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Ground states of the IRF model in two dimensions

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Abstract. Some of the ground states of Baxter's IRF model in the square lattice are constructed. It is shown that the model has an infinite series of ground states which correspond to monodisperse close-packed triangles of fixed orientation and varying size.

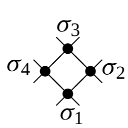
1. Introduction

Depending on the Hamiltonian, the problem of determining the ground states of a lattice model may be trivial or very difficult. In some cases, like simple Ising models, the ground states are obvious as is the case in all models without frustration. In these cases the individual terms in the Hamiltonian can be minimized separately and the ground state constructed. No such simple procedure is known for frustrated models and it may well turn out that there exists no general algorithm to solve the ground state problem for a given short range Hamiltonian.

These difficulties, however, may indicate that something interesting is happening. In fact, whereas ground states of unfrustrated models do not usually possess much structure and are 'dull' in this sense, frustrated models may have rather complicated ground states with periodicities much larger than the range of the Hamiltonian. At least one model is known which possesses an infinite number of ground states with ever larger periodicities ([**?**], see also [**?**]). Models of this kind are of particular interest in the physics of mesoscopics where structures intermediate between the microscopic and the macroscopic are studied.

The present paper stems from an attempt to construct all the ground states of Baxter's IRF model [**?**] in two dimensions. It turnes out that even this simple model (comprising all the interactions in the elementary square of the lattice) is surprisingly rich, and a complete solution of the problem has not been found. What has been found, however, is quite interesting. This model also has an infinite series of ground states and these correspond to close-packed triangles of $+(-)$ spins of ever larger size in a sea of $-(+)$ spins. This is a simple example for a strictly local Hamiltonian generating structures of arbitrary size.

2. The model

Consider the square lattice and rotate it through 45° in order to obtain more symmetrical structures. Let 

be a typical elementary square in the lattice. The energy of a configuration in the general IRF model is defined by

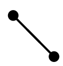
$$E = \sum_{squares} E(\sigma_1, \sigma_2, \sigma_3, \sigma_4) \tag{1}$$

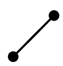
where the sum is over all elementary squares in the lattice. $E(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$ is a general function of the spins in the elementary square

$$E(\sigma_1, \sigma_2, \sigma_3, \sigma_4) = \sum_{i=1}^{10} \epsilon_i s_i. \tag{2}$$

Here the ϵ_i are energies defining the model and the s_i are the following sums of spin products in the elementary square:

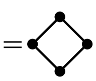
$s_1 =$ $= \frac{1}{4}(\sigma_1 + \sigma_2 + \sigma_3 + \sigma_4)$

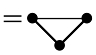
$s_2 =$  $= \frac{1}{2}(\sigma_1\sigma_4 + \sigma_2\sigma_3)$

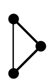
$s_3 =$  $= \frac{1}{2}(\sigma_1\sigma_2 + \sigma_3\sigma_4)$

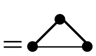
$s_4 =$ $= \sigma_2\sigma_4$

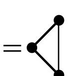
$s_5 =$  $= \sigma_1\sigma_3$

$s_6 =$  $= \sigma_1\sigma_2\sigma_3\sigma_4$

$s_7 =$  $= \sigma_1\sigma_2\sigma_4$

$s_8 =$  $= \sigma_1\sigma_2\sigma_3$

$s_9 =$  $= \sigma_2\sigma_3\sigma_4$

$s_{10} =$  $= \sigma_1\sigma_3\sigma_4.$

Since we are interested in large lattices we introduce the energy per spin $\epsilon = E/N$ where N is the number of elementary squares in the lattice. Then

$$\epsilon = \sum_{i=1}^{10} \epsilon_i x_i \tag{3}$$

where

$$x_i = \langle s_i \rangle$$

is the average of s_i over all the elementary squares of the lattice for a given global spin configuartion $\{\sigma\}$. For example, $x_1 = \frac{1}{N}\sum_\alpha \sigma_\alpha$ is the average spin on the lattice for given $\{\sigma\}$ etc.

In this way the energy per spin is a function of the configuration $\{\sigma\}$ of the lattice. The ground state problem then is the following: determine the minimum of ϵ for an arbitrary selection of the energy parameters and characterize the corresponding ground state configuration.

3. Correlation polyhedron and the ground state problem

Quite generally, consider a lattice model on a d-dimensional lattice with a Hamiltonian of the form

$$H = \epsilon_1 \langle \sigma \rangle + \epsilon_2 \langle \sigma \sigma' \rangle + \cdots$$

which depends upon a certain class of spin products

$$x_1 = \langle \sigma \rangle \qquad x_2 = \langle \sigma \sigma' \rangle, \ldots, x_\nu .$$

Here again $\{\sigma\}$ refers to a fixed configuration and the brackets $\langle\ \rangle$ mean an average over all the different positions on the lattice.

When plotted as points in a ν-dimensional space, every configuration of the spins in the lattice generates a point $\boldsymbol{x} = \{x_i\}_{1,\nu}$ in this space. Let $\mathcal{P}$ be the set of all points $\boldsymbol{x}$ obtained in this way. For a finite lattice $\mathcal{P}$ is a bounded collection of points (having $\leqslant 2^N$ points for a lattice with N sites), but for an infinite lattice $\mathcal{P}$ becomes a closed and convex set [4, 6]. This set is the correlation polyhedron and is denoted by $\overline{\mathcal{P}}$. The points of $\overline{\mathcal{P}}$ correspond to those correlations that are realizable by configurations on the infinite lattice.

For a simple example consider the one-dimensional Ising model [**?**]. Here only two correlations are relevant, the average spin $x_1 = \langle \sigma \rangle$ and the NN correlation $x_2 = \langle \sigma \sigma' \rangle$ where σ and σ' are neighbouring spins. Since $\sigma = \pm 1$, we have the inequalities $(\sigma + \sigma' \pm 1)^2 \geqslant 1$. Averaging we obtain $x_2 \pm 2x_1 + 1 \geqslant 0$. These two inequalities together with $x_2 \leqslant 1$ delimit the correlation polyhedron $\overline{\mathcal{P}}$ which in this case is a triangle.

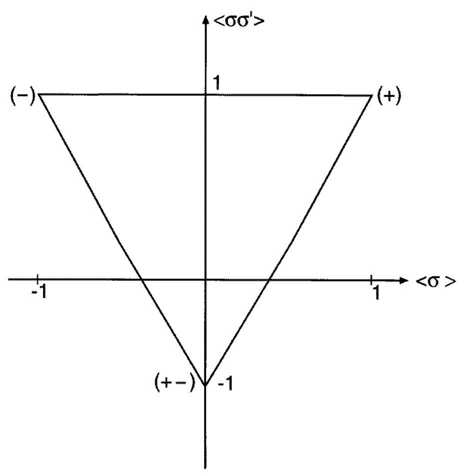


Figure 1. Correlation triangle for the one-dimensional Ising model.

The vertices of the triangle are $(1, 1)$, $(-1, 1)$, $(0, -1)$. They correspond to the two ferromagnetic $((+), (-))$ and the antiferromagnetic $(+-)$ states.

This simple case exemplifies the general situation: all configurations $\{\sigma\}$ of the lattice map via $\{\sigma\} \to \{x_i(\{\sigma\})\}$ into $\overline{\mathcal{P}}$. Conversely, every point of $\overline{\mathcal{P}}$ stems from a spin configuration on the lattice. We shall call a point $\{x_i\}$ with the latter property a *realizable* point.

The significance of $\overline{\mathcal{P}}$ for the ground state problem is the fact that the vertices correspond to the possible ground states. This is apparent for the simple Ising model discussed above, but is generally true as the following argument demonstrates. Consider a Hamiltonian of the form

$$H = \sum_{1}^{\nu} \epsilon_i x_i .$$

Geometrically $H = \epsilon$ corresponds to a hypersurface, and hypersurfaces with the same ϵ_i but different ϵ are parallel. The ground state problem can now be formulated as follows. Minimize H subject to the constraint that $\{x_i\}$ is physically realizable, i.e. that $\{x_i\}$ is located in $\overline{\mathcal{P}}$. It is geometrically obvious that H assumes its minimum at one of the vertices of $\overline{\mathcal{P}}$. Conversely, every proper vertex corresponds to the minimum of H for certain ranges of the ϵ_i.

For simple systems (one-dimensional models or IRF models without three-spin interactions, see below) $\overline{\mathcal{P}}$ is a finite polyhedron having a finite number of faces and vertices. For such systems, varying the ϵ_i generates only a finite number of groundstates.

On the other hand, suppose that $\overline{\mathcal{P}}$ has an infinite number of vertices. Then, since $\overline{\mathcal{P}}$ is a finite subset of a finite-dimensional space, these vertices must have at least one accumulation point. (In the examples below this point is one of the ferromagnetic points $\sigma_i \equiv 1$ or $\sigma_i \equiv -1$.) In every vicinity of the accumulation point there is an infinite number of vertices. The corresponding ground states must have ever larger periodicities since the number of states with bounded periodicity is finite. This also implies a kind of structural instability of the energy parameters ϵ_i: in this region of the phase diagram, arbitrary small changes of the ϵ_i result in large and different changes of the ground state.

4. Some remarks on the general IRF model

A polyhedron is uniquely specified by giving either its vertices or, dually, its facets, i.e. its faces of maximal dimension. Now it seems to be generally true that the facets of correlation polyhedra are much easier to determine than the vertices [2, 4–6]. This was true for the simple example above: the facets of the triangle are its sides and they follow from simple local inequalities. In fact, for finite-range Hamiltonians in one dimension, the remarks below are sufficient to generate all the facets [**?**].

A facet for a correlation polyhedron is a linear inequality for the average spin products of the form

$$1 + \sum_{1}^{10} \alpha_i x_i \geqslant 0. \tag{4}$$

(For definiteness the constant has been normalized to 1; it is positive since random configurations with $x_i = 0$ are located in the interior of $\overline{\mathcal{P}}$.) Inequality (4) is a facet if

(i) it is true for any spin configuration in the lattice

(ii) it becomes an equality for at least ten states $\boldsymbol{x}^{(j)}$ spanning the hypersurface

$$1 + \sum_{1}^{10} \alpha_i x_i = 0.$$

Now a simple set of linear inequalities is the following. Take any set of four integers $\tau_i = \pm 1$ and consider the product

$$\prod_{i=1}^{4} (1 + \tau_i \sigma_i)$$

for an elementary square in the lattice. This product is always non-negative. Averaging we obtain the following linear inequalities

$$0 \leqslant \left\langle \prod_{i=1}^{4} (1 + \tau_i \sigma_i) \right\rangle \qquad \tau_i = \pm 1. \tag{5}$$

These 16 inequalities determine a certain bounded convex polyhedron $\mathcal{P}^*$ in the ten-dimensional space of the x_i. $\mathcal{P}^*$ contains $\overline{\mathcal{P}}$ since $\overline{\mathcal{P}}$ can also be characterized as the intersection of *all* true inequalities.

In the one-dimensional case the set of inequalities obtained by this method is complete [**?**] in the sense that any other linear inequality is a convex combination of these. In this case $\mathcal{P}^*$ coincides with $\overline{\mathcal{P}}$. In two dimensions however, $\mathcal{P}^*$ turns out to be strictly larger than $\overline{\mathcal{P}}$. In order to see this, let us first characterize the facets of $\mathcal{P}^*$ more closely.

Consider a certain configuration $\{\sigma\}$ of spins in the infinite square lattice and focus on the elementary squares. The probability of occurrence of a particular elementary square

$$\begin{matrix} & \tau_3 & \\ \tau_4 & & \tau_2 \\ & \tau_1 & \end{matrix}$$

is given by

$$p\begin{pmatrix} & \tau_3 & \\ \tau_4 & & \tau_2 \\ & \tau_1 & \end{pmatrix} = 2^{-4} \left\langle \prod_{1}^{4} (1 + \tau_i \sigma_i) \right\rangle. \tag{6}$$

This is a very simple characterization of $\mathcal{P}^*$: in the interior of $\mathcal{P}^*$ each of the 16 different elementary squares occurs with a positive probability. Near the boundary the probability of certain squares drops to zero.

Note that the p's provide an alternative and more symmetrical characterization of a state than the $\boldsymbol{x}$. Aside from normalization

$$\sum_{\tau_1,\tau_2,\tau_3,\tau_4} p\begin{pmatrix} & \tau_3 & \\ \tau_4 & & \tau_2 \\ & \tau_1 & \end{pmatrix} = 1 \tag{7}$$

there exist the following linear relations which reduce the number of independent variables to ten.

$$\sum_{\tau_1,\tau_2} p\begin{pmatrix} & \sigma_2 & \\ \sigma_1 & & \tau_2 \\ & \tau_1 & \end{pmatrix} = \sum_{\tau_1,\tau_2} p\begin{pmatrix} & \tau_2 & \\ \tau_1 & & \sigma_2 \\ & \sigma_1 & \end{pmatrix} \tag{8}$$

$$\sum_{\tau_1,\tau_2} p\begin{pmatrix} & \tau_2 & \\ \sigma_2 & & \tau_1 \\ & \sigma_1 & \end{pmatrix} = \sum_{\tau_1,\tau_2} p\begin{pmatrix} & \sigma_2 & \\ \tau_2 & & \sigma_1 \\ & \tau_1 & \end{pmatrix}. \tag{9}$$

We will use both sets of variables p and $\boldsymbol{x}$.

Let us return to the relation between $\overline{\mathcal{P}}$ and $\mathcal{P}^*$. It is not difficult, but somewhat tedious, to determine the vertices of $\mathcal{P}^*$. It turns out that $\mathcal{P}^*$ has precisely 21 vertices which are listed in table 1.

The first 17 of these vertices are physically realizable in the sense that spin configurations exist in the infinite lattice which have the point $\boldsymbol{x}$ as spin correlations. For example, vertices $1a, b$ correspond to the ferromagnetic, vertex 2 to the antiferromagnetic and vertices $3a, b$ describe lamellar ground states.

Vertices 8 are not realizable. To see this, consider for example vertex $8a$. One finds that this vertex is located on the intersection of all facets except four and that the only allowed

Table 1. Vertices of $\mathcal{P}^*$.

Vertex	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	Unit cell
$1a, b$	± 1	1	1	1	1	1	$\pm(1$	1	1	$1)$	1×1
2	0	-1	-1	1	1	1	0	0	0	0	2×2
$3a$	0	-1	1	-1	-1	1	0	0	0	0	2×1
$3b$	0	1	-1	-1	-1	1	0	0	0	0	1×2
$4a, b$	$\pm\frac{1}{2}$	0	0	0	0	-1	$\mp(\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2})$	2×2
$5a, b$	0	0	0	$\pm(1$	$-1)$	-1	0	0	0	0	4×4
$6a, b$	$\pm\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	1	$-\frac{1}{3}$	$-\frac{1}{3}$	$\pm(\frac{1}{3}$	-1	$\frac{1}{3}$	$-1)$	3×3
$6c, d$	$\pm\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	1	$-\frac{1}{3}$	$\pm(-1$	$\frac{1}{3}$	-1	$\frac{1}{3})$	3×3
$7a, b$	0	$\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	$\pm(-\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	$-\frac{2}{3})$	2×3
$7c, d$	0	$-\frac{1}{3}$	$\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	$-\frac{1}{3}$	$\pm(-\frac{2}{3}$	$-\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3})$	3×2
$8a, b$	0	0	0	-1	0	0	$\pm(0$	1	0	$-1)$	
$8c, d$	0	0	0	0	-1	0	$\pm(1$	0	-1	$0)$	

configurations of elementary squares are the following.

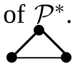
$$\begin{array}{ccc} & + & \\ - & & + \\ & + & \end{array} \qquad \begin{array}{ccc} & - & \\ + & & - \\ & + & \end{array} \qquad \begin{array}{ccc} & + & \\ + & & - \\ & - & \end{array} \qquad \begin{array}{ccc} & + & \\ - & & - \\ & - & \end{array}$$

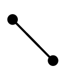
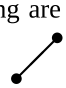
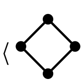
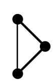
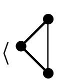
However it can be seen easily that no global spin configuration on the plane can be constructed with these squares only. Therefore vertex $8a$ and similarily the other vertices 8 are not realizable and $\mathcal{P}^*$ is strictly larger than $\overline{\mathcal{P}}$.

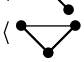
We shall now study the boundary of $\overline{\mathcal{P}}$ on certain low-dimensional subspaces.

5. The subspace $x_9 = 1$

Constraints of the form $\prod \sigma \equiv 1$ or $\prod \sigma \equiv -1$ are generally equivalent to a reduction of dimension by one. On these subspaces the spins in the whole plane are uniquely determined by the spins in a finite number of rows or columns. For the IRF model the only non-trivial case concerns subspaces involving three spins. Here some new ground states appear, different from the vertices of $\mathcal{P}^*$.

On the space $x_9 = \langle$  $\rangle = 1$ many of the spin averages coincide. The only independent variables remaining are

$z_1 = \langle$ $\rangle = \langle$  $\rangle = \langle$  $\rangle = \langle$ $\rangle = \langle$  $\rangle = \langle$  $\rangle = \langle$  $\rangle$

$z_2 = \langle$  $\rangle = \langle$  $\rangle$.

The probability for an elementary square can be written as

$$p\left(\begin{array}{ccc} & \tau_3 & \\ \tau_4 & & \tau_2 \\ & \tau_1 & \end{array}\right) = \tfrac{1}{16}(1 + \tau_2\tau_3\tau_4)[1 + z_1(\tau_1 + \tau_2 + \tau_3 + \tau_4 + \tau_1\tau_2 + \tau_1\tau_4) + z_2\tau_1\tau_2\tau_4]. \qquad (10)$$

In particular

$$p\left(\begin{array}{ccc} & + & \\ + & & + \\ & + & \end{array}\right) = \tfrac{1}{8}(1 + 6z_1 + z_2) \qquad (11)$$

$$p\left(\begin{array}{ccc} & + & \\ + & & + \\ & - & \end{array}\right) = p\left(\begin{array}{ccc} & - & \\ + & & - \\ & + & \end{array}\right) = p\left(\begin{array}{ccc} & - & \\ - & & + \\ & + & \end{array}\right) = \tfrac{1}{8}(1 - z_2). \qquad (12)$$

One finds that the +spins are always organized into triangles. As an example, figure 2 shows a triangle of length 5.

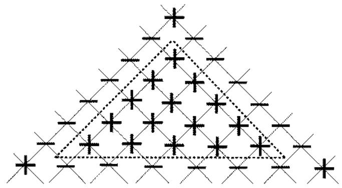


Figure 2. Triangle of +spins of length 5. +spins are always organized into triangles of varying length and fixed orientation.

The size of these triangles can vary but their orientation is fixed. Note the +spins in the three outermost corners. They imply that each triangle is connected to neighbouring triangles. The IRF model with constraint $\equiv 1$ then describes the statistical mechanics of triangles of arbitrary size which are connected to their neighbours at their corners. A typical configuration is displayed in figure 3.

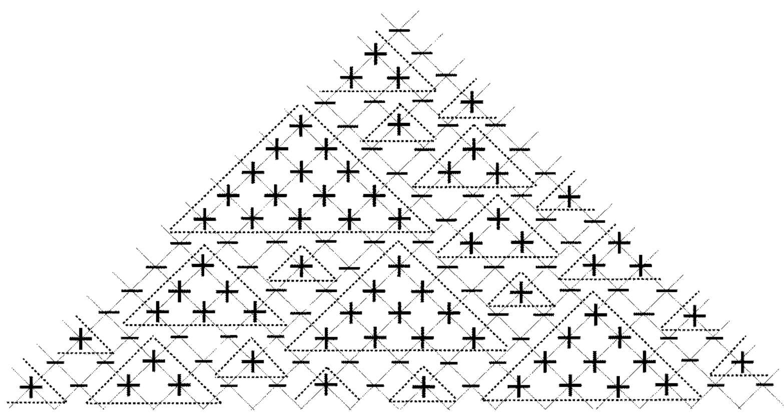


Figure 3. A typical configuration of spins.

Figure 4 depicts the (essentially unique) configurations of monodisperse triangles of length 1, 2, 3.

It will now be shown that the ground states are composed of the three states in figure 4 together with the ferromagnetic state.

The phase diagram is plotted in figure 5. In order to show that this phase diagram is complete, i.e. that there are no more ground states, the following inequalities have to be proved:

$$1 + 6z_1 + z_2 \geqslant 0 \tag{13}$$

$$1 + 4z_1 + 3z_2 \geqslant 0 \tag{14}$$

$$1 - 4z_1 + 3z_2 \geqslant 0. \tag{15}$$

Inequality (13) follows from (11). The proof of inequalities (14) and (15) is somewhat tedious and relegated to appendix A.

Let us now make a brief digression and consider the surface tension and intermediate phases.

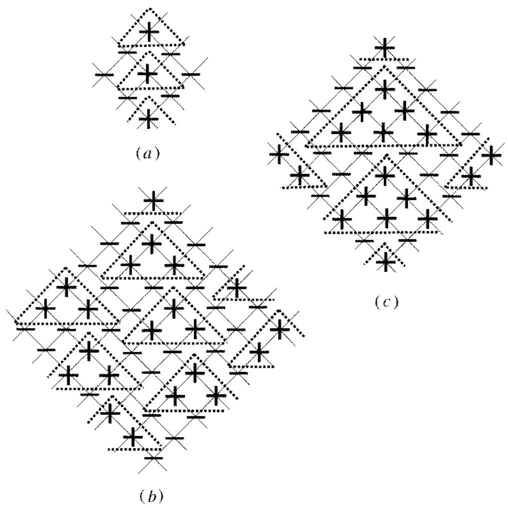


Figure 4. Close-packed monodisperse triangles of lengths $1, 2, 3$. The unit cells are 3×3 (a), 7×7 (b) and 6×6 (c).

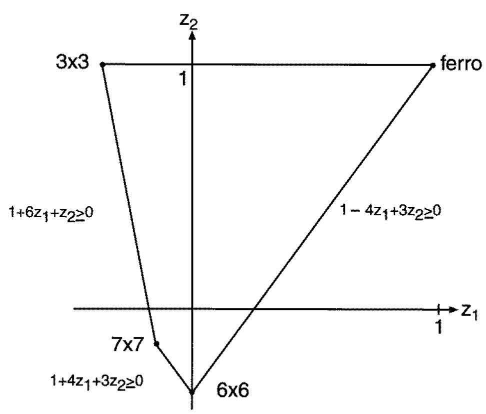


Figure 5. Phase diagram on $x_9 = 1$. There are four ground states: the ferromagnetic +state and three phases of triangles of length $1, 2, 3$.

5.1. Surface tension and intermediate phases

(i) Consider first the line segment between the 3×3 and the ferromagnetic state in the phase diagram. The surface tension between these states is positive. In order to prove this, it is suffient to show that the only configurations $\{\sigma\}$ with $x_9 \equiv z_2 \equiv 1$ are the ferromagnetic state $\sigma_i \equiv +$ or the 3×3 state. Indeed, the condition $x_9 \equiv z_2 \equiv 1$ means that $\equiv$ for any elementary square, and it is an easy exercise to convince oneself that this constraint is only satisfied by the ferromagnetic +state or the 3×3 state. Any other configuration on the subspace $x_9 \equiv 1$ must have < 1 for some elementary squares and therefore has a higher energy for certain ranges of the ϵ_i.

(ii) For the 3×3 and 7×7 ground states the left-hand side of (11) must vanish. Therefore the length of all triangles must be $\leqslant 2$. Now it is easy to verify that triangles of length 1 and 2 can never be neighbours in the above sense, if no triangles of length $\geqslant 3$ are allowed. Therefore only the endpoints can be realized and the surface tension is positive.

(iii) On the boundary segment connecting the 7×7 and 6×6 ground states the equality sign in (14) is valid. Therefore, equation (A4) of appendix A with the $+$ sign is valid as an equality and no row or column of spins may contain the sequences $++++$ or $+--+$. Since a triangle of length 1 involves the latter sequence, only triangles of length 2 or 3 are allowed on the 6×6 – 7×7 boundary. Now it is easy to verify that two neighbouring triangles of length 2 and 3 involve the forbidden sequence $+--+$. Therefore, only the endpoints can be realized and the surface tension is positive again.

(iv) Consider now the 6×6–ferromagnetic boundary. No configuration which maps upon this boundary may contain the sequences $-+--$ or $--+-$. It is shown in appendix B that an infinite number of points on the boundary can be realized. The surface tension therefore vanishes.

6. Infinitely many ground states

In appendix B we found a large number of periodic states which are almost ground states. The admissible configurations were restricted to the intersection of the eight hyperplanes $p\left(\begin{smallmatrix} & \tau_3 & \\ \tau_4 & & \tau_2 \\ & \tau_1 & \end{smallmatrix}\right) = 0$ with $\tau_2\tau_3\tau_4 = 1$. Now we restrict the configurations in such a way that the admissible squares consist of the following set.

$$\begin{matrix} \begin{smallmatrix} & + & \\ + & & + \\ & + & \end{smallmatrix} & \begin{smallmatrix} & + & \\ + & & + \\ & - & \end{smallmatrix} & \begin{smallmatrix} & - & \\ - & & + \\ & + & \end{smallmatrix} & \begin{smallmatrix} & - & \\ + & & - \\ & + & \end{smallmatrix} & \\ \begin{smallmatrix} & - & \\ - & & + \\ & - & \end{smallmatrix} & \begin{smallmatrix} & + & \\ - & & - \\ & - & \end{smallmatrix} & \begin{smallmatrix} & - & \\ + & & - \\ & - & \end{smallmatrix} & \begin{smallmatrix} & - & \\ - & & - \\ & + & \end{smallmatrix} & \begin{smallmatrix} & - & \\ - & & - \\ & - & \end{smallmatrix} \end{matrix} \tag{16}$$

This set differs from the previous one by the omission of the single square $\begin{smallmatrix} & + & \\ - & & - \\ & + & \end{smallmatrix}$ and the addition of the last two squares.

One easily verifies that again the $+$spins are organized into triangles that swim in a sea of negative spins. However, in contrast to the previous section, triangles are no longer connected.

Since every $+$spin is part of a triangle, there are three independent variables.

$$x = p\left(\begin{smallmatrix} & + & \\ + & & + \\ & + & \end{smallmatrix}\right)$$

is analogous to the area covered by triangles,

$$y = p\left(\begin{smallmatrix} & + & \\ + & & + \\ & - & \end{smallmatrix}\right) = p\left(\begin{smallmatrix} & - & \\ - & & + \\ & + & \end{smallmatrix}\right) = p\left(\begin{smallmatrix} & - & \\ + & & - \\ & + & \end{smallmatrix}\right)$$

corresponds to the interface between $+$phase in the interior and the surrounding $-$phase, and

$$z = p\left(\begin{smallmatrix} & - & \\ - & & + \\ & - & \end{smallmatrix}\right) = p\left(\begin{smallmatrix} & - & \\ + & & - \\ & - & \end{smallmatrix}\right) = p\left(\begin{smallmatrix} & - & \\ - & & - \\ & + & \end{smallmatrix}\right)$$

is the number density of triangular 'droplets'. Regarding the final two squares, we have

$$p\begin{pmatrix} & + & \\ - & & - \\ & - & \end{pmatrix} = y + z$$

and $p\begin{pmatrix} & - & \\ - & & - \\ & - & \end{pmatrix}$ is given by normalization

$$p\begin{pmatrix} & - & \\ - & & - \\ & - & \end{pmatrix} = 1 - x - 4y - 4z. \tag{17}$$

It will be proved below that all close-packed triangles of length $L = 1, 2, 3, \ldots$ are ground states and that conversely every ground state on the manifold (16) either is of this form or belongs to one of the two ferromagnetic states. Figure 6 displays the ground state for $L = 4$.

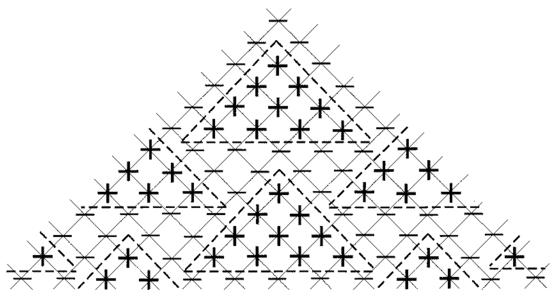


Figure 6. Part of ground state configurations for $L = 4$. The unit cell is 21×21.

The Lth ground state generates the point

$$\boldsymbol{r}_L = \left(\tfrac{1}{2}(L-1)(L-2)z_L, (L-1)z_L, z_L\right)$$

with

$$z_L = \frac{1}{\frac{3}{4}L^2 + 2L + a_L} \qquad a_L = \begin{cases} 1: & L \text{ even} \\ 5/4: & L \text{ odd.} \end{cases}$$

Figure 7 shows the projection of the points $\boldsymbol{r}_L$ onto the (y, z) plane for $L = 1, \ldots, 20$. The two ferromagnetic states collapse to the point $(0, 0)$ which is also included.

The figure already permits an easy proof that the number of ground states is infinite. Indeed, since $z_L/y_L \to 0$ for $L \to \infty$, any convex set containing these states and bounded by a finite number of straight lines must contain a part of the y-axis as a boundary. This, however, is impossible since it implies a finite concentration of +spins in the absence ($z = 0$) of triangles.

For a more complete analysis we have to find the set of inequalities delimiting the possible values of (x, y, z) that can be realized.

One set of inequalities is easy to obtain: let c_L be the probability that a particular elementary square is the upper corner $\begin{matrix} & - & \\ - & & - \\ & + & \end{matrix}$ of a triangle of length L. c_L is the concentration of triangles of length L and

$$z = \sum_{L \geqslant 1} c_L$$

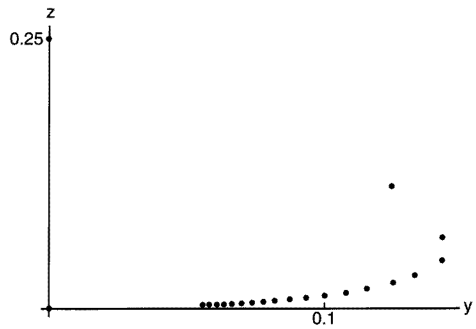


Figure 7. Projection of groundstates onto the (y, z) plane for $L = 1, \ldots, 20$.

$$y = \sum_{L \geqslant 1} (L-1) c_L$$
$$x = \tfrac{1}{2} \sum_{L \geqslant 1} (L-1)(L-2) c_L .$$

Multiplying the inequality

$$(L-k)(L-k-1) \geqslant 0$$

by c_L and summing we obtain the first set of inequalities

$$\mathcal{F}_k \geqslant 0 \qquad k = 0, 1, \ldots . \tag{18}$$

with

$$\mathcal{F}_k = x - (k-1)y + \tfrac{1}{2} k(k-1) z . \tag{19}$$

Equality holds for those configurations which possess triangles of size k or $k+1$ only.

This is sufficient to prove that monodisperse close-packed triangles are true ground states. Indeed, consider the intersection

$$(\mathcal{F}_k = 0) \cap (\mathcal{F}_{k+1} = 0).$$

This intersection is a (one-dimensional) edge of the correlation polyhedron. It corresponds to all configurations of triangles of length $k+1$ only. The extreme realizable points of this edge are ground states. One of these points is $x = y = z = 0$ which represents the ferromagnetic state of all spins negative. If we believe that the states $\boldsymbol{r}_L$ represent the closest packing of monodisperse triangles, then the $\boldsymbol{r}_L$ are indeed true ground states. This seems intuitively very plausible. A formal proof can be given using the following set of inequalities:

$$k^2 p\left(\begin{array}{ccc} & - & \\ - & & - \\ & + & \end{array}\right) - kp\left(\begin{array}{ccc} & + & \\ + & & + \\ & - & \end{array}\right) + p\left(\begin{array}{ccc} & - & \\ - & & - \\ & - & \end{array}\right) \geqslant 0 \qquad k = 0, 1, 2, \ldots . \tag{20}$$

These inequalities are demonstrated in appendix C, completing the proof.

7. Higher dimensions

The methods of this paper can be applied to higher dimensions with minor modifications. For example, the ‘interactions round the cube’ model for the cubic lattice has an infinite number of ground states corresponding to monodisperse close-packed tetrahedra of arbitrary size. Other close-packed structures like cylinders with triangular base and height 1 also generate infinite series of ground states.

Appendix A

In order to prove the inequalities (14) and (15), consider a typical configuration of the ith row and the first few rows above, subject to the constraint $x_9 = 1$. It has the form

$$\begin{array}{ccccccccccccc}
 & & & \cdots & & & \sigma_1\sigma_2\sigma_3\sigma_4 & & & \cdots & & & \\
 & & \cdots & & & \sigma_1\sigma_3 & & & \sigma_2\sigma_4 & & \cdots & & \\
 & \cdots & & \sigma_1\sigma_2 & & & \sigma_2\sigma_3 & & & \sigma_3\sigma_4 & & \cdots & \\
\cdots & & \sigma_1 & & \sigma_2 & & & \sigma_3 & & \sigma_4 & & & \cdots
\end{array}$$

Let $z_1^{(j)}$ be the spin average in the jth row. Then

$$z_1^{(i)} = \langle\sigma\rangle$$
$$z_1^{(i-1)} = \langle\sigma_k\sigma_{k+1}\rangle$$
$$z_1^{(i-2)} = \langle\sigma_k\sigma_{k+2}\rangle$$
$$z_1^{(i-3)} = \langle\sigma_k\sigma_{k+1}\sigma_{k+2}\sigma_{k+3}\rangle$$

and

$$z_2^{(i)} = \langle\sigma_k\sigma_{k+1}\sigma_{k+2}\rangle$$
$$z_2^{(i-1)} = \langle\sigma_k\sigma_{k+3}\rangle.$$

Let us form linear combinations

$$\tilde{z}_1^{(i)} = \gamma_1 z_1^{(i)} + \gamma_2 z_1^{(i-1)} + \gamma_3 z_1^{(i-2)} + \gamma_4 z_1^{(i-3)}$$

where $\sum_1^4 \gamma_i = 1$ and

$$\tilde{z}_2^{(i)} = \alpha z_2^{(i)} + (1-\alpha) z_2^{(i-1)}.$$

It will be shown below that α and the γ_i can be chosen in such a way that

$$1 + 4\tilde{z}_1^{(i)} + 3\tilde{z}_2^{(i)} \geqslant 0 \tag{A1}$$
$$1 - 4\tilde{z}_1^{(i)} + 3\tilde{z}_2^{(i)} \geqslant 0. \tag{A2}$$

Summing these inequalities yields (14) and (15).

It remains to demonstrate (A1) and (A2). These are inequalities for certain one-dimensional Hamiltonians with interaction range $r \leqslant 3$. Now the ground states for finite range Hamiltonians on one-dimensional lattices are well known [7, 6]. Hamiltonians with interaction range $\leqslant 3$ have precisely 19 ground states and it is sufficient to prove (A1), (A2) for each of them. Calculating the lhs on the 19 ground states and demanding that the result be non-negative yields a system of 19 linear inequalities for α and the γ_i. The only solution to these inequalities (which is the same for (A1) and (A2)) is given by

$$\alpha = \tfrac{2}{3} \qquad \gamma_1 = \tfrac{1}{2} \qquad \gamma_2 = \tfrac{1}{4} \qquad \gamma_3 = 0 \qquad \gamma_4 = \tfrac{1}{4}.$$

In hindsight, the corresponding inequalities

$$1 + 2\langle\sigma_k\sigma_{k+1}\sigma_{k+2}\rangle + \langle\sigma_k\sigma_{k+3}\rangle \geqslant \pm(2\langle\sigma\rangle + \langle\sigma_k\sigma_{k+1}\rangle + \langle\sigma_k\sigma_{k+1}\sigma_{k+2}\sigma_{k+3}\rangle) \tag{A3}$$

can also be proved directly from the local inequalities

$$1 + \sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_1\sigma_4 \geqslant \pm(\sigma_1 + \sigma_4 + \sigma_2\sigma_3 + \sigma_1\sigma_2\sigma_3\sigma_4)$$

which follow from

$$(1 \mp \sigma_2\sigma_3)(1 \mp \sigma_1)(1 \mp \sigma_4) \geqslant 0. \tag{A4}$$

Appendix B

In this appendix an infinite number of configurations are exhibited which map onto the 6×6–ferromagnetic boundary in figure 5. This is sufficient to prove that the corresponding surface tension vanishes.

Let us call a sequence of n $-$spins $\cdots + \underbrace{- \cdots -}_{n} + \cdots$ a $-$string of length n and similarly for $+$strings. It is not difficult to prove the following facts.

(i) In any single row or column the $-$spins are either isolated (i.e. have length 1; type A), or have an even length (type B).

(ii) Rows (and columns) of type A and B alternate.

(iii) In a row of type A all the $+$strings have odd lengths.

As a corollary it follows that the lengths of all triangles of $+$spins are odd.

Let us focus on rows of type A. A typical row of type A can be represented by a sequence of integers

$$\cdots, m_1, m_2, m_3, \cdots \tag{B1}$$

where $2m_i - 1$ is the length of the $+$strings. The next row of type A below is obtained from (B1) by applying the transformation

$$\begin{array}{c} \cdots, m, \underbrace{1, \cdots, 1}_{n}, m', \cdots \\ \downarrow \\ \cdots, m-1, n+1, m'-1, \cdots . \end{array} \qquad m > 1, m' > 1, n > 0 \tag{B2}$$

Of particular interest are the periodic states. A simple example is

$$\begin{array}{c} \vdots \\ \cdots, 4, 1, 4, 1, \cdots \\ \cdots, 3, 2, 3, 2, \cdots \\ \cdots, 2, 1, 1, 1, 2, 1, 1, 1, \cdots \\ \cdots, 1, 4, 1, 4, \cdots \\ \vdots \end{array}$$

This represents a state of period 10 in the horizontal direction. One can show that the period p as well as the number of $+$strings per period is always even and that the integers m_i represent a partition of $p/2$. We will not delve more deeply into the interesting combinatoric properties of these partitions. Suffice it to say that the sequences

$$\cdots, 2m, 1, 2m, 1, \cdots \qquad m = 1, 2, \ldots$$

as well as many others generate an infinite number of intermediate periodic states located on the 6×6–ferromagnetic boundary.

Appendix C

This appendix proves inequalities (20).

Let there be a total of M triangles of $+$spins with lengths $L_1, \ldots, L_M$. Let N_- be the total number of elementary squares of the form $\begin{smallmatrix} & - & \\ - & & - \\ & - & \end{smallmatrix}$. We have to prove

$$k^2 M - k \sum_{i=1}^{M} (L_i - 1) + N_- \geqslant 0 \qquad k = 0, 1, 2, \ldots . \tag{C1}$$

In order to estimate N_-, complete each triangle of length L to a square of length $L \times L$ as shown in figure C1.

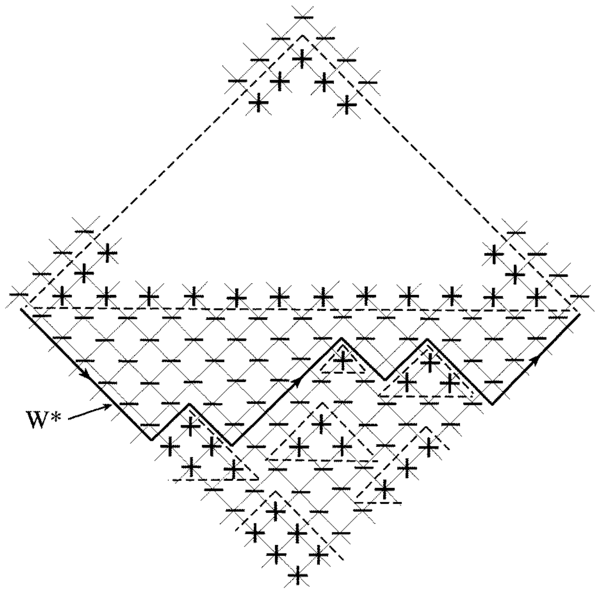


Figure C1. Triangle of $+$spins and typical spin configuration below. Path w^* delimits the region of $-$spins associated with the triangle.

Associate a number $N_-^{(i)}$ of elementary squares $\begin{smallmatrix} & - & \\ - & & - \\ & - & \end{smallmatrix}$ with this figure in the following way.

Consider all paths w from the left to the right corner with the properties

(i) the only turns allowed are $\vee$ or $\wedge$

(ii) all the triangles protruding into the lower part of the square are below w.

Let w^* be that path for which the number of $-$spins above is maximal and $N_-^{(i)}$ the number of elementary squares $\begin{smallmatrix} & - & \\ - & & - \\ & - & \end{smallmatrix}$ above w^*. Since no square $\begin{smallmatrix} & - & \\ - & & - \\ & - & \end{smallmatrix}$ is counted twice,

$$N_- \geqslant \sum_{i=1}^{M} N_-^{(i)}$$

and it is sufficient to prove

$$k^2 M - k \sum_{1}^{M} (L_i - 1) + \sum_{1}^{M} N_-^{(i)} \geqslant 0. \tag{C2}$$

In order to estimate $N_-^{(i)}$, let M_i be the number of $\wedge$ turns for path w^* for the ith triangle. Then one can show that

$$N_-^{(i)} \geqslant \frac{1}{2} \left[\frac{L_i}{M_i + 1} \right] (L_i - M_i - 1 + L_i \bmod (M_i + 1)) \tag{C3}$$

where $[x]$ is the greatest integer $\leqslant x$. Now it is sufficient to prove

$$k \sum_{1}^{M} (L_i - 1) \leqslant \frac{1}{2} \sum_{1}^{M} \left[\frac{L_i}{M_i + 1} \right] (L_i - M_i - 1 + L_i \bmod (M_i + 1)) + k^2 M$$

where

$$\sum_{1}^{M} M_i \leqslant M. \tag{C4}$$

Setting

$$L_i = P_i(M_i + 1) + Q_i \qquad 0 \leqslant Q_i \leqslant M_i$$

and minimizing with respect to P_i yields

$$P_i \in \{k, k+1\}. \tag{C5}$$

Minimizing with respect to Q_j yields

$$Q_j = \begin{cases} 0: & P_j = k+1 \\ \text{arbitrary}: & P_j = k \end{cases} \tag{C6}$$

and the inequality reduces to (C4). The conditions of equality in (20) are given by (C5), (C6), and equality in (C4).

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