Critical behaviour and ultrametricity of Ising spin-glass with long-range interactions

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Abstract. Ising spin-glass systems with long-range interactions ($J(r) \sim r^{-\sigma}$) are considered. A numerical study of the critical behaviour is presented in the non-mean-field region together with an analysis of the probability distribution of the overlaps and of the ultrametric structure of the space of the equilibrium configurations in the frozen phase. Also, in the presence of diverging thermodynamical fluctuations at the critical point the behaviour of the model is shown to be of the replica symmetry breaking type and there are hints of a non-trivial ultrametric structure. The parallel tempering algorithm has been used to simulate the dynamical approach to equilibrium of such systems.

1. The long-range spin-glass model

The greatest incentive to study spin-glasses with long-range interactions is that they are conceptually halfway between the Sherrington–Kirkpatrick model, exactly solvable in mean-field theory, and the more realistic short-range models, with nearest-neighbour interactions. Long-range spin-glass models are particularly interesting because in one dimension they already show a phase transition between the paramagnetic and the spin-glass phase. So it is possible to study this transition, also out of the range of validity of mean-field approximation, in a relatively easy way in comparison with theories with short-range interactions below upper critical dimension. Furthermore, these one-dimensional models serve as a clarifying, qualitative, analogy for short-range models in higher dimensions.

The Hamiltonian of these kind of systems is

$$\mathcal{H} = -\sum_{i<k} J_{ik} s_i s_k \tag{1}$$

where $i = 1, \dots, N$, the size of the system, the s_i are Ising spin variables and the J_{ik} are quenched, Gaussian random variables. They have mean zero and variance:

$$\overline{J_{ik}^2} = \frac{C(\sigma)^2}{|i-k|^{2\sigma}} \tag{2}$$

where $C(\sigma)$ is a normalizing factor, such that $\sum_{ik} \overline{J_{ik}^2} = N$; periodic boundary conditions have been used (i.e. $i - k = N - i + k$ for $i - k > \frac{N}{2}$).

Already in one dimension, the long-range systems show different behaviours varying the value of σ. First of all, to allow thermodynamical convergence we must have $\sigma > \frac{1}{2}$ [1].

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For $\frac{1}{2} < \sigma \leqslant \frac{2}{3}$ a continuous phase transition is present, describable in the mean-field theory approximation; the limit $\sigma_{mf} = \frac{2}{3}$ is found in the renormalization approach from the dimension of the coupling constant. Using the replica trick, in fact, we are able to get the Landau–Ginzburg effective Hamiltonian corresponding to the Hamiltonian (1). In d dimensions it is:

$$\mathcal{H} = \frac{L^d}{4} \int \frac{\mathrm{d}^d q}{(2\pi)^d} (q^{2\sigma-d} + m_0^2) \sum_{a \neq b} |\tilde{Q}^{ab}(q)|^2 + \frac{g_0}{3!} \int \mathrm{d}^d x \sum_{a \neq b \neq c} Q^{ab}(x) Q^{bc}(x) Q^{ca}(x) \quad (3)$$

where a, b and c are the replica's indices and the dimension of the coupling constant is, then,

$$d_g = 3\sigma - 2 \tag{4}$$

for $d = 1$. So the coupling constant is irrelevant for $\sigma < \frac{2}{3}$ (or marginal for $\sigma = \frac{2}{3}$). When $\frac{2}{3} < \sigma < 1$ the phase transition is supposed to still be present but we are in an infrared divergent regime causing mean-field theory to lose consistency at the critical temperature: it is then necessary to renormalize in order to find the correct critical indices. In the case $\sigma = 1$ it is not yet clear what kind of transition there is. Kotliar *et al* [2] supposed a behaviour similar to the analogous case of the long-range ordered magnetic systems with interactions decaying like $1/r^2$, in which Anderson *et al* [3] and then, in a version for general discrete models, Cardy [4], had found a Kosterlitz–Thouless-like phase transition [5]. Until now, nothing rigorous had been proved for this value of σ. Finally, for $\sigma > 1$, there is only one Gibbs thermodynamical state at all temperatures, as rigorously proved in [6].

There is, actually, an analogy with the critical behaviour of short-range systems. Starting from the lowest allowed value of the exponent driving the intensity of the bonds and increasing it, we can observe a behaviour qualitatively similar to those of short-range models in different dimensions: from mean-field ($d \geqslant 6$) to infrared divergent regime and up to the case of the absence of a phase transition.

Our contribution has been to determine the critical temperatures and the critical indices in the regime of diverging fluctuations at the critical point for different long-range systems (different values of σ). Besides, we have examined the features of the space of the equilibrium configurations for finite-volume systems, getting various hints about the existence of a replica symmetry breaking (RSB) scenery also in the region of infrared divergences. Furthermore, through the evolution in time of three independent replicas, we have obtained elements in favour of the existence of an ultrametric structure of the equilibrium states; therefore sustaining the idea that this kind of phase space belongs intrinsically to spin-glasses, and that it does not depend on mean-field theory formulation, in which framework it was initially derived.

We have performed numerical simulations of these systems with different power-law behaviours, i.e. changing the value of the exponent σ. We took $\sigma = 0.69$ and $\sigma = 0.75$, both beyond σ_{mf}. They are the same values chosen by Bhatt and Young in [7] so as to compare the common results. Every system has been simulated in different sizes to utilize the finite-size scaling (FSS) techniques: five sizes between 32 and 512 spin have been investigated for every value of σ. In this way we obtained the critical indices and compared their values with the theoretical values obtained from one-loop expansion in $\epsilon = \sigma - \sigma_{mf}$ [2]. Moreover, in every numerical run we have looked at the parallel evolution of three independent replicas (observed in the same bond configuration). In this way it has been possible to study observables built from three different overlaps, that are useful to probe the ultrametric structure of the equilibrium configurations of a spin-glass, also out of the mean-field range of validity.

To simulate the dynamical approach to equilibrium we have used the parallel tempering algorithm [8]. The evolution of every system has been simulated in a number of different random quenched samples varying between 200 (for $N = 512$) and 600 ($N = 32$), for 65 536 Monte Carlo (MC) steps each. The thermalization times, in MC steps, were all at least 30

times smaller than this value. In order to find the thermalization we, first of all, checked that the time that each configuration simulated in the parallel tempering spends in every heat bath is independent of the temperature of the bath. We also checked that the probability of exchanging two configurations between two different baths is almost the same for every couple of temperatures and it is always greater than 0.3 for the set of temperatures chosen to perform the parallel tempering simulation. Finally, the most important check on thermalization has been to look at the absence of drifting of the observables (the kurtosis of the overlap distribution and the spin-glass susceptibility) on the logarithmic timescale, after they reached their plateau values.

2. Critical behaviour

To determine the critical temperature we have used the FSS property of the observable:

$$g = \frac{1}{2}\left(3 - \frac{\overline{\langle q^4 \rangle}}{(\overline{\langle q^2 \rangle})^2}\right) \tag{5}$$

called the *Binder parameter*. Here $\langle \rangle$ stands for the mean over the thermodynamical *ensemble*, while the overline represents the mean over the random distribution of the bonds. The overlap q is defined, for our numerical goal, as

$$q = \sum_i s_i^{(1)} s_i^{(2)} \tag{6}$$

where the upper index is the real replica's one.

The FSS form of the Binder parameter is:

$$g = \overline{g}(N^{\frac{1}{\nu}}(T - T_c)) \tag{7}$$

where N is the size of the system. Since at $T = T_c$, for every size, is $g = \overline{g}(0)$, the critical temperature can be deduced from different sizes $g(T)$ intersections. To compute it, we have used the scaling behaviour of the 'critical' temperature for a finite-size system:

$$T_c(N) - T_c^\infty = B\, N^{-\theta} \tag{8}$$

where the $T_c(N)$ is the abscissa of the intersection point between the $g(T)$ for the size $N/2$ and the $g(T)$ for the size N and $\theta = 1/\nu$ [9]. Thus, fitting the curves of $T_c(N)$ for both long-range systems ($\sigma = 0.69$ and $\sigma = 0.75$) with a power-law function, we have been able to extrapolate the following values for the critical temperature in the thermodynamical limit (T_c^∞ in (8)). We have (see figure 1):

$$T_c = 0.75 \pm 0.1 \qquad \text{for} \quad \sigma = 0.69 \tag{9}$$

$$T_c = 0.63 \pm 0.08 \qquad \text{for} \quad \sigma = 0.75. \tag{10}$$

The first result is consistent with the two estimates of [7] for $\sigma = 0.69$: $T_c \sim 0.73$ and $T_c \sim 0.78$. However, they could not localize the transition temperature for $\sigma = 0.75$. Instead, we have found that there is clearly a second-order phase transition also at $\sigma = 0.75$, well besides the region of validity of the mean-field theory. In analogy with short-range models, we observe that the behaviour of the Binder parameter is qualitatively similar to that of four-dimensional short-range spin-glasses, far below the upper critical dimension and over the lower critical dimension (LCD) [10–12].

From the g's FSS properties we have also determined the critical index ν [14]. We have not used the value of the parameter $\theta = \frac{1}{\nu}$ computed from the fit (8) because of its very large
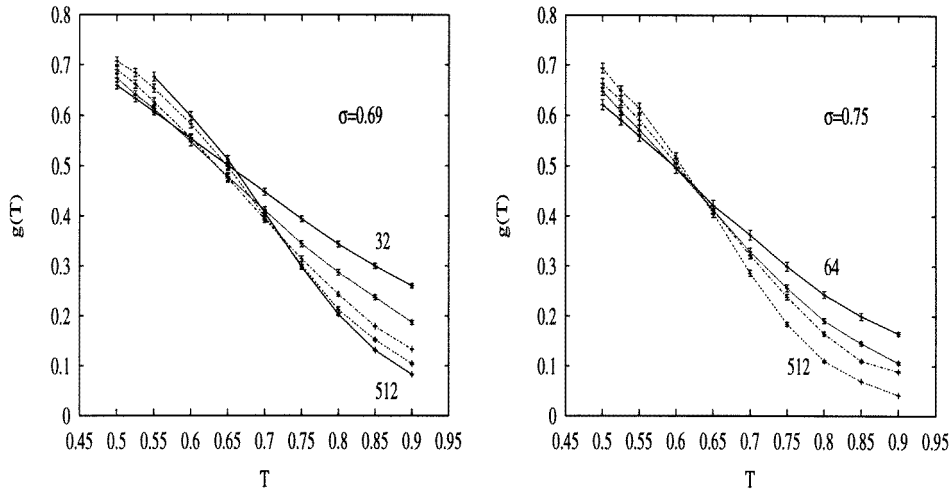
Figure 1. The Binder parameter g versus temperature for different sizes for the model with $\sigma = 0.69$ (left) and the model with $\sigma = 0.75$ (right). In the first case the 32–512 sizes are plotted, in the second case only the 64, 128, 256 and 512 are represented.

uncertainty. Instead, to estimate it, we have first calculated the derivative of g with respect to T at a given value g_0. In fact, from (7) follows:

$$\left.\frac{\mathrm{d}g}{\mathrm{d}T}\right|_{T_0: g(T_0)=g_0} \simeq AL^{\frac{1}{\nu}}. \tag{11}$$

We have computed the values of the derivative for the values of g corresponding to the confidence interval of the critical temperature. In this interval of g-values we have fitted the $g(T)$ curves, in every size, with polynomials of various order (by the fact of second or third order), each time looking for the polynomial of the lowest possible order giving a fit satisfying the χ^2 test.

For every g_0 value we have got different values of the $\frac{\mathrm{d}g}{\mathrm{d}T}|_{T_0: g(T_0)=g_0}$ for different sizes. Then for every g_0 we determine a $\nu(g_0)$. The mean value of these gives the correct exponent ν.

For our two models we have found:

$$\nu = 3.8 \pm 0.4 \qquad \text{for} \quad \sigma = 0.69 \tag{12}$$

$$\nu = 4.5 \pm 0.2 \qquad \text{for} \quad \sigma = 0.75. \tag{13}$$

The first result is consistent with [7], which gave $\nu = 4.0 \pm 0.8$, and also with the one-loop expansion result [2]: $\nu_{1l} = 3 + 36\epsilon = 3.84$ (here is $\epsilon = \sigma - \frac{2}{3} = 0.69 - \frac{2}{3}$). For $\sigma = 0.75$, instead, we are really too far from σ_{mf} for the one-loop expansion to give a good approximation ($\nu_{1l} = 6$).

To find the critical index η which gives the anomalous dimension of the two-point correlation function at the critical temperature, we have used the FSS properties of the observable χ_{sg}, the so-called spin-glass susceptibility, defined as

$$\chi_{sg} = \frac{1}{N} \sum_{ik} \overline{(\langle s_i s_k \rangle)^2} = N \overline{\langle q^2 \rangle} \tag{14}$$

whose scaling behaviour is

$$\chi_{sg} = N^{2-\eta} \overline{\chi}(N^{\frac{1}{\nu}}(T - T_c)). \tag{15}$$

We have:

$$\eta = 1.62 \pm 0.08 \qquad \text{for} \quad \sigma = 0.69 \tag{16}$$

$$\eta = 1.4 \pm 0.1 \qquad \text{for} \quad \sigma = 0.75. \tag{17}$$

The theoretical value of η in a long-range system, or, more exactly, its dependence on σ, such as that described by the Hamiltonian (3), does not vary from the mean-field value going in a region of diverging thermodynamical fluctuations, because the two-point vertex function ($\Gamma^{(2)}$) does not have any infrared divergence at the critical point. The behaviour of the vertex function of the two *fields* Q^{ab} and Q^{cd}, as derived from the Hamiltonian (1), is:

$$\Gamma^{ab,cd}(k) = \left[k^{2\sigma-d} - g_0^2(n-2) \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{1}{p^{2\sigma-d}(p-k)^{2\sigma-d}} \right] F^{abcd}$$

$$\equiv [k^{2\sigma-d} - g_0^2(n-2)I_\sigma(k)]F^{abcd}$$

$$\equiv \Gamma^{(2)}(k)F^{abcd} \tag{18}$$

where, in our case, $d = 1$, n is the number of the replicas and the tensor F^{abcd} is defined like in [13]:

$$F^{abcd} = \tfrac{1}{2}(\delta^{ac}\delta^{bd} + \delta^{ad}\delta^{bc} - T^{abcd}) \tag{19}$$

and

$$T^{abcd} = \begin{cases} 1 & \text{if} \quad a = b = c = d \\ 0 & \text{otherwise.} \end{cases} \tag{20}$$

The integral can be easily computed:

$$I_\sigma(k) \equiv \int \frac{\mathrm{d}^d p}{(2\pi)^d} \frac{1}{p^{2\sigma-d}} \frac{1}{(p-k)^{2\sigma-d}}$$

$$= \frac{(k^2)^{\frac{3d}{2}-2\sigma}}{(4\pi)^{\frac{d}{2}}} \frac{\Gamma(2\sigma - \frac{3}{2}d)}{\Gamma(2d-2\sigma)} \left[\frac{\Gamma(d-\sigma)}{\Gamma(\sigma - \frac{d}{2})} \right]^2. \tag{21}$$

Expressing the perturbative expansion in the variable $\epsilon = \sigma - \frac{2}{3}d$ we observe that the function $I_\sigma(K)$ has no pole in ϵ. Thus, the term $k^{2\sigma-d}$ in $\Gamma^{(2)}(k)$ of the free theory needs no correction from any perturbative contribution and the anomalous dimension η of the two-points correlation function does not depend on the order of the perturbation expansion.

Therefore, it always has the same dependence on the exponent σ: at any order is $\eta = d + 2 - 2\sigma = 3 - 2\sigma$. So the theoretical values are:

$$\eta_t = 1.62 \qquad \text{for} \quad \sigma = 0.69 \tag{22}$$

$$\eta_t = 1.5 \qquad \text{for} \quad \sigma = 0.75 \tag{23}$$

and our results are in total agreement with them. Using the so obtained values of the critical indices we can plot the scaling behaviour of g and of χ_{sg} as shown in figure 2.

3. $P(q)$ analysis and ultrametricity

The overlap probability distribution $P(q)$ is one of the most powerful means at our disposal to obtain information about the pure states structure of a spin-glass in its low-temperature phase. The $P(q)$, in the standard replica approach, is connected to the structure of the *finite-volume equilibrium states*. This point of view has sometimes been criticized, e.g. by Newman and Stein [15], but some of the objections raised by them have been overcome by showing that the
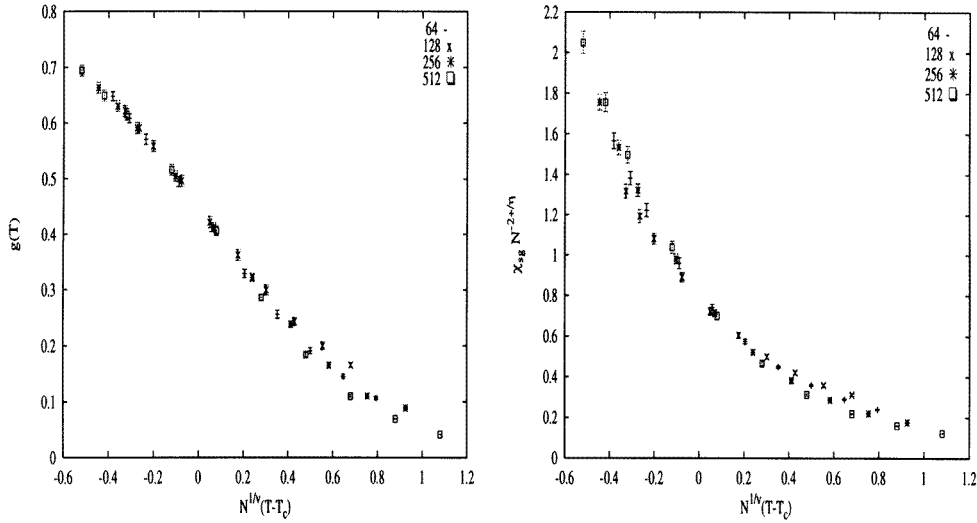
Figure 2. The scaling property of the Binder parameter (left) and of the spin-glass susceptibility (right). $g(T)$ and $\chi_{sg} N^{-2+\eta}$ versus $N^{\frac{1}{\nu}}(T - T_c)$ are plotted for all the sizes of the system with $\sigma = 0.75$ ($T_c = 0.63$, $\nu = 4.5$, $\eta = 1.4$, $N = 64, 128, 256, 512$).

behaviour of the probability distribution functions built from *window* overlaps† is identical to that of the functions $P(q)$ defined in the usual way [16].

In this paper we present the data of the numerical simulations using the standard replica approach. However, the data themselves do not depend on the definition of pure state: they are some kind of 'experimental' facts that must be explained by the theory.

An analysis of the behaviour of $P(q)$ allow us to discern between the RSB frame and the trivial one, in which only two different pure states are allowed.

Observing the behaviours of the probability distributions shown in figure 3, we realize that we are studying models, whose low-temperature phase is described by many equilibrium states, including those states which are completely different and that correspond to the region around $q \simeq 0$. The peak becomes higher as N grows, while the area under the $P_N(q)$, between $q = 0$ and the value of q corresponding to the peak of the distribution, tends to remain constant. Furthermore $P(|q| = 0)$ does not decrease, increasing the size of the system, but settles down to a non-zero value. This is the same picture we have in the mean-field case, if we are now also considering systems which cannot be treated in the mean-field approximation. The fact that these distributions do not end with a δ function like the theoretical one in RSB theory, but are non-zero in the whole interval $[0, 1]$, is an expected effect of the finite size of the simulated systems.

The most relevant and particular property of the phase space at finite volume that seems to emerge from our analysis is the ultrametricity, the special hierarchical structure of spin-glasses equilibrium configurations. We can gather hints of the existence of this property using some

† The overlap over a window of linear size B is defined as

$$q_B = \frac{1}{B^d} \sum_{i=1}^{d} \sum_{x_i}^{B-1} s^{(1)}(\{x_i\}) s^{(2)}(\{x_i\}) \tag{24}$$

where d is the dimension of the lattice, x_i are the coordinates on the lattice and B is smaller than L, the linear size of the lattice.
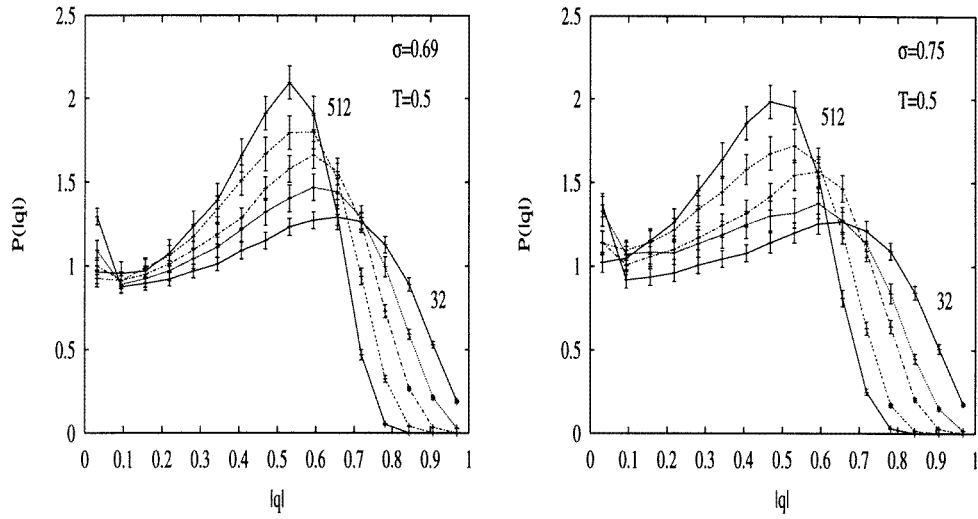
Figure 3. $P(q)$ at $T = 0.5$ for the long-range models with $\sigma = 0.69$ (left) and $\sigma = 0.75$ (right). The sizes plotted are $N = 32, 64, 128, 256, 512$. Increasing the size the distribution flattens toward a value of about one, in the region $|q| \simeq 0$, and the peak becomes increasingly sharp.
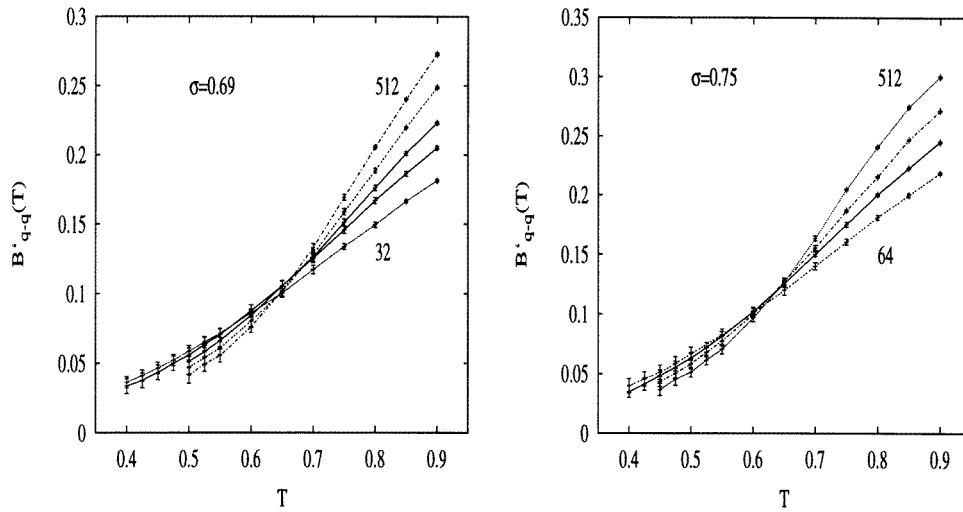
Figure 4. $B'_{q-q}(T)$ for the two long-range systems: $\sigma = 0.69$ (left), for sizes $N = 32, 64, 128, 256, 512$, and $\sigma = 0.75$ (right), for sizes $N = 64, 128, 256, 512$.
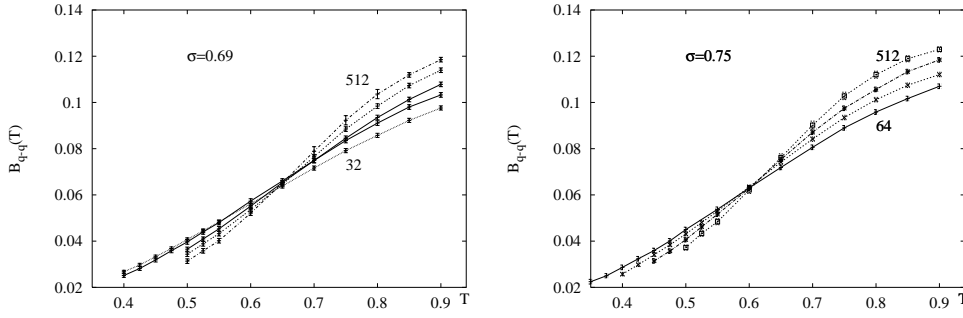
cumulants built from the overlaps q_{12}, q_{13} and q_{23} of three different, independent replicas. With this aim we have observed the behaviour of the two cumulants

$$B_{q-q} \equiv \frac{\overline{\langle(|q| - |q'|)^2\rangle}}{\overline{\langle q_M^2\rangle}} \tag{25}$$

and

$$B'_{q-q} \equiv \frac{\overline{\langle(q - q'\,\text{sign}(q_M))^2\rangle}}{\overline{\langle q_M^2\rangle}} \tag{26}$$

Figure 5. B_{q-q} versus temperature for the $\sigma = 0.69$ model (left) and the $\sigma = 0.75$ model (right). The sizes are the same as figure 4.

where q_M is the value of the overlap which has the maximum absolute value between the three, q and q' are the values of the other two overlaps ($q, q' < q_M$). The measures are made in every quenched configuration, at every temporal uncorrelated interval, once the simulated system has reached equilibrium. Like the Binder parameter g, these observables also have a FSS behaviour not depending on the index η. Their FSS form is, in fact,

$$B_{q-q}^{\#} = \overline{f}(N^{\frac{1}{\nu}}(T - T_c)). \tag{27}$$

Analysing their behaviours in the proper way we can get different checks of the existence of a complicated space of states organized in an ultrametric structure.

   If an ultrametric structure exists the cumulants B_{q-q} and B'_{q-q} should tend to zero under T_c in the thermodynamical limit. The two minor overlaps, in fact, should become equal and their difference should tend to zero. This is, really, the behaviour that we noticed and that is plotted in figures 4 and 5: the B_{q-q} and B'_{q-q} of a given system tend to zero with decreasing temperature and they do it faster the bigger the size of the system.

   At fixed temperature below the critical one, $T = 0.5$, we have fitted $B_{q-q}(N)$ with the power-law behaviour $A\,N^{-\zeta}$. In both the long-range models considered, B_{q-q}, at $T = 0.5$, appear to decrease to zero with this law. The exponents are $\zeta = 0.091 \pm 0.009$, for $\sigma = 0.69$, and $\zeta = 0.09 \pm 0.01$ for $\sigma = 0.75$. Because of these small values of ζ, we would need data about systems of greater size to guarantee that B_{q-q} tends to zero below the critical point. Nevertheless, the power-law decaying of the B_{q-q} towards zero is consistent with our data.

   Following the behaviour from the high-temperature phase the curves cross each other in the critical region (we know it from the FSS behaviour) and then tend to zero for $T \to 0$. Actually, from this crossing we can have another guess at the critical temperature, just like from the Binder parameter g (see figure 6).

   In this case, however, there is no fit of the FSS behaviour (8) satisfying the χ^2 test. Thus, we simply give the average of the last points of intersection between the $B_{q-q}(T)$ curves. The values found are:

$$\begin{aligned} T_c &= 0.65 \pm 0.08 \qquad \text{for} \quad \sigma = 0.69 \\ T_c &= 0.60 \pm 0.06 \qquad \text{for} \quad \sigma = 0.75. \end{aligned} \tag{28}$$

Anyway, this estimate agrees, within the errors, with the previous one given in (10). The errors appear to be smaller than in (10), but we underline that we could not manage to perform the FSS fit, neglecting, in this way, the shift of the $T_c(N)$ towards the T_c of the system in the thermodynamical limit: the values above experience a systematic error.

   As we can note from figures 4 and 5 the cumulant B'_{q-q} is always greater then B_{q-q}. This is due to the fact that $q'\text{sign}(q_M)$ not always has the same sign of q: there are triples
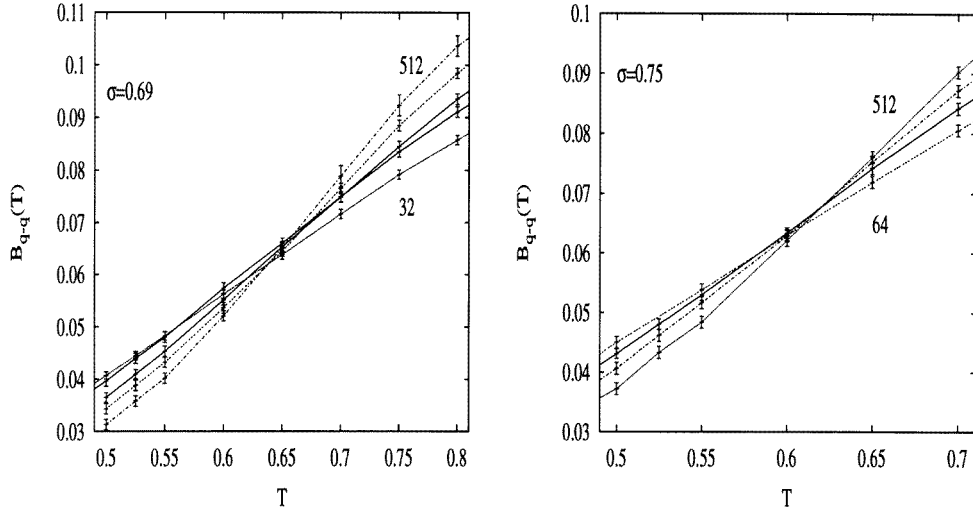
Figure 6. Detail of B_{q-q} in the critical region for the $\sigma = 0.69$ (left) and the $\sigma = 0.75$ model (right).

of spin configurations giving products $qq'q_M < 0$, that is $\text{sign}(q'\text{sign}(q_M)) \neq \text{sign}(q)$. This implies that sometimes the $(q - q'\text{sign}(q_M))^2$ contributions to the mean value are bigger than the corresponding $(|q| - |q'|)^2$ terms in B_{q-q}. The qualitative behaviour of temperature dependence, however, is not influenced in a critical way from this difference and $B'_{q-q}(T)$ tends to zero while $T \to 0$ just like $B_{q-q}(T)$. Fitting, as before, B'_{q-q} at the fixed temperature $T = 0.5$ with the power-law $A'N^{-\zeta'}$, we observe a behaviour statistically consistent with the decay to zero. The exponents are now $\zeta' = 0.12 \pm 0.01$ for $\sigma = 0.69$ and $\zeta' = 0.13 \pm 0.02$ for $\sigma = 0.75$.

4. Conclusions

In summary, the insight we get about the one-dimensional long-range ($J(r) \sim \frac{1}{r^\sigma}$) spin-glasses is that the critical behaviour satisfies the one-loop predictions for σ not too far from $\sigma_{mf} = \frac{2}{3}$, but that the first-order ϵ-expansion already fails to describe it for $\sigma = 0.75$. In both systems examined we have been able to determine a low-temperature phase, showing a non-trivial hierarchical structure of the space of the finite-volume equilibrium configurations. We have built the $P(q)$ distribution, from which we can argue the validity of the RSB ansatz also for $\sigma > \frac{2}{3}$, out of mean-field theory, and we have analysed the ultrametric structure of the equilibrium configurations with the cumulants B_{q-q} and B'_{q-q}.

To describe the behaviour of the one-dimensional long-range system with interactions decaying like $1/r$ ($\sigma = 1$) a few analytical works have been made until now [2, 17], based on the replica symmetric ansatz. Our results, however, show the inconsistency of this Ansatz in the explored region of parameters (i.e. until $\sigma = 0.75$). The ansatz of replica symmetry is, furthermore, also violated in a related model for diluted infinite-range systems [18]. Consequently, further investigation should be performed to understand the behaviour of such power-law decaying systems for $\sigma = 1$.

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