Scaling of stiffness energy for 3d $\pm J$ Ising spin glasses

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Large numbers of ground states of 3d EA Ising spin glasses are calculated for sizes up to 10^3 using a combination of a genetic algorithm and Cluster-Exact Approximation. A detailed analysis shows that true ground states are obtained. The ground state stiffness (or domain wall) energy Δ is calculated. A $|\Delta| \sim L^{\Theta_S}$ behavior with $\Theta_S = 0.19(2)$ is found which strongly indicates that the 3d model has an equilibrium spin-glass-paramagnet transition for non-zero T_c.

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Introduction The question whether three dimensional (3d) Ising spin glasses [1] have a non-zero transition temperature T_c is still not answered beyond all doubts. The best evidence for ordering below a finite T_c was found recently [2,3] by extensive Monte Carlo Simulations. But the authors could not completely rule out other scenarios.

In this work we address the question by calculating the stiffness or domain wall energy $\Delta = E^a - E^p$ which is the difference between the ground state energies E^a, E^p for antiperiodic and periodic boundary conditions [4,5]. This quantity was studied earlier only for very small system sizes using $T = 0$ transfer matrix methods [4,6] and Monte Carlo simulations [5]. The stiffness energy shows a finite size dependence

$$|\Delta| \sim L^{\Theta_S} \tag{1}$$

where L is the linear system size. A positive value of the stiffness exponent Θ_s indicates the existence of a spin glass phase for non-zero temperature. Since the direct calculation of ground states for 3d spin glasses is NP-hard there is no polynomial algorithm available. In our work we calculate ground states using a combination of Cluster-Exact Approximation (CEA) [7] and a genetic algorithm [8,9]. Similar calculations proved that the 2d spin glass, where exact ground states can be calculated using a polynomial time algorithm, exhibits no ordering for $T > 0$ [10].

We investigate systems of N spins $\sigma_i = \pm 1$, described by the Hamiltonian

$$H \equiv -\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j \tag{2}$$

In this letter we consider 3d cubic systems with periodic boundary conditions, $N = L^3$ spins and the nearest neighbor interactions (bonds) take independently $J_{ij} = \pm 1$ with equal probability. The antiperiodic boundary conditions for calculating E^a are realized by inverting one plane of bonds.

Algorithm The algorithm for the calculation bases on a special genetic algorithm [8,9] and on Cluster-Exact Approximation [7] which is an sophisticated optimization method. Now a short sketch of these algorithms is given, because later the influence of different simulation parameters on the results is discussed.

The genetic algorithm starts with an initial population of M_i randomly initialized spin configurations (= *individuals*), which are linearly arranged in a ring. Then $\nu \times M_i$ times two neighbors from the population are taken (called *parents*) and two offsprings are created using a triadic crossover: a mask is used which is a third randomly chosen (usually distant) member of the population with a fraction of 0.1 of its spins reversed. In a first step the offsprings are created as copies of the parents. Then those spins are selected, where the orientations of the first parent and the mask agree [11]. The values of these spins are swapped between the two offsprings. Then a mutation with a rate of p_m is applied to each offspring, i.e. a fraction p_m of the spins is reversed.

Next for both offsprings the energy is reduced by applying CEA. The method constructs iteratively and randomly a non-frustrated cluster of spins, whereas spins with many unsatisfied bonds are more likely to be added to the cluster. For 3d $\pm J$ spin glasses each cluster contains typically 58 percent of all spins. The non-cluster spins act like local magnetic fields on the cluster spins. For the spins of the cluster an energetic minimum state can be calculated in polynomial time by using graph theoretical methods [12–14]: an equivalent network is constructed [15], the maximum flow is calculated [16,17][1] and the spins of the cluster are set to their orientations leading to a minimum in energy. This minimization step

[1] Implementation details: We used Tarjan's wave algorithm together with the heuristic speed-ups of Träff. In the construction of the *level graph* we allowed not only edges (v, w) with level(w) = level(v)+1, but also all edges (v, t) where t is the sink. For this measure, we observed an additional speed-up of roughly factor 2 for the systems we calculated.

is performed $n_{\min}$ times for each offspring.

Afterwards each offspring is compared with one of its parents. The pairs are chosen in the way that the sum of the phenotypic differences between them is minimal. The phenotypic difference is defined here as the number of spin positions where the two configurations differ. Each parent is replaced if its energy is not lower (i.e. better) than the corresponding offspring. After this whole step is done $\nu \times M_i$ times the population is halved: From each pair of neighbors the configuration which has the higher energy is eliminated. If not more than 4 individuals remain the process is stopped and the best individual is taken as result of the calculation.

The following representation summarizes the algorithm.

```
algorithm genetic CEA({J_ij}, M_i, ν, p_m, n_min)
begin
    create M_i configurations randomly
    while (M_i > 4) do
    begin
        for i = 1 to ν × M_i do
        begin
            select two neighbors
            create two offsprings using triadic crossover
            do mutations with rate p_m
            for both offsprings do
            begin
                for j = 1 to n_min do
                begin
                    construct unfrustrated cluster of spins
                    construct equivalent network
                    calculate maximum flow
                    construct minimum cut
                    set orientations of cluster spins
                end
                if offspring is not worse than related parent
                then
                    replace parent with offspring
            end
        end
        half population; M_i = M_i/2
    end
    return one configuration with lowest energy
end
```

The whole algorithm is performed n_R times and all configurations which exhibit the lowest energy are stored, resulting in n_g statistical independent ground state configurations.

This algorithm was already applied to examine the ground state structure of 3d spin glasses [18].

Results For each system size we tried many different combinations of the simulation parameters m_i, ν, n_{min}, p_m for some sample systems. The final parameters where determined in a way, that by using four times the numerical effort no reduction in energy was obtained. Here $p_m = 0.2$ and $n_R = 10$ were used for all system sizes. Table I summarizes the parameters. Also the typical computer time τ per ground state computation on a 80 MHz PPC601 is given.

Ground states were calculated for system sizes up to $L = 10$ for N_L independent realizations (see table I) of the random variables. For each realization the ground states with periodic and antiperiodic boundary condition were calculated. One can extract from the table that the $L = 10$ systems alone required 1990 CPU-days. Using these parameters on average $n_g > 8$ ground states were obtained for every system size L using $n_R = 10$ runs per realization.

In the second part of this paragraph a detailed analysis of the influence of the simulation parameters is presented. But at first the results for the stiffness energy are shown in Fig. 1.

Also given is a fit $\Delta(L) \sim L^{\Theta_S}$ which results in $\Theta_S = 0.19(2)$. Because of the large sample sizes the error bars are small enough, so we can be pretty sure that $\Theta_S > 0$. It means that the 3d EA spin glass exhibits a non-zero transition temperature T_c. Since Δ is a small difference of large values, we have to be sure that we calculate true ground states in order to believe our results.

Fig. 2 shows the average energy per spin for 90 test systems of size $L = 6$ as function of the product of the simulation parameters $M_i \times \nu \times n_{\min}$ which is proportional to the computer time since all other parameters are kept fixed. The sets $(M_i, \nu, n_{\min}) = (8, 1, 1)$, $(8, 2, 1)$, $(8, 4, 1)$ and $M_i = 8, 16, 32, 64, 128$ for $(\nu, n_{\min}) = (4, 2)$ were investigated. The energy decreases with increasing numerical effort. For the sets with $M_i > 32$ the energy does not decrease further. We compared our results for the test systems with exact ground states which were obtained using a Branch-and-Cut program [19,20]. For the two largest parameter sets the genetic CEA algorithm found the true ground states for all 90 systems! The same result was obtained for $L = 4$ as well.[2] So we can be sure that genetic CEA and our method of choosing the parameters lead to true ground states or at least to states very close to true ground states.

The choice of the simulation parameters has only a small influence on the the energy for large values of M_i. A more sensitive indicator is the stiffness energy as function of the simulation parameters. This is shown for the same 90 test systems in Fig. 3. We also calculated the exact ground states for the realizations with antiperiodic boundary conditions and found again that genetic CEA

[2] For $L > 6$ the Branch-and-Cut needs to much computer time because of the exponential time complexity.

produced the exact results for the parameter sets with $M_i > 32$.

Since the parameters were tested always on a restricted number of systems we can not absolutely be sure that genetic CEA always finds true ground states. Since we are interested in the stiffness energy Δ we take a closer look at it. If states very close to the true ground states are found, the resulting stiffness energy may be for some realizations smaller and for others higher than the correct result. So we expect that the effect should cancel out with increasing sample size.

This is confirmed by Fig. 4 where the stiffness energy as function of the sample size N_L is shown for three different parameter sets (8,4,1), (16,4,2) and (64,4,2). The stiffness energies found using the second set, where we are very close to the true ground states, converges to the values found using the third set. The values found using the first set do not converge. So even by calculating states very close to the true ground states on gets very good estimates of the stiffness energy.

Conclusion Results have been presented from calculations of a large number of ground states of 3d Ising spin glasses. They were obtained using a combination of Cluster-Exact Approximation and a genetic algorithm. The finite size behavior of the stiffness energy has been investigated. Is has been shown that states which were obtained are true ground states or are at least very close to them. Even if one calculates only almost true ground states the resulting value of the stiffness energy is very reliable. It has been found that the stiffness energy increases with system size. So strong evidence has been obtained that the 3d Ising spin glass has a non-zero transition temperature T_c.

The only uncertainty arises from the fact that these calculations were restricted to systems sizes $L \leq 10$, it means anyway that the number of spins is more than 200 times larger than for the systems examined before ($L = 6$) [4–6]. Additionally in contrast to former publications it is possible to estimate the quality of the low energy states.

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L	M_i	ν	$n_{\min}$	τ (sec)	N_L
4	32	3	1	1	10000
6	64	4	2	20	10000
8	64	4	5	140	12469
10	128	6	10	1920	4480

TABLE I. Simulation parameters: L = system size, M_i = initial size of population, ν = average number of offsprings per configuration, $n_{\min}$ = number of CEA minimization steps per offspring, τ = average computer time per ground state on a 80MHz PPC601, N_L = number of realizations of the random variables.

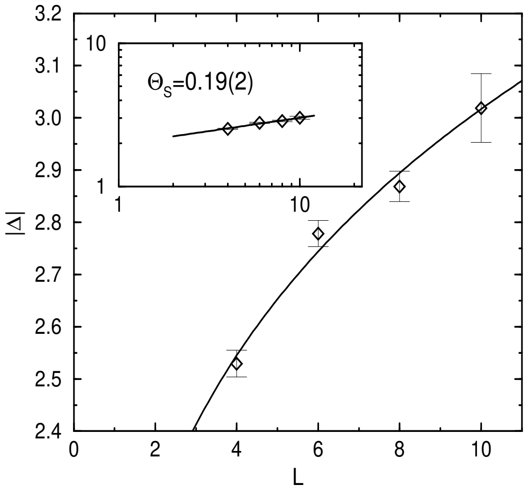

FIG. 1. Stiffness energy Δ as function of system size L. The line represents the function $\Delta(L) = aL^{\Theta_S}$ with $\Theta_S = 0.19(2)$. The inset shows the same figure on log-log scale. The increase of Δ with system size indicates, that in 3d Ising spin glasses an ordered phase exists below a non-zero temperature T_c.

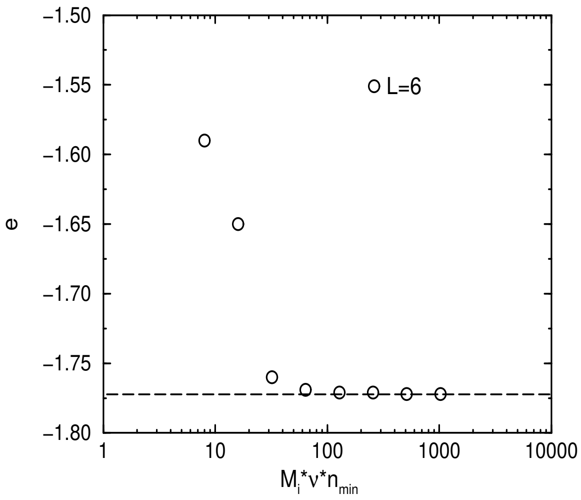

FIG. 2. Average energy as function of simulation parameters $M_i * \nu * n_{\min}$ for 90 systems of size $L = 6$. With increasing numerical effort the energy lowers. For the two rightmost points ($M_i = 64, 128$; $\nu = 4$; $n_{\min} = 2$) no further decrease of the energy is possible. A comparison with exact ground state calculations using a Branch-and-Cut algorithm confirms that in fact for all 90 systems the true ground states are found!

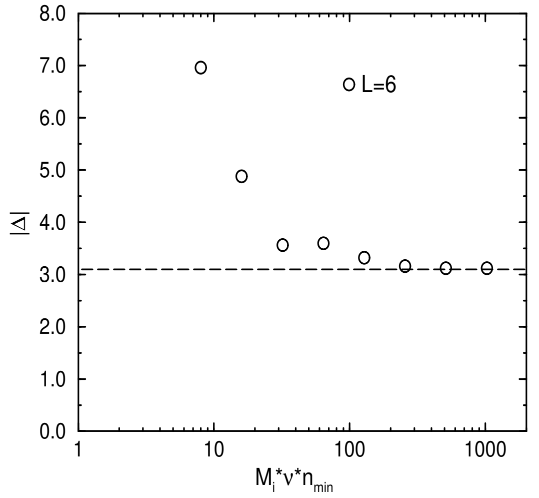

FIG. 3. Average stiffness energy Δ as function of simulation parameters $M_i * \nu * n_{\min}$ for 90 systems of size $L = 6$. This quantity is more sensitive to changes in the simulation parameters than the energy.

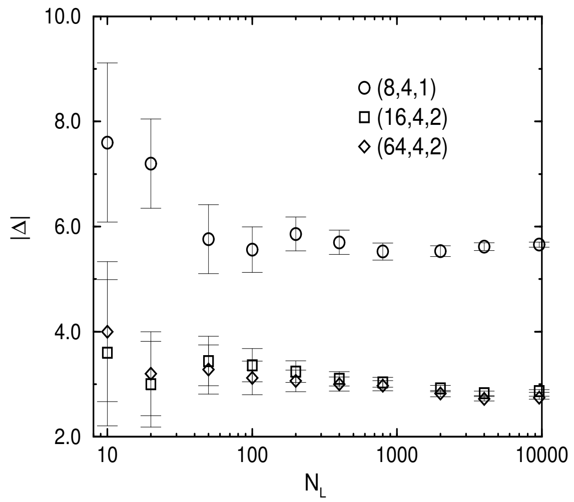

FIG. 4. Average stiffness energy Δ as function of sample size N_L for three different sets of simulation parameters for system size $L = 6$. If the calculated states are close to the true ground state (set (16,4,2)) the resulting stiffness energy is very close to the true value and converges towards it with increasing sample size. (The 90 samples from Fig. 3 are not included in the samples here, so the values for $N_L = 100$ are different from the results above.)