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On the energy minima of the Sherrington-Kirkpatrick model

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Abstract. We study properties of the energy minima obtained by quenching equilibrium configurations of the Sherrington–Kirkpatrick (SK) mean-field spin glass. We measure the probability distribution of the overlap among quenched configurations and the quenched energy, looking at the dependence on the starting equilibrium temperature, and performing a systematic analysis of finite-size effects.

1. Introduction

The local energy minima properties are analysed in several works on glass-forming liquids and they are allowing a better understanding of the behaviour of these systems. The importance of potential energy landscape in the physics of super-cooled liquids has already been pointed out by Goldstein [1]. More recently Stillinger and Weber [2] formalized the idea that the multidimensional energy surface can be partitioned into a large number of local minima, so-called *inherent structures* (IS), each one being surrounded by its attraction basin. It is now clear [3] that the low-temperature dynamics (i.e. for temperatures below the mode-coupling critical temperature T_{MCT} [4]) can be subdivided into intra-basin motion and crossing of energy barriers by activated processes, taking place on a significantly longer time-scale.

A system in equilibrium below T_{MCT} is 'almost always' trapped in one of the basins accessible at this temperature. The huge number $\mathcal{N} \propto \exp(N\Sigma)$ of these 'valleys', exponentially diverging with the system size N, suggested the scenario of an underlying thermodynamic transition due to an 'entropy crisis' at the Kauzmann temperature $T_K < T_{MCT}$ where the configurational entropy Σ goes to zero [5], which was supported by recent analytical work [6–8]. By looking at IS one can evaluate Σ numerically [8–10]. Moreover, the IS energy turns out to be an interesting quantity for studying both the static and the dynamical behaviour [9–13]. Differences between fragile and strong glasses were recently proposed to be explainable within an energy landscape description, too [14].

The outlined picture of glass-forming liquids is reminiscent of that characterizing generalized mean-field spin-glass models such as those involving p-spin interactions [15], which display a dynamical ergodicity breaking at the temperature $T_D \equiv T_{MCT}$ [16] (in this case the barriers between basins are also infinite in the thermodynamic limit for $T_K < T < T_{MCT}$ because of the mean-field approximation), and a thermodynamic entropy-driven transition at a lower temperature T_K , corresponding to a one-step replica symmetry breaking (1RSB) scenario. For $T < T_K$ one finds a non-trivial probability distribution of the overlap between

states $P(q) = m\delta(q) + (1 - m)\delta(q - q_{EA})$. Here q_{EA} is the self-overlap of a state with itself, whereas different states are orthogonal and have zero mutual overlap.

Several years ago, Kirkpatrick, Thirumalai and Wolynes [17] suggested that 1RSB spin-glass models could be a paradigm of vitreous systems. The numerical study of out-of-equilibrium dynamics in glass-forming liquids gives intriguing results [18–21]. The measurement of P(q) among 'glassy states' is a subtle task [22–24], since one faces both the problem of thermalizing the system down to very low temperatures and that of avoiding possible crystalline minima whose basin of attraction could be non-negligible for small systems. As recently proposed by Bhattacharya *et al* [23], to look at the inherent structures is helpful also from this point of view, since it allows a more precise definition of the overlap and make it easier to distinguish between glassy minima and crystalline or quasi-crystalline configurations.

On the other hand, it is not completely clear a priori which kind of behaviour one should expect for the $P_{quench}(q)$ measured among energy minima obtained by quenching equilibrium configurations instead of among equilibrium configurations themselves. To the best of our knowledge, such a quantity has never previously been studied in a spin-glass model (which is not surprising, since in this case equilibration is still feasible without difficulties for moderate system sizes). More generally, little is known about properties of 'inherent structures' in spin glasses, which (apart from analogies with glass-forming liquids) have their own interest even in the well understood Sherrington-Kirkpatrick (SK) mean-field model. In a previous work [25] one of the authors studied the energy minima of the SK model obtained starting from random initial configurations (i.e. by quenching from infinite initial temperature), whereas recently Crisanti and Ritort [26, 27] have performed both for a 1RSB spin glass and for the SK model a numerical analysis of the static and dynamical properties within the energy landscape description similar to that proposed in [9, 13] for a glass-forming liquid, by looking, in particular, at the IS energy and at the configurational entropy. Their results confirm the close similarities between 1RSB spin glass and structural glass energy landscapes and the usefulness of this kind of approach, further suggesting a systematic analysis.

In this paper, we perform an extensive numerical study of energy minima properties in the SK model, considering initial equilibrium configurations both in the high-temperature (paramagnetic) region and deep in the glassy phase. We look first of all at the behaviour of the appropriately defined $P_{quench}(q)$ which is compared with the corresponding (usual) equilibrium one. Then we extend the analysis to the overlap of the IS with the configurations from which they are obtained, which measure the (quite strong) correlations between them, and we study systematically finite-size effects on the behaviour of the IS energy.

2. Model, observables and simulations

The Sherrington-Kirkpatrick spin-glass model [28] is described by the Hamiltonian

$$\mathcal{H}_J = \sum_{i < i=1}^N J_{ij} \sigma_i \sigma_j \tag{1}$$

where $\sigma_i = \pm 1$ are Ising spins, the sum runs over all pairs of spins and J_{ij} are random independent variables with mean value $\overline{J_{ij}} = 0$ and variance 1/N. We take $J_{ij} = \pm N^{-1/2}$.

This model is exactly solvable (since interactions have infinite range) and has a glassy phase with full replica symmetry breaking (FRSB). In the case of zero magnetic field (the one we consider here), taking into account the symmetry under inversion of the spins, the

P(q) changes at the critical temperature $T_C = 1$ from a δ -function at q = 0 (characteristic of the paramagnetic phase) to the FRSB two δ -functions in $q = \pm q_{EA}$ with a non-zero *plateau* joining them. The transition is also continuous in the order parameter (at variance with 1RSB models), i.e. $\lim_{T \to T_C^-} q_{EA}(T) = 0$, and there is no distinction between the dynamical and the static transition [29], i.e. $T_D = T_C$.

The SK model is particularly suitable for the kind of study we are interested in, since its behaviour is well understood and, on the other hand, by using optimized Monte Carlo methods [30] one is able to thermalize large system sizes down to low temperatures, which allows us to study finite-size effects systematically. We simulated N = 64, 128, 256, 512 and 1024, averaging over 2048, 1024, 512, 384 and 192 different disorder realizations, respectively. The program was multi-spin coded on different sites of the system (we store 64 spins in the same word) and we used parallel tempering (PT) [30, 31], running simultaneously two independent sets of copies (replica) of the system for each sample. Up to 50 (for the two largest sizes) different temperatures between $T_{min} = 0.65$ and $T_{max} = 3$ were used, and we performed from 100.000 PT steps for the smallest value of N = 64 to 300.000 for the largest value of N = 1024.

The PT acceptance for the exchange of nearest-neighbour temperatures was never smaller than 0.6. In the second half of the run we computed the specific heat both as the derivative of the energy density with respect to temperature $c \equiv \mathrm{d}\langle e \rangle/\mathrm{d}T$, and from fluctuations $c \equiv N(\langle e^2 \rangle - \langle e \rangle^2)/T^2$, looking for compatibility of results. This means comparing one-time and two-time quantities, respectively, which is an effective way of checking thermalization, particularly when using PT (note that in this case fluctuations involve different replicas evolving at the same temperature at different times during the run). Nevertheless, we also divided the second half of the run into (four) equal intervals, checking that there were no evident differences in the values of the considered observables, P(q) and $P_{quench}(q)$ in particular. A further confirmation of the system being well thermalized comes from the perfect symmetry with respect to the exchange $q \to -q$ probability distributions that we obtained.

For each disorder realization and for each temperature, in the second half of the run, we saved 1500+1500 equilibrium configurations from the two independent sets of replicas which were subsequently quenched by a zero-temperature dynamics. The observables were computed from these configurations and the corresponding energy minima, errors being evaluated from sample-to-sample fluctuations. One should note that both P(q) and $P_{quench}(q)$ are strongly not self-averaging in the glassy phase, wherefore it was necessary to average over a large number of samples even for large system sizes. The whole simulations would have taken about 2 years of CPU time on a usual alpha-station, i.e. a few days when using 128 processors simultaneously on a Cray T3E (the code is easily parallelized with an efficiency of close to 1 by running a different disorder realization on each processor).

A subtle point concerns the quenching procedure. We are considering even values for N, which means that the local field acting on each spin because of the other ones can never be zero. Moreover, it is known [25], from the analysis of properties of quenched configurations obtained starting from infinite temperature (i.e. a random initial configuration), that different zero-temperature dynamics give qualitatively identical results. The 'greedy algorithm', where the spin corresponding to the largest energy decrease is flipped at each step, seems to stop more frequently in local high-energy minima than the 'reluctant algorithm', where one flips the spin which gives the smallest energy decrease (i.e. the opposite of the previous case). We choose to use an 'intermediate' zero-temperature dynamics, which is also easy to implement. At each step, a randomly chosen spin is suggested to flip and at least 20N steps are performed after the last successful one before stopping. The probability that

the final configuration is not a local energy minimum (under single spin flip) is therefore $\sim e^{-20}$, i.e. practically negligible. As a last remark, it should be stressed that such a quenching procedure could possibly give energy minima which are not the 'nearest' IS to the starting equilibrium configurations, i.e. which are *less* correlated but not *more* correlated than in the analoguous glass-forming liquid case, where one generates ISs by following the path of steepest descent.

Labelling by $\{\sigma_i\}$, $\{\tau_i\}$ the spins belonging to two configurations, the overlap is defined as

$$Q = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tau_i.$$
 (2)

The spin-glass order parameter, i.e. the equilibrium probability distribution of overlap among states P(q,T), is usually evaluated numerically as the histogram of the instantaneous overlap $\mathcal Q$ between two replica (with the same disorder configurations) which evolve simultaneously and independently at temperature T

$$P(q,T) = \overline{P_J(q)} = \overline{\langle \delta(q - Q) \rangle}$$
 (3)

where the thermal average $\langle \cdot \rangle$ corresponds to an average over time in the simulation, whereas $\overline{(\cdot)}$ denotes the average over J_{ij} realizations. $P_J(q,T)$ can be equivalently measured from two given sets of equilibrium configurations belonging to the two replicas, by considering the overlap of each configuration of one set with all the configurations of the other. In this work we evaluated $P_J(q,T)$ both during the simulation and from the saved configurations, obtaining perfectly compatible results, which confirm that these configurations sample the phase space accurately enough.

We define the quenched probability distribution of the overlap as

$$P_{quench}(q,T) = \frac{1}{\mathcal{N}_{IS}^2} \sum_{i_q,i_p=1}^{\mathcal{N}_{IS}} \delta(q - \mathcal{Q}_{IS})$$
(4)

where the sum runs over the $\mathcal{N}_{IS}=1500$ energy minima obtained starting from the equilibrium configurations at temperature T for each of the two replica sets. This definition, which is analogous to that introduced in [23] for a Lennard-Jones glass-forming binary mixture, implies that we are weighting each IS with the Boltzmann factor of the corresponding basin at temperature T, as is usual in numerical studies on super-cooled liquids.

3. Results

3.1. The behaviour of $P_{quench}(q)$

We present in figure 1 data for the equilibrium overlap distribution P(q) (on the left) and for the quenched overlap distribution $P_{quench}(q)$ (on the right) at a temperature very close to the critical temperature T=1.05=1.05 T_C , but still in the paramagnetic phase, for different system sizes. It was shown in [25] that the $P_{quench}(q)$ obtained from infinite-temperature configurations becomes more and more concentrated in q=0 for increasing N and it goes to a δ -function in the thermodynamic limit. We find the same qualitative behaviour in the whole high-temperature region $T>T_C=1$. It is very clear from figure 1 that there is no evidence for replica symmetry breaking in the probability distribution of overlap between IS reachable from equilibrium configurations at $T\gtrsim T_C$ and weighted with the Boltzmann factor of the corresponding basin at this temperature.

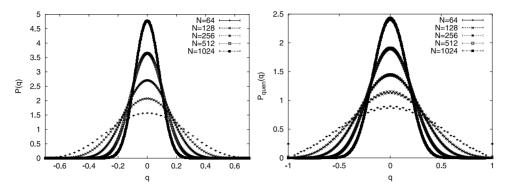


Figure 1. The equilibrium P(q) (on the left) and the quenched one (on the right) at T = 1.05, a value of the temperature slightly higher than $T_C = 1$, for different values of the system size.

In other words, we know that for $T < T_C$ there is RSB, but we cannot detect it by looking at the probability distribution of the overlap obtained with a fast quench starting from $T \gtrsim T_C$. This result implies that also in the case of a glass-forming liquid the analogously defined $P_{quench}(q,T)$ will be trivial when quenching from the paramagnetic (liquid) phase, even when quenching down to a T value where RSB occurs (if it does). This is in agreement with the behaviour reported in [23] for a Lennard-Jones binary mixture starting from $T \gtrsim T_{MCT}$.

In glass-forming liquids the overlap among IS is easier to define than the equilibrium overlap: its use releases one from the careful consideration of possible crystalline or quasi-crystalline configurations. Nevertheless, the quantity $P_{quench}(q,T)$ does not provide any evidence for the existence or absence of RSB when avoiding the hard task of thermalizing a super-cooled liquid down to low temperatures. One should also note that in 1RSB models both P(q,T) and $P_{quench}(q,T)$ are also expected to be trivial in the region $T_{MCT} > T > T_K$ (apart from finite-size effects), just because of the very large number $\sim e^{N\Sigma}$ of 'valleys' (and corresponding IS) which are *almost all* orthogonal [32], with zero overlap in the thermodynamic limit.

After clarifying this point, we note that a more careful analysis of the data shown in figure 1 (right) suggests the presence of a *weak* RSB, as already observed in $P_{quench}(q, T = \infty)$ [25]. In the whole paramagnetic phase, the 'quenched' probability distribution of the overlap approaches its delta function limit $\delta(q)$ for $N \to \infty$ much slower than the equilibrium one. To quantify the N dependence, we introduce the function

$$f(q) \equiv -\lim_{N \to \infty} \frac{1}{N} \ln \left[P_{N,quench}(q) \right]. \tag{5}$$

The replica symmetry is broken in a weak sense if f(q) is zero in an extended region I though $P_{quench}(q)$ is a δ -function in the thermodynamic limit. This implies that $P_{N,quench}(q)$ is going to zero slower than exponentially in this region and that therefore, by adding to the Hamiltonian a quantity of order N (for instance, by using appropriate boundary conditions), one could obtain any given value of the 'quenched' overlap $q \in I$. Our best numerical evidence for such a behaviour comes from the study of

$$r_N(q,T) \equiv \frac{1}{N^{\nu}} \ln \left(\int_q^1 \mathrm{d}q' \, P_{N,quench}(q',T) \right). \tag{6}$$

We obtain a practically *T*-independent estimate of the exponent for $T > T_C$, $\nu = 0.68 \pm 0.05$. This value is compatible with $\nu \simeq \frac{2}{3}$ obtained from $T = \infty$ data in [25]. Though one observes

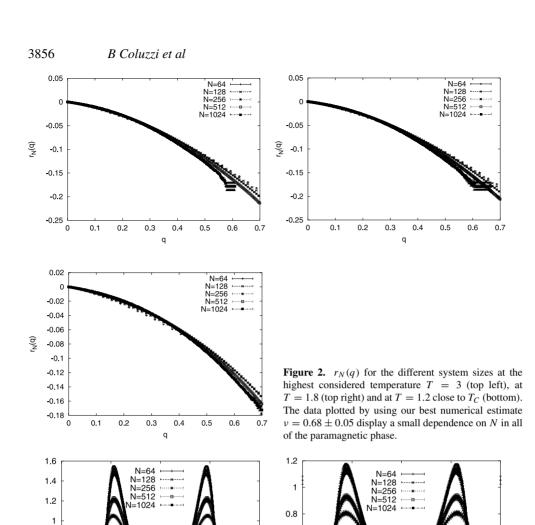


Figure 3. The equilibrium P(q) (left) and the quenched one (right) at T = 0.65 = 0.65 T_C (the lowest T-value we have considered) for different system sizes.

-0.5

0

q

0.5

0.6

0.4

0.2

some deviations at large q, the weak N dependence of r_N shown in figure 2 and the value of ν that is significantly smaller than 1, strongly suggest that f(q) is zero on a finite interval I, where possibly I = [0, 1], i.e. $P_{quench}(q)$ displays a *weak* breaking of replica symmetry.

8.0 G

0.6

0.4

0.2

-0.5

0

q

0.5

On the other hand, at temperatures lower than T_C , $P_{quench}(q, T)$ clearly shows the characteristic behaviour corresponding to a full replica symmetry breaking. This is what one would expect since RSB was already evident in the P(q) of the configurations we were starting from. The qualitative similarities between P(q) and $P_{quench}(q)$ are remarkable (see figure 3). They are present for each disordered configurations: for instance, the number of peaks found in a one-sample equilibrium $P_J(q, T)$ at a given T is preserved in the corresponding

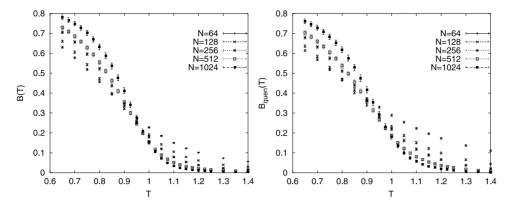


Figure 4. The Binder parameter from the equilibrium P(q) (left) and from the quenched one (right) as a function of temperature for different system sizes.

 $P_{J,quench}(q,T)$ too. FRSB features are even more evident when looking at $P_{quench}(q)$: in particular, the presence of a continuous *plateau* between the two self-overlap peaks is clearer in figure 3 on the right than in figure 3 on the left, since the 'quenched' self-overlap takes larger values, though it goes to one only for $T \to 0$.

Finite-size effects play a similar role in the equilibrium and quenched cases: for instance, it is clear from figure 3 that also the 'quenched' zero overlap probability $P_{quench}(0, T)$ does not depend on N in the glassy phase, this being a well known test when looking for FRSB [33]. To further investigate this point, we plot in figure 4 the ratio of cumulants,

$$B(T) = \frac{1}{2} \left(3 - \frac{\overline{\langle q^4 \rangle}}{\overline{\langle q^2 \rangle}^2} \right) \tag{7}$$

as a function of T. We recall that this is the usual quantity one calculates in order to locate the critical temperature, since finite-size scaling predicts that curves for different sizes intersect at T_C : this is the behaviour observed in figure 4 (left) (apart from corrections to scaling when considering the smaller system sizes). Surprisingly enough, we find that the same kind of finite-size analysis can be performed on cumulants obtained from probability distribution among IS (figure 4 (right)). Though corrections to scaling are slightly more important in this case, we see from figure 5, where the intersection points $T_C(N_1, N_2)$ for the different pairs N_1 , N_2 of considered system sizes as a function of $N_1 + N_2$ are plotted, that one obtains the correct $T_C = 1$ for $N_1, N_2 \to \infty$.

We conclude that $P_{quench}(q)$ is an interesting quantity to study. The results we have shown could be particularly relevant when looking at glass-forming liquids, but the observed behaviour suggests that this quantity could also help in further clarifying the glassy phase properties of finite-dimensional realistic spin glasses (this is a very long-standing subject, see for instance [33, 34]).

3.2. Correlations between equilibrium configurations and IS

After noting the similarities between P(q) and $P_{quench}(q)$ one expects the presence of strong correlations between equilibrium configurations and corresponding IS, particularly in the low-temperature phase. To quantify them, we measure the probability distribution of the overlaps q_{qt} between each energy minimum and the configuration from which it is obtained, $P_{qt}(q,T)$.



2

0.5

0.7

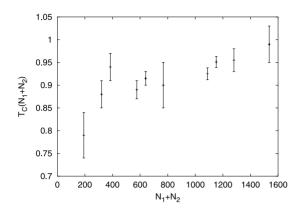


Figure 5. The intersection temperature of the quenched $B_{quench}(T)$ for the different pairs N_1 , N_2 of considered sizes as a function of $N_1 + N_2$.

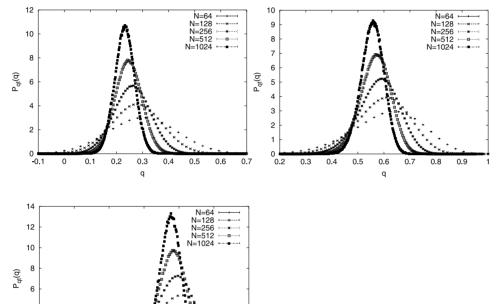


Figure 6. The probability distribution of the overlap between equilibrium configuration and corresponding IS $P_{qt}(q, T)$ for different sizes in the high-temperature region at T=3 (top left), at $T=T_C=1$ (top right) and in the glassy phase at T=0.65 (bottom).

As is shown in figure 6, we find a Gaussian-shaped distribution which goes toward a δ -function in the thermodynamic limit both in the paramagnetic and in the glassy phase. We observe that below T_C , at variance with P(q) and $P_{quench}(q)$, this probability distribution is a self-averaging quantity, which is easily understandable since we are substantially looking at overlaps between configurations related to the same state.

It is intriguing to note that there is no clear evidence for the underlying phase transition when looking at this quantity. The mean value $q_{qt}(T)$ (see figure 7) is increasing when the temperature is decreasing, and $\lim_{T\to 0}q_{qt}(T)=1$. The N dependence appears to be more pronounced in the high-temperature region, where data are well fitted by the power law

$$q_{N,qt} = q_{\infty,qt} + \frac{C}{N^{\alpha}}. (8)$$

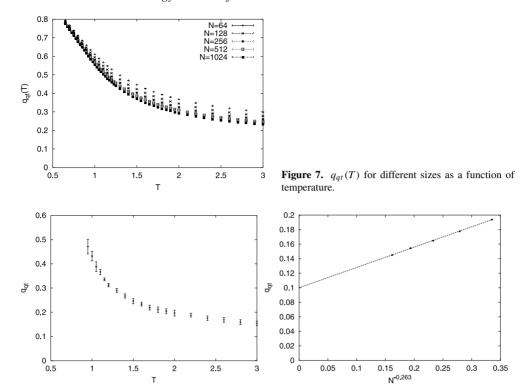


Figure 8. $q_{\infty,qt}(T)$ as obtained by fitting data for different system sizes (left) and our best fit by using data on the overlap between random initial conditions and the corresponding minima found (right), which give $\lim_{T\to\infty}q_{\infty,qt}(T)\simeq 0.1$.

We show in figure 8 our estimates for $q_{\infty,qt}(T)$ (left), which gives, in particular $,q_{\infty,qt}(T_C) \sim 0.4$, and our best fit using data for the overlap between random initial conditions and corresponding minima (right), i.e. $\lim_{T\to\infty}q_{qt}(T)$. Also in this case, we obtain a non-zero value (~ 0.1) in the thermodynamic limit. Nevertheless, it should be stressed that we are confined to a relatively small range of system sizes, which makes a reliable estimation of the error of $q_{\infty,qt}$ very hard.

It would be interesting to understand how much these correlations vary when looking at different models. In agreement with our results, in [26], for the considered volumes it was quoted $q_{qt} \sim 0.4$ for the SK slightly above T_C , to be compared with the higher value $q_{qt} \sim 0.94$ found for the 1RSB model (ROM) at a temperature higher than the mode coupling T_{MCT} , which suggests the presence of stronger correlations between equilibrium configurations and corresponding IS in the glass-forming liquid case, and therefore a $P_{quench}(q,T)$ with a behaviour even closer to the one at equilibrium.

3.3. The IS energy

In figure 9 we show the equilibrium energy e(T), as a function of the temperature T (only weakly dependent on the system size). In figure 10 (left) we present data on the IS energy $e_{quench}(T)$, i.e. the mean energy of the minima accessible from equilibrium configurations



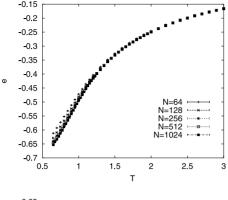


Figure 9. The equilibrium energy as a function of T for the different system sizes.

0.008

1/N

1.5

0.016

2

2.5

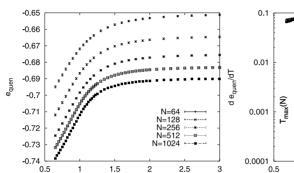


Figure 10. The quenched energy (left) and its derivative with respect to the temperature (right) as a function of T for the different system sizes N. In the inset on the right, the temperature corresponding to the maximum of de_{quench}/dT is plotted as a function of 1/N.

at a given temperature and weighted with the Boltzmann factor of the corresponding basin. The behaviour of this quantity changes abruptly from a nearly T-independent value (in the high-T regime) to the approximately $\propto T$ decreasing of the low-temperature region, where the IS energy continuously goes towards the ground-state value (which is known analytically, $e_0 = -0.7633$). Correspondingly, the derivative $de_{quench}(T)/dT$, which is plotted in figure 10 (right), displays a maximum and takes very small high-T values (note the logarithmic scale).

Data on the position $T_{max}(N)$ of the maximum of $de_{quench}(T)/dT$ as a function of N are shown in the inset and give evidence for $\lim_{N\to\infty} T_{max}(N) = 1 = T_C$. Our finite-size analysis therefore confirms [26] that in the $N\to\infty$ limit $e_{quench}(T)$ takes the constant threshold value [29] e_{th} for $T>T_C$. The behaviour in this region agrees well with the power law

$$e_N = e_{th} + C/N^{\alpha} \tag{9}$$

giving a constant $e_{th} = -0.7145 \pm 0.004$, which is our best numerical estimate for the threshold energy, down to $T \sim 1.1$ near to the critical temperature (and also still compatible with this value at T_C). We note that this estimate is in perfect agreement with $e_{th} \simeq -0.715$ quoted in [25] that was obtained by fitting data on IS reached from random initial conditions by a sequential quenching procedure (this value could depend on the considered zero-temperature dynamics). The exponent α is increases slightly when going to lower temperatures and varies between $\alpha = 0.34 \pm 0.04$ at T = 3 and $\alpha = 0.43 \pm 0.06$ at $T = T_C$.

It is interesting to stress that finite-size corrections to the asymptotic behaviour look *very* important, as shown by the small α value we have found. Correspondingly, for all the

considered sizes (up to the quite large volume, N=1024) the IS energy becomes roughly constant only at temperatures definitely higher than T_C . A similar behaviour with strong finite-size corrections is found in [26] for the considered 1RSB model at $T>T_{MCT}$ too.

Conclusions

We have presented numerical results about the properties of energy minima in the SK model. The probability distribution of the overlap between IS weighted with the Boltzmann factor of the corresponding basin at temperature T, $P_{quench}(q,T)$, turns out to be qualitatively similar to the equilibrium overlap distribution P(q,T) at the same temperature T. We found a trivially shaped $P_{quench}(q,T)$ over the whole paramagnetic $(T > T_C = 1)$ phase, whereas the FRSB behaviour characteristic of the glassy phase is evident from data on $P_{quench}(q,T)$ only when looking at energy minima obtained from equilibrium configurations at a temperature definitely lower than T_C . A finite-size analysis of the Binder parameter for $P_{quench}(q,T)$ gives the same estimate of the critical temperature as the usual (equilibrium) one.

These results can be particularly relevant for glass-forming liquids, where the overlap is more precisely definable between IS [23], but they also imply that numerical evidence for replica symmetry breaking cannot be extracted from data on $P_{quench}(q, T)$, which have been obtained from configurations at equilibrium at temperatures *above* the possible glass transition temperature (in that case $T_K < T_{MCT}$).

The analysis of finite-size corrections to the IS energy confirms [26] that it is approaching the expected thermodynamic limit behaviour $e_{IS} = \text{constant} = e_{th}$ for $T > T_C$, whereas it appears to be continuously decreasing for $T < T_C$.

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