

## Susceptibility of Two-, Three-, and Four-Dimensional Spin Glasses in a Magnetic Field

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(Received 10 June 1991)

Through Monte Carlo simulations we have studied the spin-glass susceptibility of two-, three-, and four-dimensional spin glasses in a magnetic field. We find that in four dimensions curves of constant susceptibility curve upward as the temperature is lowered, in a manner indicative of the presence of a de Almeida-Thouless (AT) line of phase transitions. In three dimensions the curves of constant susceptibility also appear to curve up, although not as sharply. In contrast, in two dimensions we do not see indications of an AT line.

PACS numbers: 75.10.Nr, 75.40.Mg

The nature of the low-temperature phase of finite-dimensional spin glasses has been a subject of some controversy recently. There are basically two differing pictures of the low-temperature state, which we will call the mean-field picture and the droplet picture: The mean-field picture is based on the replica-symmetry-breaking solution of Parisi [1] for the infinite-range Sherrington-Kirkpatrick (SK) model [2]. This solution has many novel features, one of which is that at low temperatures there are many thermodynamic states which are unrelated by symmetry. The other picture is the droplet model of Fisher and Huse [3], which is related to previous work by McMillan [4] and Bray and Moore [5]. In the droplet picture, there are only two thermodynamic states related by a global spin flip, and the important excitations at low temperatures are "droplets" of overturned spins.

It has proven difficult to establish or disprove either of these pictures. One would like to examine some measurable quantity which behaves qualitatively differently in the two models. One such quantity is the distribution of overlaps between replicas of the same system. The overlap between two replicas,  $\alpha$  and  $\beta$ , is given by

$$q_{\alpha\beta} = \frac{1}{N} \sum_i S_i^\alpha S_i^\beta. \quad (1)$$

The probability distribution of the overlaps,  $P(q)$ , is then defined to be

$$P(q) = [\langle \delta(q - q_{\alpha\beta}) \rangle], \quad (2)$$

where  $\langle \dots \rangle$  denotes a thermal average, and  $[\dots]$  denotes an average over disorder. In the Parisi solution,  $P(q)$  at low temperatures consists of two delta functions which are connected by a continuous background. In the droplet picture, since there are only two thermodynamic states,  $P(q)$  consists only of the two delta functions.

Several groups have recently looked at this quantity. Reger, Bhatt, and Young [6] have performed Monte Carlo simulations to determine  $P(q)$  in the four-dimensional spin glass, for systems of sizes up to  $6^4$ . Their results indicate that  $P(0)$  is independent of system size, although they are limited to rather small sizes. Recent  $1/d$  expansions [7] have shown that certain of the predictions of the mean-field picture are enhanced as  $d$  decreases from

infinity, but this does not directly address the question of low-dimensional spin glasses. Another recent Monte Carlo simulation [8] has looked at  $P(q)$  and other quantities and has claimed to support the mean-field picture, but does not clearly distinguish the behavior from the droplet picture [9].

A second qualitative difference between the two pictures is the behavior in a magnetic field. The SK model has a phase transition in a magnetic field at the de Almeida-Thouless (AT) line [10]. In the droplet picture, Imry-Ma arguments [3] indicate that a finite-dimensional spin glass will not have a transition in a field, since a field chooses orientations for the droplets, destroying the long-range order.

In a recent paper Singh and Huse [11] have argued that a way to distinguish between the droplet and the mean-field pictures is to look at the spin-glass susceptibility [12] in a magnetic field. The spin-glass susceptibility is defined to be

$$\chi_{SG} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i,j} [(\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle)^2]. \quad (3)$$

If there is an AT line, then curves of constant susceptibility in the  $H$ - $T$  plane must bend up as the temperature is lowered, remaining above the AT line at which the susceptibility diverges. On the other hand, in the droplet picture the susceptibility vanishes [13] for  $T=0$  and  $H \neq 0$  and is infinite for  $0 < T \leq T_c$  and  $H=0$ , and therefore curves of constant susceptibility must go to  $H=0$  as  $T \rightarrow 0$ . In one and two dimensions (where  $T_c=0$ ) they found that the curve of  $\chi_{SG}=1$  went toward zero field as  $T \rightarrow 0$ . In three dimensions the results were ambiguous, although the Padé approximants of high-temperature expansions behaved qualitatively differently than in two dimensions.

In this paper we have extended the work of Singh and Huse by performing Monte Carlo simulations to look at the susceptibility in two-, three-, and four-dimensional spin glasses. An advantage of looking at  $\chi_{SG}$  in the high-temperature phase is that one avoids the problems of trying to equilibrate the spin glass at low temperatures, where the relaxation times are very long. Furthermore, by looking at contours of constant  $\chi_{SG}$ , that is by raising

the field if  $\chi_{SG}$  is diverging at low temperatures, one reduces the correlation length, again leading to faster equilibration.

The Hamiltonian of our system is the usual Ising spin-glass Hamiltonian

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j + H \sum_i S_i, \quad (4)$$

where  $S_i = \pm 1$ , the double sum is over nearest-neighbor spins, and the  $J_{ij}$  are independent random variables. We have mainly looked at the  $\pm J$  distribution,  $P(J) = \frac{1}{2} [\delta(J-1) + \delta(J+1)]$ , but have also considered a Gaussian distribution  $P(J) = (1/\sqrt{2\pi}) \exp(-J^2/2)$ , where the results are similar. The sites are on a hypercubic lattice of linear dimension  $L$  with periodic boundary conditions.

The spin-glass susceptibility, Eq. (3), was determined by numerically computing the overlaps between three replicas [11]:

$$\chi_{SG} = \lim_{N \rightarrow \infty} [N(\langle q_{12}^2 \rangle - 2\langle q_{12}q_{13} \rangle + \langle q_{12} \rangle^2)], \quad (5)$$

where  $q_{\alpha\beta}$  is defined above in (1).

We simulated systems of different sizes to check for finite-size effects. In the two-dimensional simulations we studied systems of size  $L$  between 32 and 64, in three dimensions, between 8 and 16, and in four dimensions, between 6 and 12. We checked that the values of  $\chi_{SG}$  did not depend on system size for our biggest systems. We averaged over between 25 and 500 samples for each data point, depending on temperature and size.

In the simulations we repeatedly doubled the number of Monte Carlo steps until we were satisfied that the system had equilibrated. We have used two methods to check for equilibration of the systems. One is to monitor the variance of the susceptibility, which we determine from the spread of values computed from different samples. The variance is caused by thermal fluctuations, by changes in the values of  $\chi_{SG}$  as the system equilibrates, and by the spread in  $\chi_{SG}$  due to the different bond configurations in different samples. As the number of Monte Carlo steps is increased, the first two contributions to the variance vanish, and the variance reaches a constant value. This occurs at a fairly well-defined number of Monte Carlo steps, and we have taken this to indicate that the system has equilibrated. Another way to monitor equilibration, following an idea of Bhatt and Young [14], is to compare overlaps both between different replicas and between the same replica at different times. The two measurements underestimate and overestimate correlations and converge to the same value as the number of Monte Carlo steps is increased. We found that the two ways of checking for equilibration agreed fairly closely. We also verified that the equilibration times are indeed much shorter at high fields than at lower fields. For example, at a temperature of 1.25 and for  $H=1.45$  it took about 500 Monte Carlo steps per spin to generate an un-

correlated configuration, whereas at a lower field  $H=1.0$  it took about 4000 Monte Carlo steps.

Our main results are presented in Fig. 1, which shows the contours of  $\chi_{SG}=1$  from our two-, three-, and four-dimensional simulations, as well as for the SK model and for the one-dimensional spin glass. The error bars are 1 standard deviation. For all the systems the temperature and magnetic field are divided by the appropriate mean-field transition temperature  $T_c^{MF}$ , which in the finite-dimensional case is equal to  $\sqrt{Z}$ , where  $Z$  is the number of near neighbors. In these units, the contour  $\chi_{SG}=1$  starts off at  $1/\sqrt{2}$  for all the models at high temperature, and initially decreases as the temperature is lowered.

The two-dimensional spin glass in zero field has a zero-temperature phase transition. In a field the curve of  $\chi_{SG}=1$  decreases in  $H$  as the temperature is lowered, for the temperatures which we have simulated.

In the three-dimensional case the contour  $\chi_{SG}=1$  appears to have a broad minimum at a temperature somewhat below the mean-field transition temperature and then to turn up slightly. The actual transition temperature for the three-dimensional spin glass has been estimated in Ref. [15] to be 1.17, so  $T_c^{3D}/T_c^{MF} \approx 0.48$ . At a field of 0.6, the transition temperature  $T_c(H)$  for the SK model has been reduced by a factor of about 2 from the zero-field value. It seems compatible with the data that there is a transition in a field for the three-dimensional model, and that  $T_c$  has been reduced by roughly the same factor as in the SK model. In four dimensions it is possible to carry simulations out at a lower reduced temperature, due to the higher transition temperature. The transition temperature of the four-dimensional

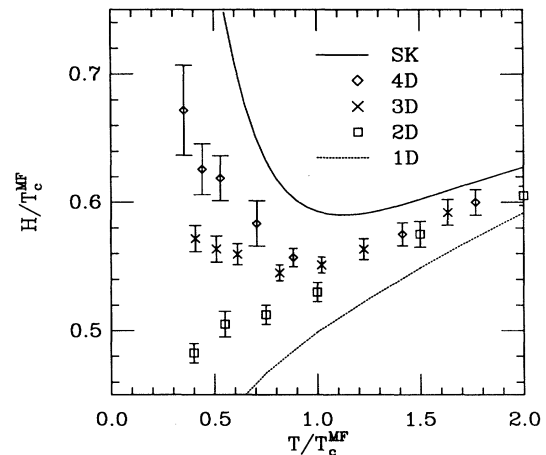


FIG. 1. Contours of  $\chi_{SG}=1$  for the SK model and for one-, two-, three-, and four-dimensional Ising spin glasses. Note that the range of  $H$  shown is rather small. The two-, three-, and four-dimensional data are from Monte Carlo simulations; the error bars are 1 standard deviation. The one-dimensional data are from Ref. [11].

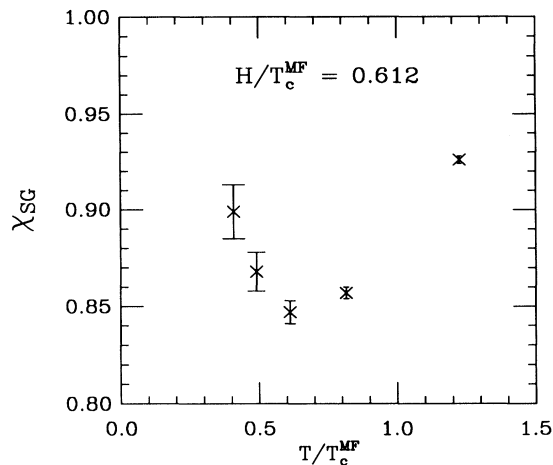


FIG. 2. The spin-glass susceptibility for the three-dimensional spin glass at a field of  $H=1.5$  ( $H/T_c^{\text{MF}} \approx 0.612$ ). The error bars are 1 standard deviation.

$\pm J$  spin glass has been estimated [16] to be about 2.0, which gives  $T_c^{4\text{D}}/T_c^{\text{MF}} \approx 0.71$ . In this case the contour of  $\chi_{\text{SG}}=1$  has a definite upturn, and again the upturn is consistent with scaling the mean-field AT line.

A slightly different way to look at the susceptibility is to look at  $\chi_{\text{SG}}$  at fixed  $H$  as a function of temperature. This is numerically simpler to perform, since one does not have to search parameters to determine where  $\chi_{\text{SG}}=1$ . In Fig. 2 we show  $\chi_{\text{SG}}$  as a function of temperature in three dimensions for  $H=1.5$ , or  $H/T_c^{\text{MF}} \approx 0.61$ . As in Fig. 1, the susceptibility is turning up in three dimensions, compatible with a divergence.

At the higher temperatures which we have simulated, the location of the contour  $\chi_{\text{SG}}=1$  becomes difficult to determine, since  $\chi_{\text{SG}}$  goes to 1 as  $T \rightarrow \infty$  for all  $H$ . We have therefore compared, in Fig. 3, our Monte Carlo data with high-temperature series expansions [11]. The contours from the series expansions are derived from particular Padé approximants. For each series, the different approximants agree with each other above  $T/T_c^{\text{MF}} \approx 1$ . Above this temperature, the Monte Carlo data also agree with the series expansions.

We have considered the possibility that even in the absence of a phase transition in nonzero field, the contours of constant  $\chi_{\text{SG}}$  might be “repelled” from the area around a finite-temperature zero-field transition, giving a spurious upturn. As a test of this possibility we have investigated the spin-glass-type susceptibility [Eq. (3)] of the three-dimensional Ising ferromagnet in a magnetic field where there is no phase transition. At high temperature the contour  $\chi_{\text{SG}}=1$  for the ferromagnet goes to a field of  $\sqrt{3}$ . As  $T \rightarrow \infty$ , all contours of  $\chi_{\text{SG}} > 1$  bend down to the  $H=0$  axis, and all contours with  $\chi_{\text{SG}} < 1$  diverge to high field. None of the contours with  $\chi_{\text{SG}} \leq 1$  show any signs of nonmonotonicity as a consequence of being near a crit-

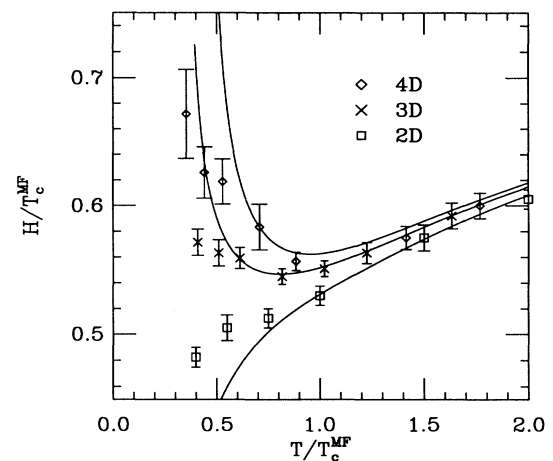


FIG. 3. Contours of  $\chi_{\text{SG}}=1$  for two-, three-, and four-dimensional spin glasses compared to series expansions from Ref. [11].

ical point.

Since we have mainly simulated the  $\pm J$  model, the degeneracy of the ground state could also lead to upturns in contours of constant  $\chi_{\text{SG}}$ . We have checked this by studying the one-dimensional  $\pm J$  spin glass. Above temperatures of about 0.15, the contour  $\chi_{\text{SG}}=1$  decreases smoothly as the temperature is lowered. (Below this temperature the effects of the degeneracies lead to increases in the susceptibility near fields of the form  $2/n$  for integer  $n$ .) Since all of our simulations are performed at temperatures well above 0.15, and since we expect that the effect of degenerate ground states will be weaker in higher dimensions, we do not think that the effects of ground-state degeneracy could cause the upturns observed in higher dimensions.

In conclusion, we have simulated the two-, three-, and four-dimensional Ising spin glass in a magnetic field and computed the contours of constant susceptibility  $\chi_{\text{SG}}=1$ . These contours provide a means of distinguishing between the mean-field and droplet pictures, as they give qualitatively different predictions as to the behavior of  $\chi_{\text{SG}}$  in a magnetic field. In two dimensions the contour drops to zero as the temperature is lowered, in agreement with the droplet picture. In contrast, the contours show a mild upturn in three dimensions and a sharper upturn in four dimensions. Our data strongly suggest the presence of a de Almeida-Thouless line of phase transitions in three and especially in four dimensions.

We would like to thank R. Bhatt, D. Huse, and R. Singh for many useful discussions. One of us (R.E.H.) was supported by the Deutsche Forschungsgemeinschaft.

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