 1061 (1961) (8th series).
 - [8] J.F. Nagle, C.S.O. Yokoi, and S.M. Bhattacharjee, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J.L. Lebowitz (Academic Press, London, 1989), Vol. 13, pp. 235–297.
 - [9] S.M. Bhattacharjee, J.F. Nagle, D.A. Huse, and M.E. Fisher, *J. Stat. Phys.* **32**, 361 (1983).
 - [10] S.M. Bhattacharjee and J.J. Rajasekaran, *Phys. Rev. A* **44**, 6202 (1991).
 - [11] A. Verberkmoes and B. Nienhuis, cond-mat/9909068.
 - [12] J. Villain, in *Ordering in Strongly Fluctuating Condensed Matter Systems*, edited by T. Riste (Plenum Press, New York, 1980), pp. 221–253.
 - [13] M. Widom, *Phys. Rev. Lett.* **70**, 2094 (1993).
 - [14] P.A. Kalugin, *J. Phys. A* **27**, 3599 (1994).