Ground-state correlations in the two-dimensional Ising frustration model

J. Phys. C: Solid State Phys., Vol. 12, 1979. Printed in Great Britain. © 1979

Ground-state correlations in the two-dimensional Ising frustration model

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Received 6 March 1979

Abstract. The ground states of the Ising spin glass with random $\pm J$ bonds on a square lattice have been studied numerically. The distribution of effective fields is obtained as a function of the concentration of negative bonds, together with the proportion of 'living' bonds (i.e. bonds which are frustrated in some ground states only). The comparison of different ground states shows the existence of large packets of solidary spins which keep the same relative orientation in all cases. For the (18×18) samples, the largest packet contains on average more than half the spins, even for maximum bond disorder. The results reveal a striking rigidity of the system at zero temperature, which is very different from the behaviour of simple paramagnets and fully frustrated models.

1. Introduction

The theoretical aspects of spin glasses are still rather confused at present, in spite of many interesting suggestions that have been put forward and calculations that have been performed. Fundamental questions about the nature of the ordering in these materials remain unanswered and the existence of a phase transition at non-zero temperature in the two-dimensional random-bond Ising model has not been proved or disproved. Conflicting results have been obtained by various approaches and even the interpretation of Monte Carlo simulations is not clear-cut (Kirkpatrick 1977, 1979, Bray *et al* 1978, Stauffer and Binder 1978).

Our approach to this problem follows directly from previous work on the frustration effect (Vannimenus and Toulouse 1977). In that paper, the ground-state energy and entropy of a two-dimensional Ising model were obtained numerically as functions of the concentration of random antiferromagnetic bonds and the energy of a topological defect (i.e. a domain boundary) was shown to vanish at the ferromagnetic–spin glass transition.

Here we use the same model and numerical methods to obtain information on other ground-state properties, namely the distribution of local effective fields, the fraction of 'living' bonds and the size of packets of solidary spins. The results are interesting because the ground states of the disordered system show much more rigidity than expected from the study of a periodic model described by Bray *et al.* We have found fairly long-range correlations between the ground states, suggesting that at zero temperature the system does not behave like a simple paramagnet. There may be a well-defined spin glass–paramagnet transition at finite temperature, but it is also possible that the system gradually freezes into a glass-like state. The study of the dynamics of the model seems to be the method best suited to resolving this question, but this lies outside the scope of the present work.

2. Model and methods

The frustration model considered here consists of Ising spins which interact via the Hamiltonian

$$\mathscr{H} = -\sum J_{ij} S_u S_j \qquad (1)$$

where the nearest-neighbour interactions J_{ij} have strength $\pm J$. The negative bonds have a concentration x and are frozen at random positions (we restrict the present study to a square lattice).

As pointed out by Toulouse (1977), this model is the simplest that shows the competitive effect that is essential in spin glasses. When an odd number of negative bonds occurs on an elementary square (plaquette), the spins cannot find a fully satisfactory arrangement and there are several choices that minimise their energy. This gives rise to a structure for the ground states and low-lying excited states that is much more complicated than is found in pure systems or systems with only dilution-type disorder.

The study of these states is made less cumbersome by the existence of a simple geometrical description (Kirkpatrick 1977, Toulouse 1977). A map of the unsatisfied bonds suffices to define a state and such a map is conveniently represented by drawing lines between the centres of the plaquettes adjacent to the frustrated bonds. A ground state corresponds to a pairing of the frustrated plaquettes with the minimum number of bonds.

Many relevant properties (but not the magnetisation) depend only on the geometry of this frustration network and not on the complete distribution of J_{ij}. This makes it possible to study samples of moderate size without the use of a computer and avoids the machinery of Monte Carlo simulations and the difficulties associated with metastable states.

In previous work (Vannimenus and Toulouse 1977), the ground-state energy and entropy for a limited number of (20 × 20) and (30 × 30) samples were obtained in this fashion and the agreement with the Monte Carlo calculations (Kirkpatrick 1977) was found to be rather good. In the present work we analyse in greater detail all the ground states of a larger number of random (18 × 18) samples, for the whole range of negative bond concentrations.

At the same time a computer program was also written to search for ground states on similar samples and its effectiveness was tested by comparison with the manual approach. The computer search is based on a Monte Carlo method: the sample is cooled progressively to $T = 0$ and the states of lowest energy thus obtained are projected to a reference state in order to find favourable spin rearrangements. This method takes advantage of local improvements, even if the total energy is not lowered by the cooling process. The process is repeated, starting from different random configurations, to generate better ground states and a map of zero-energy rearrangements. After checking the program on (18 × 18) samples and on frustrated periodic models, it was used to study a (40 × 40) sample which is too large for a direct search. 190 Monte Carlo runs were performed in this case. Analysis of the final configurations showed that the true ground state was not quite attained, although the system had considerable rigidity and very large rearrangements had to be considered to lower the energy further. The ground-state determination is thus very satisfactory in practice, as it takes into account spin configurations on all scales and not only small groups, as do the usual Monte Carlo methods.

The complementarity of both approaches is an advantage of the double-peaked distribution used here for the J_{ij}, compared to the Gaussian distribution. The particular choice made clearly affects the low-temperature properties, for instance the location of the critical concentration of negative bonds. However, it is not an oversimplification and thus the residual entropy found in the $\pm J$ model yields a finite density of low-energy excitations if the distribution is widened into a continuous one. This is of direct relevance for experimental quantities like the specific heat.

3. Numerical results

3.1. Comparison with previous results

As a first step we have compared the data from the present series of samples with previous work on the same model. In our Monte Carlo runs we found that the systematic search described above led to an improvement of about $0{\cdot}05\,J$ per spin for the ground-state energy (for $x = 0{\cdot}5$). This figure gives an indication of the range over which metastable states, with a long lifetime and a large statistical weight, are likely to affect the simulations based on simple cooling. The final results are in very good agreement with those already published ($E_0/J \sim -1{\cdot}40$ for $x = 0{\cdot}5$).

To obtain the defect energy E_D, we have compared the ground-state energies determined with periodic and antiperiodic boundary conditions on opposite sides of the sample. The difference between them vanishes at a critical concentration x_c, the frustration threshold, which is associated with the disappearance of ferromagnetic order. In the present experiments on (18 × 18) samples, x_c varied between 0·09 and 0·12, with the average somewhat larger than the threshold found in the previous study (0·09), where free boundary conditions had been used and larger samples considered.

The values deduced from both sets of results are lower than the value of $x_c = 0{\cdot}15$ favoured by other numerical studies: Monte Carlo experiments on (80 × 80) samples (Kirkpatrick 1977) and the application of a linear programming algorithm (R Rammal and R Maynard 1979 private communication). The discrepancy may come from size effects in our samples, or from the existence of metastable states in the Monte Carlo calculations. Another possible explanation is that E_D vanishes with zero slope; this would make the threshold difficult to determine in this way but would raise interesting new questions.

Further work is needed to resolve this point and we are led to ask what other properties among the wealth of microscopic information available from the ground states may signal the transition to a spin-glass phase.

3.2. Distribution of effective fields

In the theoretical work on spin glasses, much use has been made of the distribution of effective fields $P(H_e)$ which gives the spectrum of one-spin excitations (Klein 1976, Binder 1977). In the present model $|H_e|$ can only take the values 0, $2J$ and $4J$ and there is a finite fraction of spins in zero effective field (idle spins). These features are attributable to the discrete values of the interactions, and bring about considerable simplification compared with continuous interactions. It is obvious that much detail is lost, but for short-range Gaussian interactions, it has been found numerically that the density of spins in zero field does not vanish (Kirkpatrick 1979) and we expect that $P(0)$ for the $\pm J$ model gives a useful indication of the low-energy one-spin excitations for short-range interactions.

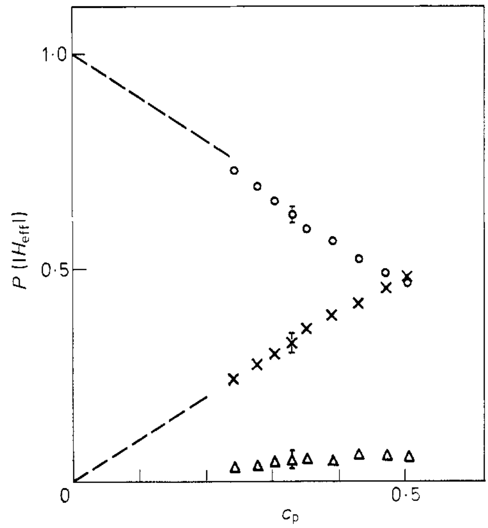

Figure 1. Distribution of effective fields as a function of the concentration c_p of frustrated plaquettes. Every point represents an average over three to five (18 × 18) samples. The broken lines indicate the slopes at the origin (equation 3). △ $H_{eff} = 0$; × $H_{eff} = 2J$; ○ $H_{eff} = 4J$.

The distribution of effective fields depends on the particular ground state considered, but the fluctuations are not too large and significant averages may be obtained with our samples. The results are shown in figure 1, where the abscissa represents the concentration of frustrated plaquettes c_p:

$$c_p = (1 - z^4)/2. \qquad (2)$$

Here $z = (1 - 2x)$ is the expectation value of the bond sign. The use of c_p as a variable is convenient as it embodies the symmetry $x \to 1 - x$ and emphasises the importance of the frustration, although the basic independent variables are the bonds and the plaquettes are independent random variables only for $x = \frac{1}{2}$.

By simple inspection of the configurations with few negative bonds, expressions valid to second order in x and c_p are easily obtained:

$$P(H_e = 0) \sim 6x^2 \sim \tfrac{3}{8}c_p^2 \tag{3a}$$

$$P(|H_e| = 2J) \sim 4x - 12x^2 \sim c_p \tag{3b}$$

$$P(|H_e| = 4J) \sim 1 - 4x + 6x^2 \sim 1 - c_p - \tfrac{3}{8}c_p^2. \tag{3c}$$

The probability $P(2J)$ is almost equal to c_p except for $x \sim 0{\cdot}5$ (see figure 1) so that equation (3*b*) provides a good approximation over the whole range.

The three probabilities appear to vary smoothly with the concentration of antiferromagnetic bonds; they present no clear break that could be associated with a transition to a spin-glass state. The most noteworthy feature is that $P(0)$ remains quite small and saturates at a value of about 0·06 for x greater than 0·15. This means that in spite of increasing frustration, the system is able to keep its total energy down and maintains a low concentration of idle spins. The proportion of idle spins found here is slightly smaller than that observed by Kirkpatrick in his Monte Carlo experiments ($P(0) \sim 0{\cdot}08$). This is linked to the slightly better ground states and the lower ground-state entropy found after manual calculation.

It is instructive to compare these results with the distribution of effective fields found in the 'odd model' studied by Villain (1977), where the bonds on every other column are negative and the frustration is complete. Let us compute the mean-square effective field, averaged over all ground states:

$$\overline{H_e^2} = \overline{(\sum_j J_{ij}S_j)^2}$$
$$= 4J^2 + 2\sum_{k \neq l} \overline{J_{ik}J_{il}S_kS_l}$$

When we sum over all sites, the terms involving two spins on the same plaquette cancel because of the frustration condition. We are left with a correlation function for the next-nearest neighbours on a row or a column:

$$\overline{H_e^2} = 4J^2(1 + \overline{S_{0,0}S_{0,2}}) \tag{4}$$

$$= 6J^2 \tag{5}$$

at $T = 0$, where we have made use of a result recently obtained by R Bidaux (1979, unpublished data) for the correlation function.

Now, the average effective field is related to the ground-state energy

$$\overline{|H_e|} = 2J \tag{6}$$

and since $|H_e|$ may take only the values 0, $2J$ and $4J$, equations (5) and (6) yield

$$P(0) = P(4J) = \tfrac{1}{4} \tag{7}$$
$$P(2J) = \tfrac{1}{2}.$$

The much lower value of $P(0)$ in the disordered system is an indication that the spin arrangements in the ground states are strongly correlated, but the distributions of effective fields only give information on the local environment and other properties must be investigated to learn more about correlations.

3.3. *Living bonds*

A quantity which is convenient to study by our methods is the 'mobility' of the bonds: a bond is mobile or 'alive' if it is satisfied in some ground states but frustrated in others.

Although the total number of frustrated bonds is fixed, their location may vary considerably between different ground states, or in contrast they may be essentially frozen. Too much work is involved in the computation of the expectation value of every bond (that is the correlation between every pair of adjacent spins), so we just record whenever a bond changes at least once. The idea is that this quantity should be more sensitive to a change in the nature of the ground states than are global properties like energy or entropy.

For low concentrations of antiferromagnetic interactions, the living bonds form small clusters. The simplest clusters arise from two- and threefold degenerate configurations that contain three negative bonds at most and they have, respectively, four and seven living bonds. Using known results for the entropy (Gabay and Garel 1978), we obtain for the concentration l of living bonds

$$l = 12x^2 + 21x^3 + \dots \quad (8)$$

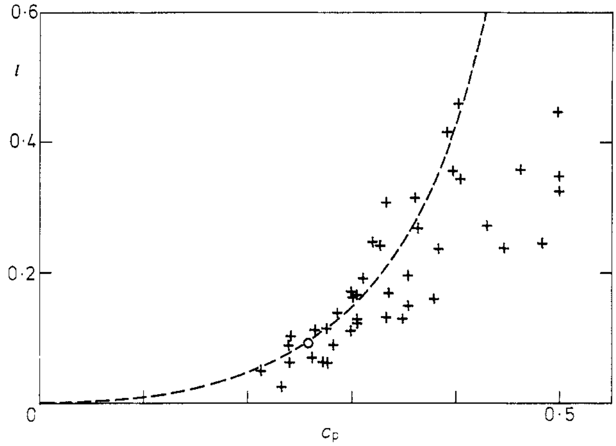

Figure 2. Fraction of living bonds l as a function of the concentration of frustrated plaquettes c_p for (18 × 18) samples. ○ represents a (80 × 80) sample; the broken curve corresponds to the low-disorder approximation (equation 8).

In figure 2, the experimental results are plotted against the concentration of frustrated plaquettes c_p (obtained from the measured value of x via equation 2). Equation (8) holds rather well for $x < 0{\cdot}10$ ($c_p < 0{\cdot}30$). For larger values of x, l increases less rapidly and saturates at a value of about 0·3–0·4 for $x = 0{\cdot}5$, compared with the value of 1 obtained for the fully frustrated odd model.

A sharp increase is observed in the fluctuations for x larger than 0·10; this arises from the appearance in some samples of ground states that are very different from those which are nearly ferromagnetic ones and where large groups of spins are flipped. This increase in the dispersion of the results is then directly related to the vanishing of the defect energy. For x larger than 0·15 ($c_p > 0{\cdot}38$), the fraction of living bonds varies little and experimentally the structure of the ground state becomes quite insensitive to the concentration of negative bonds.

We have also studied the effect of relaxing the periodic boundary conditions and allowing antiperiodic states. The dispersion in the data is further increased; in some samples states with different symmetries occur at the same energy and l is larger whereas in others an antiperiodic state of lower energy exists and l is reduced (the lower the energy, the more rigid the states). The general picture remains unchanged, however, with two well defined regimes for $x < 0{\cdot}10$ and $x > 0{\cdot}15$. In the transition region, size effects are certainly important for the determination of the threshold.

3.4. Packets of solidary spins

The same fraction of living bonds may correspond to very different physical situations, depending on whether the bonds are concentrated in clusters or whether they are scattered fairly uniformly. The geometry of the correlations is further specified by noting which groups of spins always keep the same relative orientation. These packets of solidary spins have a correlation equal to 1 at $T = 0$ and provide a measure of the rigidity of the ground states.

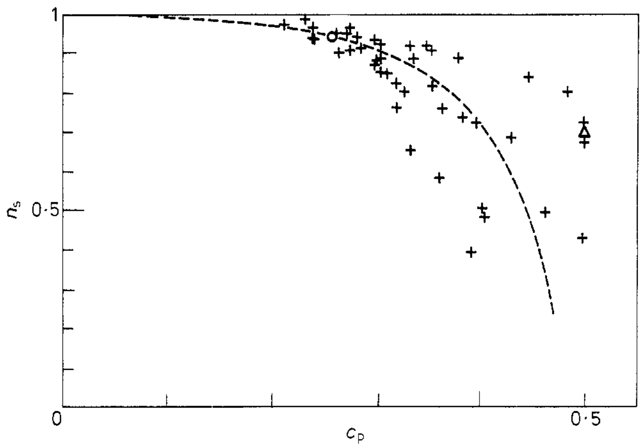

Figure 3. Fraction of spins contained in the largest packet of solidary spins. ○ denotes a (80 × 80) sample and △ a (40 × 40) sample. The low-disorder approximation (equation 5) is plotted as the broken curve.

Obviously correlations may exist between spins of different packets, because of entropy effects (Derrida *et al* 1978) and the absence of large packets above the frustration threshold would not imply the absence of long-range correlations. For the fully frustrated triangular lattice, the packets are reduced to single spins, while the spin–spin correlation decreases as a power law of distance at $T = 0$ (Stephenson 1970). The existence of an infinite packet of solidary spins would on the other hand be a very strong argument in favour of a separate spin-glass phase.

Since the interactions are between nearest neighbours only, the mechanism proposed by Adkins and Rivier (1974) for solidarity in systems with long-range oscillatory interactions cannot explain the origin of these packets. They are definitely not homogeneous ferromagnetic or antiferromagnetic clusters. Moreover they are far from being non-frustrated regions. Interpretation in terms of geometrical percolation has not proved fruitful. In the absence of a simple characterisation all ground states have to be compared; this procedure is a systematic extension of the projection concept introduced previously (Stauffer and Binder 1978) and manual analysis proves to be more efficient than a computer-aided procedure.

When few negative bonds are present, the system has ferromagnetic character and we expect that an infinite cluster will exist and contain the vast majority of spins. Indeed, the fraction n_s of spins in this cluster is, for small x

$$n_s = 1 - 6x^2 - 24x^2 + \dots \tag{9}$$

This expression is obtained from the expansion for the entropy (Gabay and Garel 1978), and is in good agreement with the experimental data (figure 3) up to $x = 0{\cdot}10$ ($c_p = 0{\cdot}30$). For larger values of the frustration the same comments as for the living bonds apply, the fluctuations show a marked increase and the size of the largest packet varies little above $c_p = 0{\cdot}38$ ($x = 0{\cdot}15$).

The surprising fact is that this size remains quite large. Typically, more than half of the spins belong to the largest packet even for $x = 0{\cdot}5$, which corresponds to maximum bond disorder. It may be expected that above the frustration threshold, many zero-energy contours cross the sample and that it becomes possible to flip small groups of spins independently, much as for the completely frustrated system (Bray *et al* 1978). This simple picture is not supported by our results. The decrease in n_s is continuous and a fragmentation of the ferromagnetic cluster is not observed, although ferromagnetism disappears. The vanishing of the interface energy per unit length is not incompatible with this behaviour, since this energy may vary as $(\text{length})^{1/2}$ for instance. It just implies that the packets are not strongly held and may easily fragment at a finite temperature.

Before we draw any conclusions, size effects must be estimated. The task of studying the ground states grows exponentially with the size of the samples, and rapidly gets out of hand (there are about 10^{11} ground states for the (18×18) samples). A more convenient way to increase the effective sample size is to relax the periodic boundary conditions and allow antiperiodic states. This has been done on all samples and the average size of the largest solidary packet is slightly decreased. However, as pointed out for the living bonds, lower energy states may appear with the less restrictive conditions and they yield larger packets, so that the net effect is not large.

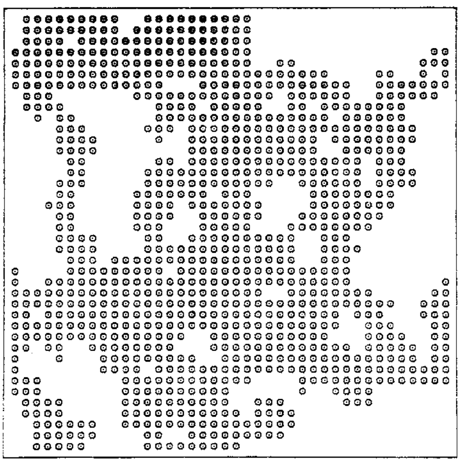

Figure 4. Map of the largest packet of solidary spins for the states of lowest energy found by a Monte Carlo method for a (40×40) sample with $c_p = 0{\cdot}50$.

We have also conducted a complete study on one (40 × 40) sample, and the computer search for ground states yielded the map of solidary spins shown in figure 4. Starting from this point, direct analysis was less formidable and other solutions could be found which differed by rearrangements of moderate size, which decreased the number of solidary spins further by 43 spins. The systematic search led to the discovery of two independent zero-energy contours crossing the sample; their combination yielded a new valley of periodic states with roughly half the spins reversed from the initial valley. Finally, states with four less frustrated bonds were found and as far as we know, they are the true ground states. They differ from the states in the initial valley by the reversal of two groups of more than 100 spins and are still more rigid: their fraction n_s of solidary spins is 0·70, which is above the average for the (18 × 18) samples (figure 3). These results, together with the findings for antiperiodic boundary conditions, do not indicate a strong size dependence for n_s. They are consistent with a slow decrease in n_s when the sample size increases and an infinite correlation length at zero temperature.

4. Discussion and conclusions

At first sight the disordered random system seems rather loose, with a finite density of idle spins and many different ground-state configurations and a finite residual entropy per spin are found. Closer inspection shows that the proportion of idle spins remains at a very low value when the bond disorder increases and that the proportion of living bonds also saturates. The ground states, far from being structureless, may be classified into a few families or valleys which are characterised by a large group of spins with a fixed relative orientation (solidary packets).

The connection with Monte Carlo investigations is interesting because the two approaches are complementary. We have studied the $T = 0$ properties in detail, while the Monte Carlo work focuses on the behaviour of some states (hopefully representative) as T varies. At low temperatures, according to our picture, the system is found near the bottom of one of the low-energy valleys. The spins belonging to the solidary packet are still highly correlated and the measured Edwards–Anderson order parameter is non-zero, in agreement with the numerical experiments. The metastability effects lead to a slow relaxation of the order parameter, but not to its vanishing.

For the sample to move into another valley, the reversal of a group containing a large number of spins is necessary. Such an event is very unlikely and, even though the energy barriers are lower than in the ferromagnetic phase, the existence of 'entropy plateaux' prevents its occurrence in realistic computer time.

The striking feature that emerges from the present work is the unexpected global rigidity in the low-energy states of the disordered system, which makes it very different from a simple paramagnet and from a fully frustrated system like the Villain model. Our main result, the existence of very large solidary packets, suggests that the correlation length is infinite at zero temperature. It also helps in understanding the fact that it is difficult for Monte-Carlo simulations to give a clear-cut answer about the existence of a sharp spin-glass transition at finite temperature.

Acknowledgments

We thank R Bidaux and B Derrida for many discussions and G Toulouse for suggesting this line of work and for lending his own go-board on which most of the analysis was carried out. The interested reader is urged to play the game of frustration, i.e. to find minimal pairings of 162 stones placed at random on the board, and to verify that its size is indeed well adapted to the capacities of the human brain.

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