Evidence for a Trivial Ground State Structure in the Two-Dimensional Ising Spin Glass

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We study how the ground state of the two-dimensional Ising spin glass with Gaussian interactions in zero magnetic field changes on altering the boundary conditions. The probability that relative spin orientations change in a region far from the boundary goes to zero with the (linear) size of the system L like $L^{-\lambda}$, where $\lambda = -0.70 \pm 0.08$. We argue that λ is equal to $d - d_f$ where d $(= 2)$ is the dimension of the system and d_f is the fractal dimension of a domain wall induced by changes in the boundary conditions. Our value for d_f is consistent with earlier estimates. These results show that, at zero temperature, there is only a single pure state (plus the state with all spins flipped) in agreement with the predictions of the droplet model.

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The nature of the ordering in spin glasses below the transition temperature, T_c, remains rather poorly understood. For the infinite range model, the replica symmetry breaking solution of Parisi[1−3] is generally believed to be correct. An important aspect of this solution is that the order parameter is a non-trivial distribution, $P(q)$, where q describes the overlap of the spin configuration between two copies of the system with identical interactions. The distribution is non-trivial because very different spin configurations occur with significant statistical weight. One loosely says that the system can be in many "pure states". Monte Carlo simulations on (more realistic) short range models on quite small lattices[4,5], find a non-trivial $P(q)$ with a weight at $q = 0$ which is independent of system size (for the range of sizes studied), as predicted by the Parisi theory.

An alternative approach, the "droplet model", has been proposed by Fisher and Huse[6] (see also Refs. 7, 8). Thermodynamic states and pure states are defined precisely by considering correlation functions of spins in a region small compared with the system size and far from the boundary, and asking whether they change or not upon changing the boundary conditions as the (linear) system size L, tends to infinity. Each different set of correlation functions corresponds to a different thermodynamic state. The droplet theory, the Parisi theory, and some other scenarios have been studied in detail by Newman and Stein[9,10].

By making some plausible and self-consistent assumptions, the droplet theory predicts that the structure of pure states is trivial in short range spin glasses below T_c. In zero field[11], trivial pure state structure means that any thermodynamic state is a combination of just two distinct pure states, related by flipping all the spins, which have the same free energy by symmetry. If one looks at the whole system, rather than a relatively small region far from the boundary, one might note that part of the system is in one pure state and the other part in the spin-flipped state, with a domain wall between them. Hence a global quantity like $P(q)$ could have a non-trivial form[12] even though the structure of pure states is actually trivial[13].

To unambiguously distinguish between the droplet and Parisi pictures it is therefore better to study correlation functions, such as the overlap distribution, in a finite region[10] far from the boundary, since the probability that the domain wall goes through this region vanishes as $L \to \infty$. More precisely, one should investigate whether these correlation functions change when the boundary conditions are changed. To our knowledge, however, this has not been done before[14].

Here, we perform such calculations numerically for the ground states of the Ising spin glass with Gaussian interactions in two dimensions. Although there is no spin glass order at finite temperature in this system, there *is* (complete) spin glass order in the *ground state*, so one can investigate the question of the number of pure states *at zero temperature*[15]. Two dimensions has the additional advantage that there are efficient algorithms for computing exact ground states[16,17] and so quite large sizes can be investigated. We find that the probability for the spin configuration in the center to change, when the boundary conditions are altered, goes to zero like $L^{-\lambda}$ as L increases, where λ can be related to the fractal dimension of a domain wall which is induced by the boundary condition change. This result shows that there is only a single pure state at $T = 0$ (*i.e.* a single ground state), plus the state with all spins flipped, in agreement with the droplet theory.

The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j, \tag{1}$$

where the sites i lie on the sites of an $L \times L$ square lattice with $L \leq 30$, $S_i = \pm 1$, and the J_{ij} are nearest-neighbor interactions chosen according to a Gaussian distribution with zero mean and standard deviation unity. Initially, we impose periodic boundary conditions, denoted by "P". Since the distribution of the interactions, J_{ij}, is continuous, the ground state is unique (apart from the equivalent state obtained by flipping all the spins).

We determine the energy and spin configuration of the ground state for a given set of bonds. Next we impose anti-periodic conditions ("AP") along *one* direction, which is completely equivalent to changing the sign of the interactions along this boundary, and recompute the ground state. Finally we change the sign of half the bonds at random along this boundary, which we denote by "R". Note that the different boundary conditions correspond to different choices of the interactions which occur with the same probability. Hence they are statistically equivalent.

For the smaller sizes, $L \leq 8$, we compute the ground state by rapidly quenching from a randomly chosen spin configuration, and repeating many times until we are confident that the ground state energy has been found. For the two largest sizes, $L = 16$ and 30, this is impractical so instead we use the Cologne spin glass ground state server[18]. We repeat the calculation of the ground state for the three copies with different boundary conditions for a minimum of 2000 samples for each size.

Next we discuss how to study the dependence of the spin configuration on boundary conditions. We consider a central block containing $N_B = L_B^2$ spins, and ask if the correlation functions between two spins, i and j say, in the block depend on the boundary conditions, *i.e.* whether $\langle S_i^\alpha S_j^\alpha \rangle_T - \langle S_i^\beta S_j^\beta \rangle_T$ is non zero for $L \to \infty$, where α and β refer to two distinct boundary conditions, P, AP, or R here, S_i^α refers to a spin in the copy with the α boundary condition, and $\langle \cdots \rangle_T$ denotes a thermal average. We consider even spin correlation functions because our boundary conditions do not distinguish between states which differ by flipping all the spins. Since the difference can have either sign, it is convenient to consider its square, $(\langle S_i^\alpha S_j^\alpha \rangle_T - \langle S_i^\beta S_j^\beta \rangle_T)^2$. If we sum over all the spins in the block, normalize, and average over disorder, it is easy to see that this becomes

$$\Delta = \left\langle \left(q_{\alpha\alpha}^B\right)^2 + \left(q_{\beta\beta}^B\right)^2 - 2\left(q_{\alpha\beta}^B\right)^2 \right\rangle, \tag{2}$$

where

$$q_{\alpha\beta}^B = \frac{1}{N_B} \sum_{i=1}^{N_B} S_i^\alpha S_i^\beta \tag{3}$$

is the overlap between the block configurations with α and β boundary conditions, and the brackets $\langle \cdots \rangle$ refer to both a thermal average and an average over the disorder. Eq. (2) can be written as

$$\Delta = \int_{-1}^{1} q^2 \left[P_{\alpha\alpha}^B(q) + P_{\beta\beta}^B(q) - 2P_{\alpha\beta}^B(q)\right] dq, \tag{4}$$

where

$$P_{\alpha\beta}^B(q) = \left\langle \delta\left(q - q_{\alpha\beta}^B\right)\right\rangle \tag{5}$$

is the probability distribution for the block overlaps. We have written these expressions in a general form, valid for $T > 0$ as well as $T = 0$. Similar arguments can be made for correlations of a larger number of spins, which leads to expressions like Eq. (4) but with higher moments of the overlap distributions. Hence the crucial quantity is the difference in the block spin overlap distributions with different boundary conditions which occurs in Eq. (4), *i.e.*

$$\Delta P_{\alpha\beta}^B(q) \equiv P_{\alpha\alpha}^B(q) + P_{\beta\beta}^B(q) - 2P_{\alpha\beta}^B(q). \tag{6}$$

If this difference tends to zero as $L \to \infty$ then the droplet picture is valid. We emphasize that this test does *not* require the size of the block to also become large.

Specializing now to $T = 0$, $P_{\alpha\alpha}^B(q)$ is just the sum of two delta functions with equal weight at $q = \pm 1$, since the ground state is unique (apart from overall spin reversal). Hence, at $T = 0$, it is sufficient to investigate the block overlap distribution $P_{\alpha\beta}^B(q)$ with $\alpha \neq \beta$. We calculate this for $\alpha =$ P, and $\beta =$ AP and R.

Now we discuss our results, for which we take $L_B = 2$. First of all, Fig. 1 shows data for the root mean square difference in ground state energy,

$$\Delta E_{\alpha\beta} \equiv \langle (E_\alpha^0 - E_\beta^0)^2 \rangle^{1/2} \tag{7}$$

with E^0 the total ground state energy (not the energy per spin), for $\alpha =$ P and $\beta =$ AP and R. One sees that $\Delta E_{P,AP}$ goes to zero like $L^{-\theta}$ as L increases, where $\theta = 0.285 \pm 0.020$. This is in agreement with earlier work[17,19]. The negative value means that large domains cost very little energy and so the order in the ground state will spontaneously break up at any finite temperature, showing that $T_c = 0$.

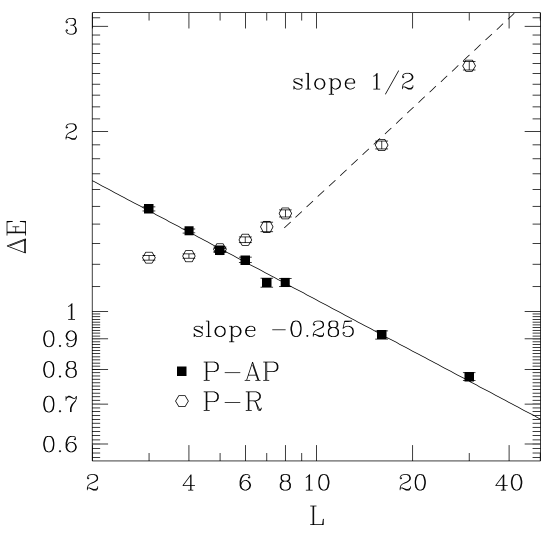

FIG. 1. A plot of the root mean square ground state energy differences $\Delta E_{P,AP}$ and $\Delta E_{P,R}$ for different sizes up to $L = 30$.

The results for $\Delta E_{P,R}$ are quite different, however, *increasing* with L, roughly as $L^{1/2}$ for large L, rather than decreasing. This difference is easily understood, since the defect (i.e. the region where the energy is locally different for the two boundary conditions) can be *locally* removed in the P-AP case, by changing the sign of the spins to one side of the boundary. The defect will then be a single domain wall somewhere in the sample not necessarily near the boundary. However, this can not be done for the P-R case and a part of the defect, with an energy which one could guess to be $L^{(d-1)/2}$ in d-dimensions, will stay close to the boundary, in addition to a domain wall which could be arbitrarily far away.

We show some of our data for the block overlaps in Fig. 2. The results for the P-AP and P-R overlaps are qualitatively similar to each other, with the weight away from the peaks at $q = \pm 1$ dropping as L increases.

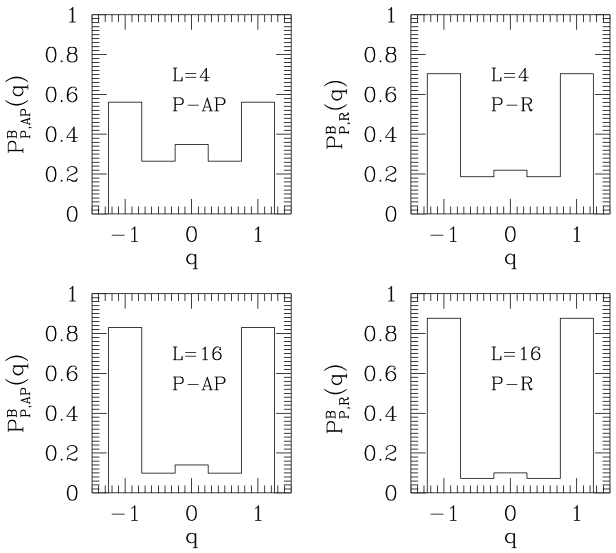

FIG. 2. A plot of the block overlaps, $P^B_{P,AP}(q)$ and $P^B_{P,R}(q)$, for $L = 4$ and 16, with block size $L_B = 2$. Note that the allowed values of q are $0, \pm 0.5$ and ± 1. The left hand column is for the P-AP overlap and the right hand column for the P-R overlap. The top row is for $L = 4$ and the bottom row for $L = 16$. The data is normalized so that the area under the histograms is unity.

We characterize this trend by the weight at $q = 0$ and show the results in Fig. 3. For both anti-periodic and random boundary condition changes, the weight at $q = 0$ vanishes like $L^{-\lambda}$, where $\lambda = -0.70 \pm 0.08$. This value is easy to understand since $P^B_{\alpha \neq \beta}(0)$ is just the probability that the domain wall bisects the block. If the fractal dimension of the domain wall is d_f then, generalizing to d-dimensions, the probability that it goes through any small region is proportional to $L^{-(d-d_f)}$. This immediately gives $d_f = 1.30 \pm 0.08$, which is consistent with other estimates for d_f: 1.26 ± 0.03 by Bray and Moore[21], 1.34 ± 0.10 by Rieger et al.[17] and 1.31 ± 0.1 (for a related model) by Gingras[20].

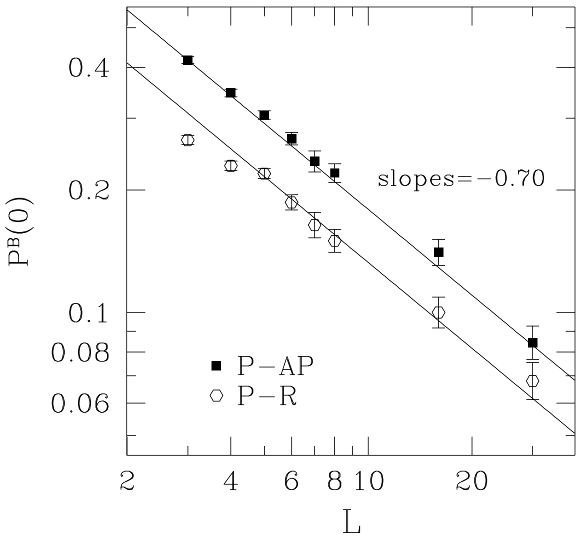

FIG. 3. A plot of the block overlaps at $q = 0$, $P^B_{P,AP}(0)$ and $P^B_{P,R}(0)$, for different sizes up to $L = 30$ with block size L_B equal to 2.

Earlier calculations have investigated some effects of changing the boundary conditions from periodic to anti-periodic, usually just the change in the ground state energy, though Bray and Moore[21] and Rieger[17] have also calculated the fractal dimension of the domain wall. They obtain a value less than d (as noted above), which implies that $P^B_{P,AP}(0)$ vanishes for large L, as we find explicitly here. However, as noted in our discussion of Fig. 1, anti-periodic boundary conditions are special since the defect can be locally removed by flipping the spins to one side of it. This is why we also investigate random boundary condition changes, for which the defect cannot be locally eliminated. An important result of our work is that the fractal dimension of the domain wall is the same in both cases.

For each configuration of the bonds in the bulk we have only studied a single random change in the boundary conditions. It would be interesting to get statistics on a large number of boundary condition changes to see if the probability for the domain wall to go through the central block obtained by averaging over boundary conditions for a single large sample is the same as we find here by averaging over samples. It would also be interesting to investigate boundary conditions which are optimized to minimize the ground state energy, i.e. which are correlated with the bonds in the bulk.

Recently, we have been able to perform calculations similar to those presented here for the three-dimensional spin glass[22], which has a finite T_c. There too we find evidence for a unique ground state.

After this work was virtually complete, we became aware of related work by Middleton[23]. Whereas we start with *periodic* boundary conditions Middleton takes *free* boundary conditions which allows him to find a ground state (for the models studied) in polynomial time, permitting the study of very large sizes, up to $L = 512$. In this approach one can only perturb the system far away from the central region by making it grow bigger. Hence there are *three* relevant lengths: the block size, which we call L^B, the size inside which the bonds are not changed (which we will call L_{mid}), and the overall size L. One needs $L_{mid} \gg L^B$ and at least some data which also satisfies $L \gg L_{mid}$. Hence the largest sizes L that Middleton studies need to be *very* large. In our work, we only have one inequality to satisfy, $L \gg L^B$, rather than two, so the sizes do not need to be as large. Overall, the two approaches are complementary and, in our view, have similar validity for the two-dimensional spin glass. However we believe that our approach is preferable for the three-dimensional spin glass, for which there are no polynomial algorithms, since it requires smaller sizes.

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[12] Note that $P(q)$ would be non-trivial in a situation with a trivial pure state structure *only* if the position of the domain wall in a given sample could fluctuate over a finite fraction of the total volume. If, as we suspect, the domain wall is pinned in some non-extensive region, then a non-trivial $P(q)$ *would* indicate a non-trivial pure state structure.

[13] It is also possible that $P(q)$ could be trivial, even though the structure of pure states is non-trivial, because $P(q)$ detects only states which differ in free energy by a finite amount from the state of lowest free energy, whereas changing the boundary conditions can alter the free energy of states by an amount which diverges with the size of the system, though less than extensively. Hence it is possible that $P(q)$ could miss some pure states.

[14] Note that E. Marinari, G. Parisi, F. Ricci-Tersenghi, and J. J. Ruiz-Lorenzo, J. Phys. A, **31** L481, (1998), have investigated the overlap distribution $P^B(q)$ in blocks of size $L_B \leq L$ for a *three*-dimensional Ising spin glass below T_c, where both copies of the system have the same (periodic) boundary conditions. They find very similar results to those for the bulk $P(q)$, in particular the weight at $q = 0$ does not diminish with size. They did not, however, consider the block spin overlap between copies with different boundary conditions.

[15] Note that $P(q)$ is not a useful quantity at $T = 0$ because both the Parisi and droplet pictures predict two delta functions with equal weight at $q = \pm 1$ in a finite system. This is a trivial consequence of the ground state being only doubly degenerate (the two states being related by time reversal) when the bond distribution is continuous.

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