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Magnetisation in some frustration models

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Abstract. In the models proposed by Longa and Oleś there exist two oppositely magnetised equilibrium states, if the temperature is sufficiently low. Spins in the frustrated cells also carry a moment, the magnitude of which is $1/\sqrt{5}$ at zero temperature.

1. Introduction

Recently, Longa and Oleś (1980) studied a family of periodic Ising frustration models on the square lattice, in which frustrated squares occupied pairs of neighbouring columns and two such pairs were separated by $m \geqslant 1$ columns of non-frustrated squares (figure 1). This distribution of frustration can be realised, for example, by choosing the bonds negative along each $(m+2)$th vertical line and positive otherwise. Applying the method of dimers, they calculated the free energy of these models and found a singularity at some $T = T_c(m) > 0$. To study the low-temperature behaviour, they performed a mean-field calculation which suggested the appearance of long-range order in areas of non-frustrated squares. In the present note, this suggestion is verified rigorously and it is shown that the spins in the frustrated cells also become partially ordered.

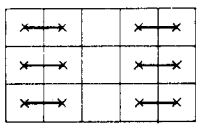

Figure 1. The $m = 1$ frustration model. Crosses mark frustrated squares and the lines connecting them indicate the wrong bonds of the ground states σ_+ and σ_- (σ_0, in general).

Very recently, Hoever *et al* (1981) extended the discussion to models with arbitrary periodic distribution of columns of frustrated squares: they calculated the free energy and found a simple and striking condition for the existence of a positive critical temperature. The study of the magnetisation is more difficult in this case and will be the subject of future work.

On physical grounds, it is easy to understand why magnetisation sets in at low temperatures in the models of Longa and Oleś. Let us adopt the choice for the bonds as indicated above and consider the ground state spin configurations (GS) of the system. The $\sigma_+ \equiv 1$ and $\sigma_- \equiv -1$ configurations are GS; in figure 1, full lines of unit length cross

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the negative bonds, indicating that they are the 'wrong bonds' in σ_+ and σ_-: those at the higher energy level. Consider, for example, σ_+. A local zero-energy transformation (LZET), which consists of flipping several non-neighbouring spins along a vertical line with negative bonds, carries σ_+ into another GS. Let F_+ be the family of those GS which can be obtained from σ_+ by performing a sequence of LZET and let F_- be the corresponding family for σ_-. Every GS in $F_+(F_-)$ shows long-range order in the sense that every spin outside the negative vertical lines has the value $+1$ (-1). Clearly, $-F_- = F_+$ and these sets are disjoint. One expects that F_+ and F_- are the continuations, to $T = 0$, of oppositely magnetised low-temperature phases. The complication arises from the existence of a family F_0 of GS which is disjoint from both F_+ and F_-. The elements of F_0 can be obtained from those of F_+ or F_- by flipping whole strips of spins; an example is shown in figure 2. The 'strip-flip' transformation is not local, but it can be

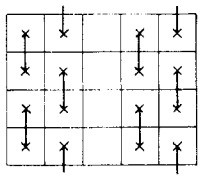

Figure 2. Wrong bonds in a ground state belonging to F_0.

performed as a sequence of local transformations at a total cost of energy proportional to the width of the strip. Therefore, F_0 provides us with a channel between F_+ and F_-, available at all small positive temperatures. A simple numerical estimate shows, however, that the mixing of F_+ and F_- via F_0 is a negligible effect: it is easy to calculate the total number of GS, $|F_{\text{tot}}|$, and the number of GS with long-range order, $|F_+| + |F_-|$. Considering a square of N sites, one finds the asymptotic results

$$|F_{\text{tot}}| \equiv |F_+| + |F_-| + |F_0| = 2(1 + c^{\sqrt{N}})^{\sqrt{N}/(m+2)}$$

and

$$|F_+| + |F_-| = 2c^{N/(m+2)}$$

where $c = (1+\sqrt{5})/2$ (see later in the text). Hence, the entropy of the mixing at zero temperature is

$$\ln|F_{\text{tot}}| - \ln(|F_+| + |F_-|) = [\sqrt{N}/(m+2)] \ln(1 + c^{-\sqrt{N}})$$

which vanishes in the thermodynamic limit, suggesting that F_+ and F_- represent different low-temperature phases.

In § 2, we make this 'physical argument' precise. In order to obtain this goal, we extend the method of Peierls which cannot be applied to the present problem, either in its original form (Peierls 1936), or in a recent generalised version aimed at covering cases of frustration (Sütö 1980).

2. Study of the magnetisation

We consider any model with frustrated squares distributed as discussed above, for some $m \geqslant 1$. Let σ_0 be one of the two GS in which the wrong bonds are those along the vertical

lines between neighbouring columns of frustrated squares (see figure 1). We prove the following proposition.

Proposition. If the temperature is sufficiently low then there exists an equilibrium state, belonging to σ_0 in the following sense:

(i) In any typical configuration, σ, of this state, one can find an infinite connected set of sites over which $\sigma = \sigma_0$.

(ii) If x is not a common site of four frustrated squares then

$$\sigma_0(x)\langle\sigma(x)\rangle_{\sigma_0} > 0$$

and goes to 1 with T going to 0.

(iii) If x is the common site of four frustrated squares (i.e. x is in a frustrated cell) then

$$\langle\sigma(x)\rangle_{\sigma_0} = (1/\sqrt{5})\sigma_0(x) \approx 0.447\sigma_0(x)$$

at $T = 0$.

We may remark the following.

(1) The equilibrium state belonging to σ_0 can be generated as the thermodynamic limit of probability distributions in finite volumes, if $\sigma(x) = \sigma_0(x)$ on the boundary of these volumes. The notation $\langle\cdot\rangle_{\sigma_0}$ refers to this construction.

(2) Except (iii), the above proposition contains the usual statements which can be obtained by a Peierls-type argument. A bound T_0, below which (i) and (ii) are verified and which is common for any $m \geqslant 1$, can be inferred from the proof; this T_0 is, however, a poor lower estimate for the critical temperatures.

(3) By reason of symmetry, there exists another equilibrium state belonging to $-\sigma_0$ in the above sense. Therefore, the properties (i)–(iii) imply the breakdown of the $\sigma \to -\sigma$ symmetry of the Hamiltonian.

To prove the proposition, we consider a finite part V of the lattice, fix the configuration σ_0 outside V and study the equilibrium probability distribution P_V for the configurations inside. By definition,

$$P_V(\text{the configuration is } \sigma \text{ in } V) = Z^{-1}_{V,\sigma_0} \exp[-\beta(H(\sigma) - H(\sigma_0))]$$

$$= Z^{-1}_{V,\sigma_0} \exp\Big(-2\beta \sum_{\langle xy\rangle \in \partial(\sigma)} J_{xy}\sigma_0(x)\sigma_0(y)\Big) \tag{1}$$

where $\partial(\sigma)$ contains those bonds $\langle xy\rangle$ for which $\sigma(x)\sigma(y) = -\sigma_0(x)\sigma_0(y)$ and Z_{V,σ_0} is the partition function corresponding to the boundary condition. If for each $\langle xy\rangle \in \partial(\sigma)$ one draws a broken line of unit length crossing the bond $\langle xy\rangle$, one finds that $\partial(\sigma)$ is represented by a collection of closed lines separating the domains of V where $\sigma = \sigma_0$ from those where $\sigma = -\sigma_0$ (an example for $\partial(\sigma)$ is shown in figure 3). Once σ_0 is fixed

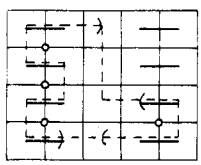

Figure 3. The ground state σ_0 and a contour with respect to it. Zero-energy sequences are put in parentheses.

outside V, there is a one-to-one correspondence between the configurations and the collections of closed lines on the dual lattice. Let Ω_0 denote the set of the wrong bonds of σ_0; these are crossed by full lines of the dual lattice. Now, the sum in the exponent of equation (1) has a simple geometric interpretation. The sets $\partial(\sigma)$ and Ω_0 may have common bonds which appear in the figure as coinciding full and broken lines; if $|\partial \cap \Omega_0|$ is the number of common bonds and $|\partial - \Omega_0|$ is the number of bonds belonging to ∂ but not to Ω_0, then

$$\sum_{\langle xy\rangle \in \partial} J_{xy}\sigma_0(x)\sigma_0(y) = |\partial - \Omega_0| - |\partial \cap \Omega_0| \equiv k_\partial. \tag{2}$$

Here we have assumed that $|J_{xy}| = 1$. Plainly,

$$0 \leqslant k_\partial \leqslant |\partial|. \tag{3}$$

We say that a set of bonds, Γ, is a contour if $\Gamma = \partial(\sigma)$ for some σ and if Γ is represented by a singly or multiply connected line. For any σ, $\partial(\sigma)$ is the union of maximal connected parts, each of them being a contour. If for some $x \in V$ we find $\sigma(x) = -\sigma_0(x)$ then there is at least one contour in $\partial(\sigma)$ which surrounds x. In the following formulae, Γ always denotes a contour and $x \in \mathrm{Int}\,\partial$ means that some part of ∂ surrounds x. Now let $0 < \varepsilon < 1$ and x be an arbitrary site in V. Then the following inequalities are true for the probability distribution (1):

$$\begin{aligned} P_V[\sigma(x) = -\sigma_0(x)] &\leqslant P_V[x \in \mathrm{Int}\,\partial(\sigma)] \\ &\leqslant \sum_{\Gamma:\, x \in \mathrm{Int}\Gamma} P_V[\Gamma] \\ &= \sum_{\substack{\Gamma:\, x \in \mathrm{Int}\Gamma \\ k_\Gamma \geqslant \varepsilon|\Gamma|}} P_V[\Gamma] + \sum_{\substack{\Gamma:\, x \in \mathrm{Int}\Gamma \\ 0 < k_\Gamma < \varepsilon|\Gamma|}} P_V[\Gamma] + \sum_{\substack{\Gamma:\, x \in \mathrm{Int}\Gamma \\ k_\Gamma = 0}} P_V[\Gamma] \\ &\equiv A_x(\varepsilon, >) + A_x(\varepsilon, <) + A_x(0) \end{aligned} \tag{4}$$

where $P_V[\Gamma]$ is the probability that Γ is a maximal connected component of some $\partial(\sigma)$. According to the usual Peierls argument (see e.g. Griffiths 1972),

$$A_x(\varepsilon, >) \leqslant \sum_{l \geqslant 4} (l/2)3^l \, \mathrm{e}^{-2\beta\varepsilon l}. \tag{5}$$

The second and third sums in equation (4) do not appear if there is no frustration present; below we elaborate their estimates.

Let $\hat{\partial}$ denote the set of those sites of the dual lattice which are visited by ∂, and let us introduce the notation

$$z = \mathrm{e}^{-2\beta}.$$

Then

$$P_V[\Gamma] = z^{k_\Gamma} \sum_{\partial':\, \hat{\partial}' \cap \hat{\Gamma} = \varnothing} z^{k_{\partial'}} \Big/ \sum_{\partial''} z^{k_{\partial''}} \tag{6}$$

where the denominator is just Z_{V,σ_0} and, if some configuration σ contributes to the LHS, then $\partial(\sigma) = \partial' \cup \Gamma$ with one of the ∂' in the numerator of the RHS.

It is obviously true that

$$\sum_{\partial''} z^{k_{\partial''}} \geqslant \sum_{\partial':\, \hat{\partial}' \cap \hat{\Gamma} = \varnothing} z^{k_{\partial'}} \sum_{\partial:\, \hat{\partial} \subset \hat{\Gamma}} z^{k_\partial},$$

which gives us

$$P_V[\Gamma] \leqslant z^{k_\Gamma} / \sum_{\partial:\, \hat{\partial} \subset \hat{\Gamma}} z^{k_\partial}. \tag{7}$$

This estimate is valid for any contour Γ. Then

$$A_x(\varepsilon, <) \leqslant \sum_{\substack{\Gamma:\, x \in \mathrm{Int}\Gamma \\ 0 < k_\Gamma < \varepsilon |\Gamma|}} \Bigg(\sum_{\substack{\partial:\, \hat{\partial} \subset \hat{\Gamma} \\ k_\partial = 0}} 1 \Bigg)^{-1}. \tag{8}$$

First, we show that

$$n_\Gamma \equiv \sum_{\substack{\partial:\, \hat{\partial} \subset \hat{\Gamma} \\ k_\partial = 0}} 1 > \left(\frac{1+\sqrt{5}}{2} \right)^{(1-3\varepsilon)|\Gamma|/2-1} \equiv f(|\Gamma|) \tag{9}$$

holds for any Γ satisfying the inequalities

$$0 < k_\Gamma < \varepsilon |\Gamma|. \tag{10}$$

For, let Γ be such a contour. We consider the line representing Γ (figure 3) and divide it into zero-energy segments (ZES) and purely positive-energy segments (PPES). A ZES is a maximal piece of Γ which begins with a wrong bond, goes on with an alternating sequence of good and wrong bonds and is terminated by a good bond (good and wrong bonds are elements of $\Gamma - \Omega_0$ and $\Gamma \cap \Omega_0$, respectively). A PPES is a maximal connected part of Γ between two ZES, and therefore it contains only good bonds. The following elementary relations hold:

$$\begin{aligned} &r_\Gamma \equiv (\text{number of ZES}) = (\text{number of PPES}) \leqslant k_\Gamma < \varepsilon |\Gamma| \\ &(1-\varepsilon)|\Gamma|/2 < |\Gamma \cap \Omega_0| < |\Gamma|/2, \end{aligned} \tag{11}$$

and, as a consequence,

$$\begin{aligned} \sum_{\mathrm{ZES} \in \Gamma, |\mathrm{ZES}| \geqslant 4} |\mathrm{ZES}| &= 2 \times (\text{number of wrong bonds belonging to ZES of length} \geqslant 4) \\ &\geqslant 2(|\Gamma \cap \Omega_0| - r_\Gamma) \geqslant (1-3\varepsilon)|\Gamma| \end{aligned} \tag{12}$$

where $|\mathrm{ZES}|$ denotes the length of a ZES.

Now consider a ZES of length $2l$ where $l \geqslant 2$; this goes through the centres of $2l$ frustrated squares. These centres surround $l-1$ sites, $x_1, \ldots, x_{l-1}$, of the lattice (denoted by circles in figure 3); the spins sitting here are in frustrated cells. To obtain the estimate (9) we have to calculate n_{l-1}, the number of ground states of these $l-1$ spins with the condition that the configuration is σ_0 outside them. Clearly, $\{\sigma_0(x_1), \ldots, \sigma_0(x_{l-1})\}$ is a GS and any configuration not containing the detail $\ldots, -\sigma_0(x_i), -\sigma_0(x_{i+1}), \ldots$ is also a GS. It is easy to see that n_l satisfies the difference equation for the Fibonacci numbers:

$$n_{l+1} = 2n_{l-1} + (n_l - n_{l-1}) = n_{l-1} + n_l \tag{13a}$$

with the initial conditions

$$n_1 = 2, \qquad n_2 = 3. \tag{13b}$$

This equation can be solved by the use of the method of generating functions, resulting in

$$n_l = \frac{2\sqrt{5}+4}{5+\sqrt{5}}\left(\frac{\sqrt{5}+1}{2}\right)^l - (-1)^l \frac{2\sqrt{5}-4}{5-\sqrt{5}}\left(\frac{\sqrt{5}-1}{2}\right)^l > \left(\frac{1+\sqrt{5}}{2}\right)^l \tag{14}$$

for any $l \geqslant 1$. Any ZES the length of which is $2l \geqslant 4$ contributes to n_Γ with a factor n_{l-1}. From (12) and (14) one then obtains (9). The bound given in (9) depends only on the length of Γ. This makes it possible to continue (8) as

$$A_x(\varepsilon, <) \leqslant \sum_l N_l / f(l) \tag{15}$$

where N_l denotes the number of contours of length l which surround x and satisfy (10). Now we give an upper bound to this number. It is easy to estimate the number of those contours which contribute to N_l and contain a given bond, b, a given number, l_0, of wrong bonds and a given number, r, of ZES. Their number will be denoted by $N_l(b, l_0, r)$. Starting from b, one can order the l bonds of the contour in a sequence so that neighbouring bonds join in a site of the dual lattice. Therefore contours correspond to random walks of length l, starting from b. In each site along a PPES, there are at most three possibilities to continue the walk; once the walk arrives at a ZES, there are altogether six possibilities until we can continue with the following PPES: two ways to choose the first good bond of the ZES and three to choose the last one. The total length of the PPES is $l - 2l_0$; therefore

$$N_l(b, l_0, r) \leqslant 3^{l-2l_0} 6^r \leqslant 3^{l-(1-\varepsilon)l} 6^{\varepsilon l} = 18^{\varepsilon l} \tag{16}$$

where we have used (11). It follows also from (11) that there are at most εl and $\varepsilon l/2$ different possibilities for choosing r and l_0, respectively. Furthermore, if one starts from x and takes $l/2$ steps to the right, one certainly crosses at least one bond of any contour contributing to N_l. Therefore, it is sufficient to choose the starting bond b from a set containing $l/2$ bonds. These facts and (16) yield

$$N_l \leqslant \tfrac{1}{4} l^3 \varepsilon^2 18^{\varepsilon l}. \tag{17a}$$

Also, (11) gives

$$N_l = 0 \qquad \text{if } l < 1/\varepsilon \tag{17b}$$

because $r_\Gamma \geqslant 1$ for any Γ satisfying (10). Equations (8), (9), (15) and (17) together result in

$$A_x(\varepsilon, <) \leqslant 0.4\varepsilon^2 \sum_{l \geqslant 1/\varepsilon} (37^\varepsilon \times 0.787)^l. \tag{18}$$

Suppose now that x is not in a frustrated cell; then $A_x(0) = 0$ and

$$P_V[\sigma(x) = -\sigma_0(x)] \leqslant \sum_{l \geqslant 4} (l/2) 3^l \, \mathrm{e}^{-2\beta\varepsilon l} + 0.4\varepsilon^2 \sum_{l \geqslant 1/\varepsilon} (37^\varepsilon \times 0.787)^l. \tag{19}$$

Choosing $\varepsilon = 0.066$ and $\beta > 3.2$, we find that the sums on the RHS of (19) are convergent. Then, from the Borel–Cantelli lemma (see e.g. Feller 1968) it follows that with probability one there is only a finite number of contours surrounding x, which is another way of formulating the percolation property (i) of the proposition. If ε is so small that $A_x(\varepsilon, <) < \frac{1}{2} - \alpha$ (where $\alpha > 0$) and β is so large that $A_x(\varepsilon, >) < \alpha/2$, then

$$P_V[\sigma(x) = -\sigma_0(x)] \leqslant (1-\alpha)/2,$$

showing that a moment, parallel to $\sigma_0(x)$, appears in x. Finally, if we keep ε fixed and let β go to infinity, we obtain that

$$\limsup_{\beta\to\infty} P_V[\sigma(x)=-\sigma_0(x)] \leqslant 0.4\varepsilon^2 \sum_{l\geqslant 1/\varepsilon} (37^{\varepsilon}\times 0.787)^l. \tag{20}$$

This inequality is true for any positive ε and volume V, implying that $\sigma(x)=\sigma_0(x)$ at $T=0$ with full probability. This concludes the proof of the statement (ii) of the proposition.

The bounds (5) and (18) are also valid for x not in a frustrated cell. However, $A_x(0)$ is not zero in that case. Let $\gamma(x)$ denote the shortest possible contour around x, that is, the contour of the four edges separating x from its nearest neighbours. Now, $k_{\gamma(x)}=0$ and $k_\Gamma>0$ for any other contour around x. We can write therefore

$$A_x(0)=P_V[\gamma(x)]. \tag{21}$$

Below we show that

$$\lim_{V\to\infty} P_V[\gamma(x)]=2/(5+\sqrt{5})\approx 0.276 \tag{22}$$

at $T=0$. Indeed, for $\beta=+\infty$,

$$z^{k_\partial}=\begin{cases}0 & \text{if } k_\partial>0,\\ 1 & \text{if } k_\partial=0,\end{cases} \tag{23}$$

and the substitution of (23) into (6) gives

$$P_V[\gamma(x)]=\sum_{\substack{\partial:\ \gamma(x)\subset\partial\\ k_\partial=0}} 1 \Big/ \sum_{\partial:\ k_\partial=0} 1. \tag{24}$$

In the numerator, the summation runs over those GS which coincide with σ_0 outside V and $-\sigma_0$ on the site x. In the denominator, we find the same summation except the restriction on $\sigma(x)$. In every GS occurring in these summations the configuration outside the frustrated cells coincides with σ_0. The number of GS is therefore the product of the numbers of GS in each column of frustrated cells. The contribution of every column cancels out in (24), except that of the one containing x. If, in this column, there are m_1 sites above x and m_2 below it, then

$$P_V[\gamma(x)]=n_{m_1-1}n_{m_2-1}/n_{m_1+m_2+1} \tag{25}$$

where n_l is given by (14). If both m_1 and m_2 go to infinity, we obtain the limit (22). The third part of the proposition follows from (22) and the fact that

$$\lim_{\beta\to\infty} P_V[\sigma(x)=-\sigma_0(x)]=\lim_{\beta\to\infty} P_V[\gamma(x)]. \tag{26}$$

3. Concluding remarks

We have rigorously shown that frustrated systems described by the above models become magnetically ordered at sufficiently low temperatures. An interesting finding is that ground states which locally transform into each other may not be equivalent from a statistical point of view. Spins in the frustrated cells become magnetised though their

moments are not fully saturated at zero temperature. Therefore, a periodic oscillation of the magnetisation appears in the horizontal direction. The continuity, at $T = 0$, of the moments in the frustrated cells still needs a proof.

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