Journal of Statistical Physics, Vol. 62, Nos. 1/2, 1991

Geometric Localization of the Threshold in Two-Dimensional Ising $\pm J$ Spin Glasses for $T=0$

J. Bendisch[1]

Received July 31, 1990

Following an approach of Toulouse, ground states in random 2D Ising $\pm J$ spin glasses (without external magnetic field), on square lattices, and with concentrations $0 \leqslant p \leqslant 0.5$ of antiferromagnetic bonds are studied by means of minimal matchings of frustrated plaquettes. Let $e(p)$ be the ground-state energy per spin in the thermodynamic limit. Then the well-known equation $e(p) = -2 + \lambda(p) f(p)$ holds, where $f(p)$ is the concentration of frustrated plaquettes and $\lambda(p)$ is the average connection length between paired frustrated plaquettes in minimal matchings. Introducing $\tau_\nu(p)$ as the probability that a frustrated plaquette is matched to another frustrated plaquette by a connection of length ν (in a minimal matching), the average length $\lambda(p)$ can be rewritten as $\lambda(p) = \sum \nu\tau_\nu(p)$. The study of $\lambda(p)$ and its components $\tau_\nu(p)$ leads to an interval $p^* \leqslant p \leqslant p_2$ ($p^* \approx 0.121 \pm 0.008$, $p_2 \approx 0.161 \pm 0.008$) where the threshold between ferromagnet and paramagnet for $T=0$ lies. Analyzing a similar so-called adjoined average length $l(p)$ admits further insight.

KEY WORDS: Random 2D Ising spin glasses; transition from ferromagnet to paramagnet at $T=0$; minimal matchings of frustrated plaquettes.

1. INTRODUCTION

We consider a random 2D Ising $\pm J$ spin glass (without external magnetic field) attached to a square lattice of size $L \times L$. Let X be a pattern of random $\pm J$ bonds on the lattice such that the probability for a bond to be antiferromagnetic is equal to a given $p \in [0, 0.5]$. To locate the critical p_c as the threshold from ferromagnet to paramagnet at $T=0$, we use a special expansion of the expected value of the average length $\langle \lambda_{p,L}(X) \rangle$ with respect to the connections between frustrated plaquettes in minimal matchings.

[1] Gesellschaft für Mathematik und Datenverarbeitung, D-5205 Sankt Augustin, Germany.

0022-4715/91/0100-0435$06.50/0

In a matching given on a finite lattice, the frustrated plaquettes are connected in disjoint pairs by strings of integer length $v \geqslant 1$ in the Manhattan metric. Passing through the centers of plaquettes, these strings begin and end in the centers of frustrated plaquettes; see Fig. 1. Clearly, there are, in general, many ways to form such pairings. A matching is minimal if the sum over all its connection lengths is minimal. Toulouse[8] introduced minimal matchings to determine ground states in $\pm J$ spin glasses (cf. also Barahona *et al.*,[2] Bieche *et al.*,[4] Kirkpatrick,[6] and Freund and Grassberger[5]).

In the following we admit only ± 1 couplings. With

$$f(p) = 4[p^3(1-p) + p(1-p)^3], \qquad 0 \leqslant p \leqslant 0.5$$

as the concentration of frustrated plaquettes for $L = \infty$ and with

$$\lambda(p) = \lim_{L \to \infty} \langle \lambda_{p,L}(X) \rangle \tag{1.1}$$

in the thermodynamic limit the ground-state energy per spin is given by the well-known equation

$$e(p) = -2 + \lambda(p) f(p), \qquad 0 \leqslant p \leqslant 0.5 \tag{1.2}$$

no matter whether the boundary conditions are free, fixed, periodic, or mixed on corresponding finite lattices.

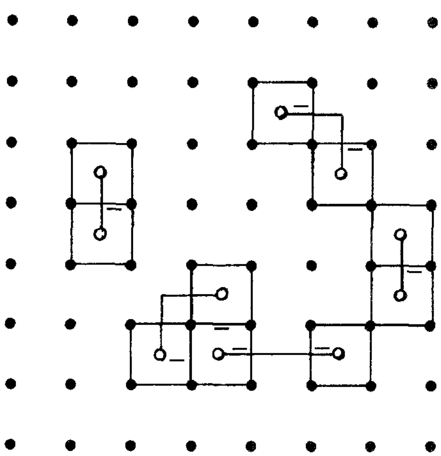

Fig. 1. An 8×8 lattice with fixed boundary conditions. The frustrated plaquettes (with exactly one or three antiferromagnetic bonds) are marked by solid contours. The connections between the open circles represent a minimal matching of length $\Lambda = 8$.

Because of (1.2) the essential information concerning ground states is related to $\lambda(p)$. Therefore a transition between ferromagnet and paramagnet (at $T=0$) should be indicated by some change in the nature of matchings.[8] For further investigation of $\lambda(p)$ we start from finite $L \times L$ lattices and, for sake of simplicity, we choose fixed boundary conditions with only ferromagnetic bonds and only positive spin values on the lattice boundary.

Given a pattern X of bonds on an $L \times L$ lattice, let $\Lambda_{p,L}(X)$ be the sum of connection lengths of paired frustrated plaquettes in a minimal matching; see Fig. 1. Then the ground-state energy per spin is

$$e_{p,L}(X) = [-b + 2\Lambda_{p,L}(X)]/L^2$$

with $b = 2L(L-1)$ the number of lattice bonds. Let $\varphi_{p,L}(X)$ be the number of frustrated plaquettes and

$$\lambda_{p,L}(X) = 2\Lambda_{p,L}(X)/\varphi_{p,L}(X) \tag{1.3}$$

be the average connection length between paired frustrated plaquettes in a minimal matching with respect to X. Taking expected values on both sides of (1.3) and increasing L to infinity, we are led to (1.1).

For a given bond pattern X we will introduce the relative frequencies $\tau^{(k)}_{v,p,L}(X)$ that in the kth minimal matching two frustrated plaquettes are connected by a path of length v in the Manhattan metric, $v = 1, 2, \ldots, 2(L-2)$. Rewriting $\lambda_{p,L}(X)$ as a special linear combination of the $\tau^{(k)}_{v,p,L}(X)$ and forming expected values, we will arrive for $L \to \infty$ at

$$\lambda(p) = \sum_{v=1}^{\infty} v\tau_v(p), \qquad \sum_{v=1}^{\infty} \tau_v(p) = 1 \tag{1.4}$$

Finally, by heuristic matching simulations and by general considerations we will localize the transition between ferromagnet and paramagnet in the interval $p^* \leqslant p \leqslant p_2$, where $\lambda(p)$, $\tau_2(p)$ are maximal at $p^* \approx 0.121 \pm 0.008$ and $p_2 \approx 0.161 \pm 0.008$, respectively.

To investigate the $\tau_v(p)$, we got helpful clues from studying the closely related "adjoined" average length

$$l(p) = \sum_{v=1}^{\infty} v\sigma_v(p), \qquad \sum_{v=1}^{\infty} \sigma_v(p) = 1 \tag{1.5}$$

where $\sigma_v(p)$ is the probability that in the thermodynamic limit the minimal distance (without any matching) between frustrated plaquettes is v. In contrast to the $\tau_v(p)$, here the $\sigma_v(p)$ can be calculated explicitly.

2. LOCALIZING THE THRESHOLD BY COMPONENTS OF $\lambda(p)$

As common in theories of critical phenomena, we assume that a transition from ferromagnet to paramagnet (at $T=0$) should be signaled by a peculiarity in the behavior of the average length $\lambda(p)$ or its components $\tau_\nu(p)$. For fixed boundary conditions we start the investigation by rewriting $\lambda_{p,L}(X)$ in (1.3) as

$$\lambda_{p,L}(X) = \sum_{\nu=1}^{2(L-2)} \nu\tau_{\nu,p,L}^{(k)}(X), \qquad k=1,2,\ldots,N_{p,L}(X) \tag{2.1}$$

where, X given, k is the index for the different minimal matchings, in any order, and

$$\tau_{\nu,p,L}^{(k)}(X) = \varphi_{\nu,p,L}^{(k)}(X)/\varphi_{p,L}(X), \qquad \varphi_{p,L}(X) = \sum_{\nu=1}^{2(L-2)} \varphi_{\nu,p,L}^{(k)}(X) \tag{2.2}$$

with $\varphi_{\nu,p,L}^{(k)}(X)$ as the number of frustrated plaquettes which are involved in a connection of length ν within the kth minimal matching. By summation of Eq. (2.1) and by averaging over the different minimal matchings (corresponding to the ground states), we obtain

$$\lambda_{p,L}(X) = \sum_{\nu=1}^{2(L-2)} \nu\bar{\tau}_{\nu,p,L}(X), \qquad \bar{\tau}_{\nu,p,L}(X) = \left(\sum_k \tau_{\nu,p,L}^{(k)}(X)\right)\Big/ N_{p,L}(X)$$

Then, forming expected values $\langle\lambda_{p,L}(X)\rangle$ and $\langle\bar{\tau}_{\nu,p,L}(X)\rangle$ with respect to random patterns X, and increasing L to infinity, we get (1.4). In particular, this expansion of $\lambda(p)$ leads to

$$\lambda(p) = \tau_1(p) + [1-\tau_1(p)]\,\delta(p), \qquad \delta(p) \geqslant 2$$

where $\delta(p)$ is a hereby implicitly defined auxiliary function used below.

We give a short survey on certain properties of $\delta(p)$ and of the $\tau_\nu(p)$. They will be used to localize the threshold between ferromagnet and paramagnet. The following statements are supported by general considerations and by results from heuristic matching simulations under periodic boundary conditions, on a 150×150 lattice and with $n=15$ samples treated for each p. We used fixed concentrations, i.e., for p given, there have been generated $round(2L^2p)$ antiferromagnetic bonds at random on the lattice.

In $0<p\leqslant 0.5$ the component $\tau_1(p)$ is dominant among the $\tau_\nu(p)$, $\tau_1(p)>0.73$,

$$\lim_{p\to 0}\tau_1(p)=1, \qquad \lim_{p\to 0}\tau_\nu(p)=0, \quad \nu\geqslant 2, \qquad \lim_{p\to 0}\delta(p)=2$$

$\tau_1(p)$ has a unique minimum at p_1 (see Fig. 2) and $\lambda(p)$, $\delta(p)$, $\tau_\nu(p)$, $\nu \geqslant 2$, have a unique maximum at p^*, p^{**}, p_ν, respectively. Hence $\min(p_1, p^{**}) \leqslant p^* \leqslant \max(p_1, p^{**})$.

Moreover, by simulations:

$$p^{**} \approx 0.077 \pm \varepsilon$$

$$p_4 \approx 0.096 \pm \varepsilon < p_3 \approx 0.110 \pm \varepsilon < p^* \approx 0.121 \pm \varepsilon \leqslant p_1$$
$$\approx 0.127 \pm \varepsilon < p_2 \approx 0.161 \pm \varepsilon$$

with $\varepsilon = 0.008$.

Let $\hat{p} = \text{infimum } p_\nu$ and $\tilde{p} = \lim_{\nu \to \infty} p_\nu$; then $0 < \hat{p} \leqslant \tilde{p}$. We guess that $p_{\nu+1} < p_\nu$ for $\nu \geqslant 2$ and thus $\hat{p} = \tilde{p}$. At $\tilde{p}$ extremely long connection lengths ν have their greatest influence on $\lambda(p)$. Our estimate is $\tilde{p} \approx 0.07 \pm 0.01$, since here the matching simulations produced significantly larger connection lengths ν than elsewhere. The $\tau_\nu(p)$, $\nu \geqslant 2$, are increasing in the interval $(0, \hat{p}]$ and decreasing in $[p_2, 0.5]$.

Only in the interval $[\hat{p}, p_2]$ do the $\tau_\nu(p)$ behave differently. This is the basic zone where we localize the transition from ferromagnet to paramagnet. At the transition itself the average length $\lambda(p)$ or its components $\tau_\nu(p)$ should exhibit an extraordinary behavior. At $\tilde{p}$ the expected absolute value of the magnetization $m(p)$ per spin is ≈ 1, but falls sharply for increasing p.[4] Therefore we continue our search to the right of $\tilde{p}$. The average length $\lambda(p)$ takes its maximum at $p^* \approx 0.121 \pm 0.008$. Note that p^*

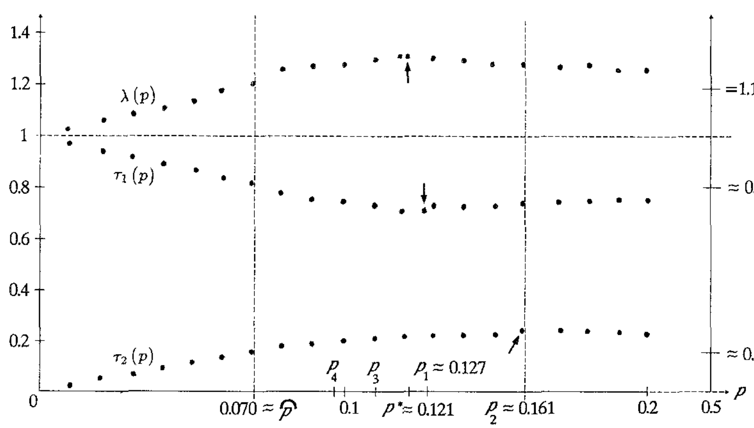

Fig. 2. Average length $\lambda(p)$ and its first components $\tau_1(p)$, $\tau_2(p)$ observed in simulations on a 150×150 lattice. The interval $\hat{p} \leqslant p \leqslant p_2$ gives the zone in which to look for the transition from ferromagnet to paramagnet.

is near p_1; there is even the possibility of coincidence. This might be understood by the following "exchange argument." Assume that $\lambda(p)$ is growing; then in the corresponding minimal matchings, on sufficiently large lattices, the connection lengths $v \geqslant 2$ appear, but to the disadvantage of the smallest length $v=1$, in particular if $\lambda(p)$ is maximal. Thus, $\tau_1(p)$ should have its minimum at least near the point where $\lambda(p)$ takes its maximum. Finally, p_2 is the rightmost maximum of the $\tau_v(p)$, $v \geqslant 2$.

From these facts we conclude that the transition takes place in the interval $[p^*, p_2]$ where in particular p^*, p_1, and p_2 are candidates for the threshold p_c. With respect to p^*, p_1 this is in good agreement with the MC estimate $p_c \approx 0.120 \pm 0.015$ by Morgenstern and Binder.[7] With respect to p_2, there is no contradiction to $p_c \approx 0.145 \pm 0.01$ given by Bieche *et al.*[4]

3. THE ADJOINED AVERAGE LENGTH $l(p)$

Now we will give some facts and results concerning the "adjoined" average length $l(p)$ in (1.5), which is similar to $\lambda(p)$, but without the constraints of a matching. It has the advantage that its components $\sigma_v(p)$, as analogues to the $\tau_v(p)$, are rational functions which can be calculated according to exact formulas. The behavior of the $\sigma_v(p)$ seemingly reflects that of the $\tau_v(p)$. The length $l(p)$ is the average minimal Manhattan distance between frustrated plaquettes, in the thermodynamic limit. We can show that

$$l(p) \leqslant \lambda(p), \qquad \sigma_1(p) \geqslant \tau_1(p) \qquad \text{for} \quad 0 < p \leqslant 0.5$$

Mathematical details are in Bendisch.[3] By (3.1) and (1.2) we are led to a lower bound for the energy per spin, namely $e(p) \geqslant -2 + l(p)\, f(p)$. Introducing $w_v(p)$ for $v \geqslant 0$ as the probability that the minimal (Manhattan) distance between frustrated plaquettes is $\geqslant (v+1)$, we obtain

$$\sigma_v(p) = w_{v-1}(p) - w_v(p) \quad \text{for } v = 1, 2,..., \qquad l(p) = \sum_{v=0}^{\infty} w_v(p)$$

where $w_0(p) \equiv 1$ and $w_v(p)$, $v \geqslant 1$, is of the form $a_v(p)/f(p)$ with $a_v(p)$ a polynomial and $f(p)$ the concentration of frustrated plaquettes. In particular $w_v(0.5) = 2^{-2(v+1)v}$ for $v = 0, 1, 2,...$. With

$$l(q^*) = \max l(p), \qquad \sigma_1(q_1) = \min \sigma_1(p), \qquad \sigma_v(q_v) = \max \sigma_v(p), \quad v \geqslant 2$$

we get

$$q_3 = 0.067 \pm 0.003 < q^* = 0.097 \pm 0.003 < q_1$$
$$= 0.1004 \pm 0.0001 < q_2 = 0.1045 \pm 0.0001$$

For regular triangular lattices there are similar results:

$$q_4 = 0.095 \pm 0.003 < q_3 = 0.128 \pm 0.001 < q^* = 0.192 \pm 0.003 < q_1$$
$$= 0.204 \pm 0.001 < q_2 = 0.217 \pm 0.001$$
$$w_\nu(0.5) = 2^{-1.5(\nu+1)\nu} \qquad \text{for} \quad \nu = 0, 1, 2, \ldots$$

The distance from the center of a triangle to the center of an adjacent triangle is considered to be 1 where adjacent triangles have one side in common.

4. FINAL REMARKS

We tacitly assumed that $\lambda(p)$, $\delta(p)$, and the $\tau_\nu(p)$ are continuous in $0 < p \leqslant 0.5$, and thus applied the notions of maximum and minimum to these functions. One reason for this assumption is that the components $\sigma_\nu(p)$ of the adjoined length $l(p)$ are continuous functions on $[0, 0.5]$. But even in the case that this is not true for $\lambda(p)$, $\delta(p)$, or a $\tau_\nu(p)$ our considerations remain valid replacing the notions of maximum and minimum by supremum and infimum, respectively.

The simulations were performed on a Siemens 7590, and the parameter p has been incremented by $\Delta p = 0.001$ in the interval $[0.07, 0.17]$. To estimate the position of a maximum (minimum) the above intervals of the form $[a - \varepsilon, a + \varepsilon]$, $\varepsilon = 0.008$, cover the 11 greatest (smallest) produced values of $\lambda(p)$, $\delta(p)$, $\tau_2(p)$, $\tau_3(p)$, $\tau_4(p)$, and $\tau_1(p)$, respectively. Using periodic boundary conditions, simulations were made for lattice and sample sizes $(L, n) = (30, 15)$, $(64, 60)$, $(150, 15)$. In order to reduce the influence from fluctuations of the concentration of frustrated plaquettes, we based our conclusions on results from 150×150 lattices. The applied heuristic matching algorithm is described in Achilles *et al.*[1]

Concerning the concentration $f_{p,L}(X)$ of frustrated plaquettes, it can be shown that under the previous fixed boundary conditions $f_{p,L}(X) = \varphi_{p,L}(X)/(L-1)^2$ stochastically tends to a one-point distribution for $L \to \infty$, in particular

$$\lim_{L \to \infty} \langle f_{p,L}(X) \rangle = f(p), \qquad \lim_{L \to \infty} \operatorname{Var}(f_{p,L}(X)) = 0$$

This allows a straightforward deduction of the limit equation (1.2) under fixed boundary conditions.[3]

The above considerations, by means of components $\tau_\nu(p)$, can be applied to triangular lattices, too (cf. Achilles *et al.*[1]).

ACKNOWLEDGMENTS

The author thanks D. Stauffer and H. v. Trotha for fruitful discussions.

REFERENCES

1. M. Achilles, J. Bendisch, K. Cassirer, and H. von Trotha, A heuristic matching algorithm and its application to 2D Ising spin glasses, GMD-Studies, Gesellschaft für Mathematik und Datenverarbeitung, D-5205 St. Augustin (1991).
2. F. Barahona, R. Maynard, R. Rammal, and J. P. Uhry, Morphology on ground states of two-dimensional frustration model, *J. Phys.: Math. Gen.* **15**:673–699 (1982).
3. J. Bendisch, On an optimization problem related to ground states in 2D Ising spin glasses, GMD-Studies (1991).
4. I. Bieche, R. Maynard, R. Rammal, and J. P. Uhry, On the ground states of the frustration model of a spin glass by a matching method of graph theory, *J. Phys. A: Math. Gen.* **13**:2553–2576 (1980).
5. H. Freund and P. Grassberger, The ground state of the $\pm J$ spin glass from a heuristic matching algorithm, *J. Phys. A: Math. Gen.* **22**:4045–4059 (1989).
6. S. Kirkpatrick, Frustration and ground-state degeneracy in spin glasses, *Phys. Rev. B* **16**:4630 (1977).
7. I. Morgenstern and K. Binder, Magnetic correlations in two-dimensional spin-glasses, *Phys. Rev. B* **22**:288 (1980).
8. G. Toulouse, *Commun. Phys.* **2**:115 (1977).

Communicated by D. Stauffer