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Are Ground States of 3d $\pm J$ Spin Glasses ultrametric ?

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Abstract. – Ground states of 3d EA Ising spin glasses are calculated for sizes up to 14^3 using a combination of a genetic algorithm and Cluster-Exact Approximation. Evidence for an ultrametric structure is found by studying triplets of independent ground states where one or two values of the three overlaps are fixed.

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. Introduction to spin glasses can be found for example in [1, 2]. 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 $\sum_{\langle i,j \rangle} J_{ij} = 0$.
This work addresses the question whether the ground states of this system exhibit an *ultrametric* structure: The distances $d^{\alpha\beta}$ between states do not only satisfy the triangular inequality $d^{\alpha\beta} \le d^{\alpha\gamma} + d^{\gamma\beta}$ but the stronger ultrametric inequality $d^{\alpha\beta} \le \max(d^{\alpha\gamma}, d^{\gamma\beta})$ as well. For an introduction to ultrametricity see [3]. The mean field solution [4] of the infinite-dimensional SK-model [5] shows an ultrametric state structure [6, 7]. Numerical work on the subject can be found in [8, 9]. For finite dimensional systems numerical evidence for ultrametricity at finite temperature but below the transition Temperature T_G was found in four dimensions [10, 11]. First attempts to find ultrametricity in three dimensions by simulation at finite temperature are given in [12, 13].
Here the first time ground states of realistic spin glasses are analyzed regarding their ultrametric structure. The ground state structure tells for example whether the usual cluster algorithms for simulating a system at *finite temperature* work efficiently [14].

In this letter we show our results for the direct calculation of spin glass ground states using a hybrid of genetic algorithms [15, 16] and Cluster-Exact Approximation (CEA) [17]. Because the computation of spin glass ground states belongs to the class of NP-hard 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.

Observables. – For a fixed realization $J = \{J_{ij}\}$ of the exchange interactions and two replicas $\{\sigma_i^\alpha\}, \{\sigma_i^\beta\}$, the overlap [4] 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 we calculate only functions $P_J(|q|)$ and $P(|q|)$.
The overlap measures the distance between two states. This can be reflected by defining a distance function

$$d^{\alpha\beta} \equiv 0.5(1 - q^{\alpha\beta}) \tag{4}$$

with $0 \leq d^{\alpha\beta} \leq 1$. For three replicas α, β, γ the usual triangular inequality reads $d^{\alpha\beta} \leq d^{\alpha\gamma} + d^{\gamma\beta}$. Expressed in terms of q it becomes

$$q^{\alpha\beta} \geq q^{\alpha\gamma} + q^{\gamma\beta} - 1 \tag{5}$$

In an *ultrametric* space [3] the triangular inequality is replaced by a stronger one $d^{\alpha\beta} \leq \max(d^{\alpha\gamma}, d^{\gamma\beta})$ or equivalently

$$q^{\alpha\beta} \geq \min(q^{\alpha\gamma}, q^{\gamma\beta}) \tag{6}$$

An example of an ultrametric space is the set of leaves of a binary tree: The distance between two leaves is defined by the number of edges on a path between the leaves. Let $q_1 \leq q_2 \leq q_3$ be the overlaps $q^{\alpha\beta}$, $q^{\alpha\gamma}$, $q^{\gamma\beta}$ ordered according their sizes. By writing the smallest overlap on the left side in Equation (6), one realizes that two of the overlaps must be equal and the third may be larger or the same: $q_1 = q_2 \leq q_3$
In a finite size system this relation may be violated. We use two ways of determining whether ground states of realistic spin glasses become more and more ultrametric with increasing size L:

The difference

$$\delta q \equiv q_2 - q_1 \tag{7}$$

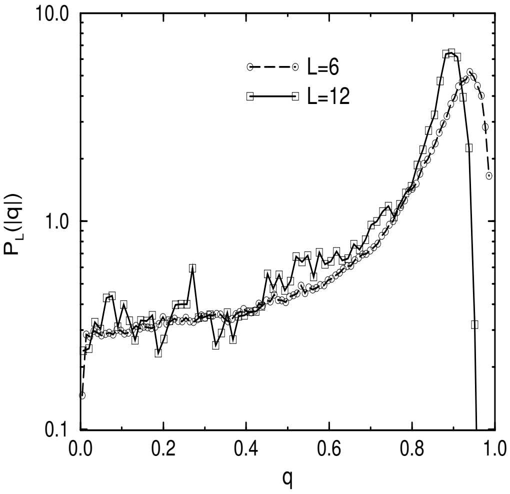
is calculated for all triplets. Because we want to exclude the influence of the absolute size of the overlaps the third overlap is fixed: $q_3 = q_{fix}$. In practice only overlap triples are used where $q_3 \in [q_{fix}, q_{fix2}]$ holds to obtain sufficient statistics . With increasing size L the distribution $P(\delta q)$ should tend to a Dirac delta function [9].

If two overlaps are fixed ($q^{\alpha\gamma} = q^{\beta\gamma} = q_{fix}$, in practice $q^{\alpha\gamma}, q^{\beta\gamma} \in [q_{fix}, q_{fix2}]$), equation (5) implies $q \equiv q^{\alpha\beta} \geq 2q_{fix} - 1$ while ultrametricity implies $q \geq q_{fix}$ which is stronger if $q_{fix} < 1$ [10]. The distribution $P_{2-fix}(q)$ of the third overlap is used to characterize the ultrametricity of a system. The fraction of the distribution outside $[q_{fix}, q_{EA}]$

$$\begin{aligned} I_L \quad \equiv \quad & \int_{-1}^{q_{fix}} P_{2-fix}(q)(q-q_{fix})^2\, dq \\ & + \int_{q_{EA}}^{1} P_{2-fix}(q)(q-q_{EA})^2\, dq \end{aligned} \tag{8}$$

(see [10]) should vanish for $L \to \infty$ in an ultrametric system.

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 for some sample systems. Using our parameters results roughly in an exponential increase of the running time as function of L. One $L = 14$ run needs typically 540 CPU-minutes on a 80MHz PPC601 processor (70 CPU-minutes for $L = 12, \ldots, 0.2$ CPU-seconds for $L = 3$). Details of the algorithm, simulation parameters and more results will be given in [18].
For small system sizes $L = 4, 6$ we could compute for 200 randomly selected systems exact ground states with a Branch-and-Cut method [19, 20] using a program which generously was made available by the group of M. Jünger in Cologne. In ALL cases our method found the exact ground states as well! So we are pretty sure that our algorithm computes true ground states or at least states very close to true ground states even for larger systems.
We calculated from 136 realizations for $L = 14$ up to 8900 realizations for $L = 3$. For each realization up to 40 independent runs were made (up to 80 for some large systems). 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 $n_{gs} = 14.9$ states per realization having the lowest energy while for $L = 3$ on average $n_{gs} = 39.97$ states were stored. This reduction of n_{gs} means that with increasing system size true ground states are harder to find, but not that the number of existing ground states is reduced:
In fig. 1 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 can be observed. But especially for $|q| \leq 0.8$ no significant reduction in the probability is visible. So with increasing sizes the width of the distribution remains finite [21]. It means that realistic spin glasses have many arbitrary different ground states which are arranged in a complex structure.
To investigate whether this structure is even ultrametric we have calculated the quantity δq (see equation (7)) for all possible triplets with $q_3 \in [0.5, 0.6]$. To improve the statistics we used the absolute value of all overlaps. The distribution $P(\delta q)$ is shown in fig. 2 for $L = 4, 10, 14$. Each realization enters the distribution with the same weight. With increasing system size



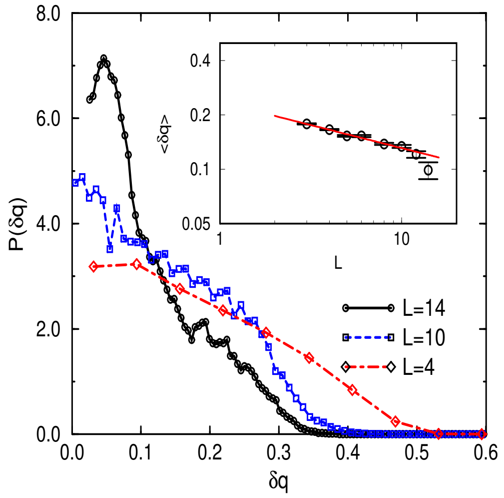


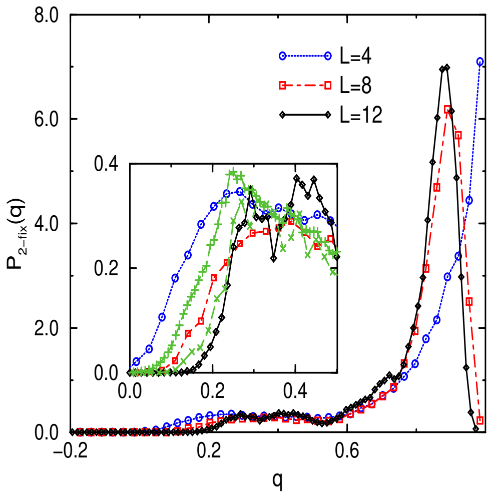
Fig. 1. – Distribution of overlaps $P(|q|)$ for ground states of 3d $\pm J$ Ising spin glass for $L = 6, 12$. Only for large values of q a difference is visible, so even for large systems there is a finite probability of overlap $q = 0$. The lines are guides for the eyes only.

Fig. 2. – Distribution $P(\delta q)$ for different system sizes $L = 4, 10, 14$ where $\delta q = q_2 - q_1$ and $q_1 \leq q_2 \leq q_3$ are triplets of absolute values of overlaps from independent triplets of ground states. Only triplets with $q_3 \in [0.5, 0.6]$ are used. For a infinite ultrametric system $\delta q = 0$ holds. With increasing system size the distributions get closer to $q = 0$ indicating the increasing ultrametricity of the ground states. The lines are guides for the eyes only. The inset shows the average value of δq as function of system size L. The straight line represents the function $\langle \delta q \rangle(L) = 0.235 \times L^{-0.255}$.

the distributions get closer to $q = 0$, indicating that the systems become more and more ultrametric. It is important to notice that the change in $P(\delta q)$ is not due to a change of $P(q)$ itself as it could not be excluded in [13]. Since the shape of $P(q)$ does not change very much with system size the effect on $P(\delta q)$ is caused by the increasing ultrametricity of the systems.

The same result is obtained by computing the average values of δq as function of the size L (see inset in fig. 2). One gets a similar figure by computing the variances of the distributions, but it is not shown here. The number of realizations is to small too perform a reasonable fit of the form $\langle \delta q \rangle(L) = \langle \delta q \rangle_\infty + cL^{-\alpha}$. So no decision is possible yet whether the average value converges to zero or not. We only provide the result of a fit with f_∞ set to zero. Then we get $c = 0.235(2)$ and $\alpha = 0.255(3)$. Since the data has a small negative curvature the assumption $\langle \delta q \rangle_\infty = 0$ seems reasonable.

By fixing two of the three overlaps of a triplet we have another way of checking ultrametricity. We took all triplets where two arbitrary overlaps fell into the interval $[0.5, 0.6]$ The resulting distributions $P_{2-fix}(q)$ of the third remaining overlap is shown in fig. 3 for $L = 4, 8, 12$. The triangular inequality gives $q > 0$ while ultrametricity leads to $q > 0.5$. The inset magnifies the values of $q \in [0.0, 0.5]$ for $L = 4, 6, 8, 10, 12$ (from left to right). The fraction of the distribution below $q = 0.5$ shrinks with increasing size. It is clearly visible that even the smallest sizes are far away from the triangular bond $q > 0$, but the system sizes are too small to decide whether



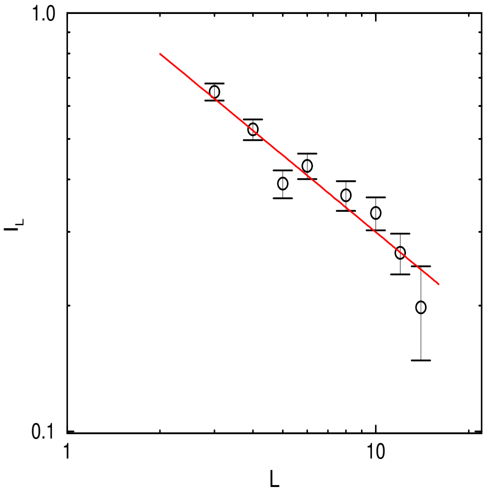


Fig. 3. – Distribution $P_{2-fix}(q)$ for different system sizes $L = 4, 8, 12$ where $q \in \{q_1, q_2, q_3\}$ and $q_1 \leq q_2 \leq q_3$ are triplets of overlaps from independent triplets of ground states. Only q-values of triplets are used where the two other overlaps are within the interval $[0.5, 0.6]$. Then for a infinite ultrametric system $q > 0.5$ holds, while for a metric system just $q > 0$ must hold. The small inset shows the part $q \in [0.0, 0.5]$ for $L = 4, 6, 8, 10, 12$ (from left to right). With increasing system size the fraction of the distribution below 0.5 shrinks, so the systems become more and more ultrametric. The lines are guides for the eyes only.

Fig. 4. – Integrated value $I_L = \int_{-1}^{0.5} P_{2-fix}(q)(q-0.5)^2\, dq + \int_{0.89}^{1} P_{2-fix}(q)(q-0.89)^2\, dq$ as function of system size L where $q \in \{q_1, q_2, q_3\}$ and $q_1 \leq q_2 \leq q_3$ are triples of overlaps from independent triples of ground states. Only q-values of triples where the two other overlaps are within the interval $[0.5, 0.6]$ are used. With increasing system size the fraction of the distribution outside $[0.5, 0.89]$ decreases, so the systems become more and more ultrametric. The straight line represents the function $I(L) = 1.2 \times L^{-0.61}$.

$q > 0.5$ really holds for large systems.

Fig. 4 shows the distributions integrated outside the interval $[q_{fix}, q_{EA}]$ as function of system size. We used $q_{EA} = 0.89$ from the results of [21]. The value I_L decreases with increasing size, but using a fit $I(L) = I_\infty + kL^{-\beta}$ no decision can be taken if it converges to zero. We only provide the result of a fit with $I_\infty \equiv 0$, where we get $k = 1.2(1)$ and $\beta = -0.61(7)$.

Conclusion. – By the calculation of ground states using genetic Cluster-Exact Approximation we find evidence for the existence of an ultrametric ground state structure in 3d $\pm J$ spin glasses. For more quantitative statements the system sizes are too small, but it is clear that the structure is more complex than simply metric. For treating larger systems more elaborate algorithms or much faster computers must be available, because even for our results 32 PPC-601 processors where busy for more than three months 24 hours a day.

For spin glasses with Gaussian distribution the ground state is not degenerate, but we expect the same behavior as for the $\pm J$ model if one allows deviations of order one from the true ground state energy,

The complex ground state structure is not just an artifact of the binary distribution of the bonds. Otherwise a simple ground state structure would result only in a large number of independent small clusters. This would lead to a peak in the distribution $P(|q|)$, as found for example for the random field Ising system with binary field distribution [22], which exhibits an exponential ground state degeneracy too. Our result is important for finite temperature as well: for 2d spin glasses, where no ordering for $T > 0$ exists, the evidences for ultrametricity presented here are indeed not found [23].
Concluding we believe that for realistic spin glasses the scenario of an ultrametric organization of the states is more probable than a scenario with a simple structure.

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