Ultrametric probe of the spin-glass state in a field

Helmut G. Katzgraber,1,2 Thomas Jörg,3 Florent Krzakała,3 and Alexander K. Hartmann4

I. INTRODUCTION

Spin glasses1,2 are paradigmatic model systems that find wide applicability across disciplines. Although studied intensely, our understanding of some of their fundamental aspects is still in its infancy. In particular, the understanding of the nature of the spin-glass state remains controversial and active discussion has emerged recently.1,3 It is unclear if the mean-field replica symmetry breaking (RSB) picture14 of Parisi describes the non-mean-field behavior of spin-glasses in an externally-applied field best. While the droplet theory1,5,16,19 states that there is no spin-glass state in a field for short-range systems, the mean-field RSB picture1,14,19,20 states that for low enough temperatures $T$ and fields $H$ (i.e., below the de Almeida-Thouless line)21, a stable spin-glass state emerges. The question lies at the core of theoretical descriptions and is of immediate importance to applications in research fields ranging from, for example, sociology to economics where terms linear in the spin variable can emerge.

One way to settle the applicability of the RSB picture to short-range spin glasses in a field while avoiding technical difficulties when measuring observables in a field12 is by testing if the phase space is ultrametric (UM). Unfortunately, the existence of an UM phase structure for short-range spin glasses on hypercubic lattices remains elusive,22 mainly because only small systems can be studied numerically. Recent results in zero field23–25 suggest that short-range systems are not UM, whereas other opinions exist.26–28

More recently29 results on one-dimensional (1D) Ising models with power-law interactions showed that short-range spin glasses might be UM after all. Therefore, a natural probe for the spin-glass state in a field is to study the UM response of 1D Ising models with power-law interactions when an external field is applied. The model has the advantage in that by tuning the exponent of the power law, the universality class can be tuned between a mean-field and a non-mean-field regime. In addition, large linear system sizes can be simulated, which allows for a better finite-size scaling analysis than for hypercubic lattices.22

Our results show that for this model in a field the phase space has an UM structure in the mean-field regime. However, in the non-mean-field regime, when an external field is applied, the UM structure seems to be much weaker for the studied system sizes, suggesting that the spin-glass state for short-range systems is fragile with respect to externally-applied fields. These results are compared to studies of spin glasses within the Migdal-Kadanoff approximation.

We study the ultrametric structure of phase space of one-dimensional Ising spin glasses with random power-law interaction in an external random field. Although in zero field the model in both the mean-field and non-mean-field universality classes shows an ultrametric signature [Phys. Rev. Lett. 102, 037207 (2009)], when a field is applied ultrametricity seems only present in the mean-field regime. The results for the non-mean field case in an external field agree with data for spin glasses studied within the Migdal-Kadanoff approximation. Our results therefore suggest that the spin-glass state might be fragile to external fields below the upper critical dimension.

PACS numbers: 75.50.Lk, 75.40.Mg, 05.50.+q, 64.60.-i

II. MODEL

The 1D Ising chain with long-range power-law interactions17,27,28 is described by the Hamiltonian

$$H = -\sum_{i<j} J_{ij} S_i S_j - \sum_i h_i S_i; \quad J_{ij} = c(\sigma) \frac{\xi_{ij}}{r_{ij}},$$  \hspace{1cm} (1)
where $S_i \in \{\pm 1\}$ are Ising spins and the sum ranges over all spins in the system. The $L$ spins are placed on a ring to ensure periodic boundary conditions and $r_{ij} = (L/\pi) \sin(i-j/L)$ is the geometric distance between the spins. $\epsilon_{ij}$ are Gaussian random couplings. The constant $\xi(\sigma)$ is chosen such that for the mean-field transition temperature $T^\text{MF}_c(\sigma \leq 0.5, L, H = 0) = 1$. In Eq. (1), the spins couple to site-dependent random fields $h_i$ chosen from a Gaussian distribution with zero mean and standard deviation $[h_i^2]_\text{av} = H$.

The model has a rich phase diagram when the exponent $\sigma$ is changed, both the universality class and the range of the interactions can be continuously tuned. In particular, $\sigma = 0$ gives the Sherrington-Kirkpatrick (SK) model whose solution is the mean-field theory for spin glasses and where a spin-glass state in a field is expected (i.e., an UM signature for low enough $H$ and temperatures $T$). More importantly, for $1/2 < \sigma < 2/3$ the critical behavior is mean-field-like, while for $2/3 < \sigma \leq 1$ it is non-mean-field-like.

Here we study in a field $H = 0.1$ the SK model $[\sigma = 0]$ to test our analysis protocol, as well as the 1D chain for $\sigma = 0.60$ (also mean-field-like), as well as $\sigma = 0.75$ ($T_c \sim 0.69$, roughly corresponding to four space dimensions) outside the mean-field regime. We choose two values of $\sigma \neq 0$ to be able to discern any trends when the effective dimensionality is reduced. In general $d_{\alpha\beta} = (2 - \eta)/(2\sigma - 1)$, where $\eta$ is the critical exponent for the short-range model at space dimension $d = d_{\text{eff}}$. Note that $\eta$ is zero in the mean-field regime and, for example, $-0.275(25)$ for $d = 4.32$.

III. NUMERICAL METHOD AND EQUILIBRATION

We generate spin-glass configurations by first equilibrating the system at low temperatures and an external random field of standard deviation $H = 0.1$ using the parallel tempering Monte Carlo method. Once the system is equilibrated we record states ensuring that the system is equilibrated we record states ensuring that these are well separated in the Markov process and thus not correlated. In practice, if we equilibrate the system for $\tau_{\text{eq}}$ Monte Carlo sweeps, we generate for each disorder realization $10^3$ states separated by $\tau_{\text{eq}}/10$ Monte Carlo sweeps. We test equilibration using the method presented in Ref. 11. We consider systems sizes up to $L = 512$, which is the same maximum size as in the zero-field case studied previously but numerically much harder than in the zero-field case because Monte Carlo methods equilibrate considerably slower in a field. For the parallel tempering simulations $T_{\text{min}} = 0.36$ and $T_{\text{max}} = 1.40$ (16 temperatures). For all values of $\sigma$ studied, and all system sizes $L$, we generate 4000 disorder realizations. For $L = 32$, the equilibration time is $2 \times 10^4$ Monte Carlo sweeps (MCS), for 64, $1.5 \times 10^5$ MCS, for 128, $5 \times 10^5$, and for 256 and 512, $10^6$ MCS.

The presented data are for $T = 0.36$. In Ref. 35 we fixed $T \approx 0.4 T_c$ for all values of $\sigma$ studied to ensure that we are deep in the spin-glass phase. However, it is unclear if one-dimensional spin glasses with power-law interactions have a spin-glass state in a field for $\sigma > 2/3$.

Using the $T_c$ estimates of Leuzzi et al. at zero and finite field ($H = 0.1$) for the diluted version of the model we estimate that if a spin-glass state exists for $H = 0.1$ it should suppress the zero-field $T_c$ by approximately 20%. For $\sigma = 0.75$ it is known that $T_c(H = 0) \approx 0.69(1)$ therefore $T = 0.36$ corresponds roughly to a 40% reduction of the critical temperature (i.e., deep in the putative spin-glass phase).

We also study spin glasses within the standard MK approximation (i.e., spin glasses on hierarchical lattices). Due to the simple lattice structure, the phase space is also expected to be simple. In fact, as shown rigorously in Ref. 39, spin glasses on MK lattices are replica symmetric. We used a variation of the standard MK recursion where, starting from one bond, iteratively each bond is replaced by $2^d$ bonds and $2^{d-1}$ spins ($d = 3$). For details, see, for example, Refs. 40 and 41.

IV. ULTRAMETRICITY

Ultrametricity appears in different fields of research ranging from linguistics to the taxonomy of animal species and is a key component of Parisi’s mean-field solution of the SK model. Therefore, if a spin glass has no UM phase-space structure there is a strong indication that Parisi’s mean-field picture might not work for this system.

In an UM space the triangle inequality $d_{\alpha\gamma} \leq d_{\alpha\beta} + d_{\beta\gamma}$ is replaced by a stronger condition where $d_{\alpha\gamma} \leq \max\{d_{\alpha\beta}, d_{\beta\gamma}\}$ (i.e., the two longer distances must be equal and the states lie on an isosceles triangle). Here, $d_{\alpha\beta}$ represents the distance between two points $\alpha$ and $\beta$ in phase space.

We use the approach developed in Ref. 12 which is closely related to the one used by Hed et al. in Ref. 22. For each disorder realization we produce $M = 10^3$ equilibrium configurations. These are sorted using the average-linkage agglomerative clustering algorithm. The clustering procedure starts with $M$ clusters containing each exactly one configuration. Distances are measured in terms of the Hamming distance $d_{\alpha\beta} = (1 - q_{\alpha\beta})$, where $q_{\alpha\beta} = N^{-1} \sum_i S_i^\alpha S_i^\beta$ is the spin overlap between configurations $\{S_\alpha\}$ and $\{S_\beta\}$. Iteratively the two closest clusters $C_a$ and $C_b$ are merged into one cluster $C_d$, reducing the number of clusters by one. The distances of the new cluster $C_d$ to the other remaining clusters have to be calculated: The distance between two clusters is the average distance between all pairs of members of the clusters. The iterative procedure stops when only one cluster remains, the results are then typically structured in a tree-like structure called a dendrogram (see Fig. 1). To probe for a putative UM space structure, we randomly select three configurations from the hierarchical cluster struc-
and an external random field \( H = 0.1 \). (a) Data for the SK model. The distribution diverges very slightly for \( K \to 0 \) and \( L \to \infty \) thus signaling an UM phase structure. (b) Data for \( \sigma = 0.60 \) (mean-field universality class). There is still a weak hint of a divergence for \( K \to 0 \). (c) Data for \( \sigma = 0.75 \) (non-mean-field universality class). There is no clear sign of a divergence in \( P(K) \) for \( K \to 0 \). Note that when \( H = 0 \) data for \( \sigma = 0.75 \) show a clear signature for UM behavior. Error bars are smaller than the symbol size.

FIG. 2: (Color online) Distribution \( P(K) \) for different system sizes (all panels have the same horizontal and vertical scale) and an external random field \( H = 0.1 \). (a) Data for the SK model. The distribution diverges very slightly for \( K \to 0 \) and \( L \to \infty \) thus signaling an UM phase structure. (b) Data for \( \sigma = 0.60 \) (mean-field universality class). There is still a weak hint of a divergence for \( K \to 0 \). (c) Data for \( \sigma = 0.75 \) (non-mean-field universality class). There is no clear sign of a divergence in \( P(K) \) for \( K \to 0 \). Note that when \( H = 0 \) data for \( \sigma = 0.75 \) show a clear signature for UM behavior. Error bars are smaller than the symbol size.

Next, we sort these Hamming distances \( d_{\max} \geq d_{\med} \geq d_{\min} \) and compute \( K = (d_{\max} - d_{\med})/g(d) \), where \( g(d) \) is the width of the distance distribution. If the phase space is UM, then we expect \( d_{\max} = d_{\med} \) for \( L \to \infty \). Thus \( P(K) \to \delta(K = 0) \) for \( L \to \infty \) and the the variance of the distribution \( \text{Var}(K) \to 0 \) for \( L \to \infty \).

FIG. 3: (Color online) Variance \( \text{Var}(K) \) of \( P(K) \) as a function of system size \( L \) for different values of \( \sigma \). The data can be fit to a power law (dashed lines). In the mean-field regime (SK and \( \sigma = 0.6 \)) a fit to a constant is unlikely (see text). The power-law decay of the variance as a function of system size suggests a divergence in \( P(K) \) for \( K \to 0 \). For \( \sigma = 0.75 \) the data are compatible with a constant behavior, showing that there is no UM phase-space structure for spin glasses within the MK approximation. The solid line is a guide to the eye.

V. RESULTS

Figure 2(a) shows the distribution \( P(K) \) for the SK model \( (\sigma = 0), T = 0.36 \), and \( H = 0.10 \). There is a slight hint for a divergence for \( K \to 0 \). Similar results are found for the mean-field regime with \( \sigma = 0.60 \) [Figure 2(b)]. The UM signature in a field is considerably weaker than when no field is applied. While for the SK model there is still a faint sign of a divergence, for larger values of \( \sigma \) it
is hard to see if the distributions diverge for \( K \to 0 \) and \( L \to \infty \). Figure 2(c) shows data for \( \sigma = 0.75 \), \( T = 0.36 \), and \( H = 0.10 \) where no clear sign of a divergence is present, suggesting that phase space might not be UM outside the mean-field regime.

Hence, drawing conclusions from the \( P(K) \) data is not sufficient. A better probe is given by the variance \( \text{Var}(K) \) of \( P(K) \) as a function of system size \( L \) (Fig. 4). The variance of the distribution for the SK model clearly decays with a power law \( \text{Var}(K) \sim b/L^\gamma \) [i.e., \( \gamma = 0.49(4) \), \( b = 0.13(2) \), and \( Q \sim 0.28 \)] [14]. If we restrict the fit to \( L \geq 128 \) we obtain \( b = 0.58(7) \) and \( \gamma = 0.16(2) \) with a \( Q \)-factor \( \sim 0.487 \). A fit to a constant gives \( Q = 0 \) if the fit is performed for all data or restricted to \( L \geq 128 \). A fit to a constant+power-law behavior \( \text{Var}(K) \sim a + b/L^\gamma \) gives a constant \( a \) compatible with zero and a clear power-law decay. Therefore, and as expected, the SK model shows an ultrametric phase space structure for small externally applied magnetic fields.

Similar results are obtained for \( \sigma = 0.60 \) where a fit to a power law is very likely with \( b = 0.395(6) \), \( \gamma = 0.074(3) \), and \( Q = 0.989 \) [restricted to \( L \geq 128 \) we obtain \( b = 0.374(1) \), \( \gamma = 0.064(1) \), and \( Q = 0.983 \)]. However, a fit to a constant gives \( Q < 10^{-5} \) [0.124 restricted to \( L \geq 128 \)]. We also attempted a fit to a constant+power-law behavior [i.e., \( \text{Var}(K) \sim a + b/L^\gamma \)]. We obtain \( a = 0.18(2) > 0 \) with \( Q = 0.989 \). This suggests that we might be at a marginal regime (i.e., close to the upper critical dimension).

For \( \sigma = 0.75 \) a fit to a very weak power law with \( b = 0.30(1) \) and \( \gamma = 0.014(6) \) is found with \( Q = 0.897 \). Thus, the exponent \( \gamma \) is extremely small, only within about two standard deviations from zero. Correspondingly, a fit to a constant is equally probable with \( Q = 0.811 \). Similar results are obtained for \( L \geq 128 \) where \( b = 0.33(2) \) and \( \gamma = 0.028(9) \) with \( Q = 0.811 \), and \( Q = 0.766 \) for a fit to a constant. A fit to a constant+power-law behavior gives a power-law exponent consistent with zero within error bars.

Summarizing, either ultrametricity in the non-mean-field regime is completely lost in a field or greatly weakened, suggesting a marginal signal for \( \sigma = 0.60 \). Larger systems would be needed to fully discern the behavior, however they are out of reach with current technology. Note that for diluted systems larger system sizes are possible, but the finite-size effects are stronger, resulting in no overall benefit.

Within the MK approximation the distributions \( P(K) \) also show no divergence for \( K \to 0 \). Figure 3 shows the variance of the distributions as a function of the system size for very large lattices. There is no discernible decrease with an increasing number of spins (i.e., no UM structure of phase space). In fact, a fit to a power-law behavior results in a slope compatible with zero (i.e., a constant behavior). This is to be expected because the model is defined on a hierarchical lattice. However, a direct comparison to the results for \( \sigma = 0.75 \) strengthens the evidence of a potential non-UM structure for the latter case, in agreement with recent results [14].

VI. SUMMARY AND CONCLUSION

We have studied numerically the low-temperature configuration landscape of long-range spin-glasses with power-law interactions. By tuning the exponent \( \sigma \) that governs the decay of the power-law interactions and therefore their range we can tune the system out of the mean-filed universality class. Using a hierarchical clustering method and analyzing the resulting distance matrices we show that when a field is applied the system is only clearly UM in the mean-field regime, unlike in the zero-field case where an UM signal was found for values of \( \sigma \) that correspond to space dimensions above and below the upper critical dimension. Therefore, our results suggest that the spin-glass state is fragile to an externally-applied field below the upper critical dimension. Larger systems would be needed to determine if the UM signature for \( \sigma = 0.75 \) (corresponding approximately to four space dimensions) persists in a field or not.

Acknowledgments

H.G.K. acknowledges support from the Swiss National Science Foundation (Grant No. PP002-114713) and the National Science Foundation (Grant No. DMR-1151387). We thank Texas A&M University, the Texas Advanced Computing Center (TACC) at The University of Texas at Austin, the Centro de Supercomputación y Visualización de Madrid (CeSViMa) and ETH Zurich for HPC resources.

1 K. Binder and A. P. Young, Spin glasses: Experimental facts, theoretical concepts and open questions, Rev. Mod. Phys. 58, 801 (1986).
2 M. Mézard, G. Parisi, and M. A. Virasoro, Spin Glass Theory and Beyond (World Scientific, Singapore, 1987).
3 R. N. Bhatt and A. P. Young, Search for a transition in the three-dimensional ±J Ising spin-glass, Phys. Rev. Lett. 54, 924 (1985).
4 J. C. Ciria, G. Parisi, F. Ritort, and J. J. Ruiz-Lorenzo, The de-Almeida-Thouless line in the four-dimensional Ising spin glass, J. Phys. I France 3, 2207 (1993).
5 N. Kawashima and A. P. Young, Phase transition in the three-dimensional ±J Ising spin glass, Phys. Rev. B 53, R484 (1996).
6 E. Marinari, C. Naitza, and F. Zuliani, Critical Behavior of the 4D Spin Glass in Magnetic Field, J. Phys. A 31,
