Non-compact local excitations in spin glasses

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Abstract. – We study numerically the local low-energy excitations in the $3d$ Edwards-Anderson model for spin glasses. Given the ground state, we determine the lowest-lying connected cluster of flipped spins with a fixed volume containing one given spin. These excitations are not compact, having a fractal dimension close to two, suggesting an analogy with lattice animals. Also, their energy does *not* grow with their size; the associated exponent is slightly negative whereas the one for *compact* clusters is positive. These findings call for a modification of the basic hypotheses underlying the droplet model.

Introduction. – In spite of over twenty years of attention, the nature of the spin glass phase is still an open question [1]. If one is guided by the mean field theory of the infinite range spin glass model [2], one is lead to a picture where three dimensional ($3d$) spin glasses have many unrelated valleys whose free-energies differ by $O(1)$. Extending this to zero temperature, one should be able to find large excitations above the ground state which cost only $O(1)$ in energy, regardless of their volume. An important problem is to characterize these excitations geometrically. In the droplet picture [3], the lowest-lying excitations are postulated to be *compact*, *i.e.*, their volume grows as the cube of their characteristic linear size ℓ. In this picture, a spin glass is like a disguised ferromagnet with just two (spin reversed) pure states. Furthermore, the lowest-lying excitations have *typical* energies that grow as a power of their size ℓ, *i.e.*, as $\Upsilon\ell^\theta$ with a positive exponent θ. Only in *rare* cases (the probability of which decreases as $\ell^{-\theta}$) will a droplet energy be $O(1)$, whereas the mean field picture suggests that this probability remains of order one even for large ℓ. The exponent θ has been estimated numerically to be about 0.2 in $3d$ by measuring the energy difference between ground states when applying periodic and antiperiodic boundary conditions [4, 5]. With this procedure, a "domain wall" of linear size L is forced through the sample and cuts it into two compact pieces. Such an approach implicitly assumes that a domain wall and the surface of a droplet are topologically similar, in which case one may hope to identify the above exponent θ describing *local* (*i.e.*, $\ell \ll L$) excitations with an a priori different exponent θ_{dw} describing domain wall

excitations (whose characteristic size is that of the whole system). Both in two [6,7] and in three [8–11] dimensions, there are now indications that this assumption is incorrect.

This work considers the *local* excitations of the $3d$ Edwards-Anderson model [12]. Our goal is to test the key ingredients of the droplet model: droplets are compact and their energies grow with their characteristic size. For our numerical investigation, we construct the connected clusters of spins of lowest energy that contain a specified number of spins and a given site, hereafter called "minimum energy clusters" (MEC). We focus on the statistical properties of the energy and geometry of a MEC as a function of its volume. In the (limited) range of volumes studied, we find that these lowest-lying excitations are actually *fractal* objects with a dimension d_f close to that of lattice animals ($d_f = 2$); this excitation branch is thus topologically unrelated to that associated with domain walls. Furthermore, the exponent θ_f describing the typical energy of these fractal MEC is measured to be small and negative, $\theta_f \simeq -0.13$. In contrast, excitations constrained to be compact have typical energies growing with their size as expected. Within a naïve argument, $\theta_f \leq 0$ seems incompatible with a spin-glass ordering at positive temperature. But such an argument assumes that excitations of different sizes are statistically independent, and we find that this assumption does not hold.

Model and Methods. –   We study the $3d$ Edwards-Anderson (EA) model with periodic boundary conditions. The Hamiltonian is defined on a cubic lattice of $N = L^3$ spins,

$$H = - \sum_{<ij>} J_{ij} S_i S_j \ . \tag{1}$$

The spins are Ising, *i.e.*, $S_i = \pm 1$, and the nearest-neighbor interactions $\{J_{ij}\}$ are quenched random variables distributed according to a Gaussian law with zero mean and unit variance.

Our measurements are performed on lattices with $N = 6^3$ and $N = 10^3$ sites; in both cases, we generated 1000 disorder samples. For each disorder sample, we first compute the ground state of the system using a genetic renormalisation algorithm [13]. After, we choose an arbitrary "reference" spin and flip it along with a cluster containing $v-1$ other spins connected to it. We then minimize the energy of this cluster by exchange Monte Carlo [14], but with the constraint that the reference spin is held flipped and the cluster is always connected and of size v. Our MEC thus differ from the droplets of Fisher and Huse [3]. Indeed, the volume of a MEC is constrained to a fixed value whereas Fisher and Huse consider the minimum amongst all clusters fitting inside a box of width 2ℓ but not of width ℓ. Because of this, the scaling of energy as a function of characteristic size can very well be different for these two definitions. However, since all of their droplets are also MEC, droplets so defined actually have energies below those of our clusters as long as one doesn't force the droplets to be compact.

To find our MEC, we use non-local Kawasaki dynamics as follows. First one randomly removes a node of the cluster and then places it back elsewhere; if the cluster is no longer connected, undo the change and try again until the modified cluster is connected; finally, apply the Metropolis condition for accepting or rejecting the change. In our exchange Monte Carlo run, we used a total of 35 temperatures uniformly spaced between $T = 0.07$ and $T = 2.45$. For each choice of v ($v_0 = 108$, $v_n = \left\lceil v_0 \times \left(\frac{3}{4}\right)^n \right\rceil$), we performed runs using different numbers of Monte Carlo "sweeps" where each sweep consists of v accept-reject tests. This allowed us to determine how many sweeps were necessary to find MEC reliably: for the final runs, we used 10^5 Monte Carlo sweeps, and then the data at $v \leq 33$ is very reliable. Unfortunately, at larger values of v, the data for 10^4 and 10^5 sometimes disagree so we are not so confident we have found the optimum there. Because of this, our analyses are restricted to $v \leq 33$, but for completeness we shall show all of our data.

Main Results. –   Our most striking result is that the average energy $\bar{E}(v)$ of MEC does not increase with their size v but actually *decreases* as shown in Fig. 1. To illustrate the effects of potential systematic errors, we also show the energy data from the runs using 10^4 sweeps only. For the largest v, it is difficult to find the optimum (^{1}), and furthermore the condition that L be much larger than the cluster's "extension" (mean end-to-end distance) is no longer fulfilled; we thus expect finite size effects to be significant for $v > 33$, and this is corroborated by the measurements of the cluster's extension and gyration radius. Because of these two systematic effects, all of our fits have been performed using the $v \leq 33$ data.

From these mean energies, we extract an estimate of θ_f. Anticipating that MEC have a fractal dimension d_f, we write $\bar{E}(v) \propto v^{\theta_f/d_f} \propto \ell^{\theta_f}$, where ℓ is the linear dimension of the cluster. A fit of the $L = 10$ data (with $v \leq 33$) to the form $\bar{E}(v) = A + B/v^\lambda$ does not work well and leads to negative values for A. On the contrary, the fit to the form $\bar{E}(v) = Av^{\theta_f/d_f}$ as shown by a dashed line is very good ($\chi^2 \approx 0.7$) and leads to $\theta_f/d_f = -0.060 \pm 0.006$.
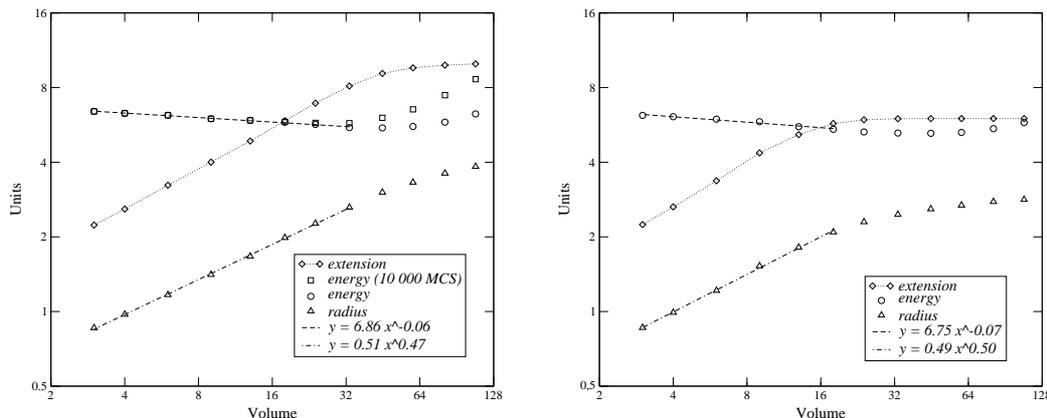

Fig. 1 – Log-log plot of energy, radius of gyration and extension versus v. Left panel: $N = 10^3$ spins; right panel: $N = 6^3$ spins. Also shown is the energy when using 10^4 rather than 10^5 Monte Carlo sweeps. The error bars are smaller than the symbols.

Next, consider the *distribution* of excitation energies (see Fig. 2). Surprisingly, the distribution hardly varies at all with v. Another feature is the suppression at energies close to zero (^{2}), in contrast to what is expected from the droplet model (if we parametrize these curves by generalized Gamma functions, fits lead to an exponent close to 2, *i.e.*, $P(E) \simeq E^2 \exp(-\beta E^2)$).

Before seeing whether these excitations are compact or not, let us now *constrain* them to be so as in the droplet model. We do this by forcing the cluster to stay within the cubic box of size $\lceil \gamma v^{1/3} \rceil$ with $\gamma = 2$, centered around the reference spin. Then we find that the energies of these compact clusters do grow significantly with their volume, in fact as $\bar{E}(v) \propto v^{0.19}$. However the value of this exponent is only indicative because: (a) the size of the cube takes integer values and therefore leads to a clear staircase effect; (b) for the relatively small sizes we considered, the value of the exponent depends on the precise value of γ used. Note that the exponent 0.19 is larger than the expected value $\theta/d = 0.07$ (with $\theta = 0.2$ and $d = 3$) from the droplet model. This disagreement may be due to the fact that we work with fixed volumes;

(^{1}) Note nevertheless that our average MEC energy for $v = 108$ is smaller than for $v = 3$.
(^{2}) The hole for small E is observed for all cluster sizes including the small ones where we are confident that we find the optimum cluster.
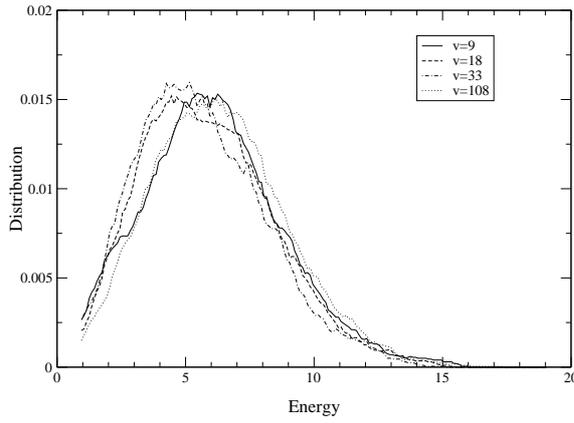
Fig. 2 – Histogram of the excitation energies for the $v = 9, 18, 33, 108$ optimal clusters. For $v = 108$, it is interesting to note that the shape of the distribution hardly changes.

such a constraint leads to cluster energies that may grow faster than those of droplets.

Finally, we turn to the geometrical characterization of MEC. Qualitatively, these lowest-energy excitations (in the absence of any compactness constraint) are quite stringy (see Fig. 3). To quantify this, we have computed the average radius of gyration, R_g, as a function of v. We find that $R_g \propto v^{1/d_f}$ with $d_f = 2.10 \pm 0.05$ (see Fig. 1). This then leads to $\theta_f = -0.13 \pm 0.02$. The same study for our compact clusters leads to $d_f = 2.7 \pm 0.1$, instead of 3, but here again the effects (a) and (b) discussed above lead to important corrections.
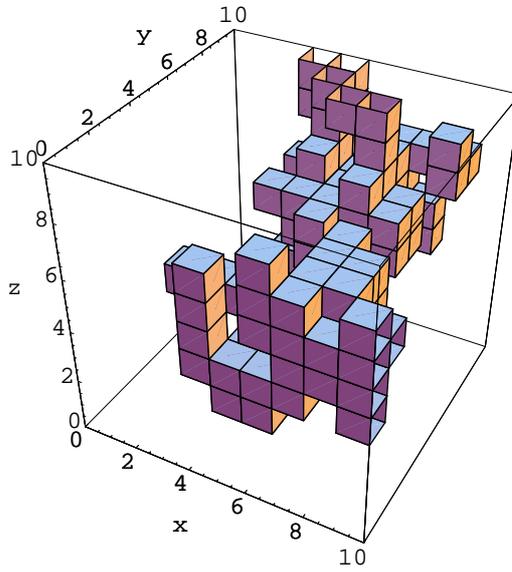

Fig. 3 – A $v = 108$ minimal excitation in a $N = 10^3$ system with periodic boundary conditions.

By comparing constrained and unconstrained clusters, we see that compact excitations are *not* the ones of lowest energy. Actually, a simple entropic argument suggests that MEC may be lattice animals (for which $d_f = 2$): the number of such animals grows exponentially with their volume, whereas the number of compact clusters only grows as the exponential of their surface. Then the non-compact clusters may perhaps reach lower energy values simply because of this greater entropy. To deepen this suggestion, recall that lattice animals can collapse and become compact when penalized by a surface energy term [15]. We have added such a penalty term to our clusters, allowing us to indeed monitor the transition of our MEC from fractal to compact. This and our measurement of d_f suggest that our MEC are in the lattice animal phase. Further indications come from geometric quantities such as the surface to volume ratio or the mass distribution within one cluster, found to be very similar in both cases (MEC and lattice animals). For example, the ratio $\langle r_i^4 \rangle / \langle r_i^2 \rangle^2$, where r_i is the distance of site i to the center of mass of the cluster saturates at a common value around 1.25 at large v.

Our results contradict the main assumptions of the droplet theory: we find non-compact excitations, decreasing instead of increasing energies with size, and a hole at zero energy in the probability distribution of energies. Such properties are compatible with the mean field picture, though at this point there have been no studies of *local* excitations in mean field models with finite connectivity. But one can assert that within such models, all excitations are non-compact in the sense of having their surface growing as their volume, and it is plausible that the low-lying excitations will be the analogs of lattice animals. Note that such a picture also seems to arise in the limit of both very strong disorder and high dimensions [16]. Finally, these local excitations may develop smoothly into system-size excitations for which mean field predicts $\theta = 0$. If this occurs in three dimensions when the extension of our MEC approaches L, then they may turn into the sponge-like system-size excitations found by Krzakala and Martin [8] for which θ is also negative or zero. It would be interesting to develop a new phenomenology based on fractal droplet excitations and to study its compatibility with the mean field picture.

Stability of the Spin Glass Phase. – Very low energy excitations of arbitrarily large size may jeopardize the stability of the spin glass phase. In fact, Fisher and Huse [3] claim that the stability of the spin-glass phase requires $\theta > 0$. Their argument assumes that the MEC are compact; when we impose that constraint, our data are indeed compatible with $\theta > 0$, but otherwise we find $\theta_f \leq 0$. Let us first re-examine their argument in the context of the droplet model (and thus keeping the hypothesis of compact droplets).

They assume that the temperature is very low and that the boundary conditions force the spins at infinity to take the same values as in the ground state. For a given site i, consider the order parameter $m_i \equiv \langle S_i \rangle$. Its value is $m_i = \sigma_i = \pm 1$ in the ground state but its magnitude is reduced at $T > 0$ by the thermally activated droplets that flip S_i with some probability. Following Fisher and Huse [3], let us neglect the interactions between the droplets; when the temperature is low, the gas of droplets is expected to be very dilute so the hypothesis of a non-interacting gas is appropriate. In this framework, the magnetization at site i depends only on the droplets containing that site and is given by [3]: $m_i(T) = \sigma_i \prod_n \tanh(E_n/2kT)$ where $E_n > 0$ is the excitation energy of droplet n containing i. Taking $n \to \infty$, m_i remains non-zero only if low-energy droplets are sufficiently rare. Mathematically, this reduces to the convergence at large L of the following integral:

$$m_i(T) \propto \exp\left(-\int_1^L d\Omega_\ell \; \frac{kT}{\Upsilon \ell^\theta} \right) \;, \tag{2}$$

where the measure $d\Omega_\ell = d\ell/\ell$ expresses the fact that the size of droplets must roughly

double before the energies become independent (^{3}). Now, as long as $\theta > 0$, the integral over ℓ converges, and $m_i \neq 0$ in the thermodynamic limit [3]. Conversely, when $\theta \leq 0$, the probability to excite a droplet becomes independent of its size ℓ for large ℓ. One then finds from Eq.(2) that $m_i(T) \propto L^{-\alpha(T)}$, with a positive exponent α that vanishes for $T \to 0$. Therefore, for any $T > 0$, $m_i(T)$ tends to zero for large system sizes. Our numerical findings suggest that $\theta_f \leq 0$ for MEC; a naïve extension of the above argument to MEC would then suggest that there is no spin-glass phase, at variance with widely accepted evidence.

However, as we now discuss, two of the assumptions needed to obtain (2) are likely not to apply to MEC. First, can MEC on different scales be treated as independent? One can measure the correlation between MEC of sizes v and $v' \geq v$ by computing the overlap $q_s(v, v') \equiv \frac{\#(\mathcal{S} \cap \mathcal{S}')}{\#\mathcal{S}}$, where $\mathcal{S}$ is the set of surface links for the excitation of volume v, and similarly for $v' > v$. By definition, one has $q_s(v, v) = 1$. If all the surface links of the smaller excitation belonged to the surface of the larger one, then one would also have $q_s(v, v') = 1$. Our results are plotted in Fig. 4 as a function of v/v' for different sizes of the largest excitation, v'. We find that $q_s(v, v')$ is nearly independent of v for a given v' and quite large (on the order of one half) for the sizes investigated. Furthermore, the value of this "plateau" only very slowly decreases with v', as a small negative power or as $1/\log v'$. This means that the MEC are extremely correlated: an
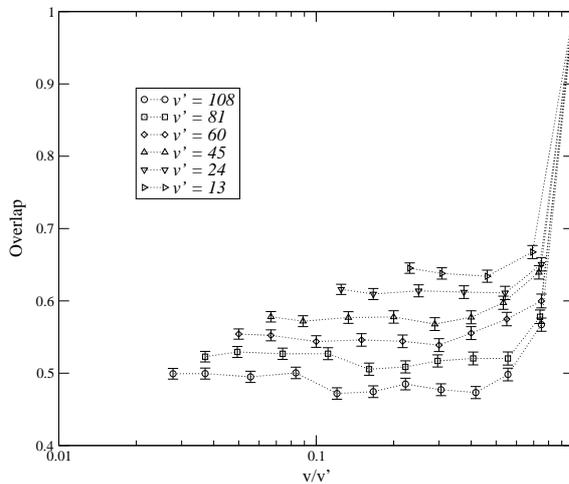

Fig. 4 – Semi-log plot of the normalized intersection $q_s(v, v')$ between surfaces of optimal clusters in the $N = 10^3$ system. We show q_s as a function of v/v' for different largest cluster sizes v'. The "plateau" value is seen to decrease slowly with v', as a small negative power-law or as $1/\log v'$.

excitation of size v serves as a good "backbone" to construct larger excitations. On the other hand, if one had two uncorrelated fractals, one should observe $q_s(v, v') \propto (v')^{1-d/d_f} \propto v'^{-1/2}$, *i.e.*, a much faster decay than the one seen in Fig. 4. These strong correlations show that our non-compact MEC are not at all independent: the number of effectively independent clusters is therefore much reduced. It is not clear at this stage how the phase space volume $d\Omega_\ell$ has to be changed to account for these correlations, and whether or not the resulting integral appearing in (2) would be convergent. The slow $1/\log v'$ decay of the correlation function

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(^{3}) The formula also assumes that the probability distribution of $E/\Upsilon\ell^\theta$ has a non-zero value at zero argument; the reasoning can be generalized if this density vanishes, leading to a different dependence on temperature of m_i, but the vanishing or not of m_i in the thermodynamic limit is unaffected.

$q_s(v, v')$ suggests that $d\Omega_\ell$ becomes $d\ell/(\ell \log \ell)$, so that the integral appearing in (2) still diverges, but only as $\log(\log L)$, leading to $m_i(T) \propto (\log L)^{-\alpha(T)}$ with α vanishing for $T \to 0$. In this case, $m_i(T)$ would therefore be zero for any $T > 0$, but the system size dependence would be so weak for small temperatures that it would be impossible to disprove this scenario numerically.

The second hypothesis underlying (2) is that the MEC are dilute enough for the interaction between two excitations centered around *different* sites can be neglected. If the integral in (2) diverges for large ℓ, then it is no longer self-consistent to neglect the interaction between the MEC. These interactions could then provide a temperature-dependent cut-off scale when $\theta \leq 0$ which would make $m_i(T)$ non-zero for $T > 0$. This, and the strong correlation between MEC of different sizes, might therefore be enough to reconcile our findings with the numerical evidence [17] of a $T > 0$ spin glass phase for the $3d$ EA model.

Conclusion. – In this paper, we have obtained numerical results on the local low-lying excitations of the $3d$ Edwards-Anderson model. We constructed the optimal connected clusters of flipped spins of a given size, and studied their energetic and geometrical properties. We find that these minimum energy clusters (MEC) have a fractal dimension close to two, suggesting an analogy with lattice animals. The energy of these clusters does not grow with their size (the corresponding energy exponent is found to be slightly negative). This is in contrast with MEC constrained to be compact, for which the energy is indeed found to grow with their size. We therefore speculate that there exists a new "fractal" excitation branch, that should be included in an extended droplet theory. To get some further insights into this theory, we are now studying these excitations in the presence of a magnetic field and in four dimensions. Clearly, the static and dynamical consequences of these objects will have to be worked out.

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