Evidence for nontrivial ground state structure of 3d $\pm J$ spin glasses

Alexander K. Hartmann
hartmann@tphys.uni-heidelberg.de
Institut für theoretische Physik, Philosophenweg 19,
69120 Heidelberg, Germany
Tel. +49-6221-549449, Fax. +49-6221-549331

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Ground states of 3d EA Ising spin glasses are calculated for sizes up to 14^3 using a combination of genetic algorithms and cluster-exact approximation. The generation of a large number of ground states allows the computation of the distribution $P(|q|)$ of overlaps. For increasing size the width of $P(|q|)$ converges to a nonzero value, indicating a nontrivial ground state structure for short range Ising spin glasses.

Keywords (PACS-codes): spin glasses (75.10.Nr), ground state calculation (75.40.Mg), graph theory (02.10.Jf).

Introduction The behavior of the Edwards-Anderson (EA) $\pm J$ Ising spin glass with short range (i.e. realistic) interactions is still not well understood. The EA Ising spin glass is a system of N spins $\sigma_i = \pm 1$, described by the Hamiltonian

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

The sum $\langle i,j \rangle$ goes over nearest neighbors. In this letter we consider 3d cubic systems with periodic boundary conditions, $N = L^3$ spins and the exchange interactions (bonds) take $J_{ij} = \pm 1$ with equal probability under the constraint $\sum_{<i,j>} J_{ij} = 0$.

One of the most important questions is, whether many pure states exist for realistic spin glasses. For the infinite ranged Sherrington-Kirkpatrik (SK) Ising spin glass this question was answered positively by the replica-symmetry-breaking mean-field (MF) scheme by Parisi [1]. Some authors [2] disbelieve that the MF theory is consistent for realistic spin glasses but no decision about the existence of many pure states is made. But also a complete different model is proposed: the Droplet Scaling (DS) theory [3–7] suggests that only two pure states (related by a global flip) exist and that the most relevant excitations are obtained by reversing large domains of spins (the droplets). From the ground state point of view the existence of many pure states means that between two ground states arbitrary differences are possible. Otherwise two ground states would only differ by the spin orientations in some finite domains, which is always possible in the $\pm J$ model because of the discrete structure of the interaction distribution.

While earlier Monte Carlo (MC) simulations [8] suffer from small system sizes or equilibrium problems [9], recent results of simulations [10] at finite temperature seem to find evidence for the MF picture. In [11] ground states were calculated using multicanonical MC sampling, but no decision between MF and DS could be made because of too small system sizes.

In this letter we show our results for the direct calculation of spin glass ground states using a hybrid of genetic algorithms [12,13] and cluster-exact approximation (CEA) [14]. Because the computation of spin glass ground states belongs to the class of NP problems, it is a tough computational task. Using this new algorithms it is possible the first time to calculated ground states of adequate size (up to $L = 14$) and with sufficient statistics (especially for the largest sizes). It is possible to calculate many strictly statistical independent configurations (replicas). In contrast to Monte Carlo methods one does not encounter ergodicity problems. It is importance to notice that no kind of temperature is involved in our method.

By calculating the distribution of overlaps for different sizes L we found that the width of the distribution remains finite for the infinite system which is an indication for the existence of many pure ground states.

Observables For a fixed realization $J = \{J_{ij}\}$ of the exchange interactions and two replicas $\{\sigma_i^\alpha\}, \{\sigma_i^\beta\}$, the overlap [1] is defined as

$$q^{\alpha\beta} \equiv \frac{1}{N} \sum_i \sigma_i^\alpha \sigma_i^\beta \tag{2}$$

The ground state of a given realization is characterized by the probability density $P_J(q)$. Averaging over the realizations J, denoted by $[\,\cdot\,]_{av}$, results in (Z = number of realizations)

$$P(q) \equiv [P_J(q)]_{av} = \frac{1}{Z} \sum_J P_J(q) \tag{3}$$

Because no external field is present the densities are symmetric: $P_J(q) = P_J(-q)$ and $P(q) = P(-q)$. So only averages of $|q|^n$ are relevant:

$$\overline{|q_J|^n} \equiv \int_{-1}^{1} |q|^n P_J(q) dq \tag{4}$$

$$\overline{|q|^n} \equiv \int_{-1}^{1} |q|^n P(q) dq \tag{5}$$

The Droplet model predicts that only two pure states exist, implying that $P(q)$ converges for $L \to \infty$ to

$P(q) = \frac{1}{2}(\delta(q-\overline{|q|}) + \delta(q+\overline{|q|}))$ (we don't indicate the L dependence by an index), while in the MF picture the density remains nonzero for a range $-q_1 \leq q \leq q_1$ with peaks at $\pm q_{\max}$ ($0 < q_{\max} \leq q_1$). Consequently the variance

$$\sigma^2(|q|) \equiv \int_{-1}^{1} (\overline{|q|} - |q|)^2 P(q) dq = \overline{|q|^2} - \overline{|q|}^2 \tag{6}$$

stays finite for $L \to \infty$ in the MF pictures ($\sigma^2(|q|) = a_1 + a_2/L^3$) [11] while $\sigma^2(|q|) \sim L^{-y} \to 0$ according the DS approach. Here y is the zero-temperature scaling exponent [3] denoted Θ in [5,6].

We have measured the energy per spin e as well. Additionally to the usual fits other scaling corrections were discussed [12], including an exponential one ($e = a_\infty + a_1 \exp(-a_2 L)$) [11].

Results We performed ground state calculations for sizes L =3, 4, 5, 6, 8, 10, 12, 14. For each size we used different parameter sets, which were determined in a way, that no decrease of the energy could be found by doubling the running time. We calculated from 100 realizations for $L = 14$ up to 4000 realizations for $L = 3$. One $L = 14$ run needs typically 540 CPU-min on a 80MHz PPC601 processor (70 CPU-min for $L = 12$, ..., 0.2 CPU-sec for $L = 3$). For each realization 40 independent runs were made. Each run resulted in one configuration, which was stored, if it exhibited the ground state energy. For $L = 14$ this resulted in an average of 13.8 states per realization having the lowest energy while for $L = 3$ on average 39.9 states were stored. Details of the algorithm, simulation parameters and more results will be given in [15].

The results of the calculations are summarized in table I. Because we want to estimate the quality of the minimization procedure, we discuss the average ground state energy at first.

We extrapolate to $L \to \infty$ by using finite size scaling (FSS) fits. For least-square fitting the Levenberg-Marquard Method implemented in [16] is used, which gives also the probability Q of finding such a bad dataset (provided that the fit function is exact). Values of $Q > 0.1$ seem acceptable, if $Q < 10^{-3}$ a fit is supposed to be not valid.

Table II show the results for FFS fits for the following three functions:

$$f(L) \equiv a_\infty + a_1/L^3 \tag{7}$$

$$g(L) \equiv a_\infty + a_1 L^{-a_2} \tag{8}$$

$$h(L) \equiv a_\infty + a_1 \exp(-a_2 L) \tag{9}$$

For $\sigma^2(|q|)$ results for fits of the first two functions $f(L)$ and $g(L)$ (with a_∞ set to 0) are given in the same table as well.

We get a ground state energy of the infinite system of $e_\infty = a_\infty = -1.7868(3)$ (Q=0.20) resp. $e_\infty = a_\infty = -1.7876(3)$ with $a_2 = 2.84(3)$ (Q=0.77). The exponential fit is ruled out (Q=10^{-7}). Our ground state energy is lower than some previous results: $e_\infty = -1.75$ [17], $e_\infty = -1.76(2)$ [18], and of the same magnitude as the most accurate study so far $e_\infty = -1.7863(4)$ [12]. In [11] a lower value was found ($e_\infty = -1.839(4)$), but that study suffers from only seven $L = 12$ realizations. By comparison with these calculations for the different sizes L we can see that we have obtained always the same or a slightly lower (i.e. better) energy (except for $L = 12$ in [11]). So we are confident that we get very close to the true ground states using our approximation procedure.

The result for the energy, together with the fits for $f(L)$ and $g(L)$, is displayed in fig. 1. In [12] a L^{-3} fit was ruled out, instead a $L^{-2.97}$ fit was preferred. Our data shows a similar tendency, but the data for the energy is not accurate enough to decide this question. The second fit supports the MF picture too, because the value $y = a_2 = 2.84$ of the exponent exceeds the limit $y \leq (d-1)/2$ proposed by DS. Since the aim of this letter is to distinguish whether only two or infinitely many pure ground states exist, we proceed by analyzing the order parameter distribution $P(|q|)$.

In fig. 2 the probability density of the overlap is displayed for $L = 6$ and $L = 12$. Each realization enters the sum with the same weight, even if different numbers of ground states were available for the calculation of $P_J(|q|)$. Only a small difference for high q-values is visible, which is reflected also in a slight shift of the average to smaller values (see table I). But especially for $|q| \leq 0.8$ no significant reduction in the probability is visible. So many different pure ground states still exist for higher L. This result is supported quantitatively by the variances of $|q|$ as function of L which are shown in fig. 3. For all sizes the magnitude of the values is higher than in [11], indicating that their MC algorithm does not explore the configuration space sufficiently. Our fits show a higher probability for the existence of many pure states ($Q = 0.79$) against the two state picture ($Q = 0.09$).

If we exclude the small system sizes ($L = 3, 4$) from the fit, the fit for $g(L)$ becomes more likely ($Q = 0.51$), but the exponent $a_2 = 0.13(3)$ is smaller than the prediction $y \approx 0.2$ [4]. This small magnitude of y and the visual impression for $L > 4$ in fig. 3 support the notion of a nonzero width of $P(|q|)$ for $L \to \infty$ as well.

Another interesting questions is whether the difference between the density functions of single realizations and the average $P(|q|)$ remains nonzero for increasing L, i.e. whether the short range spin glasses exhibit lack of self-averaging. But presently we have not computed enough ground states per realization for large sizes to address this question.

Conclusion By the calculation of ground states using genetic cluster-exact approximation we find evidence for the existence of many pure states in short range $\pm J$ spin glasses. For spin glasses with Gaussian distribution the ground state is not degenerate, $P_L(|q)|)$ are both the same in the MF and DS picture. The predictions begin to be different only by turning on the temperature. We expect the same behavior as for the $\pm J$ model if one allows deviations of order one from the true ground state energy, but for that system type ground states are much harder to calculate using our algorithm.

The major drawback of our method is that the ground states are not exact, but for these lattice sizes this is beyond the power of actual algorithms and computers. By comparison with other results and due to our experiences from changing the algorithm parameters we feel confident that the energy of our states is very close to the true ground state energy. In the moment we do not have enough ground states per realization calculated (for higher L) to decide whether short range spin glasses exhibit lack of self-averaging or not.

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Captions

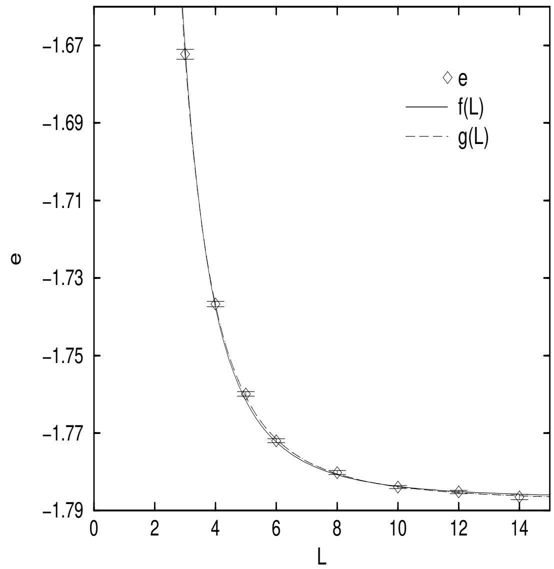
Fig. 1 Ground state energy of 3d $\pm J$ Ising spin glass for linear dimensions $3 \leq L \leq 14$ and FSS fits assuming either Mean Field (MF) $f(L)$ (7) or Droplet Scaling (DS) $g(L)$ (8) behavior. The DS fit is slightly better, but the exponent of the L^{-a_2} decay is $a_2 = 2.84$, which is much larger than the upper limit of $d/2 = 1.5$ proposed by DS.

Fig. 2 Distribution of overlaps $P(|q|)$ (3) for ground states of 3d $\pm J$ Ising spin glass for $L = 6, 12$. Only for large values of q a difference is visible, so even for large system there is a finite probability of overlap $q = 0$. The lines are guides for the eyes only.

Fig. 3 Variances $\sigma^2(|q|)$ (6) of the distributions of overlaps $P(|q|)$ as function of L for $3 \leq L \leq 14$. The function seems to converge to a nonzero limit for $L \to \infty$. Two fits assuming either MF (7) ($\sigma^2(|q|) \to c > 0$ for $L \to \infty$) or DS 8) ($\sigma^2(|q|) \to 0$ for $L \to \infty$) behavior are given. The MF picture is more likely ($Q_{MF} = 0.77 > 0.09 = Q_{DS}$, see text). So the width of $P(|q|)$ seems to remain finite for $L \to \infty$, which implies the existence of many pure ground states in the infinite system.

Tab. 1 Results of calculations of ground states for L^3 $\pm J$ Ising spin glass ($3 \leq L \leq 14$): e: energy, $\overline{|q|}$: mean value of distribution of overlaps $P(|q|)$ (3), $\sigma^2(|q|)$: variance of $P(|q|)$. The values for e are as good as the best known results, indicating that our states are very close to the real ground states.

Tab. 2 Result of FSS-fits for energy e and variance $\sigma^2(|q|)$ of $P(|q|)$ as function of L: $f(L)$ (7) assumes MF and $g(L)$ (8) DS behavior. $h(L)$ is an exponential fit for the energy. The parameters a_∞, a_1, a_2 are given by definitions of the functions. Q measures the quality of the fit (see text). For the energy both MF and DS scenarios are possible, but the value of the exponent $a_2 = 2.84$ for DS is in contradiction to the upper limit $d/2 = 1.5$. For the variance the MF fit is more likely.



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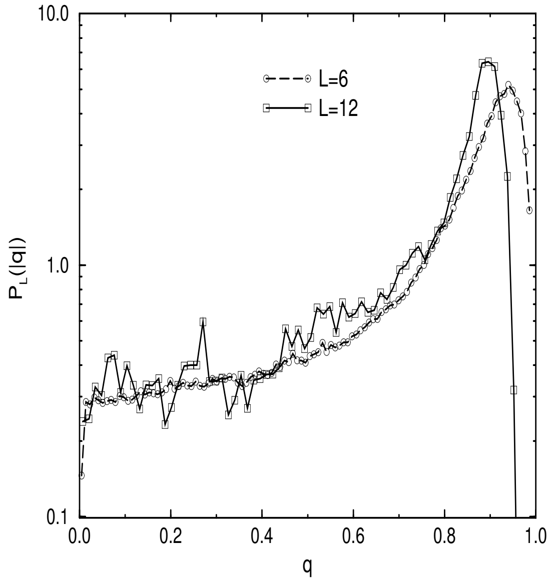

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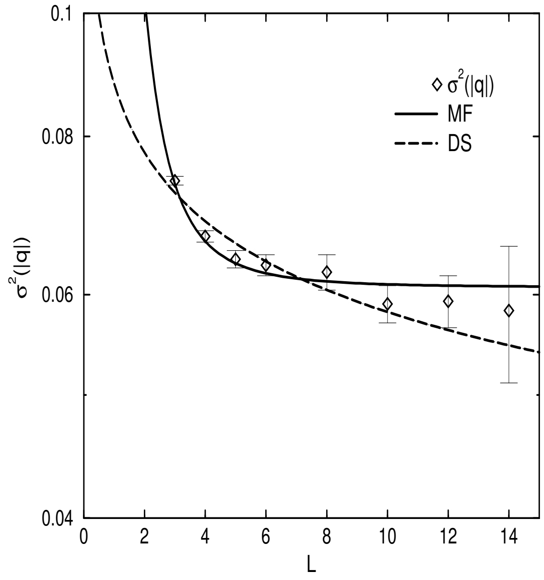

FIG. 3. Variances $\sigma^2(|q|)$ (6) of the distributions of overlaps $P(|q|)$ as function of L for $3 \leq L \leq 14$. The function seems to converge to a nonzero limit for $L \to \infty$. Two fits assuming either MF (7) ($\sigma^2(|q|) \to c > 0$ for $L \to \infty$) or DS 8) ($\sigma^2(|q|) \to 0$ for $L \to \infty$) behavior are given. The MF picture is more likely ($Q_{MF} = 0.77 > 0.09 = Q_{DS}$, see text). So the width of $P(|q|)$ seems to remain finite for $L \to \infty$, which implies the existence of many pure ground states in the infinite system.

L	e	$\overline{\|q\|}$	$\sigma^2(\|q\|)$
3	-1.6731(19)	0.742(3)	0.0731(9)
4	-1.7370(9)	0.748(3)	0.0669(9)
5	-1.7603(8)	0.743(4)	0.0628(13)
6	-1.7723(7)	0.742(4)	0.0632(15)
8	-1.7802(5)	0.726(6)	0.0621(20)
10	-1.7836(3)	0.735(4)	0.0585(16)
12	-1.7851(4)	0.709(8)	0.0593(30)
14	-1.7865(7)	0.707(17)	0.0583(72)

TABLE I. Results of calculations of ground states for L^3 $\pm J$ Ising spin glass ($3 \leq L \leq 14$): e: energy, $\overline{|q|}$: mean value of distribution of overlaps $P(|q|)$ (3), $\sigma^2(|q|)$: variance of $P(|q|)$. The values for e are as good as the best known results, indicating that our states are very close to the real ground states.

	fit	a_∞	a_1	a_2	Q
e	f(L)	-1.7869(3)	3.15(5)	-	0.20
e	g(L)	-1.7876(3)	2.60(15)	2.84(5)	0.77
e	h(L)	-1.7846(8)	1.01(17)	0.75(5)	10^{-7}
$\sigma^2(\lvert q\rvert)$	f(L)	0.0608(6)	0.34(3)	-	0.79
$\sigma^2(\lvert q\rvert)$	g(L)	0	0.088(4)	0.18(3)	0.09

TABLE II. Result of FSS-fits for energy e and variance $\sigma^2(|q|)$ of $P(|q|)$ as function of L: $f(L)$ (7) assumes MF and $g(L)$ (8) DS behavior. $h(L)$ is an exponential fit for the energy. The parameters a_∞, a_1, a_2 are given by definitions of the functions. Q measures the quality of the fit (see text). For the energy both MF and DS scenarios are possible, but the value of the exponent $a_2 = 2.84$ for DS is in contradiction to the upper limit $d/2 = 1.5$. For the variance the MF fit is more likely.