Monte Carlo Simulation of the Three-dimensional Ising Spin Glass

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Abstract. We study the 3D Edwards–Anderson model with binary interactions by Monte Carlo simulations. Direct evidence of finite–size scaling is provided, and the universal finite–size scaling functions are determined. Using an iterative extrapolation procedure, Monte Carlo data are extrapolated to infinite volume up to correlation length $\xi \approx 140$. The infinite volume data are consistent with both a continuous phase transition at finite temperature and an essential singularity at finite temperature. An essential singularity at zero temperature is excluded.

1 Introduction

Understanding the thermodynamics of spin glasses represents a challenging unsolved problem for statistical and computational physics. The very existence of a phase transition in the 3D Ising spin glass is still unclear. Previous Monte Carlo (MC) simulations give a certain evidence of a $T_c \neq 0$ continuous transition with power-law divergence of $\xi$ at $T \to T_c^+$. However, they cannot exclude completely neither an exponential divergence at $T \to 0^+$, nor a line of critical points at $T \leq T_c \neq 0$, which implies an exponential divergence at $T \to T_c^+$. Furthermore, the important topic of finite-size scaling (FSS) has not been much investigated for spin glasses.

Here, we study the 3D Ising spin glass by MC simulations of moderate–size systems in the paramagnetic phase (less hampered by long equilibration times), using the powerful FSS method. In Sect. 2 details on the simulations are given. In Sect. 3 a direct evidence of FSS, independent of the nature of the divergence of $\xi$, is provided, and the universal FSS functions are determined for the first time. The MC data are extrapolated to infinite volume up to $\xi$ one order of magnitude larger than before. In Sect. 4 the critical behavior of the extrapolated data is analyzed.

2 Model and simulation

We consider the 3D Edwards–Anderson model, whose Hamiltonian is

$$\mathcal{H} = -\sum_{(xy)} \sigma_x J_{xy} \sigma_y$$

(1)

where $\sigma_x$ are Ising spins on a simple cubic lattice of linear size $L$ with periodic
boundaries, and $J_{xy}$ are independent random interactions taking the values $\pm 1$ with equal probability. The sum runs over pairs of nearest neighbor sites.

We simulate with the heath–bath algorithm many samples of the model \( (1) \) with different $J_{xy}$. From two independent replicas ($\sigma, \tau$) with the same $J_{xy}$, we measure the overlap $q_{x} = \sigma_{x} \tau_{x}$ and $q = L^{-3} \sum_{x} q_{x}$. We compute the second-moment correlation length using the following definition:

$$\xi(T, L) = \left( \frac{S(0)/S(p) - 1}{4 \sin^{2}(p/2)} \right)^{1/2}$$

where $S(k)$ is the Fourier transform of the overlap correlation function

$$S(k) = \sum_{r} e^{ik \cdot r} \langle q_{x} q_{x+r} \rangle,$$

(3)

(the arguments $T, L$ are omitted) and $p = (2\pi / L, 0, 0)$ is the smallest non–zero wave vector. We also measure the spin–glass susceptibility $\chi_{SG}(T, L) \equiv L^{3} \langle q^{2} \rangle = S(0)$. The runs are done on a Cray T3E with a fast code (see [9] for details) that exploits the high parallelism of spin glass simulations, combining multi–processor parallelism with an efficient multi–spin coding technique. Average speed on a single processor (DEC Alpha EV5, 600 MHz) is $4.5 \times 10^{7}$ spin updates per second, and we typically used 32 to 128 PEs. We simulated 104 pairs $(T, L), (T, 2L)$ with $L$ between 4 and 48.

3 Finite size scaling analysis

According to the FSS hypothesis [10], if $O(T, L)$ is some long-distance observable (for example, $\xi(T, L)$ or $\chi_{SG}(T, L)$), then

$$\frac{O(T, L)}{O(T, \infty)} = f_{O}(\xi(T, \infty)/L),$$

(4)

where $f_{O}$ is a universal function and corrections to FSS are neglected. From (4) we obtain a useful relation involving only finite–volume observables

$$\frac{O(T, 2L)}{O(T, L)} = F_{O}(\xi(T, L)/L),$$

(5)

where $F_{O}$ is another universal function. As shown in Fig.3, our data for the observables $\chi_{SG}, \xi$, $q_{4} \equiv \langle q^{4} \rangle$ and $F \equiv V^{-3}S(p)$ verify the ansatz (5). This provides a direct test of the FSS hypothesis. Small systematic deviations, due to corrections to FSS, appear in Fig.3 for $L = 5$ and $\xi(T, L)/L \equiv x > 0.4$. We emphasize that FSS is not assumed a priori and that no adjustable parameters are contained in (5). Furthermore, no particular dependence of the observables on the temperature is assumed.

We fit the data in Fig.3, to two suitable functions $F_{\chi_{SG}}, F_{\xi}$ and then extrapolate the pair $(\xi, \chi_{SG})$ from $L \rightarrow 2L \rightarrow 2^{2}L \rightarrow \ldots \rightarrow \infty$ using (5).
For any temperature, we verify that extrapolations from different $L$ agree within the error bars. In this procedure, we assumed implicitly that (5) with a given function $F_O$ will continue to hold as $L \to \infty$. This assumption could fail if there is a crossover at large $L$. However, at high $T$ extrapolations from small $L$ are consistent with data from large $L$, which have almost no finite-size effects, and thus a crossover is unlikely. We have a good control on the extrapolated data up to $\xi \approx 140$; at lower temperatures the statistical errors become quite large, and the data are more sensitive to FSS corrections.

In Fig. 1(c,d) we show that with our extrapolated data (4) is satisfied remarkably well, providing a further test of the method. If $O \sim \xi^{\gamma O/\nu}$ as $\xi \to \infty$, then $f_O(x)$ in (4) must satisfy $f_O(x) \sim x^{-\gamma O/\nu}$ as $x \to \infty$. As shown in the insets of Fig. 1(c,d), our curves indeed have a power-law asymptotic decay. We emphasize that all the scaling functions in Figs. 1 and 2 are universal.
4 Nature of the phase transition

We now compare our extrapolated data with the three different scenarios compatible with previous simulations.

(i) Power–law singularity at $T_c \neq 0$. We fit our data to

\[ \xi(T) = c_\xi (T - T_c)^{-\nu} \left[ 1 + a_\xi (T - T_c)^\theta \right] \]

\[ \chi_{SG}(\xi) = b_\xi \xi^{2-\eta} \left[ 1 + d_\xi \xi^{-\Delta} \right] \]

with fixed $\theta$ and $\Delta$. Without corrections to scaling ($a_\xi = d = 0$), the fit parameters show small systematic variations when we vary the fit interval. The fits stabilize with $1 \leq \theta \leq 2$ and $1 \leq \Delta \leq 1.5$, the preferred values being $\theta = 1.4$ and $\Delta = 1.3$ (goodness of fit parameter $Q > 0.6$ and $Q > 0.98$ resp.). Our estimates for the critical parameters are $T_c = 1.156 \pm 0.015$, $\nu = 1.8 \pm 0.2$, and $\eta = -0.26 \pm 0.04$. Corrections to scaling are important for $\xi \leq 10$ (Fig.3).

(ii) Essential singularity at $T_c \neq 0$. Our data fit very well also to

\[ \xi(T) = f_\xi \exp \left( g_\xi/(T - T_c)^{\sigma} \right) \]

For $\xi \geq 3.8$ the best fit (shown in Fig.3b) gives $\sigma = 0.5 \pm 0.3$, $T_c = 1.08 \pm 0.04$ ($Q = 0.69$). Deviations from this fit for $\xi < 3$ are consistent with corrections to scaling of $\approx 10\%$. Since for an exponential singularity we expect multiplicative logarithmic corrections, we tried also the fit

\[ \chi_{SG}(\xi) = b_\xi \xi^{2-\eta_1} (\log \xi)^r \]

obtaining $\eta_1 = -0.36 \pm 0.03$ and $r = -0.36 \pm 0.06$ ($Q > 0.9$) (see Fig.3a).

(iii) Essential singularity at $T = 0$. Fitting our data to

\[ \xi(T) = f_\xi \exp \left( g_\xi/T^{\sigma} \right) \]
we find $\sigma \geq 9$. Such a high value is highly implausible on the basis of renormalization group arguments, from which we expect $\sigma \approx 2$ [9]. We therefore believe that an essential singularity at $T = 0$ is excluded.

![Graph](image)

**Fig. 3.** Critical behavior of the infinite volume data. (a) Best fit to (7) for $\xi \geq 1.8$ (line A), leading term from the same fit (A leading), best fit to (9) for $\xi \geq 2.2$ (B). (b) Best fit to (8) for $\xi \geq 1.9$ (A), leading term from the same fit (A leading), best fit to (10) for $\xi \geq 3.8$ (B), and best fit to (11) for $\xi \geq 14$ (C).

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