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On the Ground-State Threshold in Random Two-Dimensional Ising $\pm J$ Models

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For square, triangular, and for hexagonal lattices there is numerical and theoretical support that the ground-state threshold p_c between ferro- and paramagnetism in random 2D Ising $\pm J$ models, with p as the concentration of antiferromagnetic bonds, is identical to p^* which is characterized by minimal matching properties of frustrated plaquettes. From square lattices of size 100×100 we have got $p_{c,\mathrm{sq}} < 0.117$ by simulations which produced average groundstate magnetizations per spin by means of exact minimal matchings. Moreover, from the square $L \times L$-lattices treated ($L = 10$, 20, 50, 100) we obtained the estimate $p_{c,\mathrm{sq}} \approx 0.1$ which is in agreement with the Grinstein estimate $p_{c,\mathrm{sq}} \approx 0.099$ and $p_{c,\mathrm{sq}} \approx 0.105$ by Freund and Grassberger.

KEY WORDS: Random 2D Ising spin glasses; ground-state phase transition from ferro- to paramagnetism; minimal matching of frustrated plaquettes.

1. INTRODUCTION

The problem here is to determine numerically and if possible to characterize the critical concentration p_c of antiferromagnetic bonds for the so-called ground-state threshold from ferromagnetism to paramagnetism in random 2D Ising $\pm J$ spin glasses on square, hexagonal, and triangular lattices of size $L \times L$ in the thermodynamic limit $L \to \infty$. We put $J = 1$. With fixed $p \in [0, 1]$ a random Ising model on an $L \times L$ lattice is said to have a concentration p of antiferromagnetic bonds or (-1) bonds if for each bond of a stochastic bond pattern X (on the whole lattice) the probability to be a (-1) bond is p. For the topology of regular $L \times L$ lattices, see Table I.

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Table I. Number of Basic Structural Components of Regular $L \times L$ Lattices under Periodic Boundary Conditions

Lattice type	Spins (lattice points)	Bonds (edges)	Plaquettes (meshes)
Square	L^2	$2L^2$	L^2
Triangular	L^2	$3L^2$	$2L^2$
Hexagonal	$2L^2$	$3L^2$	L^2

For the square lattice case we roughly outline the process, still in progress, of numerically conquering $p_{c,\mathrm{sq}}$: 1976 Ono[10]: $p_{c,\mathrm{sq}} \approx 0.15$; 1977 Vannimenus and Toulouse[12]: $p_{c,\mathrm{sq}} \approx 0.09$; 1977 Kirkpatrick[8]: $p_{c,\mathrm{sq}} \approx 0.16$; 1978 Grinstein *et al.*[7]: $p_{c,\mathrm{sq}} \approx 0.099$; 1979 Bieche *et al.*[4]: $p_{c,\mathrm{sq}} \approx 0.145$; 1980 Morgenstern and Binder[9]: $p_{c,\mathrm{sq}} \approx 0.12 \pm 0.015$; 1989 Freund and Grassberger[6]: $p_{c,\mathrm{sq}} \approx 0.105$.

There are mainly two approaches to simulate energy ground states. The "primal approach" uses, in a variety of methods, the flipping of (± 1) spins to reduce the energy. The "dual approach," following a proposal of Toulouse,[11] tries to decrease the energy by so-called minimal matchings of frustrated plaquettes. [A square, triangular, or hexagonal plaquette is called frustrated if it has an odd number of (-1) bonds on its perimeter.] The primal approach refers to the minimization of the nearest neighbor (n.n.) total interaction energy

$$E(\sigma_1, \sigma_2, \ldots) = -\sum_{\text{n.n.}} J_{i,j}\sigma_i\sigma_j$$

with spin values $\sigma_i, \sigma_j = \pm 1$, given couplings $J_{i,j} = \pm 1$, and under some type of boundary conditions (e.g., periodic, fixed, or mixed b.c.).

In the dual approach there is, for instance in the square lattice case, under fixed boundary conditions, the equivalent energy minimum representation $E_{\min} = -2L(L-1) + 2\Lambda_{\min}$, where $\Lambda_{\min}$ is the minimal matching length of pairwise in Manhattan metric connected frustrated plaquettes (see Fig. 1). For the dual approach, see refs. 2, 4, 6, and 8.

A matching itself is given by pairs of frustrated plaquettes. Note that for (the here and in the following considered) fixed or periodic boundary conditions the number of frustrated plaquettes on an $L \times L$ lattice is always even. Each matched pair of frustrated plaquettes can be connected by a string which is piecewise linear from center to center of adjacent plaquettes and in general may be arranged in several ways not changing the matching. So a given matching usually leads to different "stringings." In such a stringing any two different strings must not have a line segment in

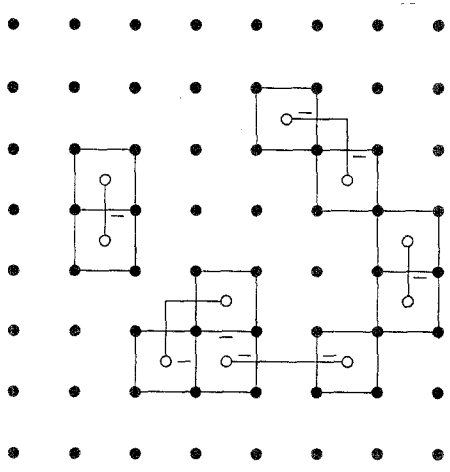

Fig. 1. An 8×8 square lattice under fixed boundary conditions (eight antiferromagnetic bonds in the interior). The frustrated plaquettes (with exactly one or three antiferromagnetic bonds) are marked by solid contours. The strings between the open circles in the plaquette centers illustrate a minimal matching of length $\Lambda_{\min} = 8$.

common. This restriction is essential when constructing, with respect to a *minimal* matching, a ground-state spin configuration (σ_ρ) whose violated bonds $(\sigma_i \sigma_j J_{i,j} < 0)$ coincide just with the bonds crossed by a stringing of this minimal matching.

We choose the dual approach. With the limit $(L = \infty)$ concentration $f(p)$ of frustrated plaquettes, the limit mean energy $e(p)$ per spin, and $\lambda(p)$ as the limit mean of average connection lengths between pairwise matched frustrated plaquettes in a minimal matching, the limit equations

$$e_{\mathrm{sq}}(p) = -2 + \lambda_{\mathrm{sq}}(p) f_{\mathrm{sq}}(p), \qquad e_{\mathrm{tri}}(p) = -3 + 2\lambda_{\mathrm{tri}}(p) f_{\mathrm{tri}}(p)$$

$$e_{\mathrm{hex}}(p) = [-3 + \lambda_{\mathrm{hex}}(p) f_{\mathrm{hex}}(p)]/2$$

hold in the square,[8] triangular, and hexagonal[1] lattice cases for $0 \leqslant p \leqslant 1$, where

$$f_{\mathrm{sq}}(p) = 4p(1-p)[p^2 + (1-p)^2], \qquad f_{\mathrm{tri}}(p) = 3p(1-p)^2 + p^3$$

$$f_{\mathrm{hex}}(p) = 6p(1-p)[(1-p)^4 + p^4] + 20p^3(1-p)^3$$

Because of the above limit equations the essential information concerning the ground states is related to the $\lambda(p)$. Bendisch,[3] following an idea of Toulouse[11] that a ground-state transition between

ferromagnetism and paramagnetism should be indicated by some change in the nature of matching, decomposed $\lambda_{sq}(p)$,

$$\lambda_{sq}(p) = \sum_{v=1}^{\infty} v\tau_{v,sq}(p), \qquad \sum_{v=1}^{\infty} \tau_{v,sq}(p) = 1 \tag{1.1}$$

where $\tau_{v,sq}(p)$ is the limit probability for connections of length v between matched frustrasted plaquettes in minimal matchings. With $p_{v,sq}$ as the site of the (unique) maximum of $\tau_{v,sq}(p)$ for $p \leqslant 0.5$ and $v \geqslant 2$ we have $p_{v+1,sq} < p_{v,sq}$. Let

$$\hat{p}_{sq} = \lim_{v \to \infty} p_{v,sq}$$

Then by (1.1) extremely great connection lengths v have their greatest influence on $\lambda_{sq}(p)$ at $\hat{p}_{sq}$. Moreover, the $\tau_{v,sq}(p)$, $v \geqslant 2$, are increasing in the interval $[0, \hat{p}_{sq}]$ and decreasing in $[p_{2,sq}, 0.5]$.

In the "basic zone" $[\hat{p}_{sq}, p_{2,sq}]$ where the $\tau_{v,sq}$, $v \geqslant 2$, behave differently, the threshold $p_{c,sq}$ from ferro- to paramagnetism is localized. By simulations of near minimal matchings on lattices of size 150×150 and with sample size $n = 15$, cf. Bendisch[3], one obtains

$$\hat{p}_{sq} \approx 0.07 \pm 0.01, \qquad p_{2,sq} \approx 0.161 \pm 0.008 \tag{1.2}$$

under periodic boundary conditions. Analogously, in Achilles *et al.*[1],

$$\begin{aligned} \hat{p}_{tri} &\approx 0.12 \pm 0.02, & p_{2,tri} &\approx 0.285 \\ \hat{p}_{hex} &\approx 0.045 \pm 0.005, & p_{2,hex} &\approx 0.069 \end{aligned} \tag{1.3}$$

so for each regular lattice type treated the threshold p_c is localized in a corresponding interval

$$\hat{p} \leqslant p_c \leqslant p_2 \tag{1.4}$$

without having directly simulated the magnetization, and it has been surmised even more restrictively that $p_c \in [p^*, p_2]$, with p^* the concentrations p where $\lambda(p)$ takes its global maximum in $0 \leqslant p \leqslant 0.5$. We formerly obtained

$$p^*_{hex} \approx 0.062, \qquad p^*_{sq} \approx 0.121, \qquad p^*_{tri} \approx 0.203 \tag{1.5}$$

Now in this work, using this time an exact matching algorithm we simulated, with an enlarged sample size $n = 120$, indeed the mean magnetization per spin on square $L \times L$ lattices ($L = 10, 20, 50, 100$) under periodic boundary conditions. Moreover we produced an improved estimate for p^*_{sq}. Note that, for instance, in the square lattice case minimal matchings have been used in simulations by, e.g., Kirkpatrick[8] for $L = 80$ [investigating $\lambda_{sq}(p)$], Bieche *et al.*[4] for $L \leqslant 22$ (simulating the magnetization), and Freund and Grassberger[6] for $L \leqslant 210$ (indirect study of the

magnetization). The simulations here, by means of "random walk stringings" between matched frustrated plaquettes (in order to generate the violated bonds), are described in Section 2. Results are presented and discussed in Section 3, in particular supporting the conjecture that the threshold $p_{c,\mathrm{sq}}$ coincides with p_{sq}^*.

2. SIMULATION OF THE MAGNETIZATION IN THE DUAL APPROACH

Let us recall that in the primal approach, for a given concentration p, given a square, triangular, or hexagonal $L \times L$ lattice and bond pattern X, the magnetization $m_{p,L}^{(k)}(X)$ per spin for the kth ground state is defined as follows. A spin configuration (σ_ρ) on the lattice is called a ground-state if $E(\sigma_1, \sigma_2, \ldots) = E_{\min}$. Let the different ground states $(\tilde{\sigma}_\rho^{(k)})$ is some way be numbered from $k=1$ to $k = x_{p,L}(X)$. Then put

$$m_{p,L}^{(k)}(X) = \left| \sum_\rho \tilde{\sigma}_\rho^{(k)} \right| \Big/ d(L) \qquad \text{for} \quad k = 1, \ldots, x_{p,L}(X)$$

where $d(L) = L^2$ for square and triangular lattices and $d(L) = 2L^2$ in the hexagonal lattice case. Averaging $m_{p,L}^{(k)}(X)$ over all ground states of X, set

$$\bar{m}_{p,L}(X) = \left[\sum_k m_{p,L}^{(k)}(X) \right] \Big/ x_{p,L}(X)$$

Taking the expected value of $\bar{m}_{p,L}(X)$ with respect to the stochastic bond pattern X, let $m_L(p) = \langle \bar{m}_{p,L}(X) \rangle_X$ and, finally, $m(p) = \lim_{L \to \infty} m_L(p)$ for $0 \leqslant p \leqslant 1$, the thermodynamic limit magnetization per spin.

Now in the dual approach we arrive at $m(p)$ in the following way. For fixed p, L, and given bond pattern X number the different minimal matchings in some manner from $i=1$ to $i = i_{\mathrm{last}}(X)$. Then for each of these matchings M_i the different stringings (as introduced in Section 1) are numbered in some way from $j=1$ to $j = j_{\mathrm{end}}(X, M_i)$. The bonds crossed by such a stringing S_j are chosen to be the violated ones. Putting some spin to $+1$, for each of these stringings we recursively calculate a global spin configuration $(\sigma_\rho^{*(i,j)})$ by means of the previously generated violated bonds. Now, in analogy to the primal approach, let

$$\mu_{p,L}^{(i,j)}(X) = \left| \sum_\rho \sigma_\rho^{*(i,j)} \right| \Big/ d(L), \qquad \bar{\mu}_{p,L}^{(i)}(X) = \left[\sum_j \mu_{p,L}^{(i,j)}(X) \right] \Big/ j_{\mathrm{end}}$$

$$\bar{\bar{\mu}}_{p,L}(X) = \left[\sum_i \bar{\mu}_{p,L}^{(i)}(X) \right] \Big/ i_{\mathrm{last}}, \qquad \mu_L(p) = \langle \bar{\bar{\mu}}_{p,L}(X) \rangle_X$$

In the thermodynamic limit we have $m(p) = \lim_{L \to \infty} \mu_L(p)$.

For fixed p, L the mean magnetization $\mu_L(p)$ per spin is estimated by a corresponding $\hat{\mu}_{p,L,n,r,s}$ from n random bond patterns X, r random minimal matchings (X given), and s random walk stringings (X and a minimal matching given). Note that, since a fixed (random) minimal matching has, in general, a great many different stringings (see Section 1), each stringing leading to a ground-state spin configuration, we generate s stringings at random in order to get an estimate for the average magnetization with respect to the minimal matching considered. In practice we have chosen $(n, r, s) = (120, 1, 15)$. The restriction $r = 1$ is because of the difficulty of creating a *representative* sample of minimal matchings for given X. Note that in principle even $r = s = 1$ and n sufficiently large should lead to a satisfactory estimate for $\mu_L(p)$. These simulations were achieved by an efficient matching algorithm described in Derigs *et al.*[5]

3. RESULTS AND DISCUSSIONS

For $L = 10$, 20, 50, 100 we give simulated means $\hat{\mu}_{p,L,n,r,s,\mathrm{sq}}$ of the magnetization per spin on square $L \times L$ lattices under periodic boundary conditions. For reasons of accuracy we present, for small values of p, the produced $\hat{\mu}_{p,L,n,r,s,\mathrm{sq}}$ in the form of Table II; for $p > 0.08$ the presentation is graphical.

In Fig. 2 we see that, increasing the lattice size parameter from $L = 10$ to $L = 100$, there is a distinct shift to the left concerning the fall of the magnetization, and the "tail to the right" shrinks with decreasing finite-size effects. The thermodynamic limit $m_{\mathrm{sq}}(p)$, of the form $m_{\mathrm{sq}}(p) > 0$ for $p < p_c$

Table II. Estimates $\hat{\mu}_{p,L,n,r,s,\mathrm{sq}}$ of Ground-State Magnetizations per Spin for Small Concentrations p of Antiferromagnetic Bonds on Square $L \times L$ Lattices under Periodic Boundary Conditions

p	$\hat{\mu}_{p,L,n,r,s,\mathrm{sq}}$ $(n = 120, r = 1, s = 15)$			
	$L = 100$	$L = 50$	$L = 20$	$L = 10$
0.010	0.9994	0.9994	0.9997	1.0000
0.020	0.9973	0.9974	0.9975	0.9993
0.030	0.9939	0.9940	0.9944	0.9964
0.040	0.9885	0.9890	0.9884	0.9920
0.050	0.9803	0.9807	0.9835	0.9854
0.060	0.9703	0.9708	0.9733	0.9780
0.070	0.9548	0.9520	0.9594	0.9725
0.080	0.9324	0.9305	0.9332	0.9530

and $m_{\mathrm{sq}}(p)=0$ for $p \geqslant p_c$, should have no turning point, in contrast to the $m_{L,\mathrm{sq}}(p)$ curves associated with finite lattices.

Let $\tilde{p}_{L,\mathrm{sq}}$ be the turning point of $m_{L,\mathrm{sq}}(p)$. Then, under the above assumption that $m_{\mathrm{sq}}(p)$ is turning point free and because of the empirical turning point drift to the left (see Fig. 2) with increasing L, we conclude that $p_{c,\mathrm{sq}} < \tilde{p}_{L,\mathrm{sq}}$ and that

$$p_{c,\mathrm{sq}} \equiv \lim_{L \to \infty} \tilde{p}_{L,\mathrm{sq}} \tag{3.1}$$

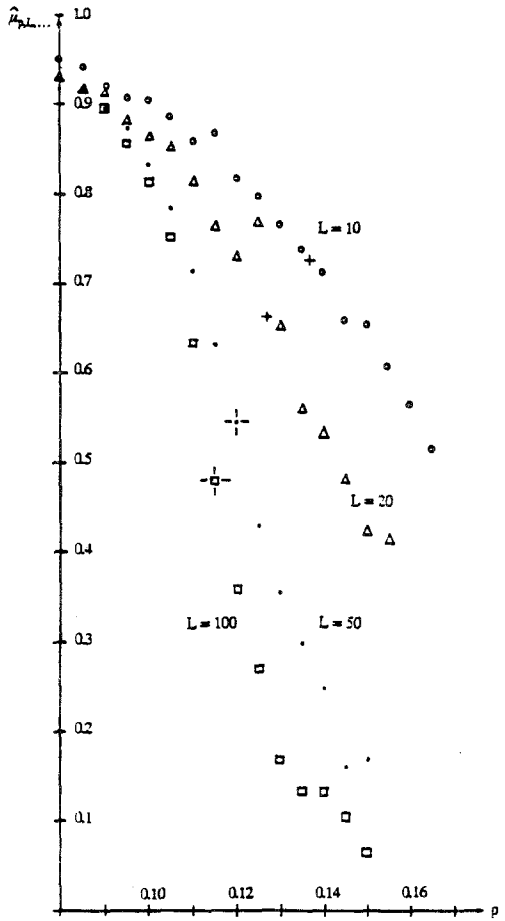

Fig. 2. The presentation of estimates $\hat{\mu}_{p,L,n,r,s,\mathrm{sq}}$ ($s=15$, $r=1$, $n=60$ for $L=100$ and $p>0.12$, otherwise $n=120$) is graphically continued for $p>0.08$. Small circles, triangles, dots and squares mark $\hat{\mu}_{\ldots,\mathrm{sq}}$ from simulations for $L=10$, 20, 50, and 100, respectively, on square $L \times L$ lattices. The plus signs mark empirical turning points for the $m_{L,\mathrm{sq}}(p)$-curves.

Table III. CPU Time (without Paging) in Seconds Used on an IBM RS6000/550 when Calculating $\hat{\mu}_{p,L,n,r,s,\mathrm{sq}}$ for Selected Values of L and p and with Sample Sizes $n=120$, $r=1$, $s=15$, for Square $L\times L$ Lattices under Periodic Boundary Conditions

	$L=20$			$L=50$			$L=100$		
p	0.01	0.05	0.10	0.01	0.05	0.10	0.01	0.05	0.10
CPU	2	5	12	20	94	350	192	1762	5348

From Fig. 2, we estimate

$$\tilde{p}_{10,\mathrm{sq}}\approx 0.137,\quad \tilde{p}_{20,\mathrm{sq}}\approx 0.127,\quad \tilde{p}_{50,\mathrm{sq}}\approx 0.120,\quad \tilde{p}_{100,\mathrm{sq}}\approx 0.115 \tag{3.2}$$

and extrapolate by means of a concave empirical "turning point curve" that $\lim_{L\to\infty}\tilde{p}_{L,\mathrm{sq}}\approx 0.1$ and so by (3.1) we obtain

$$p_{c,\mathrm{sq}}\approx 0.1 \tag{3.3}$$

Our estimate is in good agreement with the estimates $p_{c,\mathrm{sq}}\approx 0.099$ by Grinstein et al.[7] and $p_{c,\mathrm{sq}}\approx 0.105$ by Freund and Grassberger.[6]

Now let $\lambda_{L,\mathrm{sq}}(p)$ in $0\leqslant p\leqslant 0.5$ be the finite lattice analogue to $\lambda_{\mathrm{sq}}(p)$ and let $\lambda_{L,\mathrm{sq}}(p)$ take its global maximum at $p^*_{L,\mathrm{sq}}$. Then the $p^*_{L,\mathrm{sq}}$ drift with increasing L to the left to p^*_{sq} as indicated by

$$p^*_{10,\mathrm{sq}}\approx 0.130,\quad p^*_{20,\mathrm{sq}}\approx 0.128,\quad p^*_{50,\mathrm{sq}}\approx 0.125,\quad p^*_{100,\mathrm{sq}}\approx 0.119$$

Since for $L\geqslant 20$ the estimates (3.2) of turning points $\tilde{p}_{L,\mathrm{sq}}$ are close to the corresponding estimates of $p^*_{L,\mathrm{sq}}$ we infer that

$$p^*_{\mathrm{sq}}=\lim_{L\to\infty}p^*_{L,\mathrm{sq}}=\lim_{L\to\infty}\tilde{p}_{L,\mathrm{sq}}=p_{c,\mathrm{sq}} \tag{3.4}$$

regarding (3.1).

As for the computing time used when estimating groundstate properties, see Table III.

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