Triviality of the Ground State Structure in Ising Spin Glasses

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We investigate the ground state structure of the three-dimensional Ising spin glass in zero field by determining how the ground state changes in a fixed finite block far from the boundaries when the boundary conditions are changed. We find that the probability of a change in the block ground state configuration tends to zero as the system size tends to infinity. This indicates a trivial ground state structure, as predicted by the droplet theory. Similar results are also obtained in two dimensions.

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Controversy remains over the nature of ordering in spin glasses below the transition temperature, T_c, and two scenarios have been extensively discussed. In the "droplet model" proposed by Fisher and Huse[1] (see also Refs. 2–5), the structure of "pure states" is predicted to be trivial. This means that there is a unique state[6] in the sense that correlations of the spins in a region far from the boundaries are independent of the boundary conditions imposed. As a consequence, the order parameter distribution function[7–9], $P(q)$, is also trivial, i.e. is a pair of delta functions at $q = \pm q_{EA}$ where q_{EA} is the Edwards-Anderson order parameter. In the alternative approach, one assumes that the basic structure of the Parisi[7–9] solution of the infinite range model applies also to realistic short range systems. In this picture, $P(q)$ is a non-trivial function because many thermodynamic states contribute to the partition function, i.e. the pure state structure is non-trivial. Monte Carlo simulations on short range models on small lattices[10–13], 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.

Most numerical work has concentrated on $P(q)$. By contrast, here we attempt to determine the pure state structure by investigating whether spin correlation functions in a *finite* region[5] far from the boundary, change when the boundary conditions are changed. It is interesting to investigate this question even at $T = 0$, where there are efficient algorithms for determining ground states, even though $P(q)$ is trivial in this limit (for a continuous bond distribution). Here we show that the Ising spin glass in *three dimensions* which has a *finite transition temperature*[14–17] T_c, has a trivial ground state structure. We also find a trivial ground state structure in the *two-dimensional* Ising spin glass which has a transition at *zero temperature* with long-range order at $T = 0$. Some of our results in two dimensions have also been reported elsewhere[18] (referred to as PY). Similar results for two dimensions, as well as results for some three-dimensional models (but none for a spin glass with a finite T_c) have also been found by Middleton[19].

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 a simple cubic ($d = 3$) or square lattice ($d = 2$) with $N = L^d$ sites ($L \le 10$ in $3d$, $L \le 30$ in $2d$) , $S_i = \pm 1$, and the J_{ij} are nearest-neighbor interactions chosen according to a Gaussian distribution with zero mean and standard deviation unity. We determine the energy and spin configuration of the ground state for a given set of bonds, initially for periodic boundary conditions denoted by "P". Next we impose anti-periodic conditions ("AP") along *one* direction, which is equivalent to keeping periodic boundary conditions and 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".

To determine the ground state in three dimensions we use a hybrid genetic algorithm introduced by Pal[20,21]. Starting from a population of random configurations ("parents"), new configurations ("offspring") are generated by recombination (triadic crossover) and mutation. The population is progressively reduced, with a bias towards the offspring with lower energy. The algorithm is hybridized with a local optimization of the offspring (see Ref. 20 for details). For each sample and boundary condition, we repeat the algorithm n_r times, see Table I, and take the lowest energy state found. Our values for the average ground state energy are in agreement with those of Ref. 21. For $L \le 6$, we checked all our results with a different method, which consists in repeating many times the microcanonical simulated annealing algorithm introduced in Ref. 22. This algorithm was also used to prepare the initial populations of the genetic algorithm for $L \ge 8$. We discuss later additional checks that we performed for the largest sizes $L = 8$ and 10.

In two dimensions, we used the Cologne spin glass server[23], which calculates *exact* ground states of the Ising spin glass with periodic boundary conditions.

In order to study the dependence of the spin configuration on boundary conditions we consider a central block containing $N_B = L_B^d$ spins. We compute the block spin overlap distribution $P^B_{\alpha\beta}(q)$, where α and β denote two boundary conditions, P, AP or R here, and

$$P^B_{\alpha\beta}(q) = \left\langle \delta\left(q - q^B_{\alpha\beta}\right)\right\rangle, \tag{2}$$

in which

L	N_s	n_r	$\langle E \rangle$	$\langle E \rangle$ Ref. 21
4	20000	3	$-106.59(4)$	$-106.609(9)$
5	15000	3	$-210.26(7)$	$-210.22(3)$
6	9450	3	$-364.9(1)$	$-364.89(5)$
8	6646	2	$-868.1(2)$	$-868.1(2)$
10	3010	1	$-1697.5(4)$	$-1698.8(8)$

TABLE I. Parameters of the simulation and results for the ground state energy in $d = 3$. As a function of the size L we show: number of samples N_s, number of runs per sample n_r, and the average ground state energy $\langle E \rangle$, from our data and that of Pal[21].

$$q^B_{\alpha\beta} = \frac{1}{N_B} \sum_{i=1}^{N_B} S_i^\alpha S_i^\beta \qquad (3)$$

is the overlap between the block configurations with α and β boundary conditions, S_i^α is the value of S_i in the ground state with the α boundary condition, and the brackets $\langle \cdots \rangle$ refer to an average over the disorder.

Since we work at $T = 0$, each sample and pair α, β gives a single value for q. The self overlap distribution, $P^B_{\alpha\alpha}(q)$, has weight only at $q = \pm 1$, since the ground state is unique for a given boundary condition. $P^B(q)$ is normalized to unity i.e. $\int P^B(q)\, dq = 1$, it is symmetric, and the allowed q-values are discrete with a separation of of $\Delta q = 2/N^B$, so $P^B_{\alpha\alpha}(\pm 1) = N^B/4$.

If the configuration in the block changes when the boundary conditions are changed from α to β, then the block overlap, $q^B_{\alpha\beta}$, will no longer be ± 1. Hence $1 - P^B_{\alpha\beta}(1)/P^B_{\alpha\alpha}(1)$ is the probability that the block ground state changes on changing the boundary conditions. We will see that

$$1 - \frac{P^B_{\alpha\beta}(1)}{P^B_{\alpha\alpha}(1)} \sim L^{-\lambda}, \qquad (4)$$

with $\lambda > 0$, showing that the block ground state configuration is unchanged in the thermodynamic limit. Our interpretation[18,19] of this result is that the boundary condition change induces a domain wall of fractal dimension $d_f = d - \lambda$, and $L^{-\lambda}$ is then the probability that the domain wall intersects the block.

Now we discuss our numerical results, for which ake $L_B = 2$. First of all, Fig. 1 shows the root mean square energy difference, ΔE, between P and AP and between P and R boundary conditions in $d = 3$. Apart from the smallest size, $L = 3$, the data for $\Delta E_{P,AP}$, are consistent with the power law variation

$$\Delta E_{P,AP} \sim L^\theta \qquad (5)$$

with

$$\theta = 0.23^{+0.02}_{-0.04}, \qquad (6)$$

where the asymmetric error bar comes from systematic effects discussed below. The positive value of θ shows

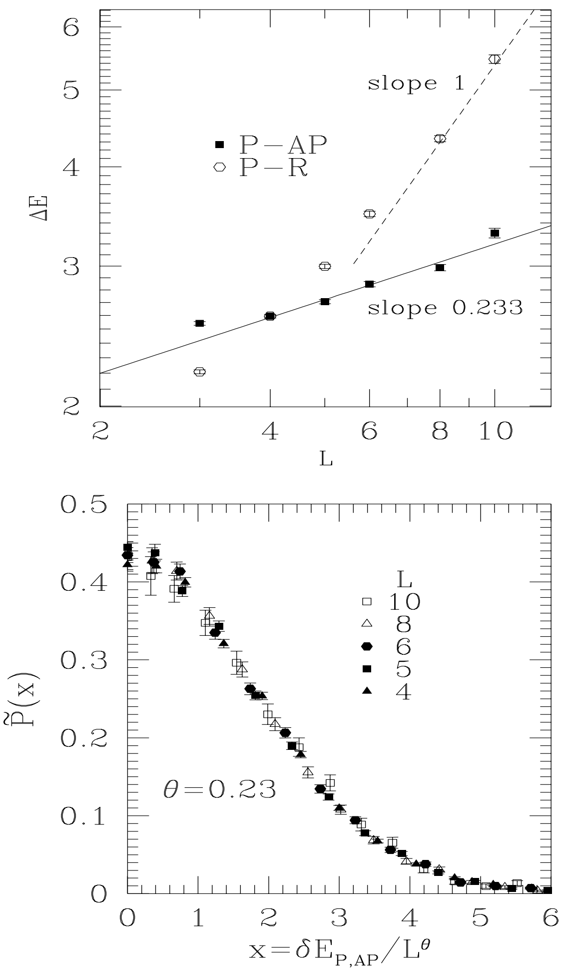

FIG. 1. Upper figure: a plot of the root mean square ground state energy differences $\Delta E_{P,AP}$ and $\Delta E_{P,R}$ for different sizes up to $L = 10$ in $d = 3$. The fit for the P-AP data omits the $L = 3$ point. Lower figure: a scaling plot of the symmetrized distribution of the values for $\delta E_{P,AP}$, the energy difference between periodic and anti-periodic boundary conditions for a single sample. The distribution scales quite well with the value of θ obtained from the fit to $\Delta E_{P,AP}$.

that the system is stable against breaking up into large domains of little energy, which implies that $T_c > 0$, in agreement with earlier work[14–17]. The value for θ is a little larger than earlier estimates[24] for the Gaussian distribution considered here, but these calculations used a much smaller range of sizes. For the $\pm J$ distribution, Hartmann[16] studied sizes up to $L = 10$ and found $\theta = 0.19 \pm 0.02$, which is just consistent with the value here. It is expected[1] that the distribution of energy differences, $\delta E_{P,AP}$ has the scaling form $P(\delta E_{P,AP}) = L^{-\theta} \widetilde{P}(\delta E_{P,AP}/L^\theta)$ and this works quite well as shown in the lower part of Fig. 1. As discussed in PY, $\Delta E_{P,R}$ is expected to vary as $L^{(d-1)/2}$, $(= L$ here), for large L. Fig. 1 shows that our results are consistent with this behavior.

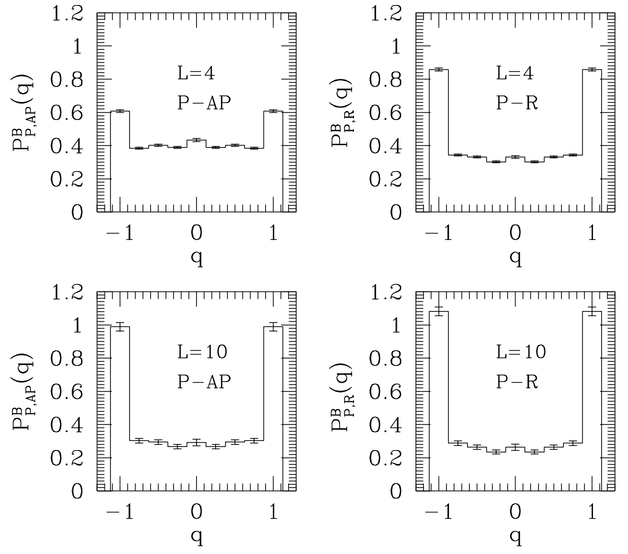

FIG. 2. A plot of histograms of block spin overlaps for $L = 4$ and 10 in $d = 3$, with block size $L_B = 2$. Note that the allowed values of q are 0, ± 0.25, ± 0.5, ± 0.75 and ± 1. The left hand column is for the P-AP overlap and the right hand column for the P-R overlap. The top row is for $L = 4$ and the bottom row for $L = 10$. The data is symmetrized and normalized so that the area under the histograms is unity.

Some representative histograms of the block overlap distributions are shown in Fig. 2 for $d = 3$. One sees that for both P-AP and P-R overlaps the weight at $q = \pm 1$ increases with increasing L.

The probability that the configuration of the block changes when the boundary conditions are changed, see Eq. (4), is plotted for a range of sizes in the upper part of Fig. 3. For comparison, the lower part of the figure shows similar data in $d = 2$ (see PY for related results).

In $d = 3$, the data for P-AP overlaps lies on a good straight line with a slope $-\lambda$ where $\lambda = 0.32 \pm 0.02$. This leads to a fractal dimension of the domain walls given by

$$d_f = d - \lambda = 2.68 \pm 0.02 \tag{7}$$

The data for P-R overlaps for larger sizes lies parallel to this, as shown in the figure, but with some deviations for smaller sizes. However, given the statistical uncertainties, one can also fit *all* the P-R data to a power law with a different slope giving $\lambda = 0.23 \pm 0.02$. If the ground state structure in $d = 3$ were non-trivial the data for the P-R boundary conditions in the upper part of Fig. 3 would eventually saturate at a finite value for $L \to \infty$. There is no sign of such a saturation for the sizes that we are able to study. We also considered fits of the form $a + bL^{-\lambda}$, finding that, although a range of positive values of a is not ruled out by the data, the value $a = 0$ is statistically preferred.

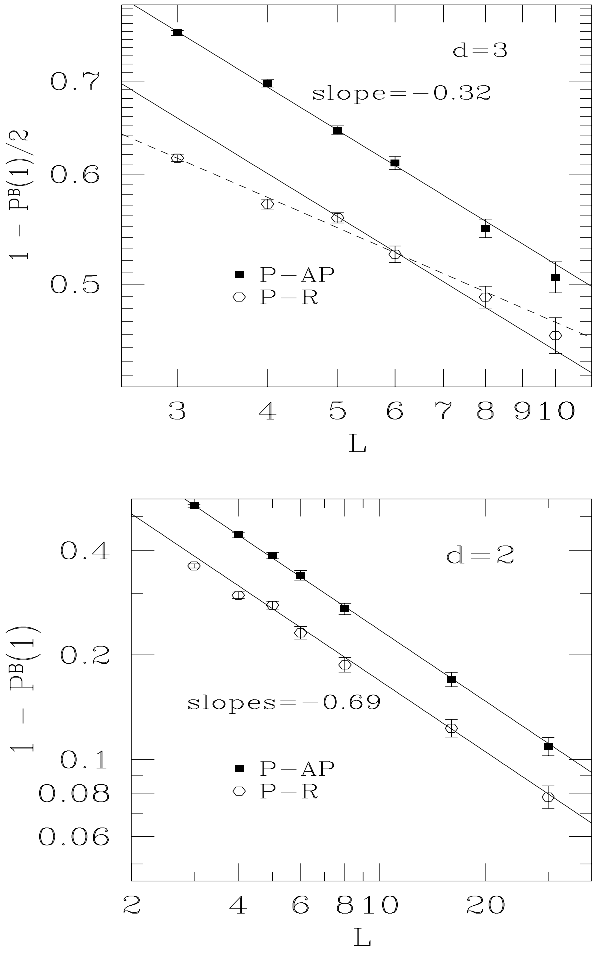

FIG. 3. The figures show the probability that the spin configuration of the central block changes when the boundary conditions are changed. Upper figure: Data for three dimensions, for different sizes up to $L = 10$ with block size L_B equal to 2. The solid line through the P-R data is parallel to the fit for the P-AP points (slope = -0.32), and fits the results for large L. The dashed line is fit to *all* the P-R data and has a different slope of -0.23. Lower figure: a similar plot but for $d = 2$, with sizes up to $L = 30$ and $L^B = 2$.

We also investigated the effects of changing the bonds on one boundary to other random values (rather than just changing the *sign*) and also changed the bonds on *all three* boundaries to new random values. The results for these boundary conditions give similar results to those for the R boundary condition.

It is important to estimate the size of the errors which arise because the algorithm is not guaranteed to find the exact ground state. This is a problem only for the larger sizes so we estimated the errors carefully for $L = 8$ and 10 for P-AP boundary conditions by doing a smaller number of samples for a larger number of runs, $n_r = 10$, than before (see Table I) and assuming that the difference in results is a reasonable measure of the error in the original data. For $L = 8$, the result for whether the block spin configuration changed upon changing the boundary conditions was the same after 2 runs as after 10 runs in 367 out of the 370 samples considered, with 1 sample giving $|q| = 1$ after 2 runs but $|q| < 1$ after 10 runs, and 2 samples the other way round. Hence our estimate of the relative error in the data in Fig. 3 (due to not finding the correct ground state) is in the range $(-1 \pm \sqrt{5})/370$, i.e. between -0.7% and $+0.2\%$, which is well within the statistical error bar of $\pm 1.5\%$ shown in Fig. 3. For $L = 10$ the corresponding figures are: 11 out of the 266 samples considered gave $|q| = 1$ after 1 run but $|q| < 1$ after 10 runs, and 13 samples the other way round. The estimate of the error is therefore $(-2 \pm \sqrt{24})/266$, i.e. the true answer should lie between -2.5% and $+1.1\%$ of the value given, compared with the statistical error bar of $\pm 2.5\%$ in Fig. 3. The error from the algorithm is therefore no bigger than the statistical error, and is significantly less than that on the positive side. Hence the decreasing trend in the $3d$ data in Fig. 3, is *not* due to inaccuracies in the algorithm. Altogether, we find no evidence for a *systematic* error in the data in Fig. 3 due to not always finding the true ground state. A similar analysis for the defect energy with P-AP boundary conditions finds that, for $L = 8$, the error is negligible compared with the statistical error, but that for $L = 10$ the result is about 5% too high, compared with the error bar in Fig. 1 of about $\pm 1.5\%$. This is probably why the $L = 10$ data point lies above the fit. The best fit with the $L = 10$ point 5% lower has $\theta = 0.21$, rather than 0.23, which is why we give asymmetric error bars in Eq. (6).

In $d = 2$, the data for P-AP and P-R lie nicely parallel to each other and we find $\lambda = 0.69 \pm 0.02$, and hence $d_f = 1.31 \pm 0.02$, for both sets of boundary conditions, in agreement with PY who get $\lambda = 0.70 \pm 0.08$ and also in agreement with Middleton[19]. Note that λ is substantially smaller in $d = 3$ than in $d = 2$. It would be interesting to know how it varies in higher dimensions, but the numerics of such a calculation are challenging.

The only other calculation of d_f in $d = 3$ that we are aware of is that of Huse[25] who studied domain growth at finite temperatures by Monte Carlo simulations, obtaining $d_f \simeq 2.2$. However, his method "only measures the size of domains which are *compact*", which may explain why his value is lower than ours.

To conclude we have seen that the ground state structure appears to be trivial in a spin glass model with a finite T_c, the three-dimensional Ising spin glass. It remains to understand why Monte Carlo simulations at finite temperature find, by contrast, evidence for a non-trivial pure state structure.

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