Groundstate Properties of the 3d Ising Spin Glass\textsuperscript{1}

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Abstract

We study zero–temperature properties of the 3d Edwards–Anderson Ising spin glass on finite lattices up to size $12^3$. Using multicanonical sampling we generate large numbers of groundstate configurations in thermal equilibrium. Finite size scaling with a zero–temperature scaling exponent $y = 0.74 \pm 0.12$ describes the data well. Alternatively, a description in terms of Parisi mean field behaviour is still possible. The two scenarios give significantly different predictions on lattices of size $\geq 12^3$.

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The theoretical problem to determine the equilibrium groundstate structure of spin glasses has remained an important, but elusive, question. It is generally agreed that the statistical mechanics of the infinitely ranged Sherrington–Kirkpatrick Ising spin glass is essentially understood. The replica–symmetry breaking mean field (MF) scheme discovered by Parisi [1] exhibits infinitely many low–temperature states whose properties are consistent with simulations [2], see [3] for a recent overview. Whether, for temperatures below the spin glass phase transition point $T_c$, the more realistic short–ranged 3d Edwards–Anderson Ising spin glass model (EAI) also exhibits Parisi mean field behaviour has become a central question. It was answered in the negative by proponents of a simple scaling ansatz [4–7]. These droplet scaling (DS) theories suggest that no more than two pure states (related via a global flip) exist at any temperature. The MF approximation is surely valid for $d \to \infty$, and it has been suggested [5] that $d = 6$ is the upper critical dimension which separates the MF from the DS scenario.

The EAI Hamiltonian is given by

$$H = -\sum_{<ij>} J_{ij} s_i s_j.$$  \hspace{1cm} (1)

Here the sum $<ij>$ goes over nearest neighbours. We consider 3d systems with periodic boundary conditions and $N = L^3$ spins. The exchange interactions $J_{ij} = \pm 1$ between $N$ spins $s_i = \pm 1$ are randomly distributed over the lattice with the constraint $\sum_{<ij>} J_{ij} = 0$. For each system there are $(3N)!/[(3N/2)!]^2$ realizations of the quenched random variables $J = \{J_{ij}\}$. Recent simulations [8] in a magnetic field favour the mean field picture rather than the alternative droplet model. However, it has been pointed out that equilibrium at sufficiently low temperatures has not been reached [9].

A quantity of decisive importance is the probability density $P(q)$ of the Parisi order parameter $q$:

$$P(q) = \langle P(q) \rangle_J = \frac{[(3N/2)!]^2}{(3N)!} \sum_j P_J(q).$$  \hspace{1cm} (2)

By $\langle \cdot \rangle_J$ we denote averaging over the realizations $J$. For a fixed realization $P_J(q)$ is the
probability density of the overlap

\[ q = q_J = \frac{1}{N} \sum_i s_i^1 s_i^2 \mid J. \]  

(3)

Here \( s_i^1 \) and \( s_i^2 \) denote two replica (i.e. statistically independent configurations) of the realization \( J \) at temperature \( T \). Due to magnetic field zero we have the symmetry \( P(-q) = P(q) \), such that \( \int_{-1}^{+1} q^n P(q) dq = 0 \) for \( n \) odd. We therefore define averages over the range \( 0 \leq q \leq 1 \):

\[ \bar{q}^n = \langle q^n \rangle = 2 \int_0^1 q^n P(q) dq. \]  

(4)

For the spin glass susceptibility \( \chi_q = N \langle q^2 \rangle \) the MF as well as the DS scenario suggest divergence \( \chi_q \sim N \) for \( T < T_c \). However they give significantly different predictions for the variance

\[ \sigma^2(\bar{q}) = \langle (\bar{q} - q)^2 \rangle. \]  

(5)

In the limit \( N \to \infty \) one has \( \sigma^2(\bar{q}) \to \text{finite} \) in MF theory, while \( \sigma^2(\bar{q}) \sim L^{-y} \to 0 \) within the DS approach. Here \( y = -y_T \) is the zero–temperature scaling exponent \([3]\), denoted \( \theta \) in \([3]\), which governs also the finite size scaling (FSS) corrections of the expectation values\(^1\):

\( \bar{q}^n_L - \bar{q}^n \sim L^{-y} \) for DS, whereas we assume \( 1/\text{Volume} \) corrections for MF theory.

Lack of self–averaging is one prominent feature of MF behaviour. In reference \([8]\) \( \langle f(P(q) - P_J(q))^2 dq \rangle_J \) was studied. This was criticised by the authors of \([3]\). Following their suggestion we estimate

\[ \sigma^2_J(\bar{q}^2) = \langle (\bar{q}^2 - \bar{q}^2_J)^2 \rangle_J. \]  

(6)

Again, this quantity stays finite in MF theory, but drops off \( \sim L^{-y} \) in the DS picture.

With the development of multicanonical techniques for disordered systems \([10]\) it has become feasible to generate spin glass groundstates in thermal equilibrium; see \([11]\) for a brief, general review, and \([12]\) for the earlier umbrella sampling. A pilot study for the model at hand has been presented in \([13]\). In essence a multicanonical spin glass simulation proceeds in three steps. First Monte Carlo (MC) weights are recursively constructed which

\(^1\)If necessary we indicate the lattice size by an additional subscript \( L \), which is otherwise dropped.
will allow to simulate an ensemble, the “multicanonical”, which yields canonical expectation values in the temperature range \(0 \leq T \leq \infty\) through use of the spectral density. Secondly, equilibrium configurations with respect to the multicanonical ensemble are generated by means of standard MC. In a third step canonical expectation values at desired temperatures are obtained from the analysis. Multicanonical sampling circumvents the notorious ergodicity problems of canonical low temperature spin glass simulations through regular excursions into the disordered phase, while staying in equilibrium.

In this paper we focus on the investigation of groundstate properties. A lower bound on the number of statistically independent groundstates sampled is obtained by counting how often the system moves from the energy \(E \geq 0\) region to the groundstate energy \(E_{\min}\), and back to the \(E \geq 0\) region. This has been termed “tunneling” [10] and we follow this notation, but one should bear in mind that the free energy barriers are actually not overcome by a tunneling process. With present techniques the tunneling time approximately increases \(\sim V^{3.4}\) in 3d [13]. This slowing down limits our investigation to rather moderately sized lattices.

We have performed simulations for \(L = 4, 6, 8, 12\) (\(N = 64, 216, 512, 1728\)). For \(L \leq 8\) the sum (2) is approximated through 512 randomly chosen realizations of the \(\{J_{ij}\}\), whereas we have only 7 realizations for \(L = 12\). For all 1,543 cases multicanonical parameters were determined recursively. Then each system was simulated twice with independent random starts and random numbers. This constitutes our two independent replica per realization. In these production runs iterations were stopped when a preset number of tunneling events \(n_\tau\) had occurred: \(n_\tau = 128\ (L = 4), 64\ (L = 6), 32\ (L = 8)\) and 10 \((L = 12)\). Despite this decrease in tunneling events, the average number of updates per spin \(n_s\) (sweeps) did steadily increase. Approximate values are: \(n_s = 8 \cdot 10^4\ (L = 4), 10^5\ (L = 6), 7.6 \cdot 10^6\ (L = 8)\) and \(50 \cdot 10^6\ (L = 12)\). The average CPU time spent on one \(L = 8\) replica was approximately 800 minutes on an IBM 320H workstation.

Per replica we have stored up to 2,048 groundstate configurations. Due to correlations
the number of encountered groundstates is, of course, much larger than \( n_r \). If the number exceeded 2,048, the stored configurations were randomly selected from the total set. For groundstate configuration \( n \) this is elegantly done on–line by picking a random integer \( i_r \) in the range \( 1 \leq i_r \leq n \). Configuration \( n \) is stored at position \( i_r \) if \( i_r \leq 2,048 \) and discarded otherwise. For both replica the same groundstate energy has to be found between all tunneling counts. This is a strong, albeit not rigorous, criterium to ensure that the correct groundstate energy has not been missed.

On a semi–log scale figure 1 depicts the thus obtained probability densities (2) for the Parisi order parameter. The \( L = 12 \) probability density, presented without error bars, is very bumpy due to the small number of realizations, and will only be reliable for a few of the considered physical quantities. Note, altogether the data respect the \( P(q) = P(-q) \) symmetry well. For \( L = 8 \) figure 2 plots the \( P_J(q) \) probability densities of two rather extreme \( L = 8 \) realizations: two peak shape versus continuous distribution. Various different shapes in–between these extremes are also found. Figure 3 shows all \( L = 8 \) realizations together. From figures 1–3 it is evident that only a careful quantitative analysis of these distributions may give hints concerning the \( L \to \infty \) groundstate distribution.

Our estimates for various measured quantities are summarized in table 1. The error bars are with respect to the different realizations, which are statistically independent and enter with equal weights. Table 2 summarizes two–parameter fits of the data, assuming alternatively MF theory or the DS ansatz to be true. If MF and DS scenario lead to the same functional form, the fit is marked “All”. The \( \infty \) column gives the infinite volume extrapolations of the considered quantity, \( Q \) is the goodness of fit, and \( R_{12} \) comments Yes or No on the reliability of the \( L = 12 \) data for the purposes of the particular fit. With an exception for \( P_{\text{max}} \), the MF and ALL fits are of the form \( a_1 + a_2/L^3 \). In the MF as well as in the DS scenario the self–overlap gives rise to a \( \delta \)–function singularity. Therefore \( P_{\text{max}} \) is supposed to grow \( \sim V \) and the appropriate fit is \( a_1L^3 + a_2 \). Including all data points the fit is still consistent. Although, omitting the smallest lattice indicates that \( L = 4 \) may not fully
exhibit the asymptotic behaviour.

Let us now discuss $\sigma^2(q)$ and $\sigma^2_J(q^2)$. The DS fit is $a_1 L^{-a_2}$. Fits and data are depicted in figure 4. For each case we give two fit curves. The upper one relies on three data points ($L = 4, 6, 8$), whereas the lower one includes also the $L = 12$ result. When only three data are used, MF and DS fits are both consistent ($Q = 0.10$ and $Q = 0.43$). Once the $L = 12$ data point is included, the consistency of the MF fit becomes marginal ($Q = 0.04$). However, from the $L = 8$ data we have the experience that 10% of the realizations amount to 99% of the $P(0)$ contribution. Consequently, the $L = 12$ data suffer not only from large statistical fluctuations, but are altogether unreliable for quantities which are sensitive to the small $q$ distribution. The above fits were also used for $P(0)$, but the data are too inaccurate to yield meaningful results. We now rely on the three–point fits for $\sigma^2(q)$ and $\sigma^2_J(q^2)$. The two $y = a_2$ estimates are still compatible, and we summarize them to $y = 0.74 \pm 0.12$. The error bar is not reduced as both estimates rely on the same data set.

Assuming that our $L = 4 - 8$ lattices show already typical scaling behaviour, we conclude from figure 4 that similarly accurate data on lattices up to size $L = 16$ would discriminate between the MF and the DS ansatz. Due to the slowing down, our new data indicate $\sim V^{3.9}$, the needed CPU time would be about 1,000 times larger than the one spent on the present investigation. With upcoming massively parallel devices in the teraflop range such a factor can be achieved.

The not yet discussed DS fits are of the form $a_1 + a_2 L^{-y}$ with $y = 0.74$. Let us first comment on the groundstate energy fits. The energy is self–averaging, $L = 12$ contributes reasonably accurate results, and we rely on all data sets. Most interesting, the DS fit is consistent, whereas the MF fit with $1/\text{Volume}$ corrections is ruled out. Unfortunately, there is still a catch to it. It may well be that the corrections to the uncritical MF behaviour are exponentially small. Although FSS corrections for larger systems would then be greatly reduced, the disadvantage at the present level is that the appropriate $a_1 + a_2 \exp(-a_3 L)$ fit has three free parameters. A consistent ($Q = 0.19$) fit is then still possible. Again, accurate
data on lattices up to $L = 16$ would allow to differentiate this behaviour from DS.

Let us remark that the groundstate entropy stays finite, as about 5% of the spins can still be freely flipped due to the exact degeneracy of the ±1 quenched random variables [14]. Because of this pathology of the model non–critical FSS correction seem to be appropriate in either scenario, and 1/Volume corrections work indeed well.

A relevant consistency check for the correctness of the DS picture is that the infinite volume estimates of $\overline{q}_{\text{max}}$, $\sqrt{\overline{q}^2}$ and $\overline{q}$ have to agree. Figure 5 shows the MF and DS fits for these quantities. For $L$ a log–scale is used to exhibit $L \to \infty$ clearly, and the infinite volume estimates are depicted towards the end off the scale. With the previously determined zero–temperature exponent the values are indeed consistent. For the MF fits $\overline{q}_\infty < \sqrt{\overline{q}^2_\infty} < \overline{q}_{\text{max}}$, as it should be then. It is notable that fitting with a wrong zero–temperature exponent may produce entirely inconsistent results. For instance with $y = 0.2$ one finds $\overline{q} > 1 > \overline{q}_{\text{max}}$.

In summary, the DS ansatz is so far consistent. Our investigation presents the first MC estimate of the zero–temperature scaling exponent. Obviously, our lattices are too small to allow seminal results. In particular, the MF picture is still a valid alternative. It is clear that, either by brute computer power or by algorithmic improvements, simulations on larger lattices will become feasible. It seems, we are approaching a numerical conclusion about the correct groundstate picture of the 3$d$ EAI model.

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\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|}
\hline
 & $L = 4$ & $L = 6$ & $L = 8$ & $L = 12$ \\
\hline
$-\epsilon^0$ & 1.7378 (28) & 1.7674 (13) & 1.7799 (08) & 1.7936 (27) \\
$s^0$ & 0.0740 (09) & 0.0535 (05) & 0.0479 (03) & 0.0437 (24) \\
$\sigma(e^0)$ & 0.00373 (25) & 0.000749 (51) & 0.000277 (19) & 0.000057 (34) \\
$\sigma(s^0)$ & 0.000784 (53) & 0.000190 (13) & 0.0000709 (48) & 0.0000046 (27) \\
$\bar{q}$ & 0.785 (07) & 0.800 (06) & 0.817 (06) & 0.880 (28) \\
$\frac{q^2}{\bar{q}}$ & 0.669 (09) & 0.685 (08) & 0.703 (07) & 0.786 (38) \\
$\bar{q}_{\text{max}}$ & 0.939 (06) & 0.9252 (25) & 0.9160 (15) & 0.901 (10) \\
$P_{\text{max}}$ & 4.08 (15) & 6.04 (21) & 8.38 (26) & 16.0 (5.0) \\
$P(0)$ & 0.206 (30) & 0.231 (41) & 0.140 (37) & 0.007 (07) \\
$\sigma^2(\bar{q})$ & 0.0532 (26) & 0.0446 (27) & 0.0354 (27) & 0.013 (13) \\
$\sigma^2_j(q^2)$ & 0.0385 (17) & 0.0258 (15) & 0.0214 (15) & 0.006 (06) \\
\hline
\end{tabular}
\caption{Data.}
\end{table}

Tables

Figure Captions

**Fig. 1** Probability densities $P(q)$ for the Parisi order parameter ($L = 4, 6, 8$ and 12).

**Fig. 2** Probability densities $P_j(q)$ for two very different $L = 8$ realizations.

**Fig. 3** All $P_j(q)$ probability densities for $L = 8$.

**Fig. 4** Fits for $\sigma^2(\bar{q})$ (Data q) and $\sigma^2_j(q^2)$ (Data q2).

**Fig. 5** Fits and extrapolations for $\bar{q}_{\text{max}}$ (up), $\sqrt{q^2}$ (middle) and $\bar{q}$ (down).
\[
\begin{array}{|c|c|c|c|c|c|c|c|c|}
\hline
L = 4 \rightarrow 8: & L = 4 \rightarrow 12: \\
\hline
-e^0 & -e^0 & Q & -e^0 & e_0 & -e^0 & e_0 & -e^0 & e_0 \\
\hline
a_1 & 1.78541 (92) & -3.23 (21) & 0.01 & 1.78637 (88) & -3.23 (21) & 10^{-5} & Y & MF \\
\hline
s^0 & 1.84051 (42) & -0.279 (18) & 0.16 & 1.8389 (40) & 0.274 (16) & 0.29 & Y & DS \\
\hline
L^a (e_0) & 0.04419 (46) & 1.947 (97) & 0.49 & 0.04413 (46) & 1.954 (97) & 0.64 & Y & All \\
\hline
L^a (s^0) & 0.0352 (25) & 0.98 (31) & 0.56 & 0.0353 (25) & 0.97 (31) & 0.55 & Y & All \\
\hline
\sigma^2 (\bar{q}) & 0.0359 (25) & 1.15 (25) & 0.10 & 0.0349 (25) & 1.22 (26) & 0.04 & N & MF \\
\hline
\sigma^2 (\bar{q}) & 0.0195 (15) & 1.23 (16) & 0.59 & 0.0188 (14) & 1.28 (16) & 0.06 & N & MF \\
\hline
\sigma^2 (q^2) & 0.129 (25) & 0.88 (12) & 0.44 & 0.137 (26) & 0.92 (12) & 0.29 & N & DS \\
\hline
\bar{q} & 0.8168 (53) & -2.18 (62) & 0.20 & 0.8196 (51) & -2.41 (62) & 0.01 & N & MF \\
\hline
\bar{q}^2 & 0.863 (17) & -0.225 (61) & 0.44 & 0.873 (16) & -0.258 (59) & 0.09 & N & DS \\
\hline
q^2 & 0.7029 (64) & -2.32 (78) & 0.20 & 0.7059 (63) & -2.58 (78) & 0.02 & N & MF \\
\hline
\bar{q}^2 & 0.752 (21) & -0.239 (76) & 0.48 & 0.764 (20) & -0.278 (74) & 0.08 & N & DS \\
\hline
P^\max & 3.58 (17) & 0.00974 (67) & 0.04 & 3.60 (17) & 0.00958 (65) & 0.08 & Y & All \\
\hline
P^\max & - & L = 6, 8, 12: & 4.39 (39) & - & 0.0077 (11) & 0.66 & Y & All \\
\hline
P(0) & 0.168 (35) & 2.8 (3.3) & 0.13 & 0.002 (07) & 14.9 (2.1) & 10^{-6} & N & MF \\
\hline
P(0) & 0 & 0.36 (22) & 0.38 (36) & 0.17 & 0.76 (39) & 1.21 (24) & 10^{-11} & N & DS \\
\hline
\end{array}
\]

Table 2: Fits.