Universal dynamic scaling in three-dimensional Ising spin glasses

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We use a nonequilibrium Monte Carlo simulation method and dynamical scaling to study the phase transition in three-dimensional Ising spin glasses. The transition point is repeatedly approached at finite velocity v (temperature change versus time) in Monte Carlo simulations starting at a high temperature. This approach has the advantage that the equilibrium limit does not have to be strictly reached for a scaling analysis to yield critical exponents. For the dynamic exponent we obtain $z = 5.85(9)$ for bimodal couplings distribution and $z = 6.00(10)$ for the Gaussian case. Assuming universal dynamic scaling, we combine the two results and obtain $z = 5.93 \pm 0.07$ for generic 3D Ising spin glasses.

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I. INTRODUCTION

Understanding spin glasses analytically has proved difficult, and there are only very few exact results beyond Parisi's solution [1–3] of the infinite-range Sherrington-Kirkpatrick model [4]. Furthermore, Monte Carlo (MC) simulations in three dimensions proved challenging because $d = 3$ turns out to be close to the lower critical dimension d_l, below which fluctuations destroy the transition. For Ising spins, which we study here, $d_l \simeq 2.5$ [5]. Nonetheless, there has been substantial progress in recent years, aided by increased computer power, the technique of parallel tempering [6] (exchange MC) to speed up equilibration and reduce autocorrelations, and better methods of performing finite-size scaling. In particular, Hasenbusch *et al.* [7] extracted not only the leading singular behavior at the transition but also the dominant correction to scaling. This gives confidence that the asymptotic critical region has been reached (which it had not in much of the earlier work, see, e.g., discussion in Ref. [8]), and hence that the critical exponents are accurate. Subsequently, massive simulations by Baity-Jesi *et al.* [9], using a special-purpose computer, obtained even more accurate results, which are consistent with the earlier work of Ref. [7].

These impressive developments have given a good understanding of the *static* critical behavior of spin glasses, but our knowledge of their *dynamic* critical behavior is much less well developed. To understand critical dynamics of spin glasses (and other similar computationally hard problems) it is useful to employ new techniques. Here we explore MC simulations out of equilibrium in combination with a powerful dynamic scaling theory [10] building on the Kibble-Zurek (KZ) mechanism [11–19]. We will demonstrate that this approach is particularly well suited for studies of spin glasses because it avoids the normally very difficult problem of ensuring that the simulations are fully equilibrated. Rather, as we shall explain, deviation from equilibrium is turned into a *feature* of the scaling methodology. Using this approach we will obtain the dynamic exponent z of spin glasses with quite high accuracy.

Universality is a cornerstone of the theory of critical phenomena according to which critical exponents and many other quantities do not depend on microscopic system details. Thus, the exponents for a spin glass should not depend on the distribution of interactions, so results obtained for, e.g., a bimodal distribution should be the same as those from a continuous distribution such as Gaussian. An interesting question, raised by Campbell and collaborators [20–22], is whether universality may be violated in spin glasses. While these works claim numerical evidence that the exponents *do* depend on the distribution of interactions, other works, e.g., Ref. [8], found universal behavior, though with some inconsistencies due to corrections to scaling not being incorporated. The work of Refs. [7,9] only used a bimodal distribution of nearest-neighbor interactions, because considerable speedup in the MC code can be obtained in this case. Unfortunately, simulations of comparable quality to those in Refs. [7,9], i.e., which systematically incorporate the leading correction to scaling, have not yet been done for a continuous distribution of the interactions.

A major focus of the present paper is to test universality of spin glasses by determining the *dynamic* exponent for both Gaussian and bimodal distributions with high accuracy. Several earlier estimates of the dynamical exponent z are summarized in Table I. It is seen that there there are significant differences in the results from different works, and claims are again made [21,22] that the dynamical exponent, like the static ones, depend on the distribution of interactions. However, we will see that our results for 3D Ising spin glasses with bimodal and Gaussian distributions show the *same* value for z within small error bars, thus supporting universality.

In the remainder of the paper, we discuss the model, simulation method, and dynamical critical scaling scheme in Sec. II and present results in Sec. III. We end with a brief discussion in Sec. IV.

II. MODEL AND METHODS

We study Ising spin glasses that can be described by the Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j, \tag{1}$$

where $\sigma_i \in \{-1,1\}$ and $\langle i,j \rangle$ stands for the nearest neighbors on a simple cubic lattice of linear size L. We consider (i) a bimodal distribution in which $J_{ij} = \pm 1$ with equal probability and (ii) J_{ij} drawn from a Gaussian with mean 0 and standard

TABLE I. Estimates of the dynamical critical exponent z for 3D Ising spin glasses with local updates (metropolis dynamics) with a bimodal ($\pm J$) or Gaussian coupling distribution (G). The papers indicated by an asterisk determine a nonequilibrium coherence length $\xi(t)$ below or at T_c. This increases with time t like $t^{1/z_{\rm eff}(T)}$, where an effective exponent $z_{\rm eff}(T)$ is found empirically to vary as T^{-1} and is also found to merge smoothly into the critical exponent z at T_c, i.e., $z_{\rm eff}(T) = (T_c/T)z$. The value of z quoted by the authors was obtained by using the best accepted value of T_c at that time. Reference [25] plots values for a temperature-dependent $x(T)$, related to $z_{\rm eff}(T)$ by $x(T) = (d-2+\eta)/2z_{\rm eff}(T)$. The value quoted in the table is obtained from the data point for $x(T)$ closest to the currently accepted T_c, and the currently accepted value of η was used [9].

Study	Model	Exponent z
Pleimling and Campbell (Ref. [22])	$\pm J$	5.7(2)
	G	6.2(1)
Nakamura (Ref. [23])*	$\pm J$	5.1(1)
Katzgraber and Campbell (Ref. [24])*	G	6.80(15)
Rieger (Ref. [25])*	$\pm J$	$\simeq$6
Ogielski (Ref. [26])	$\pm J$	6.0(8)
Belletti *et al.* (Ref. [27])*	$\pm J$	6.86(16)
This study	$\pm J$	5.85(9)
	G	6.00(10)

deviation 1. The relevant quantity to characterize the spin-glass transition is the Edward-Anderson order parameter:

$$q = \frac{1}{N}\sum_{i=1}^{N}\sigma_i^{(1)}\sigma_j^{(2)}, \tag{2}$$

where $N = L^3$, and (1) and (2) stand for two independent simulations ("replicas") of the same coupling realizations. We will study the mean-squared order parameter $\langle q^2\rangle$.

The spin-glass transition temperature T_c for the bimodal case has been determined to very high numerical accuracy [9,28]: $T_c = 1.102(3)$. T_c for the Gaussian case is not as well determined, although a reasonable estimate is also available [24,29]: $T_c = 0.94(2)$. The static exponents for the bimodal case are also well studied in Refs. [7,9], which gave the correlation length exponent $\nu = 2.562(42)$ and correlation function exponent $\eta = -0.3900(36)$. We will here regard the T_c values and static critical exponents quoted above as known values, given as input in our scaling analysis to be discussed below. The effects of the uncertainties given by the error bars, treated as one standard deviation of a normal distribution, will be taken into account using a detailed error propagation analysis.

A. Dynamic simulation scheme

The simulations start from an initial temperature $T_i = 2$, roughly twice T_c where the system is easily equilibrated prior to each dynamic ("quench") simulation. We proceed with a linearly varying T as a function of the simulation time τ (measured in units of a standard MC sweep consisting of $N = L^3$ metropolis spin-flip attempts) until a final temperature $T_f = 0.5$ is reached. Thus, our quench velocity is defined as $v = 1.5/\tau$ and the temperature is lowered by $\Delta_T = v$ after each MC step. We choose the total quench time $\tau = 150 \times 2^n$ with $n = 0,1,2,\ldots$. This kind of process is also known as *simulated annealing* [30], but in that case one normally has in mind a very slow reduction of T with the goal of finding an energy minimum or reaching equilibrium. We are interested in both slow and fast processes and carry out detailed studies of the behavior of averages over many quenches as a function of v and L.

We use 64-bit multispin coding to simulate 64 replicas with the same interactions J_{ij} in a single run (using different random numbers for the acceptance probabilities for each replica, to avoid correlations). To compute the order parameter in Eq. (2) we consider overlaps between 32 replica pairs. Since the fluctuations among different realizations of J_{ij} will in general be much larger than the statistical errors within a given realization, we only perform one such 64-replica quench for each disorder realization. For small sizes and short quenches, we generate $\mathcal{O}(10^5)$ realizations and for larger sizes and longer quenches we have at least $\mathcal{O}(10^2)$ realizations.

For simplicity of notation, we use $\langle\ldots\rangle$ to denote all averages involved. After the simulations we use polynomial interpolation to obtain $\langle q^2\rangle$ at any T within $[T_i, T_f]$. We focus on the squared order parameter $\langle q^2\rangle$ at or in the close vicinity of the known T_c. An alternative would be to perform quenches that stop at exactly T_c (instead of continuing below T_c). However, since we will also consider the propagation of errors from the uncertainties of T_c, we need at least a corresponding window of temperatures around T_c. We actually continue to still lower temperatures, at not much cost of CPU time, since our results in this region could then be used in a future analysis of the dynamics of the spin-glass phase without needing to run new simulations.

B. Dynamic scaling

According to now well-established equilibrium finite-size scaling theory [31], the critical order parameter in the neighborhood of T_c depends asymptotically on the linear system size L of a d-dimensional system and the distance $\delta = (T - T_c)/T_c$ from the critical point as

$$\langle q^2\rangle_{\rm eq} = L^{-(d-2+\eta)} f(\delta L^{1/\nu}), \tag{3}$$

where the function f is nonsingular. We now have the quench velocity v as an additional parameter. The KZ framework [11–19] then suggests that there is a characteristic velocity,

$$v_{\rm KZ}(L) \sim L^{-(z+1/\nu)}, \tag{4}$$

separating slow (quasistatic) and fast processes, and that a generalized finite-size scaling ansatz applies with $v/v_{\rm KZ}$ as a second scaling argument:

$$\langle q^2\rangle_v = L^{-(d-2+\eta)} f(\delta L^{1/\nu}, vL^{z+1/\nu}). \tag{5}$$

We focus on results when the quench has reached the critical temperature, i.e., $\delta = 0$ and the above form reduces to a much simpler scaling function of a single argument:

$$\langle q^2\rangle_v = L^{-(d-2+\eta)} f(vL^{z+1/\nu}). \tag{6}$$

This form should hold for v small and L large for any value of the argument $x = vL^{z+1/\nu}$. Data for large v, $v \gtrsim 1$, is not described by the scaling form in Eq. (6). Rather there is a crossover to a constant value of $\langle q^2\rangle_v$, which depends on the

initial state at temperature T_i. For example, when $v \to \infty$ the system does not evolve at all and its properties are just those in equilibrium at T_i [10]. This crossover is interesting but we will not discuss it here, focusing instead on the slow dynamics.

For $v \to 0$ at fixed L, the argument of the scaling function $f(x)$ in Eq. (6) tends to zero, and we must have $f(x \to 0) =$ const. in order that equilibrium finite-size scaling behavior at T_c be obtained. In the opposite limit, $v \gg v_{\rm KZ}(L)$ (but still $v \ll 1$), where $x \to \infty$, the scaling function crosses over to a universal power-law behavior. To determine the power, note that in this region the correlation length ξ_v at T_c satisfies $\xi_v \ll L$, so the finite size does not limit the correlations. Hence the dependence of $\langle q^2 \rangle_v$ on L is just the trivial prefactor L^{-d} in the definition in Eq. (2). Consistency between this behavior and the general scaling form in Eq. (6) requires that

$$\langle q^2 \rangle \propto \frac{1}{L^d} \frac{1}{v^{(2-\eta)/(z+1/\nu)}}, \tag{7}$$

which should apply for $v \ll 1$ down to some $v \propto v_{\rm KZ}$ before the crossover into the quasistatic regime as v is further lowered. The scaling function itself in the scaling regime is given by

$$f(x) \propto x^{-(2-\eta)/(z+1/\nu)}, \qquad (x \to \infty). \tag{8}$$

We will use Eq. (8) below to constrain data fits for scaling collapse onto the function f in the appropriate regime.

The dynamic finite-size scaling form in Eq. (6) has been thoroughly tested on standard Ising models [10] and yielded high-precision results for z for different types of dynamics (local and cluster updates) and dimensionality. In the case of a spin glass, in particular, as anticipated in Ref. [10] and as will be demonstrated with results in the present work, a major additional advantage of the quench approach combined with dynamic scaling is that uncertainties related to poor equilibration due to critical slowing down are avoided. In standard approaches one has to make sure that equilibrium indeed has been reached, and this can be very difficult to confirm in practice. In our approach, equilibration only has to be carried out at the high initial temperature T_i (or, one could also start with some other initial condition). In the subsequent quench process, equilibration, or lack thereof, is manifested as the scaling behavior in Eqs. (6) and (8), and the simulation results themselves are never questionable. Of course, one still has to make sure that the simulation times are long enough that the system probes sufficiently large length scales that corrections to scaling are small, but it is highly advantageous that we do not need to ensure equilibration.

III. RESULTS

We use many different velocities and system sizes $L = 8, 12, \ldots$ up to $L = 128$ for the bimodal case and up to $L = 96$ for the Gaussian case. With the static exponents ν and η known (we use the values quoted above for both the bimodal and Gaussian cases), the dynamic exponent z enters as the only unknown exponent in fitting our data to Eq. (6). We present our data in Fig. 1. We quantify the quality of the collapse using χ^2 per degree of freedom relative to a function fitted to all the data. As fitting function we choose a high-order polynomial at lower velocities, which is matched to a linear function at high velocities with a slope equal to the exponent in Eq. (8).

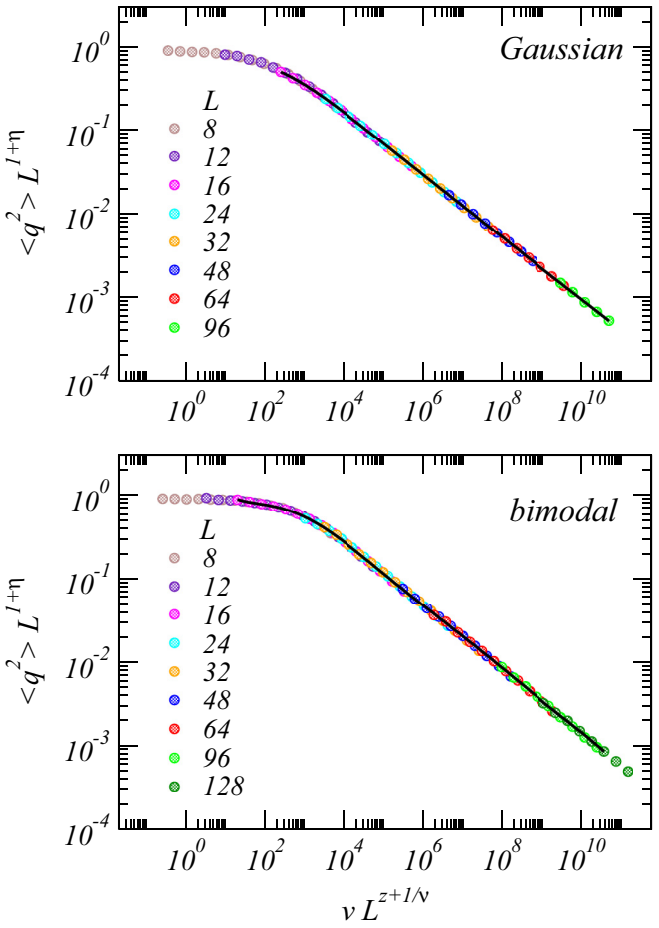

FIG. 1. (Color online) Scaling after quenching to T_c, using the form Eq. (6). The static exponents ν and η have been fixed so the only exponent to be optimized for scaling collapse is the dynamic exponent z, for which we obtain $z = 5.85(9)$ and $6.00(10)$ for bimodal (top) and Gaussian (bottom) distributions, respectively. The error bars on the data points are not visible as they are much smaller than the plotting symbols.

After z is determined this way, we introduce Gaussian noise to the MC data points as well as to the parameters T_c, ν, and η, with standard deviation equal to the corresponding error bars, repeating the scaling analysis with such altered data many times to obtain error estimates for z.

Results of the data collapse procedure are shown for both coupling distributions in Fig. 1. Here high-velocity points were removed for each L until the data collapse was satisfactory, and only the points included are shown in the figure. The removed high-v points gradually split off from the power-law scaling regime in a way very similar to the behavior in ferromagnets found in Ref. [10]. We obtain $z = 5.85(9)$ for the bimodal case and $z = 6.00(10)$ for the Gaussian case. The plateau on the low-velocity side indicates the quasistatic regime, while the straight line on the high-velocity side in these log-log plots shows the universal scaling governed by the power-law in Eq. (8).

We have, thus, demonstrated dynamic scaling at the spin-glass transition and its cross-over into the standard equilibrium finite-size scaling. The fits have excellent reduced χ^2 values

close to 1 and the values of z are also stable with respect to removing small system sizes.

Note that the way the fitting function is parametrized is not important in practice, provided that the function is capable of reproducing the true scaling function and that the number of parameters is much less than the total number of data points included in the fit (which here is easily satisfied because the number of data points is of the order 100 and the number of parameters is less than 10). We have not found any significant discrepancies between fits using different values of the break point between the polynomial and linear regimes, as long as it is in the beginning of the linear scaling regime where a straight line is an appropriate fit.

The above analysis did not consider any scaling corrections, as the data for the larger system sizes follow the expected forms very precisely despite the error bars being very small. We have also carried out fits using various correction terms but have not found any statistically significant corrections within the data set used in Fig. 1. We conclude that the dynamic scaling corrections must be very small, as can also be visually observed in the very linear behavior over several orders of magnitude of the scaling variable. The internal consistency built in as a constraint on the fitting function obeying power-law scaling exactly with the exponent in Eq. (8) in the scaling regime is also an indication of the soundness of the procedures without corrections.

IV. DISCUSSION

The nonequilibrium MC simulations and accompanying scaling analysis we have used here in large-scale studies of 3D Ising spin glasses demonstrate the utility of this method for highly frustrated systems. We have used existing knowledge of the T_c values and static exponents of the systems studies and found remarkably good fits with the dynamic exponent z as the only adjustable parameter. We note that the dynamic MC scheme can also be used to *extract* critical points and static exponents, as has recently been done for quantum models in Refs. [32,33].

The results presented in Fig. 1 for two different coupling distributions are in agreement with each other within fairly small error bars, thus supporting universality for the dynamic exponent for Ising spin glasses with single-spin metropolis MC updates. We naturally expect this to extend to any local dynamics. If we *assume* universality, we can combine our two independent estimates of the dynamic exponent (see the caption of Fig. 1) to obtain a more precise value for the 3D Ising spin-glass universality class:

$$z = 5.93 \pm 0.07. \tag{9}$$

Looking back at Table I, our results are in good overall agreement with those of Pleimling and Campbell [22], though the spread in their values is wider and the error bars are somewhat larger. Our results are quite far away (up to 5–10 error bars) from many of the other estimates which have similar or only slightly larger statistical errors. The discrepancy illustrates the difficulties in reliably studying systems with a large dynamic exponent. Our method circumvents problems related to insufficient equilibration, and our scaling plots extend all the way from the equilibrium behavior to a wide region of universal power-law scaling, with confirmed negligible scaling corrections. We therefore do not expect our results to be affected by any errors beyond purely statistical ones.

The complete description of all our data by the simple scaling function Eq. (6) also demonstrates that the spin-glass transition, when approached from $T > T_c$, is not qualitatively different from a ferromagnetic transition as far as scaling is concerned, only the values of the exponents are different, with the dynamic exponent being very much larger in the spin glass. Even the form of the scaling functions shown in Fig. 1 are very similar to those of ferromagnetic Ising models [10]. From the perspective of the generic derivation of KZ scaling behavior recently presented in Ref. [10], this simply reflects the fact that there is a single dominant divergent length scale ξ in the system, and the characteristic time scale τ is just a power of this length-scale: $\tau \sim \xi^z$. The situation may be completely different when approaching the spin-glass transition from the ordered side, where the dynamic exponent is temperature dependent; see, e.g., Ref. [34] for a recent discussion. It would be interesting to also study such quenches using generalized KZ scaling, but from a technical perspective this is much more difficult as the advantage of fast equilibration at T_i no longer applies when $T_i < T_c$.

After the completion of all calculations reported in this paper another nonequilibrium study appeared [34] for the $J = \pm 1$ model in which a random ($T = \infty$) state was suddenly quenched to the temperature of interest and the growth of correlations versus simulation time was monitored. Close to T_c a dynamic exponent $z \approx 6.0$ was found in this way, in excellent agreement with our results. The good agreement further supports our assertion made above that corrections to dynamic scaling are very small in this system.

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