

## Spin Domains Generate Hierarchical Ground State Structure in $J = \pm 1$ Spin Glasses

Guy Hed,<sup>1</sup> Alexander K. Hartmann,<sup>2</sup> Dietrich Stauffer,<sup>3</sup> and Eytan Domany<sup>1</sup>

<sup>1</sup>*Department of Physics of Complex Systems, Weizmann Institute of Science, Rehovot 76100, Israel*

<sup>2</sup>*Institut für Theoretische Physik, Universität Göttingen, Bunsenstrasse 9, 37073 Göttingen, Germany*

<sup>3</sup>*Institute for Theoretical Physics, University of Cologne, Zùlpicher Straße 77, D-50937 Köln, Germany*

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Unbiased samples of ground states were generated for the short-range Ising spin glass with  $J_{ij} = \pm 1$ , in three dimensions. Clustering the ground states revealed their hierarchical structure, which is explained by correlated spin domains, serving as cores for macroscopic zero energy “excitations.”

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Mean-field (MF) theory [1] provides a commonly accepted description of the low- $T$  phase of infinite-range spin glasses [2]. It predicts many pure states with a hierarchical ultrametric organization and a nontrivial state overlap distribution  $P(q)$ . Although this structure was suggested to hold also for short-range spin glasses (SRSG) [3], the equilibrium properties of these are still controversial. The main dispute concerns the number of different thermodynamic (pure) states of the system below  $T_c$ . Fisher and Huse (FH) [4] studied SRSG with continuously distributed couplings. According to them, a finite region embedded in an infinite system will be in one of two pure states. They describe the system’s low energy excitations above the local ground state as *finite* flipped spin domains. By flipping compact *macroscopic* domains one can generate other pure states. This structure of pure states (which we call the FH scenario) yields, *for any finite region of the infinite system*, a trivial  $P(q)$  distribution. Numerical evidence for nontrivial  $P(q)$  in *finite* systems [5–7] does *not* contradict the FH scenario [8].

We present here evidence for a new picture of the spin glass phase. *It possesses some characteristics of the MF description, such as nontrivial  $P(q)$  and a hierarchical (but nonultrametric) structure of the pure states; nevertheless, it is also consistent with the FH scenario.*

*The model.*—We study the ground states (GS) of the Edwards-Anderson model [9] of an Ising spin glass

$$\mathcal{H} = \sum_{\langle ij \rangle} J_{ij} S_i S_j, \quad J_{ij} = \pm 1. \quad (1)$$

$\langle ij \rangle$  denotes nearest neighbor sites of a simple cubic lattice; the values  $J_{ij} = \pm 1$  are assigned to each bond independently and with equal probabilities [10]. Although this model is very special—it has highly degenerate GS [11]—we expect that its low- $T$  properties are generic, i.e., not qualitatively different from other  $\{J_{ij}\}$  distributions (such as Gaussian). On the other hand, the low- $T$  properties of (1) are most probably dominated by the structure of its GS. Hence we hope that the GS of the  $J = \pm 1$  model provide insight about the low- $T$  behavior of generic short-range Ising spin glass. In any case, the GS structure of this model is interesting on its own merit.

By combining very efficient algorithms [12] that produce ground states of this model, with simulated tempering (ST) [13], we generated *unbiased* samples of the GS; i.e., we “equilibrated” our system at  $T = 0$ . We studied the model (1) with periodic boundary conditions in three dimensions, with  $N = L^3$  spins, for  $L = 4, 5, 6, 8$ . For each size  $L$  we produced 800 to 1000 realizations  $\{J\}$ ; for each realization an unbiased sample of  $M = 500$  GS has been generated and analyzed.

We now summarize the main results:

(i) For any given  $\{J\}$ , the GS do *not* cover the hypercube  $\mathbf{S} = (S_1, S_2, \dots, S_N)$  uniformly; rather, there is a *hierarchical structure*, as shown schematically in Fig. 1 and in detail in Fig. 2 (the clustering of spins is shown in Fig. 3). The set of all GS splits into two *state clusters*  $C$  and  $\bar{C}$ , related by *spin reversal*;  $C$  splits into  $C_1$  and  $C_2$ , and so on.

(ii) This structure is generated by domains of highly correlated spins [14], with very different sizes. Separation of GS into  $C$  and  $\bar{C}$  is determined by the largest *spin domain*  $\mathcal{G}_1$ , whose size is typically larger than  $N/2$ . Two states in which  $\mathcal{G}_1$  has the same orientation have a much

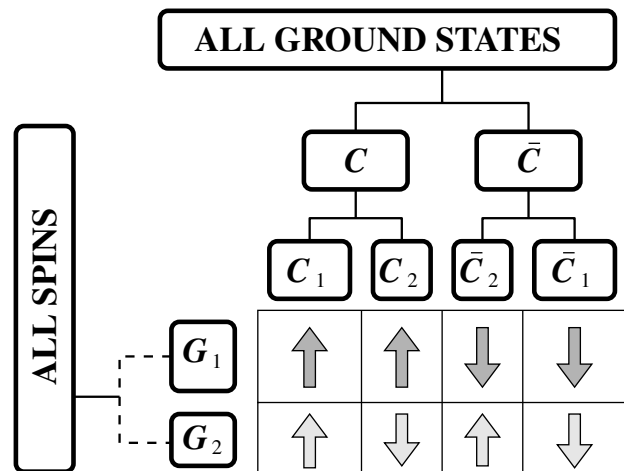


FIG. 1. Schematic representation of our picture; the two largest spin domains and the first two levels in the hierarchical organization of the GS are shown. The structure of the GS is explained by the spin domains’ orientations; e.g., in the GS of the two sets  $C_1, C_2$ , the spins of  $\mathcal{G}_1$  have the same orientation, whereas the spins of the smaller cluster,  $\mathcal{G}_2$ , have flipped.

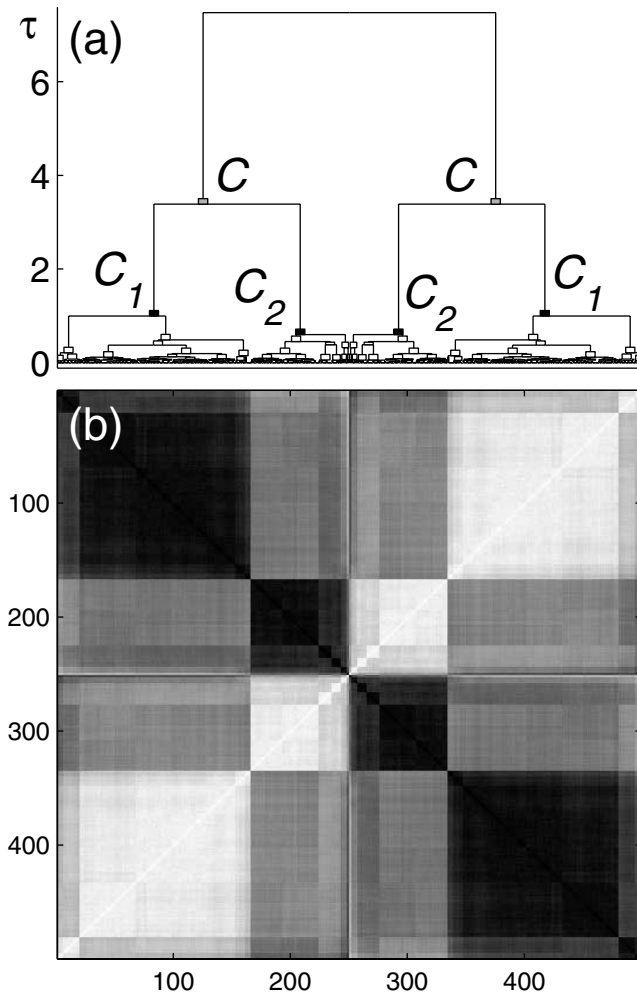


FIG. 2. (a) The dendrogram obtained by clustering the ground states, for a particular set of  $J_{ij}$ , for  $N = 6^3$  spins. (b) When the states are ordered according to the dendrogram, a clear block structure is seen in  $D_{\mu\nu}$ , the distance matrix of the GS. Darker shades correspond to shorter distances.

higher overlap than two states in which the spins of  $\mathcal{G}_1$  are inverted. This implies formation of two clusters of states,  $C$  and  $\bar{C}$ , corresponding to the two possible orientations of  $\mathcal{G}_1$ . The same structure persists at the next level, where the second largest *spin domain*  $\mathcal{G}_2$  determines the partition of  $C$  into  $C_1$  and  $C_2$  (see Fig. 1). Note that  $\mathcal{G}_1$  has the same orientation in these two clusters.

(iii) The hierarchical structure of the GS is due to large differences between the sizes of the spin domains (typically  $|\mathcal{G}_1| > 4|\mathcal{G}_2|$ ). For domains of equal sizes no hierarchy would have been observed.

(iv) This picture *differs* from MF; the correlated domains determine the overlap distribution, and the GS do not exhibit ultrametricity. On the other hand, *if* in the  $L \rightarrow \infty$  limit all but a vanishing fraction of the spins belong to compact [15] macroscopic correlated domains  $\mathcal{G}_a$ , then any finite region of the infinite system will exhibit a trivial  $P(q)$ , in agreement with the FH scenario (we have not tested the compactness of  $\mathcal{G}_a$ ).

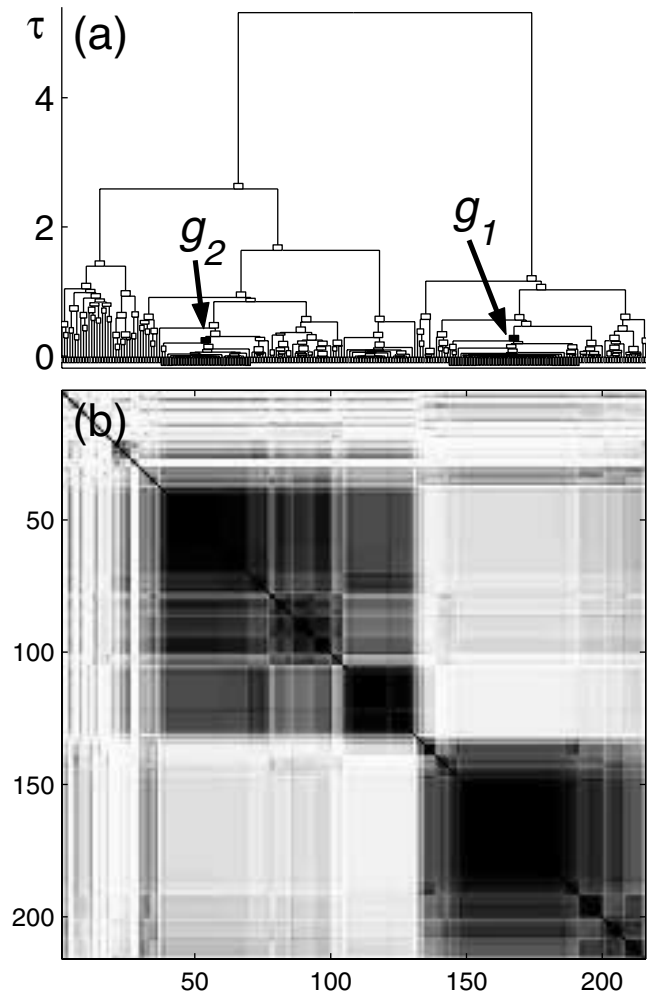


FIG. 3. (a) The dendrogram  $\mathcal{D}$  obtained by clustering the spins of the system of Fig. 2. For this realization  $g_a = \mathcal{G}_a$  for both  $a = 1, 2$ . (b) When the spins are ordered according to the dendrogram, a structure of correlated spin domains emerges; darker shades correspond to shorter distances and higher correlations.

We explain how this picture of GS structure and spin clusters has been found; we present evidence that substantiates our findings, investigate their dependence on system size, and discuss their implications.

*Generating unbiased samples of ground states.*—For every realization  $\{J_{ij}\}$  we used the *genetic cluster exact approximation* (CEA) algorithm [12] to sample the GS. Samples obtained by CEA are, however, biased [16], overweighting GS from small *valleys* (a valley  $V$  consists of all the GS that can be traversed flipping one spin at a time)—therefore the probability to miss a valley is *lower* than that of an unbiased method. We used three methods to overcome this bias. For  $L = 4, 5$ , and  $6$  we succeeded, for most realizations  $\{J\}$ , to enumerate exactly all GS within each valley; selecting at random  $M$  of the GS ensures that each valley is represented according to its size. For some  $\{J\}$  enumeration was not possible; then we used ST [13] to generate samples (our Glauber dynamics had a

decorrelation time of less than two sampling periods for each spin). For  $L = 8$  we estimated the size of each valley by the method of [17] and generated a sample of GS in a valley by a Metropolis Monte Carlo procedure. To test that this method [17] indeed yields unbiased GS, we sampled 60 realizations with ST and ascertained that for the quantities of significance for our claims (the size of  $\mathcal{G}_2$  and the average correlation  $\bar{c}_{12}$  of the domains—see below) the estimates obtained by the two ways did not differ significantly and systematically.

*Clustering methodology.*—Clustering is a powerful way to perform an exploratory analysis of all kinds of data. In general, one calculates a *distance matrix*  $d_{ij}$  between the  $i = 1, \dots, n$  data points and determines the underlying hierarchy of partitions (clusters) in the data. We used Ward's agglomerative algorithm [18]; it starts with each data point as a separate cluster and at each step fuses the pair of clusters  $\alpha, \beta$  that are at the shortest effective distance  $\rho_{\alpha\beta}$  from each other, stopping when all points are in one cluster. Initially  $\rho_{\alpha\beta} = d_{\alpha\beta}$ ; when two clusters  $\alpha, \beta$  are fused, the distances of the new cluster  $\alpha'$  to all unchanged clusters  $\gamma \neq \alpha, \beta$  are updated [18]:

$$\rho_{\alpha'\gamma} = \frac{(n_\alpha + n_\gamma)\rho_{\alpha\gamma} + (n_\beta + n_\gamma)\rho_{\beta\gamma} - n_\gamma\rho_{\alpha\beta}}{n_\alpha + n_\beta + n_\gamma}, \quad (2)$$

where  $n_x$  is the number of points in cluster  $x$ . The algorithm produces a dendrogram such as Fig. 2(a). Leaves represent individual data points. The boxes at the nodes represent clusters; they are ordered horizontally in a way that reflects their proximity. The vertical coordinate of cluster  $\alpha'$  is  $\tau(\alpha') = \rho_{\alpha\beta}$ , i.e., the *effective distance* between the two clusters that were fused to form  $\alpha'$ . For the initial (single state) clusters we set  $\tau = 0$ . When we fuse two “natural” clusters, whose separation exceeds significantly their linear extent, the branch *above* them is long. Hence we can identify natural subpartitions of a cluster; as is evident from Fig. 2(a),  $C_1, C_2$  are such natural subpartitions of  $C$ , and also  $C, \bar{C}$  are natural subclusters of the set of all GS. For each realization we analyzed the data in *two ways*: (a) viewing the GS as  $M$  data points and (b) viewing the spins as  $N$  data points.

*Clustering the ground states.*—Define  $D_{\mu\nu} = (1 - q_{\mu\nu})/2$  as the *distance between states*  $\mathbf{S}^\mu$  and  $\mathbf{S}^\nu$ ;  $q_{\mu\nu} = \sum_i S_i^\mu S_i^\nu / N$  is their overlap. The dendrogram obtained by clustering 500 GS for a system with  $6^3$  spins is shown in Fig. 2(a). Hierarchical GS structure is evident. To provide a quantitative measure of the extent to which a partition (of, say,  $C$  to  $C_1$  and  $C_2$ ) is natural, we evaluate the average distance *between* points in  $C$  and  $\bar{C}$ ,

$$D(C, \bar{C}) = \frac{1}{|C||\bar{C}|} \sum_{\mu \in C} \sum_{\nu \in \bar{C}} D_{\mu\nu}, \quad (3)$$

and compare it to  $D(C)$ , the average distance *within*  $C$ . In the same manner we define  $D(C_1, C_2)$ ,  $D(C_1)$ , and  $D(C_2)$ . For  $L = 6$  we obtained  $D(C) = 0.094$ (mean)  $\pm$

0.067(standard deviation);  $D(C, \bar{C}) = 0.906 \pm 0.067$ ;  $D(C_1) = 0.057 \pm 0.045$ ;  $D(C_2) = 0.058 \pm 0.036$ ;  $D(C_1, C_2) = 0.178 \pm 0.143$ . For  $L = 8$  we obtained  $D(C) = 0.078 \pm 0.050$ ;  $D(C, \bar{C}) = 0.921 \pm 0.050$ ;  $D(C_1) = 0.049 \pm 0.028$ ;  $D(C_2) = 0.049 \pm 0.020$ ;  $D(C_1, C_2) = 0.162 \pm 0.135$ . The results clearly show that the hierarchical structure is real and not a mere artifact of Ward's algorithm.

A striking demonstration of this point can be seen in Fig. 2(b), which shows the distance matrix  $D_{\mu\nu}$  between the GS that were ordered in Fig. 2(a). Dark shading represents short distances and light shading represents long distances. If we cluster states with  $S_i = \pm 1$  at random, the reordered distance matrix is a greyish square. Only when the clustered states form a real, well defined hierarchy does the reordered distance matrix reveal the structure so clearly seen in Fig. 2(b). To understand this hierarchy of GS we investigated the organization of the  $N$  spins in the  $M$  GS.

Figure 2(b) resembles the state distance matrix of the MF picture. There is, however, one crucial difference. In the MF scenario the off-diagonal submatrices of the distance matrix are *uniform*, which leads to ultrametricity [1]. For example, if the *submatrix*  $\bar{D}_{ij}$  for  $i \in C_1$  and  $j \in C_2$  is uniform, the *width*  $w(C_1, C_2)$  of the distribution  $P(\bar{D}_{ij})$  should vanish as  $L \rightarrow \infty$ . We performed a fit of the form  $w(C_1, C_2, L) = w_\infty + AL^{-y}$ , with  $A$  and  $y$  as fit parameters. The minimum of  $\chi^2 = 6.7 \times 10^{-7}$  was found for  $w_\infty = 0.025(2)$  with  $y = 3.4(8)$ . Setting  $w_\infty = 0$  we get a worse fit, with  $\chi^2 = 1.9 \times 10^{-5}$ . Our data supports a nonvanishing value of  $w_\infty$ , in disagreement with the ultrametricity of the MF picture.

*Clustering the spins.*—We cluster  $i = 1, \dots, N$  spin vectors  $\mathbf{S}_i = (S_i^1, S_i^2, \dots, S_i^M)$ , looking for correlated spin domains. Define a *distance between spins*  $i$  and  $j$  by  $d_{ij} = 1 - c_{ij}^2$ , where  $c_{ij} = \mathbf{S}_i \cdot \mathbf{S}_j / M$  is the correlation between spins  $i$  and  $j$ . Note that  $c_{ij}^2$  is the relevant measure of correlations in a spin glass. A typical outcome of clustering the spins with this distance matrix is the dendrogram  $\mathcal{D}$  of Fig. 3(a), obtained for the same system, whose GS were studied in Fig. 2. In Fig. 3(b) we show the distance matrix obtained *after* the spins have been reordered according to  $\mathcal{D}$ . Nontrivial structure in spin space is evident; dark squares along the diagonal represent highly correlated clusters.

*Identifying  $\mathcal{G}_1$  and  $\mathcal{G}_2$ .*—In order to identify  $\mathcal{G}_1$ , the largest domain of correlated spins, we go over all pairs of GS,  $\mu, \nu$ , with  $\mu \in C$  and  $\nu \in \bar{C}$ , and identify  $\mathcal{G}_{\mu\nu}$ , the set of spins that have opposite signs in  $\mu$  and  $\nu$ . For all  $L$  and  $\{J\}$ , the set  $\mathcal{G}_{\mu\nu}$  is contiguous for more than 99.5% of the pairs. Thus,  $\mathcal{G}_{\mu\nu}$  can be related to the low energy excitations found for SRSB with Gaussian couplings [5,15].

For a given  $\{J\}$  we identify as  $\mathcal{G}_1$  the largest contiguous group of spins shared by at least a fraction  $\theta = 0.95$  of the sets  $\mathcal{G}_{\mu\nu}$ . Thus, inside  $\mathcal{G}_1$   $c_{ij}^2 \geq 0.81$  (for  $L = 8$  the

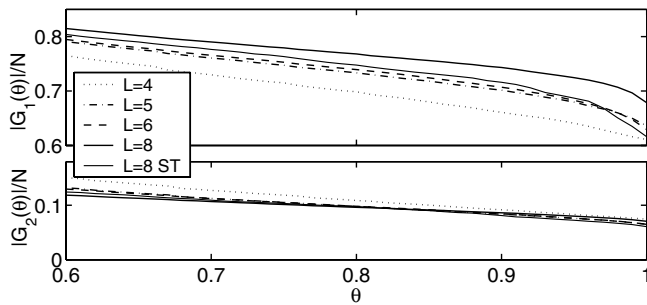


FIG. 4. The average sizes of  $\mathcal{G}_1(\theta)$  and  $\mathcal{G}_2(\theta)$ . The thin solid line presents only ST data for  $L = 8$ , which are unbiased but highly noisy due to the relatively small number of (60) realizations.

average correlation inside  $\mathcal{G}_1$  is always larger 0.94). The second largest spin domain,  $\mathcal{G}_2$ , is found in a similar way, by scanning all pairs of GS with  $\mu \in C_1$  and  $\nu \in C_2$ . As seen in Fig. 4, the average sizes of  $\mathcal{G}_1, \mathcal{G}_2$  do not change a lot for  $0.60 < \theta < 0.95$ .

According to our picture we expect  $|\mathcal{G}_a| \propto L^d$  for both  $a = 1, 2$ . We present the distributions of  $|\mathcal{G}_a|/L^3$  for  $4 \leq L \leq 8$  in Fig. 5. Our results show that the sizes of the two largest spin clusters do scale as  $L^3$ .

We turn now to identify those clusters  $g_1, g_2$  in our spin dendrogram, which can be associated most naturally with the domains  $\mathcal{G}_1, \mathcal{G}_2$ .  $g_1$  is that cluster which is most similar to  $\mathcal{G}_1$ , i.e., has the largest fraction of shared spins  $S(g_1, \mathcal{G}_1) = 2|g_1 \cap \mathcal{G}_1|/(|g_1| + |\mathcal{G}_1|)$ . The similarity is high: for  $L = 8$  on the average we have  $S(g_a, \mathcal{G}_a) = 0.99(1)$  for  $a = 1$  and  $0.97(4)$  for  $a = 2$ . This means that  $\mathcal{G}_1$  and  $\mathcal{G}_2$  do have a meaningful role in spin space and are not just an artifact of our analysis.

*Overlap distribution.*—Figure 5 strongly suggests that  $\mathcal{G}_2$  does *not* vanish as  $L$  increases, as one can conclude from [5]. Still, the distribution may become trivial if

$$\bar{c}_{12} = \frac{1}{|\mathcal{G}_1||\mathcal{G}_2|} \sum_{i \in \mathcal{G}_1} \sum_{j \in \mathcal{G}_2} c_{ij}^2 \rightarrow 1 \quad \text{as } L \rightarrow \infty. \quad (4)$$

In this case  $\mathcal{G}_1$  and  $\mathcal{G}_2$  will always flip together. We carried out fits of the form  $\bar{c}_{12}(L) = \bar{c}_{12}(\infty) - AL^{-\phi}$  with  $A$  and  $\phi$  as fit parameters. The minimum of  $\chi^2$  is  $1.7 \times 10^{-4}$  for  $\bar{c}_{12}(\infty) = 0.54$ . For  $\bar{c}_{12}(\infty) = 1$  we have  $\chi^2 = 3.4 \times 10^{-4}$ . Our result  $\bar{c}_{12}(\infty) < 1$  should be tested further for larger systems. The results  $|\mathcal{G}_2(\infty)| > 0$  and  $\bar{c}_{12}(\infty) < 1$  yield a nontrivial  $P(q)$  [19].

*Summary.*—The ground states of the  $\pm J$  short-range Ising spin glass have a hierarchical, treelike structure. This structure is induced by correlated spin domains, which are the cores of macroscopic zero energy excitations, taking the system from one state-cluster to another. This structure of the GS and the associated barriers has some features of the MF picture but is inconsistent with it, since it

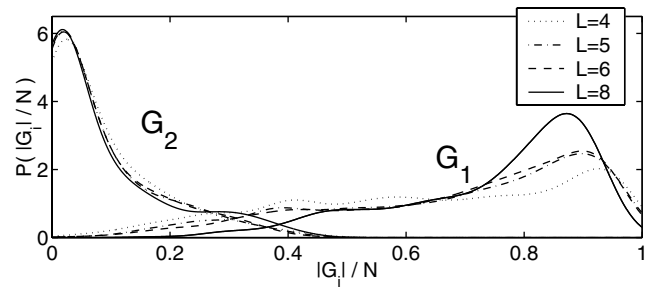


FIG. 5. Size distribution of  $\mathcal{G}_1$  and  $\mathcal{G}_2$ . Note that the distribution of  $\mathcal{G}_2$  seems to converge already for  $L = 8$ . The distribution of  $\mathcal{G}_1$  converges for sizes between  $0.5N$  and  $0.7N$ .

lacks ultrametricity. It is, however, consistent with the FH scenario.

Note that evidence for low energy macroscopic excitations has been found by [5]; we presented here detailed statistics of these domains, investigated their correlations, and demonstrated that they produce a hierarchical structure in state space.

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- [1] M. Mézard, G. Parisi, N. Sourlas, G. Toulouse, and M. A. Virasoro, *J. Phys.* **45**, 843 (1984).
  - [2] D. Sherrington and S. Kirkpatrick, *Phys. Rev. Lett.* **35**, 1792 (1975).
  - [3] E. Marinari, G. Parisi, and J. J. Ruiz-Lorenzo, *Phys. Rev. B* **58**, 14 852 (1998).
  - [4] D. S. Fisher and D. A. Huse, *Phys. Rev. B* **38**, 386 (1988).
  - [5] F. Krzakala and O. C. Martin, *Phys. Rev. Lett.* **85**, 3013 (2000).
  - [6] H. G. Katzgraber, M. Palassini, and A. P. Young, *cond-mat/0007113*.
  - [7] S. Franz and G. Parisi, *cond-mat/0006188*.
  - [8] D. A. Huse and D. S. Fisher, *J. Phys. A* **20**, L997 (1987).
  - [9] S. F. Edwards and P. W. Anderson, *J. Phys. F* **5**, 965 (1975).
  - [10] In fact, we ensured to have equal numbers of positive and negative bonds.
  - [11] S. Kirkpatrick, *Phys. Rev. B* **16**, 4630 (1977).
  - [12] A. K. Hartmann, *Physica (Amsterdam)* **224A**, 480 (1996); *Phys. Rev. E* **59**, 84 (1999).
  - [13] W. Kerler and P. Rehberg, *Phys. Rev. E* **50**, 4220 (1994).
  - [14] F. Barahona, R. Maynard, R. Rammal, and J. P. Uhty, *J. Phys. A* **15**, 673 (1982).
  - [15] M. Palassini and A. P. Young, *Phys. Rev. Lett.* **85**, 3017 (2000).
  - [16] A. W. Sandvik, *Europhys. Lett.* **45**, 745 (1999).
  - [17] A. K. Hartmann, *J. Phys. A* **33**, 657 (2000).
  - [18] A. K. Jain and R. C. Dubes, *Algorithms for Clustering Data* (Prentice-Hall, Englewood Cliffs, NJ, 1988).
  - [19] For a more elaborate investigation of  $P(q)$ , see G. Hed, A. K. Hartmann, and E. Domany, *cond-mat/0012451*.