Multicanonical Study of the 3D Ising Spin Glass

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Abstract:

We simulated the Edwards-Anderson Ising spin glass model in three dimensions via the recently proposed multicanonical ensemble. Physical quantities such as energy density, specific heat and entropy are evaluated at all temperatures. We studied their finite size scaling, as well as the zero temperature limit to explore the ground state properties.

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One of the great challenges in numerical simulations is the study of spin glasses. These systems display a rather peculiar structure due to the effects of disorder and frustration, for reviews see [1, 2]. Recently two of the authors explored the multicanonical ensemble [3] for simulations of spin glasses. Results for the 2D Edwards-Anderson Ising spin glass were encouraging [4]. Similar concepts were also tested in [5]. In this letter we present a preliminary multicanonical simulation of the physically more interesting 3D Edwards-Anderson Ising spin glass.

The Hamiltonian of the model is given by

$$H = - \sum_{<ij>} J_{ij} s_i s_j,$$

where the sum goes over nearest neighbours and the exchange interactions $J_{ij} = \pm 1$ between the spins $s_i = \pm 1$ are randomly distributed over the lattice with the constraint $\sum J_{ij} = 0$ for each realization. Despite its simplicity the model is supposed to be sufficiently realistic. Recent simulations [6] of the 3D model in a magnetic field favour the mean field picture rather than the alternative droplet model [7, 8]. However, it can be argued that equilibrium at sufficiently low temperatures has not been reached [9]. For previous simulations of Ising spin glasses in 3D see [10, 11, 12, 13, 14].

The multicanonical ensemble [3] can be defined by weight factors

$$P_M(E) = \exp \left[ -\beta(E) E + \alpha(E) \right],$$

(2)

where $\alpha(E)$ and $\beta(E)$ are to be determined such that for the chosen energy range $E_{\text{min}} \leq E \leq E_{\text{max}}$ the resulting multicanonical probability density is approximately flat:

$$P_{\text{mu}}(E) = c_{\text{mu}} n(E) P_M(E) \approx \text{const}$$

(3)

where $n(E)$ is the spectral density. In the present study we take $E_{\text{max}} = 0$ ($\beta(E) \equiv 0$ for $E \geq E_{\text{max}}$) and $E_{\text{min}} = E^0$ the ground state energy of the considered spin glass realization. The purpose of the function $\alpha(E)$ is to give $\beta(E)^{-1}$ the interpretation of an effective temperature. This leads to the recursion relation

$$\alpha(E - 4) = \alpha(E) + [\beta(E - 4) - \beta(E)] E, \quad \alpha(E_{\text{max}}) = 0.$$

(4)

The multicanonical function $\beta(E)$ is obtained via recursive multicanonical calculations. One performs simulations with $\beta^n(E)$, $n = 0, 1, 2, \ldots$, which yield probability densities $P^n(E)$ with medians $E_{\text{median}}^n$. We start off with $n = 0$ and $\beta^0(E) \equiv 0$. The recursion from $n$ to $n + 1$ reads

$$\beta^{n+1}(E) = \begin{cases} 
\beta^n(E) \text{ for } E \geq E_{\text{median}}^n; \\
\beta^n(E) + 0.25 \times \ln \left[ P^n(E + 4)/P^n(E) \right] \text{ for } E_{\text{median}}^n > E \geq E_{\text{min}}^n; \\
\beta^{n+1}(E_{\text{min}}^n) \text{ for } E < E_{\text{min}}^n.
\end{cases}$$

(5)

The recursion is stopped for $m$ with $E_{\text{min}}^{m-1} = E^0$ being groundstate.
By weighting with \( \exp[-\hat{\beta}E + \beta(E)E - \alpha(E)] \) canonical expectation values \( \mathcal{O}(\hat{\beta}) = Z(\hat{\beta})^{-1} \sum_{E} \mathcal{O}(E)n(E) \exp(-E) \), where \( Z(\hat{\beta}) = \sum_{E} n(E) \exp(-E) \) is the partition function, can be reconstructed for all \( \hat{\beta} \) (the canonical inverse temperature). The normalization constant \( c_{max} \) in equation (3) follows from \( Z(0) = \sum_{E} n(E) = 2^{N} \), where \( N \) is the total number of spin variables. This gives the spectral density and allows to calculate the free energy as well as the entropy.

We simulated the Edwards-Anderson Ising spin glass model on 3D cubic lattices with linear size \( L = 4, 6, 8 \) and 12. We performed simulations of \( 2 \times 10^{6} \) iterations on \( 4^{3} \) lattice with 32 different realizations of random variables \( J_{ij} \). We carried out up to \( 4 \times 10^{6} \) iterations on \( 4^{3}, 6^{3} \) and \( 12^{3} \) lattices with 16, 8 and 4 realizations, respectively. Thermal averages were evaluated after the first additional \( 2 \times 10^{5} \) iterations being discarded, although with a disordered starting configuration the multicanonical ensemble is immediately in equilibrium.

Our results for physical quantities are summarized in Table 1. The final mean values and their error bars are obtained by combining the results from the different realizations. Different realizations are statistically independent and enter with equal weights. The final error bars are enlarged by a Student multiplicative factor, such that the probability content of two standard deviations is Gaussian (95.5%).

| \( \hat{\beta}_{\text{max}} \) | \( L = 4 \) | \( L = 6 \) | \( L = 8 \) | \( L = 12 \) |
|---|---|---|---|---|
| \( \beta_{\text{max}} \) | 1.04 ± 0.03 | 1.52 ± 0.12 | 2.04 ± 0.18 | 2.30 ± 0.38 |
| \( \tau_{L} \) | 685 ± 95 | 30166 ± 16383 | 117038 ± 40630 | 1580230 ± 882686 |
| \( e^{0}_{\text{L}} \) | -1.7403 ± 0.0114 | -1.7741 ± 0.0074 | -1.7822 ± 0.0081 | -1.7843 ± 0.0030 |
| \( s^{0}_{\text{L}} \) | 0.0724 ± 0.0047 | 0.0489 ± 0.0049 | 0.0459 ± 0.0030 | 0.0491 ± 0.0023 |
| \( \chi^{0}_{q} \) | 0.65 ± 0.05 | 0.71 ± 0.05 | 0.56 ± 0.10 | 0.68 ± 0.10 |

Table 1:

The energy density \( e(\hat{\beta}) \), the specific heat \( c(\hat{\beta}) \), and the entropy per spin \( s(\hat{\beta}) \) follow in a straightforward manner by constructing the canonical ensemble. Fig. 1 depicts the energy density and the entropy per spin versus inverse temperature for \( L = 8 \). The indicated error bars are with respect to the eight different realizations. For the temperature range \( 0.8 \leq T \leq 1.6 \) we collect in Fig. 2 our \( L = 4, 6, 8 \) and 12 results for the specific heat. This is of interest as a spin glass phase transition is claimed to take place at \( T_{c} \approx 1.2 \) \cite{10, 11}. However, this picture was recently questioned by Bhanot and Lacki \cite{14} on the basis of exact partition function calculations on fairly small systems (up to \( 5 \times 5 \times 9 \)). The critical exponent estimate \( \nu = 1.3 \) \cite{10, 11} implies \( \alpha = -1.9 \) via the hyperscaling relation \( D\nu = 2 - \alpha \). The finite size scaling (FSS) of the specific heat \( T = T_{c} \) is \( e \sim L^{\alpha/\nu} \). Clearly, Fig. 2 is inconsistent with this \( L \)-dependence and exhibits instead almost negligible finite size effects as would be typical for non-critical behaviour.

Let us now concentrate on the zero temperature (\( \hat{\beta} \rightarrow \infty \)) limit. The groundstate energy density is \( e^{0} = E^{0}/N \), and we obtain its entropy per spin as \( s^{0} = S^{0}/N = \ln[n(E^{0})]/N \). FSS fits of the form \( f^{0}_{\infty} = f^{0}_{\infty} + c/N \) are used to estimate the infinite volume groundstate energy density and entropy per spin. Fig. 3 displays these fits. Our groundstate energy density result \( e^{0} = -1.7863 \pm 0.0028 \) is consistent with the previous estimates \( e^{0} = -1.76 \pm 0.02 \) \cite{10} and \( e^{0} = -1.75 \) \cite{14}. Our value for the groundstate entropy per spin \( s^{0} = 0.046 \pm 0.002 \).
Figure 1: Energy density and entropy per spin versus $\beta$ (from the $L = 8$ lattices).
is consistent with \( s^0 = 0.04 \pm 0.01 \) given by Morgenstern and Binder [16] and lower than Kirkpatrick’s value \( s^0 = 0.062 \) which was estimated from a single sample of \( 20^3 \) spins [14]. Our groundstate entropy value translates, even for moderately sized systems, into large numbers of distinct groundstates. For instance \( s^0 = 0.046 \) implies approximately \( 3.3 \times 10^{34} \) groundstates for a \( 12^3 \) lattice. We also tried the entropy fit \( N s^0_L = \ln(N) + c \), which corresponds to a power law ansatz for the groundstate degeneracy. Unacceptable \( \chi^2 \) values rule out this fit even if the lattice range is restricted to \( L = 4 - 8 \).

To visualize the low temperature behaviour, we show in Fig. 4 the spin glass order parameter distribution of one of our \( L = 8 \) realizations. Its calculation follows the lines of [4]. One clearly sees five configuration space valleys which are separated by high tunneling barriers. The multicanonical simulation overcomes these energy barriers by connecting back to the disordered high temperature states. The realization from which Fig. 4 is depicted showed nine tunneling events. Here tunneling means that starting from the high temperature disordered phase the algorithm finds a true ground state and then travels all the way back to the disordered phase. The average number of sweeps needed for this process is our ergodicity time \( \tau^L_e \). Table 1 shows how the ergodicity times increase with the lattice size for our simulations. The data corresponds in CPU time to a slowing down \( \sim V^{3.4(2)} \) which is similar to the one involved in our previous 2D simulations.

Further, we have included in Table 1 our zero temperature (groundstates) results \( \chi^0_q \) for the spin glass susceptibility density \( \chi_q = <q^2>/V \) (note that \( <q> = 0 \) due to the symmetry of the Hamiltonian). The numbers are modestly indicative for a non-trivial \( P_0(q) \) distribution (lack of self-averaging). We also looked at the temperature dependence of the spin glass susceptibility and the corresponding Binder parameter. In the neighbourhood of the suspected \( T_c \) our results are consistent with [10,11], but our present accuracy does not allow a detailed finite size scaling investigation. Considerable future improvements are feasible.
Figure 3: FSS estimates of the infinite volume groundstate energy density and entropy per spin.
Let us state the conclusions. Our results on specific heat, shown in Fig. 2, raise some additional doubts about the standard picture of the spin glass phase transition. But on a qualitative level we find a bifurcation of the spin glass order parameter, as depicted in Fig. 4. A future, more quantitative, investigation of this quantity is desirable. Fig. 4 and our preliminary results for the spin glass susceptibility favour the mean field picture of spin glasses. To reach seminal results one has to investigate larger lattices and, first of all, to clarify the nature of the transition.

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