

Monte Carlo Study of the Order-Parameter Distribution in the Four-Dimensional Ising Spin Glass

J. D. Reger

Institut für Physik, Universität Mainz, D-6500 Mainz, West Germany

R. N. Bhatt

AT&T Bell Laboratories, Murray Hill, New Jersey 07974

A. P. Young

Physics Department, University of California, Santa Cruz, California 95064

(Received 30 November 1989)

We investigate the order-parameter distribution, $P(q)$, of the Ising spin glass with nearest-neighbor interactions in four dimensions using Monte Carlo simulations on lattices of linear dimension up to $L=6$. We find that, below the transition temperature, T_c , the weight at small q seems to saturate to a nonzero value as the size increases, similar to the infinite-range Sherrington-Kirkpatrick model. We discuss our results in the light of recent theoretical predictions for the nature of the spin-glass phase.

PACS numbers: 05.50.+q, 75.10.Nr, 75.30.-m

There is by now a fair amount of data supporting the existence of a nonzero transition temperature in three-dimensional spin glasses, at least for Ising or anisotropic systems.¹⁻⁸ The nature of the low-temperature, spin-glass phase remains unclear, however. For the infinite-range Sherrington-Kirkpatrick (SK) model,⁹ the prediction of the Parisi solution¹⁰⁻¹² is that there are distinct thermodynamic states, unrelated by symmetry, with free energies which differ from one another by an amount of order unity in the thermodynamic limit. Hence many states contribute to the statistical sum and should be incorporated into a description of the problem.

Of course the infinite-range interactions in the SK model are quite artificial so its properties are not necessarily similar to those of more realistic models with short-range interactions. In fact, recent ideas based on a droplet model¹³ and a related picture arising from domain-wall renormalization-group (DWRG) arguments,¹⁴ augmenting the ideals of McMillan,¹⁵ suggest that short-range systems are quite different in that they have only two thermodynamic states related by a global spin flip. With free or periodic boundary conditions, these states may be characterized by an order-parameter distribution, $P(q)$, defined in Eq. (1) below, which consists only of δ functions at the values $q = \pm q_{EA}$, where q_{EA} is nonzero below the transition. In contrast, the Parisi result for $P(q)$ in the SK model has, in addition to the δ functions, a continuous part extending to $q=0$, i.e., $P(0) \neq 0$ in the thermodynamic limit.¹¹ In this paper we use Monte Carlo simulations to investigate whether the Parisi result holds for the four-dimensional nearest-neighbor Ising spin glass or whether it instead follows the behavior predicted by the droplet-DWRG picture according to which $P(0) \rightarrow 0$ in the thermodynamic limit.

One convenient way to determine if many states contribute to the equilibrium statistical-mechanics description of the system is through the order-parameter distri-

bution $P(q)$ defined by

$$P(q) = \frac{1}{N} \sum_{\alpha, \beta} [P_{\alpha} P_{\beta} \delta(q - q^{\alpha\beta})]_{\text{av}}, \quad (1)$$

where α and β denote thermodynamic states and P_{α} is the Boltzmann statistical weight of this state; i.e.,

$$P_{\alpha} = \exp(-\beta F_{\alpha}) / Z, \quad (2)$$

with F_{α} the free energy of the state and Z the partition function defined by

$$Z = \sum_{\alpha} \exp(-\beta F_{\alpha}), \quad (3)$$

and $q^{\alpha\beta}$ is the "overlap" between states α and β ; i.e.,

$$q^{\alpha\beta} = \frac{1}{N} \sum_i m_i^{\alpha} m_i^{\beta}, \quad (4)$$

where m_i^{α} is the magnetization of site i when the system is constrained to be in the state α , and N is the number of spins. We use $\langle \dots \rangle$ to denote the statistical-mechanics average for a single sample, and $[\dots]_{\text{av}}$ to indicate the average over bond configurations.

If there is just a single thermodynamic state other than states related by a global symmetry, as happens in conventional systems, then $P(|q|)$ is just a single δ function at $q^{\alpha\alpha}$, which we shall call q_{EA} from now on, the "self-overlap" of the state with itself. Clearly in this limit it is unnecessary to describe the order parameter by a distribution and the single number q_{EA} suffices. However, the Parisi solution of the SK model predicts that, in addition to a δ -function peak at q_{EA} , there is a continuous part extending down to zero q (in zero field) coming from overlaps between different states. For any one bond configuration there are only a finite number of states contributing with significant statistical weight,¹² so $P(q)$ for one sample has only a finite set of δ functions of significant weight, but the position and weight of

these differ for different bond configurations so the bond average smears out all peaks into a continuum, except for the one at q_{EA} which is self-averaging.

It has been pointed out¹⁶ that the question of many thermodynamic states and the existence of a nontrivial $P(q)$ are not precisely the same and one can find examples, such as the random-field Ising model below T_c , for which $P(q)$ has just a single δ function but there are actually two inequivalent thermodynamic states. The one with higher free energy does not appear in $P(q)$ because it is higher by an amount of order $N^{1/2}$, and so does not contribute to the Boltzmann average. Nonetheless, we feel that $P(q)$ is an interesting quantity to calculate for the following reason. The question of the nature of the low-energy excited states in a spin glass and their correlation with the ground state is of paramount importance. If $P(q)$ has a tail down to $q=0$ below T_c , then there are clusters containing a finite fraction of the spins of the system which can be flipped with only a finite cost in energy. Thus $P(q)$ is a useful probe of low-energy excitations at large length scales. In addition, it is easy to calculate microscopically, as we shall see, without having to determine the different thermodynamic states for each bond configuration, which appears to be very difficult from simulations on small lattices.

We consider the standard model of Edwards and Anderson¹⁷ for which the Hamiltonian is

$$H = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j, \quad (5)$$

where S_i are Ising spins, $S_i = \pm 1$, on each site of a regular lattice and J_{ij} are independent random interactions with a symmetric distribution and are nonzero for nearest neighbors only. We use a Gaussian distribution and choose the temperature scale by setting the standard deviation to unity. Periodic boundary conditions are applied. We work on a four-dimensional simple cubic lattice, rather than in three dimensions, because $d=3$ is fairly close to the lower critical dimension so T_c in 3D is rather low, the relaxation times are very long, and, as a result, even locating the transition itself is difficult. Here we wish to investigate the region below T_c where the problem of long relaxation times is even more severe. In addition, the droplet-DWRG picture^{13,14} predicts that $P(0)$ vanishes with the linear lattice size, L , as $L^{-\theta}$, where the exponent θ vanishes at the lower critical dimension and so is expected to be much smaller in three than in four dimensions. Hence, even apart from equilibration problems, it would be very hard to see the vanishing of $P(0)$ on small lattices in three dimensions. In four dimensions, the transition temperature is higher and easy to locate by Monte Carlo simulations even with modest computer time.⁷ Hence a study below T_c is possible, though this now needs a substantial numerical effort because of the longer relaxation times. Furthermore, we expect that there is a lower critical dimension below which $P(0)$ vanishes, so that if we see a vanishing

of $P(0)$ in four dimensions, it should also vanish in 3D. Hence 4D results can tell us about the likely behavior in three dimensions.

To calculate $P(q)$ it is convenient to simulate two copies of the system with the same bonds but with no interaction between them. After equilibrating with t_0 sweeps the simulation proceeds for an additional t_M sweeps, where $t_M \geq t_0$, and $P(q)$ is calculated from

$$P(q) = \left[\frac{1}{t_M} \sum_{t=1}^{t_M} \delta[q - Q(t)] \right]_{av}, \quad (6)$$

where

$$Q(t) = \frac{1}{N} \sum_i S_i^{(1)}(t_0+t) S_i^{(2)}(t_0+t) \quad (7)$$

is the instantaneous mutual overlap between the spins in the two replicas. Here $S_i^{(1)}(t_0+t)$ denotes spin i in copy "1" after t_0+t sweeps. It is straightforward to show, using the result that connected correlation functions vanish at large separations in a single pure state, that this microscopic definition goes over to the macroscopic one, Eq. (1), in the thermodynamic limit. We used the same technique for equilibration described in our earlier work,^{3,7} namely, to compute $P(q)$ and its moments both by the overlap between two replicas at the same time, as in Eq. (6) above, and from the same replica at two different times. These two measurements give results which approach the equilibrium value from opposite sides.

The mean-field transition temperature is given by $T_c^{mf} = \sqrt{z}$, where z is the coordination number, which yields $T_c^{mf} \cong 2.83$ with $z=8$, which is appropriate here. This should be compared with the actual transition temperature, $T_c \cong 1.75$. Here we study temperatures from the vicinity of T_c down to $T=1.2$, which is the lowest temperature at which we can equilibrate a reasonable range of sizes. The sizes studied are $2 \leq L \leq 6$ and we generally took the measurement time t_M to be twice the equilibration time t_0 . For $L=6$ and $T=1.2$ we set $t_0=10^6$, while higher temperatures and smaller sizes needed shorter runs. The number of samples taken varied between 1000 and 4800 depending on size and temperature. It is essential to run a large number of samples because there are big sample-to-sample variations in $P(q)$, particularly in the small- q tail, which is perhaps not surprising because the sample-to-sample fluctuations are predicted to *diverge* for the SK model in the thermodynamic limit.¹² The computations were carried out on forty T414 Transputers operating in a parallel array with a performance of about 2×10^6 updates per second.

In Fig. 1 we show our results for $P(q)$ at $T=1.2$ for sizes $L=4$ and 6, obtained both by the overlap between the two replicas and by the two different times for one replica, as discussed above. The two methods give very close agreement for the whole distribution, which we

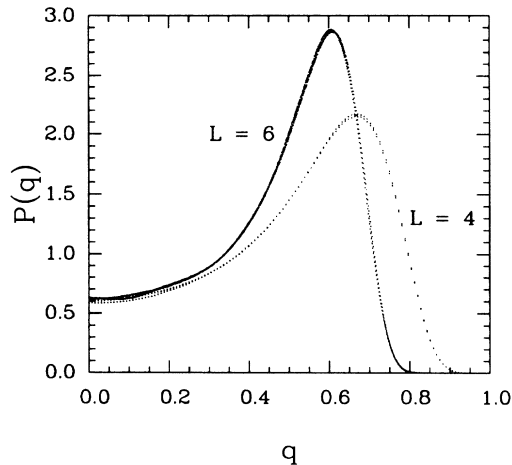


FIG. 1. A plot of $P(q)$ for $T=1.2$. Data are shown for two sizes: $L=4$ and 6. For each size there are *two* sets of points representing data calculated by the two methods described in the text, which are expected to agree with each other only when the system has reached equilibrium. Since they do agree with each other so well that the difference is barely resolvable in the figure, we infer that the system is well equilibrated.

take as evidence that the results represent thermal equilibrium. It will be seen that there is a tail in the distribution down to $q=0$ for both these sizes. Results for $P(0)$, averaged over a small range of q where the results appear to be independent of q , are plotted against L in Fig. 2 on a log-log plot for different sizes and temperatures. In the vicinity of T_c , $P(0)$ increases as a power of L , as expected from standard finite-size scaling theory which predicts $P(0) \sim L^{(d-2+\eta)/2}$ at the critical point. The solid line in Fig. 2 has a slope 0.75, which corresponds to $\eta = -0.5$, close to the earlier estimate⁷ of $\eta = -0.3 \pm 0.15$. At the lowest temperatures, however, $P(0)$ seems to be independent of size, as was found for the SK model but different from the droplet-DWRG prediction that $P(0) \sim L^{-0}$. Note the downward curvature of the results for $T=1.6$, i.e., just below T_c , which comes from the crossover between critical behavior (for small L and T close to T_c) and the low-temperature region (for larger sizes and lower temperatures). However, the curvature for temperatures $T=1.2$ and 1.4 is *opposite* to that for $T=1.6$ so we do not feel that the size independence of the results at lower temperatures can be explained by the proximity of the critical region. Hence we believe that our results at the lower temperatures are representative of the ordered state unless there are *two* crossovers in the low- T phase.

In order to see if the apparent size independence of the results is significant, we need to estimate roughly the expected value of θ . McMillan¹ finds that $\theta = -0.31$ in $d=2$ and 0.17 in $d=3$, while the corresponding values given by Bray and Moore² are similar, namely, -0.29 and 0.2. Estimating θ in $d=4$ by linearly extrapolat-

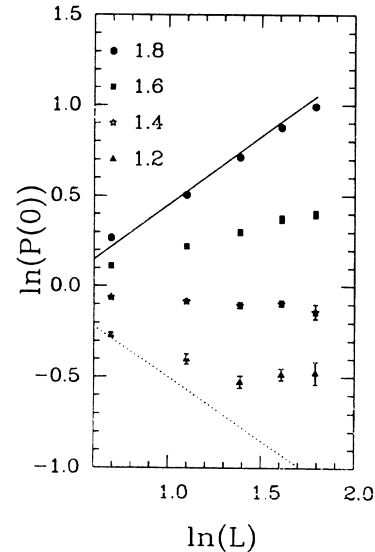


FIG. 2. A plot of $\ln(P(0))$ vs $\ln(L)$ for sizes L between 2 and 6 and different temperatures, as indicated. The behavior at $T_c = 1.75 \pm 0.05$ is expected to be a straight line with a slope $1 + 0.5\eta$ (in four dimensions) as discussed in the text. The solid line has a slope 0.75 which corresponds to $\eta = -0.5$, which is to be compared with the earlier estimate (Ref. 7) of -0.30 ± 0.15 . According to the droplet-DWRG theory, the behavior below T_c should be a straight line with a slope $-\theta$, where θ is an exponent which controls the (nontrivial) behavior in the low- T phase. The dotted line has a slope -0.7 , which is a rough estimate of $-\theta$, as described in the text. The data at low temperatures are clearly decreasing much slower than this and are, indeed, essentially size independent except for the smallest sizes.

ing these results or from the plausible formula $\theta \cong \frac{1}{2} \times (d - d_l)$, where the lower critical dimension, d_l , is roughly equal to 2.6, one gets $\theta \sim 0.7$. Figure 2 shows a dotted line with a slope -0.7 which is clearly inconsistent with the data at low T . Over this range of sizes the data rule out a θ larger than about 0.2, which is roughly the value found in $d=3$.

To conclude, we have found that the order-parameter distribution in a short-range Ising spin glass in four dimensions looks surprisingly like what one obtains for the SK model; namely, there is a finite weight at $q=0$. This means that there are large clusters making up a finite fraction of the total number of spins which can be flipped with only a finite cost in energy. This appears to be in contradiction to the droplet-DWRG theories which predict that the energy to flip a cluster of linear dimension L varies as L^θ , which diverges as $L \rightarrow \infty$, unless $\theta \lesssim 0.2$ in 4D. Of course, we cannot definitely rule out the possibility that the sizes studied are too small, and that there may be a crossover to different behavior at larger sizes. It is unclear to us, however, why there should be a large crossover length scale. Another possibility is that, while the droplet-DWRG theories describe the majority of

cluster excitations correctly, there may be more clusters which can be flipped with a low-energy cost than would be naively expected. Whether, *in the thermodynamic limit*, some large clusters can be flipped with zero-energy cost cannot be unambiguously determined from results on finite lattices. However, some results in this direction have recently been obtained by Georges, Mezard, and Yedidia,¹⁸ who find that $P(0)$ of an infinite-range model with finite coordination number z *increases* within a $1/z$ expansion. To conclude, our results show that there is some new and unexpected physics happening in the low-temperature state of spin glasses: either there is a new length scale or the droplet picture is missing some important ingredient.

It is a pleasure to thank Josh Deutsch and David Huse for many helpful discussions. The work of J.D.R. and A.P.Y. was supported in part by NSF Grant No. DMR 87-21673. We are grateful to the INMOS Corporation for partial support of the Transputer project at the University of California, Santa Cruz.

¹W. L. McMillan, Phys. Rev. B **30**, 476 (1984).

²A. J. Bray and M. A. Moore, J. Phys. C **17**, L463 (1984).

³R. N. Bhatt and A. P. Young, Phys. Rev. Lett. **54**, 924 (1985).

⁴A. T. Ogielski and I. Morgenstern, Phys. Rev. Lett. **54**, 928 (1985).

⁵A. T. Ogielski, Phys. Rev. B **32**, 7384 (1985).

⁶R. R. P. Singh and S. Chakravarty, Phys. Rev. Lett. **57**, 245 (1986).

⁷R. N. Bhatt and A. P. Young, Phys. Rev. B **37**, 5606 (1988).

⁸J. D. Reger and A. Zippelius, Phys. Rev. Lett. **57**, 3225 (1986).

⁹D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1972 (1975).

¹⁰G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979); J. Phys. A **13**, 1101 (1980); **13**, 1887 (1980); **13**, L115 (1980).

¹¹G. Parisi, Phys. Rev. Lett. **50**, 1946 (1983); A. Houghton, S. Jain, and A. P. Young, J. Phys. C **16**, L375 (1983).

¹²M. Mézard, G. Parisi, N. Sourlas, G. Toulouse, and M. Virasoro, Phys. Rev. Lett. **52**, 1156 (1984); J. Phys. (Paris) **45**, 843 (1984).

¹³D. S. Fisher and D. A. Huse, Phys. Rev. Lett. **56**, 1601 (1986); J. Phys. A **20**, L1005 (1988); Phys. Rev. B **38**, 386 (1988).

¹⁴A. J. Bray and M. A. Moore, in *Heidelberg Colloquium on Glassy Dynamics*, edited by J. L. Van Hemmen and I. Morgenstern, Lecture Notes in Physics Vol. 275 (Springer-Verlag, Heidelberg, 1987), p. 121; A. J. Bray, Comments Condens. Matter Phys. **14**, 21 (1988).

¹⁵W. L. McMillan, J. Phys. C **17**, 3179 (1984).

¹⁶D. S. Fisher and D. A. Huse, J. Phys. A **20**, L997 (1988).

¹⁷S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

¹⁸A. Georges, M. Mézard, and J. Yedidia, in Proceedings of STATPHYS 17, Rio de Janeiro, 1989 (to be published); (to be published).