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LETTER TO THE EDITOR

Small window overlaps are effective probes of replica symmetry breaking in three-dimensional spin glasses

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Abstract. We numerically compute small window overlaps in the three-dimensional Edwards–Anderson spin glass. We show that they behave in the way implied by the replica symmetry breaking ansatz, that they do not qualitatively differ from the full volume overlap and do not tend to a trivial function when increasing the lattice volume. In contrast we show that they are affected by small finite-volume effects, and are interesting tools for the study of the features of the spin-glass phase.

In this letter we shall try to give an unambiguous answer to an important question, concerning overlaps in spin glasses. On the one hand recent numerical simulations [1–10] make it clear that finite-dimensional spin glasses behave in a way very reminiscent of the replica symmetry breaking (RSB) solution [11, 12] of the mean-field Sherrington–Kirkpatrick (SK) model [13]. Also recent experimental results seem to hint that the RSB feature can be detected in real materials [14]. On the other hand there has been much progress based on rigorous and heuristic results: the validity of the RSB solution of the SK model is supported (but not yet proven) by the work of [15–17], while potential problems in applying RSB ideas to finite-dimensional spin glasses have been stressed in [18] (but see [19] for ideas pointing in the opposite direction).

It is useful, for making the issues raised in [18, 19] precise, to distinguish among the full volume overlap and the small window overlap. In the standard case the (full volume) overlap is computed among all of the spins of two configurations of the system (under the same realization of the quenched disorder), typically with periodic boundary conditions. The small window overlap is defined on a box of size much smaller than the volume of the system.

The first kind of overlap plays an important role in RSB theory, and it is the one that is usually measured in numerical simulations. Only out-of-equilibrium, dynamical

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measurements of the second kind of overlap have been reported [1, 5], and they are consistent with a RSB behaviour of the finite-dimensional system.

The small window overlap plays an important role in attempting a rigorous analysis of the behaviour of the system. Interfaces can make the probability distribution of the order parameter look non-trivial even in a situation where there is no spin-glass ordering, but small window overlaps detect the difference: if there are only two equilibrium states (related by a global flip of all the spins) the probability distribution of the overlap in a (large) window much smaller than the (large) size of the system will be the sum of two delta functions at $q = \pm q_{\text{EA}}$, where q_{EA} is the Edward–Anderson order parameter [12].

Let us quote from the second of [18]: [...] *Essentially all the simulations of which we are aware compute the overlap distribution in the entire box. [...] we suspect that the overlaps computed over the entire box are observing domain wall effects arising solely from the imposed boundary conditions rather than revealing spin glass ordering. [...] In other words, if overlap computations were measured in ‘small’ windows far from any boundary, one should find only a pair of δ -functions. One way to test this would be to fix a region at the origin, and do successive overlap computations in that fixed region for increasingly larger boxes with imposed periodic boundary conditions; as the boundaries move farther away, the overlap distribution within the fixed region should tend toward a pair of δ -function.*

In our investigations we have gathered numerical evidence to show that what happens is not what is described from the point of view which we have just quoted. To start from the end, in figure 1 we show (which we shall discuss in more detail in the rest of the paper) the probability distribution in a block of size $B = 4$ around the origin for two different lattice sizes, $L = 8$ and $L = 12$. Here T is lower than T_c , and the systems are at thermal equilibrium (these are static measurements) thanks to the tempering Monte Carlo approach [20]. The two probability distributions are non-trivial, and they do not have any

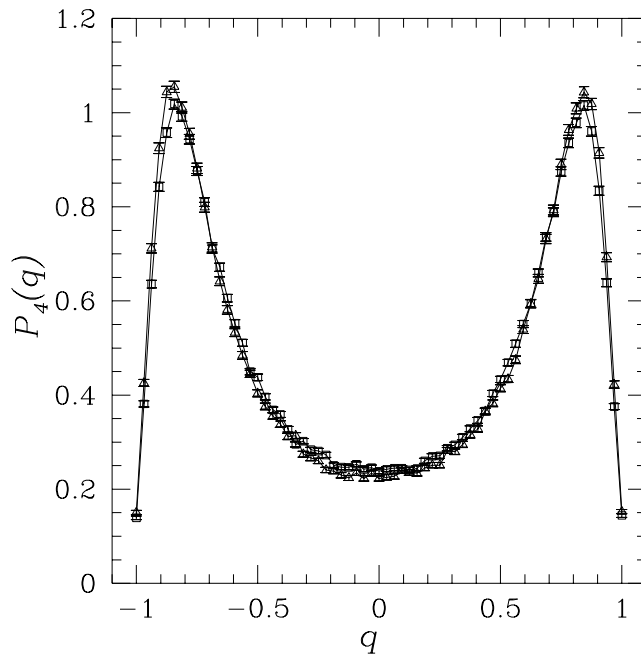


Figure 1. $P_4(q)$: triangles for $L = 8$ and squares for $L = 12$ and $T = 0.7$.

substantial dependence over L . In no way do they approach δ -function when the lattice volume increases, but they have the typical shape of RSB probability distributions. In contrast, it seems (as one would maybe expect when reasoning according to a usual point of view) that they have smaller finite-size effects than the full volume overlap probability distribution, that feels the use of periodic boundary conditions more. We suggest that small window overlaps could turn out to be a precious tool for the numerical study of RSB-like phases: that would surely be a pleasant remainder of the present disagreements about the behaviour of finite-dimensional spin-glass systems [18, 19].

We have simulated the three-dimensional Edward–Anderson spin glass defined on a cubic box of size L with periodic boundary conditions. The quenched couplings J_{ij} have a Gaussian distribution with zero mean and unit variance. The Hamiltonian of the model is

$$\mathcal{H} \equiv - \sum_{\langle ij \rangle} \sigma_i J_{ij} \sigma_j \quad (1)$$

where the sum runs over couples of first neighbouring sites. In the following we shall also denote the spin at the point (x, y, z) using $\sigma(x, y, z)$. We have simulated two real replicas (σ and τ) in the same realization of the quenched disorder.

We define the overlaps (that we denote as B -overlaps) on a finite cubic window (of linear size B), that is part of the lattice of size L

$$q_B \equiv \frac{1}{B^3} \sum_{x=0}^{B-1} \sum_{y=0}^{B-1} \sum_{z=0}^{B-1} \sigma(x, y, z) \tau(x, y, z). \quad (2)$$

We also define $Q_B \equiv B^3 q_B$. We shall denote the probability distribution of q_B using $P_B(q)$. When $B = L$ one recovers the standard overlap. For every couple of spin configurations we have only measured the B -overlap related to a single origin: in principle one could average among all the B -overlaps (with a fixed value of B) centred around different sites.

We have used a $L = 8$ and $L = 12$ lattice, and we have measured the B -overlaps for $B = 2, 3, 4, 5$ and 6 . We have used the parallel tempering Monte Carlo method [20, 5] and a set of 13 temperatures, from $T = 1.3$ to $T = 0.7$ with a step of 0.05 . All of the figures we shall present here show data at $T = 0.7$, the lowest temperature we have studied. We have used the APE-100 parallel computer [21], and simulated 2048 samples. The acceptance factor for the β swap of the tempering update has always been in the range of 0.2 – 0.5 . The parallel tempering β swap has been used from the start of the thermal run.

We have used all the described approaches to check thermalization, for example, in [4], and we are sure of a good thermalization for our samples. In order to give a hint to the reader about the situation in figure 2 we show $\log \langle Q_6^2 \rangle$ at $T = 0.7$ on the $L = 12$ lattice versus the Monte Carlo time. $Q^2(t)$ needs to have reached a *plateau* as a minimal test of thermalization. We chose thermalization time $t_{\text{eq}} = 150\,000$. We have redone the analysis shown here with a larger thermalization time, $t_{\text{eq}} = 300\,000$, and our data do not change within the statistical error. We have used in the analysis of the $L = 8$ run $t_{\text{eq}} = 150\,000$. The total length of the $L = 8$ and $L = 12$ runs was of the order of $900\,000$ Monte Carlo sweeps.

Another strong thermalization test is to obtain a symmetric probability distribution $P_B(q)$ for the B -overlaps under the transformation $q \leftrightarrow -q$ [20]. We show the different window probability distributions at $T = 0.7$ on the $L = 12$ lattice in figure 3: all of them are fully symmetric under the transformation $q \leftrightarrow -q$.

We have compared our window overlaps with the full volume overlap distributions computed in [4]. These results were based on 2048 samples. In that case for each sample we ran 10^6 Metropolis steps without β swap just to initialize the system, followed by

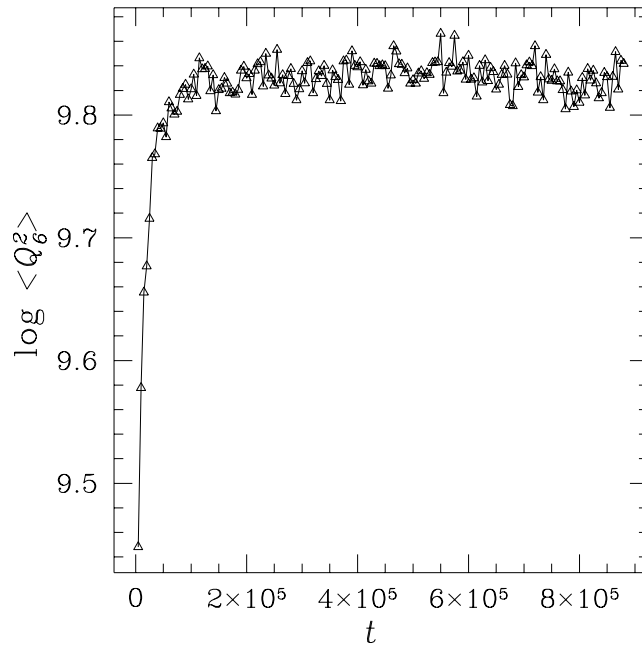


Figure 2. $\overline{\log \langle Q_6^2 \rangle}$ versus the Monte Carlo time t . $L = 12$ and $T = 0.7$.

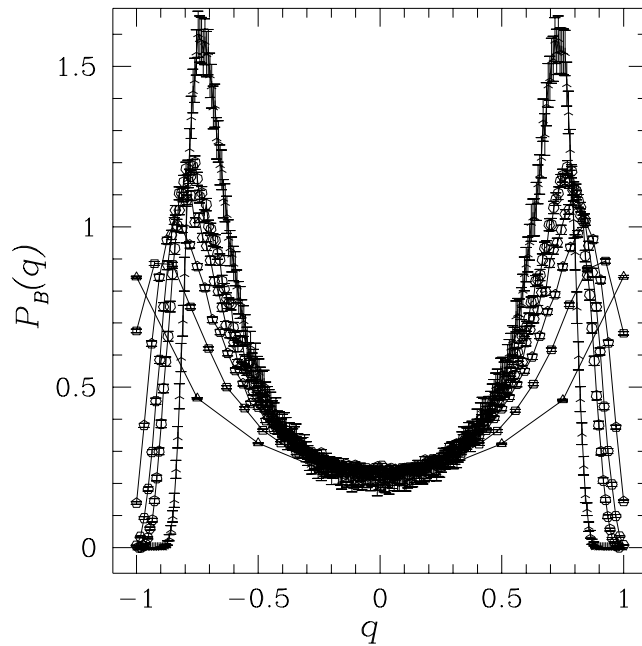


Figure 3. $P_B(q)$ for $T = 0.7$ and $L = 12$ and $B = 2$ (triangles), 3 (squares), 4 (pentagons), 5 (hexagons), 6 (heptagons) and 12 (three line stars). B is increasing for higher curves.

10^6 thermalization steps with parallel tempering and by the real thermal run of 2×10^6 parallel tempering steps, where we measured the relevant quantities (for details about the

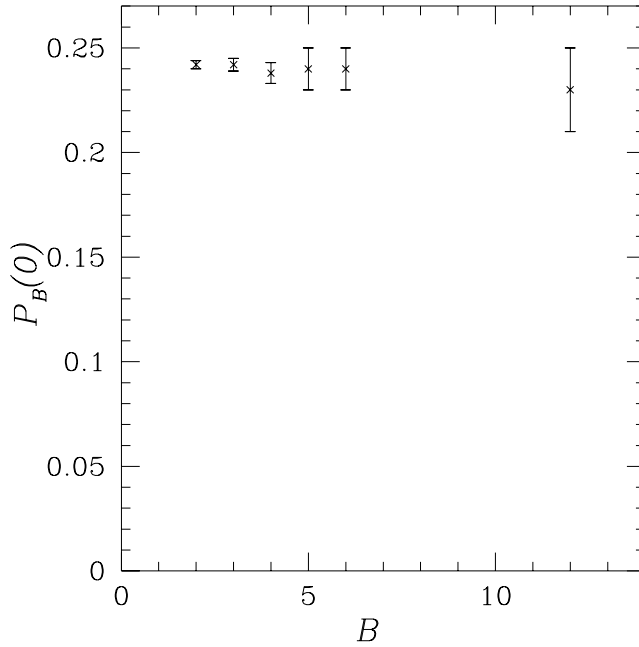


Figure 4. $P_B(0)$ versus the block size B for $L = 12$, $T = 0.7$.

thermalization of the system we refer the interested reader to [4], where the issue was discussed in detail). The $P_{12}(q)$ computed in [4] appears in figure 3.

Our first comments are about figure 1, which makes it clear that window overlaps do not have a trivial behaviour (i.e. two δ -functions at $\pm\bar{q}$) when the lattice volume increases. The probability distribution of a block of size 4 has the typical RSB shape, and basically does not change when increasing the lattice volume from $L = 8$ to $L = 12$. For this comparison we have chosen B as a compromise between wanting a large window, but wanting it still much smaller than the lattice volume. This behaviour also demonstrates that block overlaps are very good estimators of RSB-like effects, and they will probably play an important role in numerical simulations of spin glasses.

When measuring $P_B(q)$ in a finite-volume simulation there are two different sources of finite-size effects, the finiteness of the lattice (L size) and the finiteness of the block used for the measurement (B size). We have found that the major changes in $P_B(q)$ appear when increasing the block size B , as shown in figure 3. This effect is related to the usual L -dependence of the full volume overlap probability distribution (see for example figure 6 of [4]). The great advantage of using blocks of fixed size (much smaller than the lattice size) is that, in this case, $P_B(q)$ have a very small dependence on L , so that we can assume that their shape is very similar to the one they would have in a $L = \infty$ lattice and we can focus our attention on their B -dependence.

In figure 3 we show the $L = 12$, $T = 0.7$ probability distribution of the overlap q_B , for $B = 2, 3, 4, 5, 6$ and 12. The shape of $P_B(q)$ changes only smoothly with the window size. The window overlap distributions have the same qualitative behaviour of the full volume distribution, contradicting the expectations of [18] and strongly supporting the presence of a RSB-like behaviour.

The value of $P_B(q_B \simeq 0)$ has only a very small dependence on B . In the RSB point

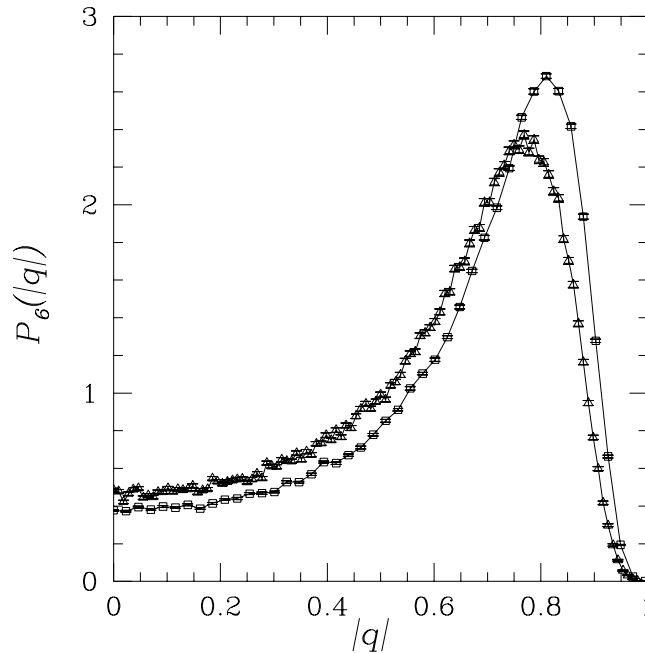


Figure 5. $P_6(|q|)$ for $L = 12$ (triangles) and for $L = 6$ (squares), $T = 0.7$. The error bars are comparable with the symbol width.

of view it is a crucial quantity, since it gives the probability of finding two equilibrium configurations with very small overlap. We plot the values of $P_B(0)$ for different B values in figure 4. In the scenario of [18] this number should asymptotically go to zero for $B \ll L$, while, if any, we are observing the opposite phenomenon, i.e. a small enhancement, owing to the finiteness of the block, at small window sizes B .

Finally in figure 5 we show two probability distributions: the first is the probability distribution computed in a lattice $L = 6$ with $B = 6$ (i.e. it is the full volume overlap probability distribution on a $L = 6$ lattice), while the second is computed on a lattice with $L = 12$ and $B = 6$. From figure 5 it is clear that the shape of the two probability distributions is the same. Selecting small window overlap instead of full volume overlaps does not imply any dramatic quantitative change. We note three small effects. (i) The overlap where the probability distribution presents the maximum is (slightly) lower for $P_6(q)$ with $L = 12$ than for $P_6(q)$ with $L = 6$. (ii) The peak of $P_6(q)$ with $L = 12$ is lower than the one of $P_6(q)$ with $L = 6$. (iii) The value of $P_6(0)$ (on the lattice with $L = 12$) is slightly greater than the value of $P_6(0)$ (on the lattice with $L = 6$). The latter two effects are in contradiction with the predictions of [18]: if $P_6(q)$ measured on an infinite lattice ($L = \infty$) was really a delta function, the value of $P_6(0)$ should decrease when increasing the lattice size, and the height of the peak should increase, with a behaviour opposite to the one observed.

The results we have shown here are quite clear, and they support the idea that the RSB picture accurately describes the low-temperature phase of the three-dimensional Ising spin glass. We will attempt in a following work [19] to understand better from a theoretical point of view why the scenario proposed in [18] does not seem to apply.

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