

Ultrametricity in three-dimensional Edwards-Anderson spin glasses

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(Received 10 March 1999)

We perform an accurate test of ultrametricity in the aging dynamics of the three-dimensional Edwards-Anderson spin glass. Our method consists in considering the evolution in parallel of two identical systems constrained to have fixed overlap. This turns out to be a particularly efficient way to study the geometrical relations between configurations at distant large times. Our findings strongly hint towards dynamical ultrametricity in spin glasses, while this is absent in simpler aging systems with domain growth dynamics. A recently developed theory of linear response in glassy systems allows us to infer that dynamical ultrametricity implies the same property at the level of equilibrium states.

PACS number(s): 05.50.+q, 75.10.Nr, 75.40.Mg

The dispute about the nature of the spin glass phase of finite-dimensional spin glasses has lasted by now almost twenty years. The droplet model [1] has challenged the predictions of mean field theory (MFT) [2].

In the last years a large collection of numerical data have tested, with positive answer, the applicability of spin glass mean field picture to finite-dimensional ($d=3,4$) systems [3–5]. However, some of these numerical evidences have been recently reinterpreted as finite volume effects by the authors of Ref. [6] and so many questions on the low-temperature phase of finite-dimensional spin glasses still remain unanswered.

One of the most characteristic aspects of mean field theory is the prediction of ultrametricity (UM) [7]. At low temperature the ergodicity is broken and many low free energy states are present. Ultrametricity implies that the distances between these states verify an inequality stronger than the triangular one (see below). However, this property has been rather elusive to a direct probe. The best evidences in favor of this property have been given (to our knowledge) in Refs. [8,9]. In the former it was studied the equilibrium of a four-dimensional (4D) spin glass model using small samples. In the latter very-low-energy configurations of a 3D model were used, again for relatively small samples. In both cases an extrapolation to large volumes was needed in order to check ultrametricity. In this paper we present results for the 3D spin glass model with a method that allows us to reach much larger sizes.

Another fundamental aspect of MFT is the prediction of slow dynamics and aging [10–12]. This is a nonstationary asymptotic regime, following a quench from a high temperature, which persists forever in infinite systems. In this out-of-equilibrium regime, the equilibrium property of ultrametricity has a dynamical counterpart in ultrametric relations among time dependent autocorrelation functions. Recent results of linear response theory succeeded to relate in a unique way properties of statics and dynamics, relying on the recently introduced hypothesis of stochastic stability [13]. This property states the continuity of the average correlation functions under weak random perturbation of the Hamiltonian. The validity of the property in three- and four-dimensional spin glasses has been numerically verified in Ref. [4]. A

remarkable consequence of stochastic stability is that dynamical ultrametricity implies the static one [14].

In this paper we investigate the possibility for dynamical UM in the three-dimensional Edwards-Anderson (EA) model. For comparison we also perform the same test on models with domain coarsening off-equilibrium dynamics, where UM should not be expected.

The high evidence we can achieve is based on a new dynamical method where we evolve in parallel two identical systems (replicas for short) with fixed value of the mutual overlap. This is analogous to a conserved-order-parameter dynamics in a ferromagnetic system and it is similar to the one already used in Ref. [8] to study the equilibrium behavior.

The EA model is defined by the Hamiltonian $H(\mathbf{S}) = \sum_{\langle i,j \rangle} J_{ij} S_i S_j$ where the spins are Ising variables, the sum spans the nearest neighbors pairs on a cubic lattice, and the couplings J_{ij} are normally distributed quenched independent random variables. We define the overlap among two spin configurations \mathbf{S}^1 and \mathbf{S}^2 as $q_{12} = L^{-3} \sum_i S_i^1 S_i^2$, which is directly related to the Hamming distance d_{12} through $q_{12} = 1 - d_{12}$.

The mean field equilibrium solution of this model has the ultrametric property at low temperature; for each three configuration \mathbf{S}^1 , \mathbf{S}^2 , and \mathbf{S}^3 chosen with Boltzmann probability, the following inequalities hold:

$$q_{12} \geq \min\{q_{13}, q_{23}\}, \quad d_{12} \leq \max\{d_{13}, d_{23}\}, \quad (1)$$

which are much stronger than the usual triangular one $d_{12} \leq d_{13} + d_{23}$. Moreover in Ref. [15] it has been shown that, if some kind of ultrametricity holds in the low-temperature phase of the EA model, it must be of the same kind of that present in the mean-field solution.

In the off-equilibrium dynamical solution a relation analogous to Eq. (1) holds for the two-time autocorrelation functions $C(t, t') = L^{-3} \sum_i S_i(t) S_i(t')$. Taken three large times $t_1 \ll t_2 \ll t_3$, one finds that

$$C(t_1, t_3) = \min\{C(t_1, t_2), C(t_2, t_3)\}. \quad (2)$$

The precise statement is that the relation among the correlations *should tend* to the one of Eq. (2) in the infinite time

limit [11,12]. In the simulations the relation among the three correlations is plagued by strong finite time effect, so that a direct verification would be difficult with the present computer resources. We therefore decided to probe a relation which for long times is consequence of, and equivalent to, Eq. (2). We consider the dynamics of two replicas of the system with the same disorder \mathbf{S}^1 and \mathbf{S}^2 , which evolve in parallel with different thermal noises and constrained at each time to have a fixed mutual overlap q_0 . The dynamics follows a quench at time zero and we measured the auto-correlation and cross-correlation functions

$$C(t, t') = \frac{1}{L^3} \sum_i S_i^1(t) S_i^1(t') = \frac{1}{L^3} \sum_i S_i^2(t) S_i^2(t'),$$

$$D(t, t') = \frac{1}{L^3} \sum_i S_i^1(t) S_i^2(t') = \frac{1}{L^3} \sum_i S_i^2(t) S_i^1(t'). \quad (3)$$

Note that $C(t, t) = 1$ for Ising variables, while the constraint implies $D(t, t) = q_0$.

We would like to argue, with a hand waving argument, that the relation in Eq. (2) entails the following ultrametric constraint on the cross-correlation function if the value of q_0 is between 0 and the value of the Edwards-Anderson parameter q_{EA} :

$$D(t, t') = \min\{C(t, t'), q_0\}. \quad (4)$$

During the relaxation the free energy of the system decreases monotonically towards its equilibrium value. This will be higher or equal to the one of the unconstrained system at the same temperature. The basic observation is that, if q_0 is one of the values allowed for the overlap among equilibrium states, i.e., $q_0 \in [0, q_{EA}]$, the equilibrium free-energy of the constrained system should coincide with the one of the unconstrained one [16]. Equation (2) expresses the fact that for large times, the directions in which the system can go without increasing the free-energy must be compatible with ultrametricity. The constrained system can lower its free-energy down to the equilibrium value only if all the possible correlations one can form (auto and cross) verify for long times UM inequalities. As two of the four correlations that can be formed with the configurations $\mathbf{S}^1(t)$, $\mathbf{S}^1(t')$, $\mathbf{S}^2(t)$, and $\mathbf{S}^2(t')$ are fixed to q_0 , Eq. (4) should follow. A formal argument leading to the same conclusions can be formulated [17], extending to constrained systems the correspondence among statics and dynamics mentioned above.

In order to see how restrictive relation in Eq. (4) is, let us discuss what one can expect on a general ground for the relation among D and C in a relaxational system. In Fig. 1 we display the set of allowed values for $C(t, t')$ and $D(t, t')$ (shaded area), simply assuming the triangular relation and a monotonic decrease of both functions when the time argument's difference increases. The set of values allowed by the UM relation is represented with the bold dashed line.

In order to check whether Eq. (4) holds in the 3D EA model, we have simulated, by Monte Carlo method (Metropolis update), two coupled systems with a soft constraint $\sum_i S_i^1 S_i^2 \approx L^3 q_0$, imposed modifying the Boltzmann weight with a Gaussian of width proportional to $L^{-3/2}$, such that the

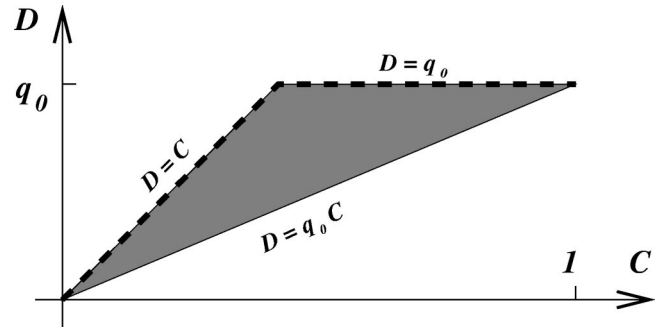


FIG. 1. Schematic draw of the region of allowed values for C and D (shaded area). The ultrametric relation force them on the bold dashed line.

weight of a configuration would be $\exp\{-\beta[H(\mathbf{S}_1) + H(\mathbf{S}_2)] - \lambda L^3 (q_{12} - q_0)^2 / 2\}$. The value of the λ parameter must be appropriately tuned: a too small value would not force enough the systems and their overlap will be systematically different from the one we fixed (q_0). On the other hand a too large value would render movements too unprobable and the dynamics would evolve very slowly. In the whole set of runs we fixed $\lambda = 5$ for the EA model and $\lambda = 2$ for the other models. The choice has been made with the aim of maximizing the Monte Carlo acceptance rate, avoiding the systematic errors just described. We have checked (see Fig. 2) that, for these values of λ , $q_{12}(t)$ tends to the desired value q_0 .

As we study the behavior of the model in the aging regime, we do not need to reach thermalization and we can simulate large sizes ($L=24$). For such volume, finite size effects do not affect the dynamical regime we study. The critical temperature of a single uncoupled model is $T_c = 0.95(4)$ [5] and we simulate the system in the spin glass phase at $T=0.7$. The large size, the low temperature, and the starting configuration, which is randomly chosen, ensure that the system stays in the aging regime all along the simulation

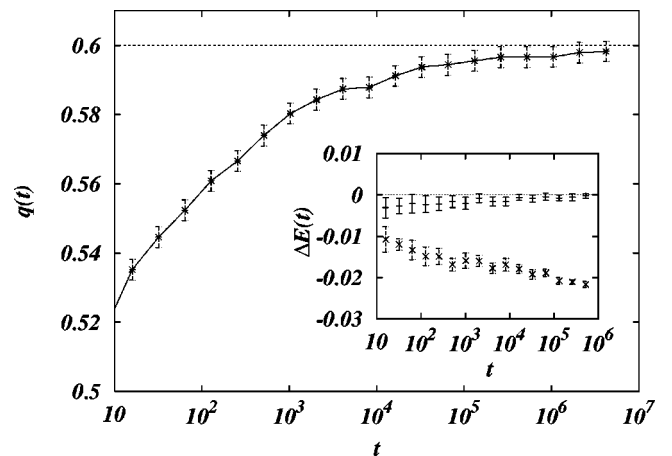


FIG. 2. The time evolution of the overlap between the pairs of EA systems at temperature $T=0.7$ with $q_0=0.6$. In the inset we show the energy difference between a constrained and a free system at the same temperature. The upper data correspond to $T=0.7$ and $q_0=0.6 < q_{EA}$ and are clearly compatible with zero. The lower data correspond to $T=0.9$ and $q_0=0.9 > q_{EA}$ and show how the energy of the constrained system is lower.

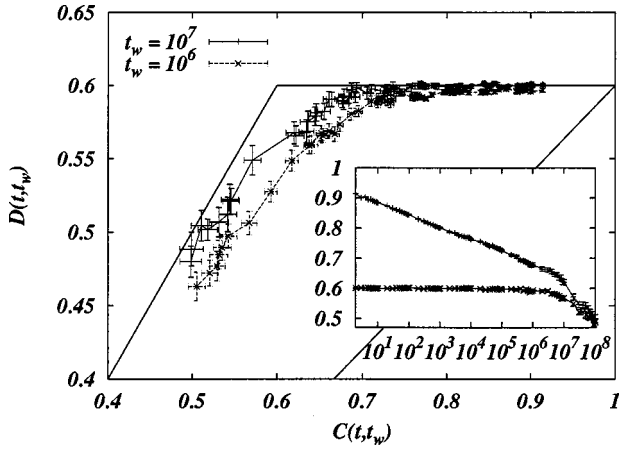


FIG. 3. Plot of the cross-correlation function versus the autocorrelation one in the 3d EA model at temperature $T=0.7$ for two waiting times $t_w=10^6, 10^7$. The curves approach the UM bound as t_w grows. The solid lines are the boundaries of the shaded area of Fig. 1. In the inset we display the time dependence of the two functions.

which can be as long as 10^8 MCS. These high performances have been achieved using the parallel computer APE100 [18].

All the correlation functions we measure are extensive and self-averaging quantities, so we do not need a large number of disorder realizations. Their fluctuations are small thanks to the large volume used and we average the results on a quite small number of samples ($N_S=10$). The error on the data is always calculated as the sample-to-sample fluctuation.

The first quantities we have studied are the overlap of the two replicas and the internal energy as a function of time. As announced, we see in Fig. 2 that the overlap converges towards the value q_0 we have fixed. The “soft” way of imposing the constraint is evident in the behavior of the overlap, which is not equal to q_0 during all the run, but clearly converges to it. In the forthcoming analysis we will use only the data obtained in the time range where the overlap is statistically compatible with q_0 , that is $t_w \geq 10^5$. The data in the inset of Fig. 2 show the difference between the energy of the constrained system and that of a free system evolving at the same temperature after a quench at time zero. As we expected, the energy difference tends to zero, as it should if the value q_0 is allowed at equilibrium, while for $q_0 > q_{EA}$ the energy difference goes to a finite value.

In Fig. 3 we show our main result: plotting the cross correlation as a function of the auto correlation we obtain, for relatively long times, that the data points are quite close to the UM bound. A perfectly ultrametric system would stay on the line $D=q_0=0.6$ as long as $C \geq q_0$ and then would follow the line $D=C$ (both lines are plotted in Fig. 3). The data for the 3D EA model are clearly converging to the UM bound: we remind the reader that the data cannot leave the shaded area of Fig. 1, that is they cannot cross any of the boundary lines reported in Fig. 3, and so we expect that they naturally converge to the UM bound.

To understand better how probing are our data, we have also simulated two models where UM is not expected to hold: the 2D ferromagnetic Ising model, and its site diluted

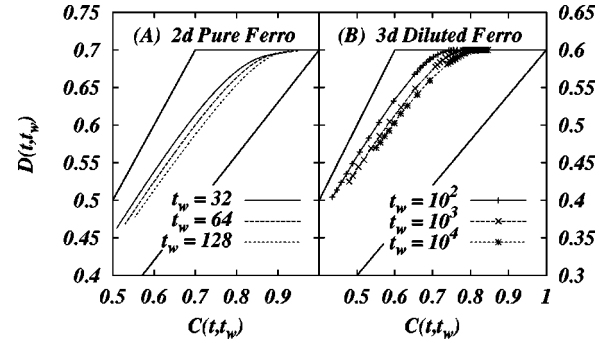


FIG. 4. The same plot as Fig. 3 for (A) the pure ferromagnet in 2d at $T=1.5$ and (B) the 3d diluted ferromagnet at $T=1.67$. The waiting time effect is opposite to the one observed in the spin glass.

version in 3D. The off-equilibrium dynamics of both models shows a domain coarsening regime where the correlation function depends on both times as $C(t, t') \approx C(t'/t)$, a scaling form incompatible with ultrametricity.

We have simulated a 2D pure ferromagnetic Ising model of linear size $L=2000$ at a temperature $T=1.5$ ($T_c^{2D} \approx 2.27$). We choose a very large size and small waiting times ($t_w=32, 64, 128$) in order to avoid that the system gets out from the aging regime we are interested in. These times are sufficiently large to be close to the scaling regime. The data are averaged on $N_S=100$ different noise realizations.

The data from the pure ferromagnetic system are plotted in Fig. 4(a) in the usual $D(t, t_w)$ versus $C(t, t_w)$ plot. We also report the bounds of the allowed region (the shaded region of Fig. 1). Note that the data are far away from the UM bound and they seem to converge to some t_w -independent curve.

Maybe one can think that the comparison of a spin glass with the pure ferromagnet is not enough. So we have simulated also a 3D site-diluted ferromagnetic Ising model, which has a coarsening dynamics similar to that of the pure model, but much slower [19] and complicated by interface pinning. We have simulated two samples (each one consisting of a pair of interacting systems) of linear size $L=200$ and spin concentration $c=0.65$. The temperature is well deep in the frozen phase, $T=1.67$, the critical temperature being $T_c^{3d}(c=0.65) \approx 2.70$ [20].

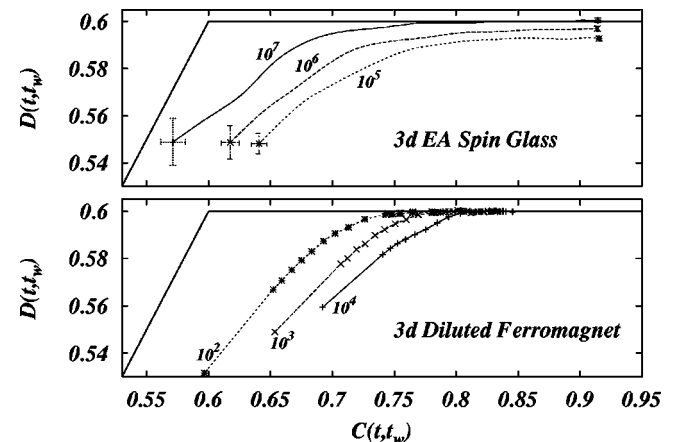


FIG. 5. Zooms of Figs. 3 and 4(b) in the region of D close to the upper boundary $D=q_0$. The comparison of the two plots makes clear that the effect of the waiting time is opposite in the two cases, and the long time extrapolation is certainly very different.

In Fig. 4(b) we see that the behavior of the data from the diluted ferromagnetic model may resemble that of the EA model, because it seems to be somehow close to the UM bound.

Looking carefully at the figure we note, however, that the t_w dependence of the data in Fig. 3 and in Fig. 4(b) are opposite. In fact increasing the waiting time, the value of the autocorrelation function at the point where the data leave the horizontal line decreases in the spin glass case, while it increases in the diluted ferromagnetic case. To make this effect clearer we zoomed the region of Figs. 3 and 4(b) near the horizontal line (see Fig. 5).

Summarizing, we have used a new numerical method to

test ultrametricity in short range spin glasses. We find evidence that for long times the ultrametric equality between two time correlations become fulfilled. As we already stressed the property of stochastic stability implies then static ultrametricity. The behavior of spin glasses is strikingly different from the behavior of ordered and disordered models with domain coarsening, where we find incompatibility with ultrametricity.

We would like to thank Giorgio Parisi for continuous interactions and advises, the “INFN sezione di Roma I” for the use of the APE100 computer and the “Università di Roma La Sapienza” for kind hospitality. We thank also M. A. Virasoro and R. Zecchina for useful discussions.

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