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Ground State Structure of Spin Glasses

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We investigate the ground state structure of Ising spin glasses in zero magnetic 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, both in two and three dimensions, 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.

KEYWORDS: Spin glasses, ground states, optimization methods.

§1. Introduction

In this talk we discuss some recent work that tries to shed light on the nature of the spin glass state. It is now fairly clear that there is a finite temperature spin glass transition in three dimensions[1–5] (3-d) though a transition only occurs[6,7] at $T = 0$ in 2-d. However, the nature of the spin glass phase below the transition temperature T_c is not clear. We will review the two principal scenarios that have been proposed for the spin glass phase, which differ in how many "states" contribute to the correlation functions, and will mention briefly existing numerical results which probe this region. Then we describe a new approach[8,9] to investigate the problem which involves looking at how sensitive the region far from the boundaries is to changes in the boundary conditions. The idea can be applied both to ground states and to finite temperature studies, but initially we have just considered $T = 0$.

§2. Scenarios for the spin glass phase

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 first approach, one assumes that the basic structure of the replica symmetry breaking (RSB) in Parisi's[15–18] solution of the infinite range model applies also to realistic short range systems. In this picture, the order parameter is not just a single number, as is the case for a ferromagnet for example, but is a probability distribution, $P(q)$. This distribution gives the

probability that two spin configurations, weighted by the Boltzmann factor, have overlap given by q. To be precise $P(q)$ is defined by

$$P(q) = \langle \delta \left(q - q_{12} \right) , \tag{2.1}$$

where $\langle \cdots \rangle$ denotes both a thermal average and an average over disorder, and

$$q_{12} = \frac{1}{N} \sum_{i=1}^{N} S_i^{(1)} S_i^{(2)}, \tag{2.2}$$

where (1) and (2) denote two copies of the system with the same interactions.

In the Parisi picture $P(q)$ is a non-trivial function because many thermodynamic states contribute to the partition function, i.e. they have differences in total (free) energy which are of order unity and yet have very different spin configurations from each other. As a result, $P(q)$ has a delta function at q_{EA} coming from ordering in a single state, and a tail down to $q = 0$ from overlap between different states, which does not vanish for $L \to \infty$.

In the alternative approach, the "droplet model", proposed by Fisher and Huse[10] (see also Refs.[11–14]), one starts by defining the concept of "thermodynamic states" and "pure states". For a given set of boundary conditions, one looks at the correlation functions of the spins in the bulk, i.e. in a finite region far from the boundary. Each different set of correlation functions defines a separate thermodynamic state.

However, many thermodynamic states defined in this way are related to each other. To see this, consider, for example, a ferromagnet below T_c. Clearly two of the thermodynamic states are $|\uparrow\rangle$ and $|\downarrow\rangle$, where the spins are aligned up and down respectively. These can be generated by fixing the spins on the boundary to be up (or down). However, if we use *periodic* boundary conditions, then the system is in a linear combination of $|\uparrow\rangle$ and $|\downarrow\rangle$ with equal weight (assuming no external field, which will be case for all the discussions in this paper). States like $|\uparrow\rangle$ and $|\downarrow\rangle$, which are "extremal", in the sense that other states can be expressed as linear combinations of them, are called pure states. An important question is the number of these pure states. For the ferromagnet, there are just two. In such a situation, where there is just one pure state (plus other(s) related by a global symmetry of the Hamiltonian), we say that the pure state structure is trivial. If this occurs at $T = 0$ we refer to a "trivial ground state structure".

One other issue relating to the ferromagnet needs to be addressed before we go on to spin glasses. It is possible that the boundary conditions generate a "domain" state which is $|\uparrow\rangle$ in some region of space and $|\downarrow\rangle$ in the rest. If the domain wall intersects the region where we are computing the correlation functions, we would have another pure state, since it is not a linear combination of $|\uparrow\rangle$ and $|\downarrow\rangle$ (more precisely it is one linear combination in part of the region and a different linear combination in the rest). Since these domain states are closely related to the pure states $|\uparrow\rangle$ and $|\downarrow\rangle$ we will still denote the pure state structure as trivial. In order to eliminate domain states,

which do not really alter the nature of the ground state structure, but still enable us to detect other possible states, we look at correlation functions in a fixed *finite* box, far from the boundaries, as the (linear) system size L tends to infinity. The probability that the domain wall intersects the block vanishes as $L \to \infty$, and so the ground state structure is trivial if we get the same state in the box (or the reversed state) with probability one for $L \to \infty$ when the boundary conditions are changed.

Returning now to spin glasses, Fisher and Huse[10] find, under certain assumptions, that the pure state structure in spin glasses is trivial. More precisely, they argue that the elementary excitations are compact objects called "droplets" such that the minimum energy of a droplet of linear extent L which encloses a given site is $\sim L^\theta$, where θ is a "stiffness" exponent. For the spin glass state to be stable at finite temperature one must have $\theta > 0$. Since it costs a lot of energy to turn over a large number of spins, the state far from the boundary will not change upon changing the boundary conditions, as in a ferromagnet where in that case $\theta = d-1$. As an additional consequence, $P(q)$ 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 describing order in the (single) pure state. For a finite system, there will be a weight in the tail but this vanishes in the thermodynamic limit as $1/L^\theta$.

It should be pointed out that although the volume of a droplet is assumed to be compact, i.e. $V \sim L^d$, the surface of the droplets will be a fractal of fractal dimension, d_f where $d-1 < d_f < d$. Furthermore, in the droplet picture, the spin glass state *is* much richer than the ferromagnet, even though the pure state structure is trivial, because the relative spin orientations at large distances change when the temperature is changed by even a small amount. This is sometimes called "chaos".

Fisher and Huse have also argued that $P(q)$ is not necessarily a good indicator of the number of pure states. For example an antiferromagnet with an odd lattice size L must have a domain wall built in. This domain wall will fluctuate in position and so give a non-trivial $P(q)$, although the pure state structure is trivial. An opposite example, where $P(q)$ is trivial but there is more than one pure state is the random field Ising model. The two pure states are $|\uparrow\rangle$ and $|\downarrow\rangle$, but these are no longer related by symmetry and have a (free) energy difference of order $L^{d/2}$. Because this difference diverges for $L \to \infty$ one state will dominate the statistical sum so $P(q)$ will just be a single delta function.

§3. Earlier Numerical Work

First of all we discuss earlier numerical work at zero temperature. In two dimensions, it is clear[6,7] that θ is about -0.28, the negative value indicating that spin glass order does not persist to finite temperature because large domains, which cost very little energy, will be excited at arbitrarily low temperatures. In three dimensions, θ is about[4,5] 0.20, which is positive, implying a finite T_c which has also been found directly. However, it is also small which means that it is hard to distinguish the droplet theory from the RSB picture from simulations of $P(q)$. In four dimensions, recent work[21]

has found a fairly large positive value of θ of around 0.7. Hence 4-d should be the easiest case in which to distinguish droplet from RSB predictions for $P(q)$.

At finite temperature, Monte Carlo simulations on short range models on small lattices in three and four dimensions,[19,20,22,23] 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. Some of the 4-d results show a $P(q)$ which is size independent up to around $L = 8$ at about 2/3 T_c, which is surprising if the droplet theory is correct. Perhaps the droplet theory is correct but there is some length scale, greater than a lattice spacing, below which the RSB picture works better. This length could, perhaps, be the critical correlation length, but naively, it should be quite small at 2/3 T_c since the correlation length exponent ν is less than one.[24]

§4. New Approach

Most numerical work up to now has concentrated on $P(q)$ but here,[8,9] by contrast, we focus directly on the the pure state structure. It is interesting to investigate this 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).

We look at how the spin correlations in a central block of fixed size $N_B = L_B^d$, change when the boundary conditions change. Remember, if the probability of a change tends to zero for $L \to \infty$, then the ground state structure is trivial. Here we just consider $T = 0$ and consider a central block of size $L_B = 2$. Note that there is no need for the block size to tend to infinity. This would be very inconvenient to implement since we need $L_B \ll L$ and yet the largest size L that can be studied is not extremely large..

According to the droplet theory, the change in boundary conditions will induce a domain wall of size L plus possibly some smaller domains near the boundary. The configuration of the central block will change if the the surface of the droplet of size L passes through the block. The probability that this happens is proportional to

$$\frac{1}{L^{d-d_f}}, \tag{4.1}$$

where d_f is the fractal dimension of the surface of the droplet (i.e. the domain wall). Hence this probability tends to zero for $L \to \infty$, at least as long as $d_f < d$.

According to the RSB picture, changing the boundary conditions will shuffle the order of the low energy states (in general we expect by an amount proportional to $L^{(d-1)/2}$). Anti-periodic boundary conditions, see below, will have a smaller effect. Since there are assumed to be states which differ in energy by a finite amount, and which have very different spin configurations (since the overlap is less than unity), the new ground state will be quite different from the old one. Hence the probability that the spin configuration in the block changes is non-zero for $L \to \infty$.

§5. The Model

The Hamiltonian is given by

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j, \tag{5.1}$$

where the sites i lie on a simple cubic ($d = 3$) or square lattice ($d = 2$) with $N = L^d$ sites ($L \leq 10$ in $3d$, $L \leq 30$ 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. Then we change the sign of half the bonds at random along this boundary, which we denote by "R". Finally we replace the bonds on *all* the surfaces by a new set of random variables (so the magnitude as well as the sign is changed). We denote this by "R3".

In 2-d we used sizes up to $L = 30$ while for 3-d the largest size was $L = 10$. To determine the ground state in two dimensions we used the Cologne spin glass ground state server[31] which computes *exact* ground states using a branch-and-cut algorithm. In three dimensions we used a heuristic "genetic" algorithm discussed by Pal,[28,29] see also Refs.[9,30] We did some checks[9] to verify that errors due to the genetic algorithm sometimes not giving the exact ground state are negligible.

In order to study the dependence of the spin configurations in the central block on boundary conditions we compute the block spin overlap distribution $P^B_{\alpha\beta}(q)$, where α and β denote two boundary conditions, and

$$P^B_{\alpha\beta}(q) = \left\langle \delta\left(q - q^B_{\alpha\beta}\right) \right\rangle, \tag{5.2}$$

in which

$$q^B_{\alpha\beta} = \frac{1}{N_B} \sum_{i=1}^{N_B} S_i^\alpha S_i^\beta \tag{5.3}$$

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 this quantity vanishes as $L \to \infty$,

§6. Results

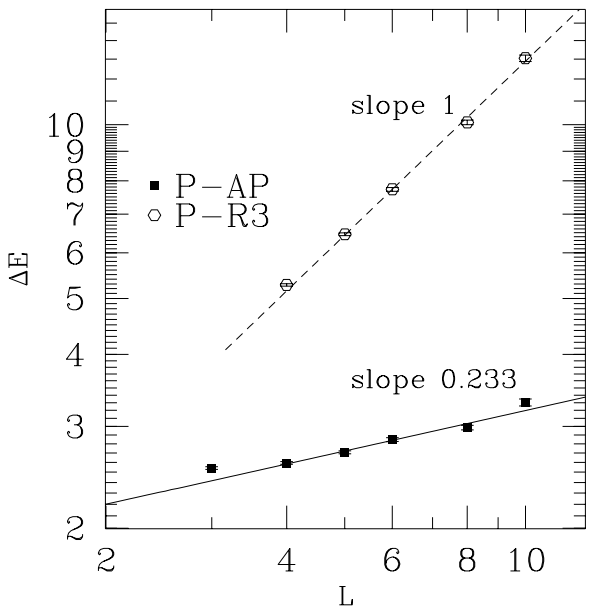

Fig. 1. Defect energies in 3-d.

Fig. 1 shows results for the defect energies in 3-d for P-AP and P-R3 boundary conditions. For P-AP, the boundary condition change can be removed locally by a gauge transformation[8,9] and one is left with a single domain wall, in general far from the boundary, of size L. For P-AP boundary conditions we estimate that the data point for $L = 10$ is about 5% too high because the genetic algorithm does not always find the exact ground state. Correcting for this, we get $\theta = 0.21 \pm 0.02$ in agreement with other estimates.[4,5] For the P-R3 boundary conditions, the change cannot be removed locally by a gauge transformation and small droplets, in the vicinity of the boundary, will also be induced, giving an energy change of order $L^{(d-1)/2} \sim L$ which agrees with the numerics.

Fig. 2 shows block spin overlaps in 3-d for P-AP and P-R3 boundary conditions for two different sizes. One clearly sees that the peaks at $q = \pm 1$ (whose weight gives the probability that the configuration did *not* change) increase significantly for larger L. The probability that the block configuration changes when the boundary conditions are changed is shown in Fig. 3 for 3-d for P-AP

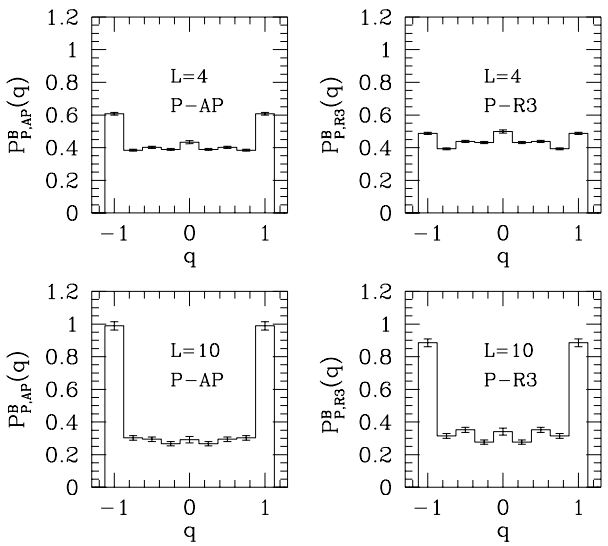

Fig. 2. Block overlaps in 3-d. The probability that the block configuration is unchanged is the weight in the bins at $q = \pm 1$.

and P-R3 changes. The data for P-R boundary conditions is similar but shows some corrections for smaller sizes.[9] The data in Fig. 3 fit straight lines with the same slope for the whole range of sizes. Fitting to the form $a + bL^{-\lambda}$, the chi-squared is higher for any positive a than for $a = 0$. However, we cannot definitely rule out that the data might extrapolate to a small positive value for $L \to \infty$.

In 3-d data for both sets of boundary conditions is consistent with the probability of a change in the block configuration tending to zero as $L^{-\lambda}$ with $\lambda \equiv d - d_f = 0.32 \pm 0.02$. These results imply that the ground state structure is trivial in Ising spin glasses in three (and also in two) dimensions. We believe that our value for d_f is the first reliable prediction for this quantity in 3-d. The data for 2-d shows[8,9] good power law behavior according to Eq. (4.1) with $d - d_f = 0.69 \pm 0.02$, in good agreement with Middleton[25] and earlier estimates of d_f.[6,26,27]

§7. Conclusions

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

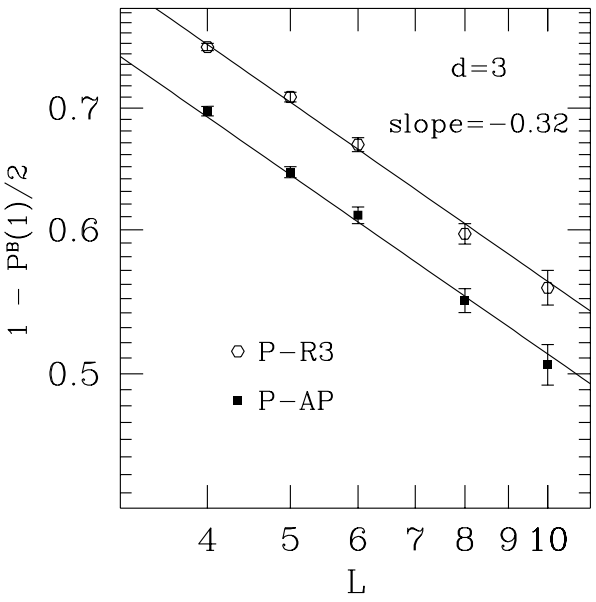

Fig. 3. Probability that the block configuration changes in 3-d for a range of sizes on a log-log plot.

structure. It seems likely either that the droplet theory is correct and a trivial $P(q)$ is only seen for larger sizes at finite-T, or, possibly, that there are other low energy excitations which are not seen by changing the boundary conditions and which could give a non-trivial $P(q)$ in the thermodynamic limit.

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