Absence of an Almeida-Thouless Line in Three-Dimensional Spin Glasses

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We present results of Monte Carlo simulations of the three-dimensional Edwards-Anderson Ising spin glass in the presence of a (random) field. A finite-size scaling analysis of the correlation length shows no indication of a transition, in contrast with the zero-field case. This suggests that there is no Almeida-Thouless line for short-range Ising spin glasses.

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Since the work of Ballesteros *et al.* [1], there has been little doubt that a finite-temperature transition occurs in three-dimensional spin glasses [2]. However, the behavior of a spin glass in a magnetic field is less well understood. In mean-field theory [5], which is taken to be the solution of the infinite-range Sherrington-Kirkpatrick (SK) model [6], an Ising system [3] has a line of transitions in a magnetic field [7], known as the Almeida-Thouless (AT) line. This line separates the paramagnetic phase at high temperatures and fields from the spin-glass phase at lower temperatures and fields. Although there is *no* change of symmetry at this transition, the relaxation time diverges (and for short-range systems so does the correlation length as we shall see). In the spin-glass phase below the AT line, there is "replica symmetry breaking" in which the free energy landscape breaks up into different regions separated by infinite barriers, and the distribution of relaxation times extends to infinity.

It is important to know whether the AT line also occurs in more realistic short-range models, since the two main scenarios that have been proposed for the spin-glass state differ over this issue. In the "droplet picture" [8–11] there is *no* AT line in *any* finite-dimensional spin glass. By contrast, the "replica symmetry breaking" (RSB) picture [12–15] postulates that the behavior of short-range systems is quite similar to that of the infinite-range SK model which *does* have an AT line as just mentioned. Both scenarios are illustrated in Fig. 1.

Experimentally, it has proved much more difficult to verify the transition in a field than for the zero-field transition. For the latter, the divergence of the nonlinear susceptibility gives clear experimental evidence of a transition, but unfortunately this divergence no longer occurs in a magnetic field. Experiments have therefore looked for a divergent relaxation time, and a careful analysis by Mattsson *et al.* [16] finds that this does *not occur* in a field. However, not all experimental work has come to the same conclusion [17].

In simulations, it is most desirable to perform finite-size scaling on *dimensionless* quantities for reasons that we will discuss below. One such quantity, the Binder ratio, gave some evidence for the zero-field transition [18,19]. However, the Binder ratio turns out to be very poorly behaved in a field [20] in short-range systems, while for the SK model it does indicate a possible transition [21], although not with any great precision. Results of out of equilibrium simulations on large lattices in four dimensions [22] were interpreted as evidence for RSB, although it is not completely clear that the true equilibrium behavior is probed by this procedure [23]. By contrast, simulations [24] corresponding to experimental protocols in (nonequilibrium) aging experiments have been analyzed in terms of a "dynamical crossover" consistent with the droplet picture.

Houdayer and Martin [25] carried out interesting calculations at $T = 0$ to determine $H_{\rm AT}$, the critical field at $T = 0$, see Fig. 1, for a simple cubic lattice in three dimensions. Their results indicated that $H_{\rm AT} = 0$, i.e., there is no AT line, although a subsequent zero-temperature study by Krzakala *et al.* [26] found some evidence of a critical field for $H \simeq 0.65$, which is much less than the "mean-field" value for this lattice [27] of around 1.86. However, Krzakala *et al.* [26] could not exclude the possibility that the critical field is zero.

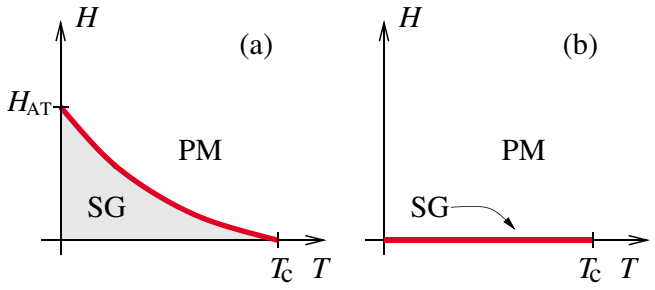

FIG. 1 (color online). (a) H–T phase diagram expected according to RSB for the short-range case. For $T < T_c(H)$ there is a spin-glass phase (SG), whereas for $T > T_c(H)$ the system is in the paramagnetic (PM) state. The value of the critical field at $T = 0$ is called $H_{\rm AT}$. (b) H–T phase diagram following the predictions from the droplet picture. A spin-glass phase exists only for $H = 0$.

As noted above, the (dimensionless) Binder ratio has provided some evidence for zero-field transition at finite T. However, a *much sharper* signature of the zero-field transition in three dimensions is provided by the correlation length [1] from which a dimensionless quantity is formed by dividing by the system size L. This approach should also provide evidence *from equilibrium calculations* for a transition in a field, if one occurs, and in this Letter we use it to determine whether there is an AT line in a three-dimensional Ising spin glass. Our conclusion will be that there is not, at least down to fields significantly smaller than the value of 0.65 suggested by Krzakala *et al.* [26].

The Hamiltonian we study is given by

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

in which the Ising spins $S_i = \pm 1$ lie on the sites of a simple cubic lattice of size $N = L^3$ ($4 \le L \le 12$) with periodic boundary conditions, and the nearest neighbor interactions J_{ij} are independent random variables with a Gaussian distribution with mean zero and standard deviation unity. At each site there is a field h_i which, like the bonds, *is randomly drawn from a Gaussian distribution*, and whose mean and standard deviation are given by

$$[h_i]_{\rm av} = 0, \qquad [h_i^2]_{\rm av}^{1/2} = H_r, \tag{2}$$

where $[\cdots]_{\rm av}$ denotes an average over the disorder. For a symmetric distribution of bonds, the *sign* of h_i can be "gauged away" so a uniform field is completely equivalent to a bimodal distribution of fields with $h_i = \pm H$. Our choice of a Gaussian distribution, which still has an AT line in mean-field theory, also puts disorder into the *magnitude* of the h_i. We use a Gaussian distribution, rather than a uniform field, in order to apply a very helpful test for equilibration, discussed below.

To determine the correlation length we calculate the wave vector–dependent spin-glass susceptibility which, for nonzero fields, is defined by

$$\chi_{\rm SG}(\mathbf{k}) = \frac{1}{N}\sum_{i,j}[(\langle S_i S_j\rangle_T - \langle S_i\rangle_T\langle S_j\rangle_T)^2]_{\rm av} e^{i\mathbf{k}\cdot(\mathbf{R}_i - \mathbf{R}_j)}, \tag{3}$$

where $\langle\cdots\rangle_T$ denotes a thermal average. As in earlier work [1,28] the correlation length of the finite system is defined to be

$$\xi_L = \frac{1}{2\sin(k_{\rm min}/2)}\left[\frac{\chi_{SG}(0)}{\chi_{SG}(\mathbf{k}_{\rm min})} - 1\right]^{1/2}, \tag{4}$$

where $\mathbf{k}_{\rm min} = (2\pi/L, 0, 0)$ is the smallest nonzero wave vector.

Now ξ_L satisfies the finite-size scaling form

$$\frac{\xi_L}{L} = \widetilde{X}(L^{1/\nu}[T - T_c(H_{\rm r})]), \tag{5}$$

where ν is the correlation length exponent and $T_c(H_r)$ is the transition temperature for a field strength H_r. Note that there is no power of L multiplying the scaling function $\widetilde{X}$, as there would be for a quantity with dimensions. This greatly simplifies the analysis since the critical point can be seen by inspection as the temperature where data for different sizes intersect.

On the AT line, $T = T_c(H_r)$, the "connected correlation function" $\langle S_i S_j\rangle_T - \langle S_i\rangle_T\langle S_j\rangle_T$ becomes long range and so, for an infinite system, the correlation length and $\chi_{\rm SG}(0)$ diverge while for a finite system, ξ_L/L is independent of L. Below the AT line, according to RSB the correlation functions no longer have a "clustering property," i.e., $\lim_{|\mathbf{R}_i - \mathbf{R}_j|\to\infty}(\langle S_i S_j\rangle_T - \langle S_i\rangle_T\langle S_j\rangle_T) \neq 0$, so $\chi_{\rm SG}(0) \propto L^d$ and ξ_L/L increases with L. Hence, according to RSB, the behavior of ξ_L/L should be *qualitatively the same* as at the zero-field transition, namely, it decreases with increasing L above the transition, is independent of L at the transition, and increases with increasing L below the transition.

We use parallel tempering to speed up the simulations but unfortunately it is less efficient in a field than in zero field [29,30], because "chaos" with respect to a field is stronger than chaos with respect to temperature. As a result, the computer time increases very rapidly with increasing L, so it is unlikely that we will be able to study larger sizes in the near future without a better algorithm. In order to compute the products of up to four thermal averages in Eq. (3) without bias we simulate four copies (replicas) of the system with the same bonds and fields at each temperature.

Parameters of the simulation are shown in Table I. Most of our work is for $H_r = 0.3$ since this is smaller than the predicted [26,31] zero-temperature value of $H_{\rm AT} = 0.65$, but is not so small that the results would be seriously influenced by the zero-field transition. The lowest temperature is 0.23 well below the zero-field transition temperature which is about [32] 0.95.

For a Gaussian distributions of bonds *and* fields, the expression for the average energy, $U = [\langle\mathcal{H}\rangle_T]_{\rm av}$, can be integrated by parts with respect to the disorder distribu-

TABLE I. Parameters of the simulations for $H_r = 0.3$. $N_{\rm samp}$ is the number of samples, $N_{\rm sweep}$ is the total number of Monte Carlo sweeps for each of the $4N_T$ replicas for a single sample, $T_{\rm min}$ is the lowest temperature simulated, and N_T is the number of temperatures used in the parallel tempering method. For other values of H_r, we used the same parameters but only simulated $L = 4$, 6, and 8.

L	$N_{\rm samp}$	$N_{\rm sweep}$	$T_{\rm min}$	N_T
4	5000	6.0×10^4	0.23	18
6	5319	6.0×10^5	0.23	18
8	5000	6.0×10^5	0.23	18
12	304	6.0×10^7	0.23	18

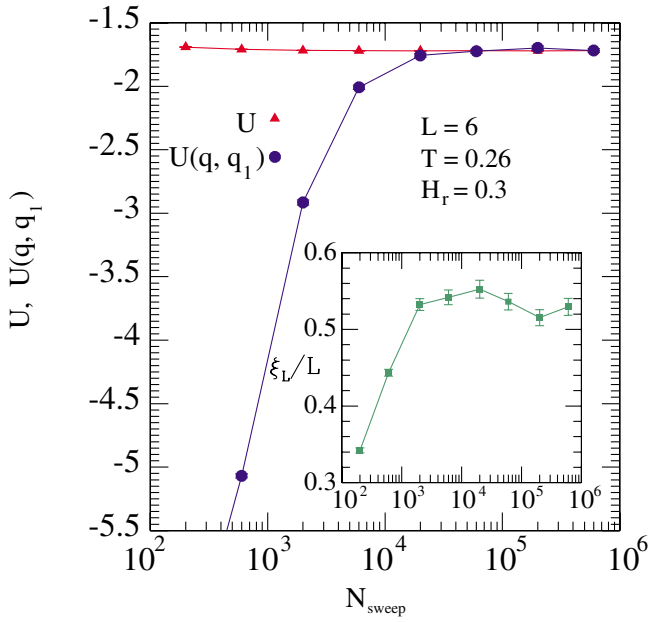

FIG. 2 (color online). An equilibration plot for $L = 6, H_r = 0.3, T = 0.3$ showing that the data for the average energy U and the quantity $U(q, q_l)$, defined in Eq. (7), approach their common equilibrium value from opposite directions as the number of Monte Carlo sweeps N_{sweep} increases. The inset shows data for ξ_L/L indicating that it has equilibrated when U and $U(q, q_l)$ have become equal.

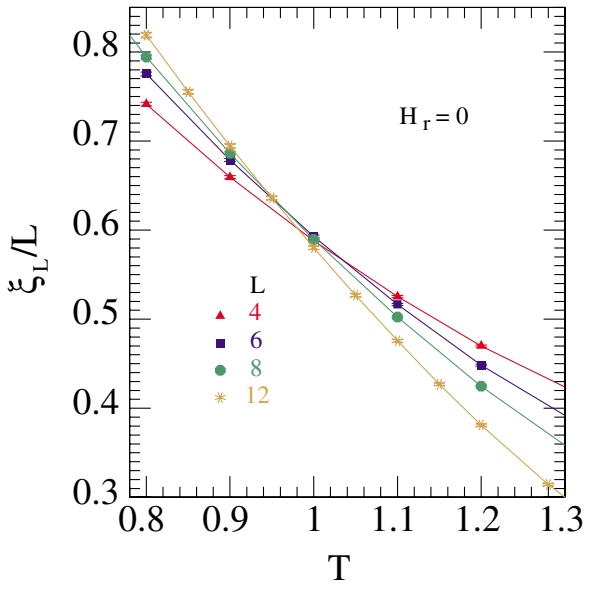

FIG. 3 (color online). Data for ξ_L/L for $H_r = 0$ for different sizes. Note that there are clear intersections at roughly a common temperature, with the data splaying out at lower temperatures. The temperature of the intersections is the zero-field transition temperature, marked T_c in Fig. 1. In this data, 5000 samples are used for the disorder average in each system size.

tion, with the result

$$U = U(q, q_l), \tag{6}$$

where

$$U(q, q_l) = \frac{z}{2}\frac{q_l - 1}{T} + \frac{q - 1}{T}H_r^2, \tag{7}$$

where z ($= 6$ here) is the number of neighbors, q is the spin overlap given by

$$q = \frac{1}{N}\sum_{i=1}^{N}[\langle S_i^{(1)} S_i^{(2)}\rangle_T]_{\text{av}}, \tag{8}$$

and q_l is the "link overlap" given by

$$q_l = \frac{2}{z}\frac{1}{N}\sum_{\langle i,j\rangle}[\langle S_i^{(1)} S_j^{(1)} S_i^{(2)} S_j^{(2)}\rangle_T]_{\text{av}}. \tag{9}$$

In Eqs. (8) and (9), "(1)" and "(2)" refer to two copies of the system with the same bonds and fields. Because U will *decrease* as the system approaches equilibrium and q and q_l will *increase* (since we initialize the spins in the two copies in random configurations), U and $U(q, q_l)$ approach their common equilibrium value *from opposite directions* and so Eqs. (6) and (7) can be used as an equilibration test. This is a generalization to finite fields of a test used previously [33]. Figure 2 shows that these expectations are born out. We accept a set of runs as being equilibrated if $U = U(q, q_l)$ within the error bars. The inset to the figure shows that ξ_L/L has equilibrated when U and $U(q, q_l)$ have become equal.

It is useful to compare results in a field with those at the zero-field transition. Hence in Fig. 3 we show data for ξ_L/L for $H_r = 0$ for sizes up to $L = 12$. For these results we set $\langle S_i\rangle_T = 0$ in Eq. (3). There are clear intersections, with data splaying out at lower temperatures, indicating a transition at $T = T_c \equiv T_c(H_r = 0)$, in the region 0.95–1.00, in agreement with Marinari *et al.* [32].

However, the analogous results for $H_r = 0.3$ shown in Fig. 4 have no sign of an intersection for sizes up to $L = 12$ at temperatures down to $T = 0.23$, which is considerably below the zero-field transition temperature of about 0.95. This provides quite strong evidence that there is no AT line, except possibly for fields less than 0.3. In order to test this possibility we have also performed simulations down to $H_r = 0.05$ (for $4 \le L \le 8$), and again found no intersections. We have also performed simulations in a uniform field, finding that data are very similar to those for the random fields, and have no intersection down to the lowest field studied, $H = 0.1$.

To go to low fields without passing too close to the zero-field transition, we also tried a diagonal "cut" in the H_r–T plane with H_r/T kept fixed at the constant value of 0.7. However, the equilibration problems were even more severe than for H_r fixed at 0.3, and so we have not been able to get useful data for this case.

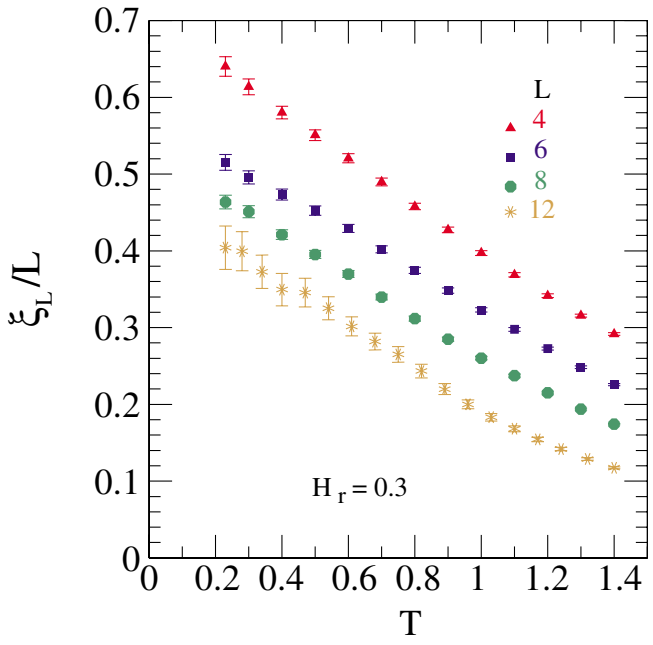

FIG. 4 (color online). Data for ξ_L/L for $H_r = 0.3$ for different sizes. Note that in contrast to the zero-field data in Fig. 3 there is no sign of intersections down to the lowest temperature $T = 0.23$.

To conclude, our finite-temperature Monte Carlo simulations provide *simple, direct* evidence from *equilibrium* calculations that there is no AT line in three dimensions. Of course, the numerical data cannot rule out a transition at exceptionally small fields, or the possibility of a crossover at much larger sizes to different behavior, but we see no particular reason for these scenarios to occur.

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