Small Window Overlaps Are Effective Probes of Replica Symmetry Breaking in 3D Spin Glasses

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Abstract

We compute numerically 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. On the contrary we show they are affected by small finite volume effects, and are interesting tools for the study of the features of the spin glass phase.

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In this note we will try to give an unambiguous answer to an important question, concerning overlaps in spin glasses. On one side recent numerical simulations [1]-[10] are making 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 model (SK) [13]. Also recent experimental results seem to hint that RSB feature can be detected in real materials [14]. On the other side there have been progresses 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, 16, 17], while potential problems in applying RSB ideas to finite dimensional spin glasses have been stressed in [18] (but see [19] for ideas pointing to 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 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 measurements of the second kind of overlap have been reported [1, 5], and they are consistent with a RSB behavior of the finite dimensional system.

The small window overlap plays an important role in trying a rigorous analysis of the behavior 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 $q = \pm q_{\mathrm{EA}}$, where q_{EA} is the Edward-Anderson order parameter [12].

Let us quote from the second of references [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.*

This is exactly what we have done, finding numerical evidence that what happens is not what is described from the point of view we have just quoted. To start from the end, we show in figure (1) (that we will 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 substantial dependence over L. In no way they are approaching δ-function when the lattice volume is increasing,

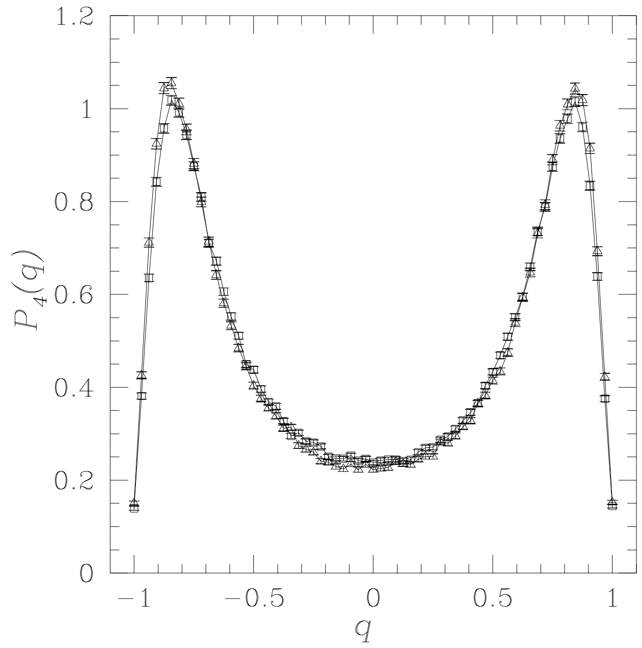

Figure 1: $P_4(q)$: triangles for $L = 8$ and squares for $L = 12$. $T = 0.7$.

but they have the typical shape of RSB probability distributions. On the contrary, it seems (as one would maybe expect when reasoning according to an usual point of view) that they have smaller finite size effects than the full volume overlap probability distribution, that is feeling more the use of periodic boundary conditions. We suggest indeed 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 behavior 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

$$\mathcal{H} \equiv - \sum_{<ij>} \sigma_i J_{ij} \sigma_j \ , \tag{1}$$

where the sum runs over couples of first neighboring sites. In the following we will also denote by $\sigma(x,y,z)$ the spin at the point (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

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

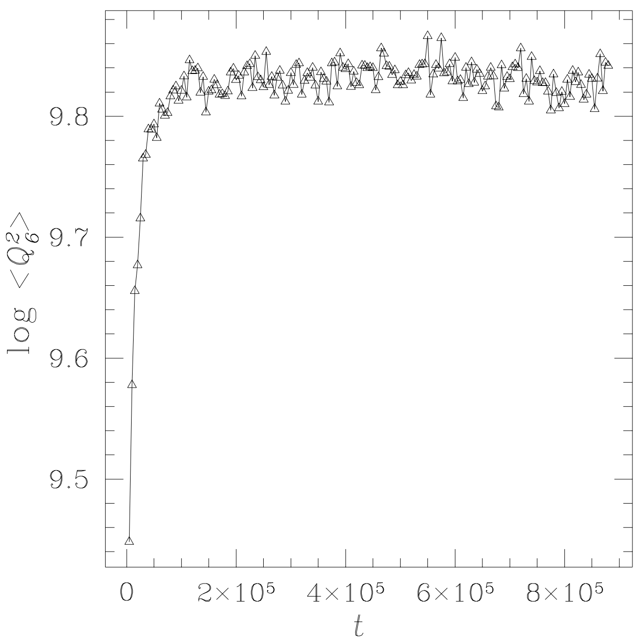

Figure 2: log $\overline{\langle Q_6^2 \rangle}$ versus the Monte Carlo time t. $L = 12$ and $T = 0.7$

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

We have used a $L = 8$ and a $L = 12$ 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]. We have used a set of 13 temperatures, from $T = 1.3$ to $T = 0.7$ with a step of 0.05. All the figures we will present here show data at $T = 0.7$, the lower temperature we have studied. We have used the APE-100 parallel computer [21], and we have simulated 2048 samples. The acceptance factor for the β swap of the tempering update has always been in the range $0.2 - 0.5$. The parallel tempering β swap has been used from the start of the thermal run.

We have used all the approaches to check thermalization that are described, for example, in [4], and we are sure of a good thermalization of our samples. In order to give a hint to the reader about the situation we show in figure (2) log $\overline{\langle Q_6^2 \rangle}$ at $T = 0.7$ on the $L = 12$ lattice versus the Monte Carlo time. We need $Q^2(t)$ to have reached a *plateau* as a minimal test of thermalization. We have chosen as thermalization time $t_{\text{eq}} = 150000$. We have redone all the analysis shown here with a larger thermalization time, $t_{\text{eq}} = 300000$, and our data do not change within the statistical error. We have used in the analysis of the $L = 8$ run $t_{\text{eq}} = 150000$. The total length of the $L = 8$ and $L = 12$ runs was of the order of nine hundred thousand Monte Carlo sweeps.

Another strong thermalization test is to obtain a symmetric probability distribution

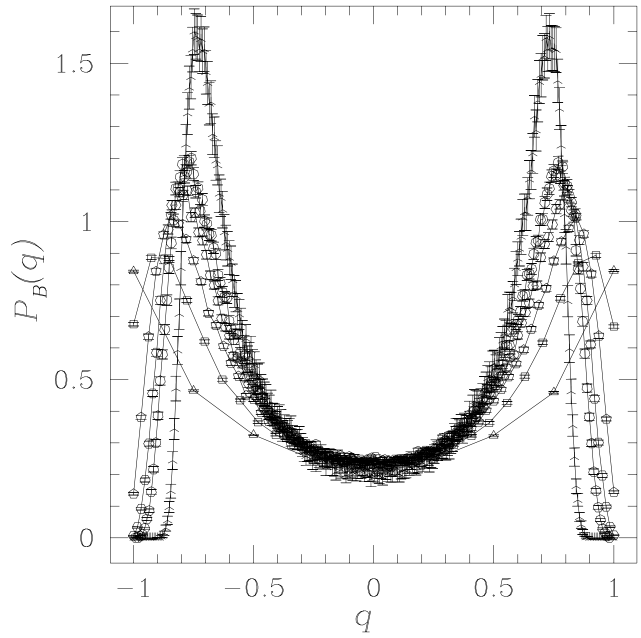

Figure 3: $P_B(q)$ for $T = 0.7$ and $L = 12$ and $B = 2$ (triangles), 3 (squares), 4 (pentagons), 5 (hexagons), 6 (heptagons) and 12 (three line stars). B is increasing for higher curves.

$P_B(q)$ 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 to the full volume overlap distributions computed in [4]. These results were based on 2048 samples. In that case for each sample we had run 10^6 Metropolis steps without β swap just to initialize the system, followed by 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 detail about the thermalization of the system we refer the interested reader to reference [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), that makes clear that window overlap do not have a trivial behavior (i.e. two δ-functions at $\pm\overline{q}$) 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 among wanting a large window, but wanting it still much smaller than the lattice volume. This behavior also denounces that block overlaps are a very good estimator 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

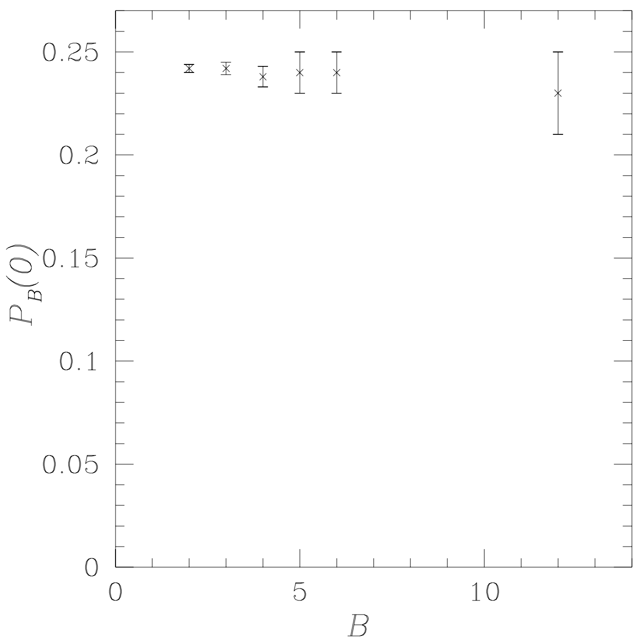

Figure 4: $P_B(0)$ versus the block size B for $L = 12$, $T = 0.7$.

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 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 behavior of the full volume distribution, contradicting the expectations of [18] and strongly supporting the presence of a RSB like behavior.

The value of $P_B(q_B \simeq 0)$ has only a very small dependence on B. In the RSB point 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, due to the finiteness of the block, at small window sizes B.

Finally in figure (5) we show two probability distributions: the first one 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 one is computed on a lattice

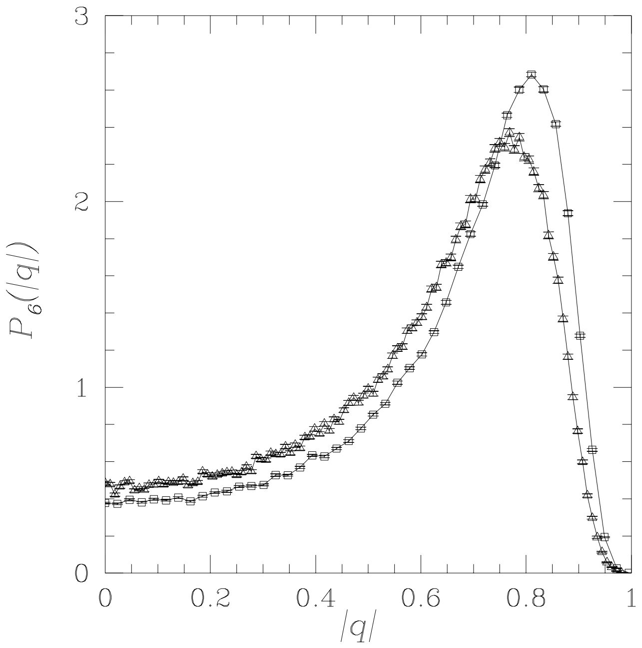

Figure 5: $P_6(|q|)$ for $L = 12$ (triangles) and for $L = 6$ (squares). $T = 0.7$. The error bars are comparable to the symbol width.

with $L = 12$ and $B = 6$. From figure (5) is clear that the shape of the two probability distributions is the same. Selecting small window overlap instead than full volume overlaps does not imply any dramatic quantitative change. We note three small effects. The first one is that 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 $L = 6$. The second one is that the peak of $P_6(q)$ with $L = 12$ is lower than the one of $P_6(q)$ with $L = 6$. The third one is that 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 $L = 6$). These last two effects are in contradiction with the predictions of reference [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 behavior opposite to the one observed.

The results we have shown here are quite clear, and they support again the idea that the RSB picture describes accurately the low temperature phase of the three dimensional Ising spin glass. We will try 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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