Ultrametricity and long-range correlations in the Edwards-Anderson spin glass

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In recent times, the theoretical study of the three-dimensional Edwards-Anderson model has produced several rigorous results on the nature of the spin-glass phase. In particular, it has been shown that, as soon as the overlap distribution is non-trivial, ultrametricity holds. However, these theorems are valid only in the thermodynamical limit and are therefore of uncertain applicability for (perennially off-equilibrium) experimental spin glasses. In addition, their basic assumption of non-triviality is still hotly debated. This paper intends to show that the predictions stemming from ultrametricity are already well satisfied for the lattice sizes where numerical simulations are possible (i.e., up to $V = 32^3$ spins) and are, therefore, relevant at experimental scales. To this end we introduce a three-replica correlation function, which evinces the ultrametric properties of the system and is shown to scale in the same way as the overlap correlation function.

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During the last decade, the understanding of the properties of the low-temperature phase of model spin glasses [1–3] has made significant progress, thanks both to theoretical advances and numerical simulations. The Mean Field solution [4–6] is known since the eighties, but its relatively recent rigorous proof has been lacking for more than twenty years [7]. The debate remains [8, 9] whether the peculiar features of the Mean Field solution are present in realistic, finite-dimensional model spin glasses (the Replica Symmetry Breaking scenario, RSB) or whether a completely different picture, the droplet model [10–13] describes the spin-glass phase. Indeed, the central issue of whether the spin-glass order parameter has a non-trivial distribution is still very much the subject of active discussion (see, e.g., [14–18] for recent examples). Thus, the detailed investigation into the properties of the spin-glass phase remains an active field.

In this paper, we build on recent advances in the study of the structure of correlations in the spin-glass phase [15, 19, 20] in order to test one of the most conspicuous features of the RSB picture: the ultrametric structure of the low-temperature phase. We shall define a (would-be) ultrametric correlation function and show that it scales just as the standard spin autocorrelation, validating the prediction of the RSB theory. To this end we shall take advantage of the unprecedented statistics afforded to us by the use of the Janus computer [21–23].

In what follows we consider the Edwards-Anderson model, a long-studied paradigm for realistic spin glasses:

$$H = - \sum_{i,j} J_{ij} S_i S_j$$ (1)

where $S_i$ are Ising spins and $J_{ij}$ are i.i.d. random quenched couplings between nearest-neighbor sites $i,j$ on a finite-dimensional cubic lattice. We define as usual the total overlap of an equilibrium configuration at a given temperature of model (1) as the microscopic average of local (single-site) overlaps $q(i) = S_i^a S_i^b$, $q = \langle \sum_i q(i) \rangle/V$ where $i$ is a cubic lattice site label, $V = L^3$ is the system volume and $a,b$ are labels for two independent replicas of the system. This model undergoes a second-order phase transition [24–26] at temperature $T_c = 1.1019(29)$ [27]. The RSB and droplet pictures provide very different descriptions of the $T < T_c$ spin-glass phase.

In the droplet model, the low-temperature phase is governed by a single pair of states (related by a global spin inversion) and excitations are produced by coherently flipping compact regions. If $\ell$ is the typical size of such droplets, the energy of the excitations grows as a power of $\ell$, making system-wide excitations unaccessible in the thermodynamic limit. All peculiar dynamical and equilibrium features of the spin-glass phase come from the complex interaction of droplet excitations. In the off-equilibrium regime, the spin-glass order builds in a super-universal coarsening dynamics [12]. The order parameter of the spin-glass transition is the overlap, whose value is well defined below the transition temperature so the probability distribution $P(q)$ in the thermodynamic limit is a pair of delta functions: $P(q) = \delta(q^2 - q_{EA}^2)$. The introduction of any external driving field completely destroys the spin-glass phase and the system is paramagnetic at all $T > 0$.

In the Replica Symmetry Breaking scenario, infinitely many states contribute to the thermodynamics; excitations cost a finite amount of energy and fill all the available space [8, 28]. The probability distribution of the overlap at a given non-zero temperature in the spin-glass phase has a delta function at $q = 2q_{EA}$ as well as a finite weight down to $q = 0$. The probability distribution of the overlaps is strongly constrained by the requirement of stochastic stability [29–32]. The latter has been shown to be a quite general property: in the case of the the Edwards-Anderson model it has been both proved [33] and observed numerically [34]. As a consequence of a very general theorem of Panchenko [35], the many states are hierarchically organized and the phase space is ultrametric: if we take the overlap as a measure of distance between states, and we pick three equilibrium configurations at random, they always form an isosceles triangle. Their probability distribution, including the fraction of equilateral triangles...
is fixed by stochastic stability.

The differences in the droplet and RSB pictures reflect on their predictions for long-range correlations. In what follows we are interested in space correlation functions of local overlaps. The usual non-connected overlap-overlap correlation function is

$$C_q(r) = \frac{\langle q(i)q(i+r) \rangle}{\langle q^2 \rangle},$$

(2)

where \(\langle \ldots \rangle\) denotes the average over all disorder samples and \(\langle \ldots \rangle\) the thermal average for a single sample. The correlation function at a fixed value of \(q\)

$$C_q(r|q = Q) = \frac{\langle q(i)q(i+r)\delta(q-Q) \rangle}{\langle \delta(q-Q) \rangle}$$

(3)

declines with a power law at long distance so that

$$C_q(r|q = Q) \sim Q^2 + A(Q)r^{-\eta(Q)}, \quad Q \leq q_{EA},$$

(4)

with non-negative \(\theta\) at all values of \(Q\) up to \(q_{EA} = \langle S_i \rangle^2\) (and \(\theta < 3\)).

On the other hand, for \(Q > q_{EA}\) the system is in a very forced state and the correlations decrease exponentially, characterized by a correlation length \(\xi_q\). In the large-\(L\) limit, the crossover between these two regimes becomes a phase transition when \(Q \to q_{EA}\) from above: \(\xi_q \propto (Q^2 - Q_{EA})^{-\nu}\). Finally, the exponents \(\nu\) and \(\theta_q = \theta_q(\xi_q)\) are related by a hyperscaling law: \(\theta_q(\xi_q) = 2/\nu\).

The droplet and RSB pictures agree on the above description, but differ on the shape of \(\theta_q(Q)\) for \(Q < q_{EA}\). In the mean field theory \([23]\) we expect \(\theta_q(Q)\) to be a non-trivial function of \(Q\). Above the upper critical dimension \(D > D_u = 6\), a zero-loop computation starting from the Mean Field approximation predicts three distinct values of the correlation exponent in the sectors \(Q = q_{EA}\) (\(\theta = D - 2\), \(Q = 0\) (\(\theta = D - 4\)) and \(0 < Q < q_{EA}\) (\(\theta = D - 3\)). Below \(D_u\), these expectations should renormalize (in fact, the given exponents are inconsistent with the clustering property below \(D = 4\): for any choice of \(Q\) we must have a correlation function decaying to a well defined value). Therefore, in \(D = 3\) connected correlation functions should decay as in Eq. (4) but little can be said a priori on the shape of \(\theta_q(Q)\) for \(Q < q_{EA}\), other than it should be strictly positive. At critical the temperature the exponent is discontinuous and \(\delta\theta(0) = 1 + \eta_q\), where \(\eta_q\) is the anomalous dimension \([26, 29, 30]\).

In the droplet picture we expect a completely different scenario. There is a unique state (apart from time-reversal symmetry) in the thermodynamic limit with \(q = q_{EA}\) at any \(T \to T_c\). The space correlation function in the small-\(Q\) sectors behaves as \(Q_{EA}^2 g(r/L)\) with \(g\) a scaling function of order \(\sim 1\) in the intermediate-distance region \(r \ll L\) where \(L\) is the typical linear sizes of coexistent droplets of the two symmetric phases. Therefore \(\theta_q(Q < q_{EA}) = 0\) in the droplet picture. For \(Q = q_{EA}\), the connected correlation function decays to zero and the power is given by the stiffness exponent \(\theta(q_{EA}) = y_{13}\), whose value has been computed to be \(y = 0.24(1)\) in \(D = 3\) (from \(T = 0\) studies \([41]\)).
This last point is crucial: if the weight of the triangles with a negative side were significative, the rest of our analysis would not rest on a solid foundation (the system would either not be ultrametric or we would be too far from the asymptotic regime for our results to have any value). In order to test this issue we define the following quantity:

$$S^{(-)} = \frac{\int_{-1}^{0} dq^c q^c (q^c)^2 p(q^c)}{\int_{-1}^{1} dq^c (q^c)^2 p(q^c)}.$$  \hspace{1cm} \text{(5)}$$

As we can see in Figure 1 the value of $S^{(-)}$ is indeed very small below the critical temperature and, furthermore, it decreases with increasing lattice size. Notice that $S^{(-)}$ decreases very quickly (exponentially) when we decrease the temperature. Therefore, in what follows we shall work at the lowest temperature for which we have data up to $L = 32$, $T = 0.703$.

As we have said, ultrametricity requires that triangles must be isosceles and $q^{bc} = q^{ac}$. It is therefor interesting to consider the difference

$$x = q^{ac} - q^{bc} = \frac{1}{V} \sum_i q_i^{ac} - q_i^{bc} = \frac{1}{V} \sum_i x_i.$$  \hspace{1cm} \text{(6)}$$

In particular, we define

$$Q_i^2 = (q_i^{ac} - q_i^{bc})^2 = (x_i)^2 = \frac{1}{\sqrt{2}} \sum_i \sum_k (x_i x_k),$$  \hspace{1cm} \text{(7)}$$

which should vanish in the thermodynamical limit. We then define a three-replica correlation function from the autocorrelation of $x$ (analogous to $C_q$):

$$C_3(r) = \frac{1}{V} \sum_i \langle x_i x_{i+r} \rangle.$$  \hspace{1cm} \text{(8)}$$

which verifies $Q_i^2 = \frac{1}{V} \sum_r C_3(r)$.

A rapidly vanishing $C_3(r)$ at large distance would then be a signature of ultrametricity. We are tempted to conjecture that the behavior is not dissimilar from the one of the connected

FIG. 2: The three-replica correlation function $C_3(r)$ for several system sizes at $T = 0.703$. Lines are only a guide to the eye. The corresponding plot for the connected overlap correlation function $C_q$, which has a similar behavior (see, e.g., [15]).

FIG. 3: Scaling of the three-replica correlation function $C_3$ of \textcolor{red}{[6]} at $T = 0.703$. In the top panel, we show the $C_3$ computed with all the triplets of configurations, which scales with an exponent $\alpha \approx 0.6$. These data are just the same as those in Figure 1 rescaled with $\alpha$. In the middle panel, we show that if we recompute $C_3$ only for triplets where all the $q_i^c < 0.3$, then $\alpha \approx 0.4$. Finally, at $T_c$, $\alpha$ is compatible with $1 + \eta = 0.6100(36)$ \textcolor{red}{[27]}. This behavior is compatible with that of the exponent $\theta(Q)$ that controls the scaling of the connected spin overlap function $C_q$, as shown in the insets. In particular, notice that the most recent computation gives $\theta(Q < 0.3) = 0.38(2)$, with $\theta(Q = q_{EA}) = 2\theta(Q = 0)$ \textcolor{red}{[28,42]}.
overlap-overlap correlation function, and that at long distance $C_3(r)/C_3^q(r) \sim O(1)$, where $C_3^q(r) = C_q(r) - \langle q^2 \rangle$ is the connected version of $C_3$. In the droplet picture, since no states with $q \neq q_{RA}$ survive in the thermodynamic limit, all triangles all equilateral and $Q^2$ is trivially null.

We show data for $C_3^q$ and $C_5$ in Figure 2 for various system sizes at temperature $T = 0.703$. Both functions decay to zero at large distances. We can now look for an algebraic decay of the form

$$C_3(r) = \frac{1}{r^\alpha} f(r/L).$$

We have attempted this in Figure 3. In the upper panel we show $C_3$ computed with all the triplets of configurations. We are able to obtain a reasonably good collapse of the data for the largest system sizes with $\alpha \approx 0.6$. However, should $C_3$ really scale as $C_q$, we expect that number to be only an effective exponent, combining the effect of the different $q$ sectors. In principle, we would like to study the dependence of $\alpha$ on $Q$ and, in particular, whether $\alpha(Q) = \theta(Q)$. Unfortunately, since $C_3$ is a three-replica function we cannot write it as a function of a single overlap, as in $C_q$. However, recall the numerical observation that $\theta(Q < C) = \theta(0)$, where $C$ is a finite cutoff value (expected to be $C = q_{RA}$ in the thermodynamical limit, but $C \approx 0.3$ for our system sizes [42]). Assuming that $\alpha$ has a similar behavior we have recomputed $C_3$ considering only the triplets where all the $q^j$ are smaller than $C = 0.3$. We see in the middle panel of Figure 2 that now the value of $\alpha$ that produces the best collapse is $\alpha \approx 0.4$, compatible with the value $\theta(0) = 0.38(2)$ found for $C_q$.

In the lower panel of Figure 3 we also show collapsed data at a $T = T_c$. In this case we do not need to impose any cutoff and the collapse for $L > 12$ is compatible with the ansatz $\alpha = \theta_{T_c}^c = 1 + \eta$, with $\eta = -0.3900(36)$ from [27].

We can get more information on the distribution of triplets of configurations with ordered overlaps from a study of the probability distribution of $x$, which should approach a delta function as the system size increases. In order to test this hypothesis, we can study the variance of $x$. We have represented this quantity in Figure 4 normalized by $\text{Var}(q) = \langle q^2 \rangle$ (this is to absorb the effect of the narrowing peaks in the $p(q)$ as the system size grows). Considered as a function of $L$, $\text{Var}(x)/\text{Var}(q)$ has a clearly different behavior at low and high temperature. Below $T_c$ we can see that $\text{Var}(x)$ decreases with $L$ at a rate that cannot be explained simply by a narrowing of the $q$ distribution. Indeed, if we consider $T = 0.703$ and fit $\text{Var}(x)/\text{Var}(q) = A L^{-\alpha}$, we obtain a value of $\alpha = 0.33(4)$, with $\chi^2$/d.o.f. $= 0.84/3$. Notice that in the thermodynamical limit $\text{Var}(q)$ is finite, while, according to the previous study, we should expect $\text{Var}(x)$ to decay algebraically with an exponent $\alpha = \theta(0) = 0.38(2)$, which is very close to the value of $\alpha$ from the fit (there are probably some preasymptotic effects due to the narrowing of the $q$ distribution). This is a clear quantitative sign that all the overlap triangles are isosceles (or equilateral) in the thermodynamical limit, but not in a trivial way.

In conclusion, we have presented an analysis of statistics taken from triplets of independent configurations and found clear signatures of ultrametricity. We introduce a three-replica ultrametric correlation function that decays algebraically with distance with an exponent compatible with the predictions of the RSB theory. In the thermodynamical limit it is always possible to flip configurations to have contributions only from non-frustrated triplets. The variance of the difference between minimum and mid-value overlap in these triplets is vanishing in the thermodynamical limit.

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