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

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
(March 20, 2018)

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.

Keywords (PACS-codes): Spin glasses and other random systems (02.10.Jf), General mathematical systems (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. 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

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

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 $d_{\alpha\beta} \leq d_{\alpha\gamma} + d_{\gamma\beta}$ but the stronger ultrametric inequality $d_{\alpha\beta} \leq \max(d_{\alpha\gamma}, d_{\gamma\beta})$ as well. For an introduction to ultrametricity see [3]. The mean field solution [3] of the infinite-dimensional SK-model [4] shows an ultrametric state structure [5]. Numerical work on the subject can be found in [6,7]. For finite dimensional systems numerical evidence for ultrametricity at finite temperature but below the transition Temperature $T_G$ was found in four dimensions [8,9]. First attempts to find ultrametricity in three dimensions by simulation at finite temperature are given in [10,11]. Here the first time ground states of realistic spin glasses are analyzed regarding their ultrametric structure. The ground state structure has a strong influence on the overall behavior of a system: an ultrametric ground state structure implies a complex free energy landscape so that no efficient variant of the usual cluster algorithms exists, i.e. that there is a critical slowing down [12].

In this letter we show our results for the direct calculation of spin glass ground states using a hybrid of genetic algorithms [13,14] and Cluster-Exact Approximation (CEA) [15]. 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 algorithm 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 important 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 $\{\sigma^\alpha_i\}, \{\sigma^\beta_i\}$, the overlap $q$ is defined as

$$q^{\alpha\beta} = \frac{1}{N} \sum_i \sigma^\alpha_i \sigma^\beta_i$$

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)

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

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

$$d^{\alpha\beta} = 0.5(1 - q^{\alpha\beta})$$

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

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

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

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

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 (4), 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

\[
\delta q \equiv q_2 - q_1
\]

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 \( q_3 \in [q_{fix}, q_{fix+2}] \) holds to obtain sufficient statistics. With increasing size \( L \) the distribution \( P(\delta q) \) should tend to a Dirac delta function [1].

- If two overlaps are fixed (\( q^{x\gamma} = q^{y\gamma} = q_{fix} \), in practice \( q^{x\gamma} , q^{y\gamma} \in [q_{fix}, q_{fix+2}] \)), equation (5) implies \( q \equiv q^{x\beta} \geq 2q_{fix} - 1 \) 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 \( [q_{fix}, q_{EA}] \) 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 for some sample systems. By writing the smallest overlap on the left side in Equation (4), 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

\[
\delta q \equiv q_2 - q_1
\]

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 \( q_3 \in [q_{fix}, q_{fix+2}] \) holds to obtain sufficient statistics. With increasing size \( L \) the distribution \( P(\delta q) \) should tend to a Dirac delta function [1].

- If two overlaps are fixed (\( q^{x\gamma} = q^{y\gamma} = q_{fix} \), in practice \( q^{x\gamma} , q^{y\gamma} \in [q_{fix}, q_{fix+2}] \)), equation (5) implies \( q \equiv q^{x\beta} \geq 2q_{fix} - 1 \) 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 \( [q_{fix}, q_{EA}] \) 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 \( L = 12 \), ..., 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:

![FIG. 1. Distribution of overlaps \( P(|q|) \) for ground states of 3d \( ±J \) 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.](image)

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 $\delta q$ (see equation (7)) for all possible triplets with $q_3 \in [0.5, 0.6]$. For a infinite ultrametric system $\delta q = 0$ holds. With increasing system size the average decreases, which indicates the increasing ultrametricity of the ground states. The straight line represents the function $\langle \delta q \rangle(L) = 0.235 \times L^{-0.255}$.

The same result is obtained by computing the average values of $\delta q$ as function of the size $L$ (see fig. 3). One gets a similar figure by computing the variances of the distributions, but it is not shown here. The number of realizations is too small to perform a reasonable fit of the form $\langle \delta q \rangle(L) = \langle \delta q \rangle_\infty + c L^{-\alpha}$. So no decision is possible yet whether the average value converges to zero or not. We only provide the result of a fit with $f_\infty$ 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.
FIG. 4. Distribution $P_{2-\text{fix}}(q)$ 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 $q \in [0, 0.5]$ 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.

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 $P_{2-\text{fix}}(q)$ of the third remaining overlap is shown in fig. 4 for $L = 4, 8, 12$. The triangular inequality gives $q > 0$ while ultrametricity leads to $q > 0.5$. The inset magnifies the values of $q \in [0, 0.5]$ 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 $q > 0.5$ really holds for large systems.

![Graph showing distribution $P_{2-\text{fix}}(q)$](image)

FIG. 5. Integrated value $I_L = \int_{-1}^{0.5} P_{2-\text{fix}}(q)(q - 0.5)^2 dq + \int_{0.89}^{1} P_{2-\text{fix}}(q)(q - 0.89)^2 dq$ 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 triplets of overlaps from independent triplets of ground states. Only $q$-values of triplets 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 $I(L) = 1.2 \times L^{-0.61}$.

Fig. 5 shows the distributions integrated outside the interval $[q_{\text{fix}}, q_{\text{finit}}]$ as function of system size. We used $q_{\text{finit}} = 0.89$ 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 short range $\pm J$ 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. 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.

Acknowledgements We thank H. Horner and G. Reinelt for manifold support. We are grateful to M. Jünger, M. Diehl and T. Christof who made us available a Branch-and-Cut Program for the exact calculation of spin glass ground states of small systems. We thank R. Kühn for critical reading the manuscript and for giving many helpful hints. We took much benefit from discussions with H. Kinzelbach, S. Kobe, H. Rieger, A.P. Young, N. Kawashima, N. Sourlas, J.-C. Anglès d’Auriac, M. Mézard and R. Monasson. We are grateful to the Paderborn Center for Parallel Computing for the allocation of computer time as well. This work was supported by the Graduiertenkolleg “Modellierung und Wissenschaftliches Rechnen in Mathematik und Naturwissenschaften” at the Interdisziplinäres Zentrum für Wissenschaftliches Rechnen in Heidelberg.

1 K. Binder and A.P. Young, Rev. Mod. Phys. 58, 801 (1986)
2 K.H. Fisher and J.A. Hertz, Spin Glasses, Cambridge University Press, 1991
3 R. Rammal, G. Toulouse and M.A. Virasoro, Rev. Mod. Phys. 58, 765 (1986)
4 G. Parisi, Phys. Rev. Lett. 43, 1754 (1979); J. Phys. A 13, 1101 (1980); 13, 1887 (1980); 13, L115 (1980); Phys. Rev. Lett. 50, 1946 (1983)
5 D. Sherrington und S. Kirkpatrick, Phys. Rev. Lett. 35, 1792-1796 (1975)
6 M. Mézard, G. Parisi, N. Sourlas, G. Toulouse and M.A. Virasoro, Phys. Rev. Lett. 52, 1156 (1984); J. de Phys. 45, 843 (1984)
7 S. Franz, G. Parisi and M.A. Virasoro, Europhys. Lett.
[8] N. Parga, G. Parisi and M.A. Virasoro, J. de Phys. Lett. 45, L1063 (1984)
[9] R.N. Bhatt and A.P. Young, J. Mag. Mag. Mat. 54-57, 191 (1986)
[10] A. Cacciuto, E. Marinari and G. Parisi, J. Phys. A 30, L263 (1997)
[11] E. Marinari, G. Parisi and J.J. Ruiz-Lorenzo, in: Spin Glasses and Random Fields, Ed. A.P. Young, World Scientific 1998
[12] N. Sourlas, J. de Phys. Lett. 45, L969 (1984)
[13] S. Caracciolo, G. Parisi, S. Patarnello and N. Sourlas, J. de Phys. 51, 1877 (1990)
[14] N. Persky and S. Solomon, Phys. Rev. E 54, 4399 (1996)
[15] K.F. Pál, Physica A 223, 283 (1996).
[16] Z. Michalewicz, Genetic Algorithms + Data Structures = Evolution Programs, (Springer, Berlin 1992).
[17] A.K. Hartmann, Physica A, 224, 480 (1996).
[18] A.K. Hartmann, to be submitted
[19] C. De Simone, M. Diehl, M. Jünger, P. Mutzel, G. Reinelt and G. Rinaldi, J. Stat. Phys. 80, 487 (1995)
[20] C. De Simone, M. Diehl, M. Jünger, P. Mutzel, G. Reinelt and G. Rinaldi, J. Stat. Phys. 84, 1363 (1996)
[21] A.K. Hartmann, Europhys. Lett. 40, 429 (1997)