Energetics of clusters in the two-dimensional Ising spin glass

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(Dated: April 25, 2003)

We study numerically the properties of local low-energy excitations in the two-dimensional Ising spin glass. Given the ground state, we determine the lowest-lying connected cluster of flipped spins containing one given spin, either with a fixed volume, or with a volume constrained to lie in a certain range. Our aim is to understand corrections to the scaling predicted by the droplet picture of spin glasses and to resolve contradictory results reported in the literature for the stiffness exponent. We find no clear trace of corrections to scaling, and the obtained stiffness exponent is in relatively good agreement with standard domain wall calculations.

PACS numbers: 75.50.Lk, 75.40.Mg, 05.50.+q

I. INTRODUCTION

According to one of the principal scenarios for the spin glass state, the "droplet picture"[1–4], the minimum energy excitation of linear dimension L containing a given spin, a droplet, has an energy proportional to L^{θ}. The "stiffness exponent" θ is positive if one assumes that the transition temperature T_c is finite. It follows that, in the thermodynamic limit, excitations that flip a finite fraction of the spins cost an infinite energy. However, the results of several numerical calculations[5–12], on small system sizes, imply that the amount of energy needed to generate system-size droplet excitations is independent of size, so that θ for droplet-like excitations is zero. This is consistent with the alternative replica symmetry breaking (RSB)[13–16] picture. Note that numerics simultaneously finds that the stiffness exponent for domain-wall excitations is positive and therefore apparently different from the exponent for droplets, an unexpected feature.

To explain the discrepancy between those two different estimates of the stiffness exponent, it has been proposed[17,18] that the droplet theory is correct on large scales, i.e. the stiffness exponent θ is the same for droplets and domain walls, and that the apparently contradictory numerical data can be explained by corrections to scaling. More precisely Refs. 17,18 propose that the droplet energy ΔE has the form

$$\Delta E = AL^{\theta} + BL^{-\omega}, \qquad (1)$$

where $\theta > 0$ (if $T_c > 0$ which is the case for $d \geq 3$), ω is a correction to scaling exponent, and A and B are positive constants. If $\theta > 0$, ΔE has a minimum at some value of L and if this occurs in the range of sizes where numerical data is taken, the numerical values could be roughly independent of size in the range studied. In general, only a modest range of sizes, $L \lesssim 10$, can be studied in dimension d equal to 3.

To quantitatively check this proposal, simulations have recently been carried out[19] on a one-dimensional model with long range interactions which fall off as a power of the distance, in a region of parameters for which $T_c > 0$. A much larger range of sizes can be studied than in three dimensions but even up to $L = 512$ the energy of system-size excitations was found to be independent of size. Hence, for Eq. (1) to be correct with $\theta > 0$ the values of θ, ω, A and B must conspire to give an almost constant ΔE over a very wide range of sizes.

Another model where large sizes can be studied is the two-dimensional Ising spin glass at $T = 0$, where efficient algorithms[20–22] can be applied to determine exact ground states. Now $\theta < 0$ in $d = 2$, with $T = 0$ "domain-wall" calculations giving[22–27] $\theta \simeq -0.28$. However, finite-T simulations[28,29] and $T = 0$ studies in a magnetic field[30], both of which excite droplets rather than domain walls, find $\theta \simeq -0.47$. A good review of this situation is given in Ref. 31. Since $\theta < 0$ in $d = 2$, both the L^{θ} and $L^{-\omega}$ contributions to the droplet energy in Eq. (1) decrease with increasing L, but Refs. 17,18 argue that they could combine to give an effective exponent of about -0.47 for small L crossing over to the asymptotic value of about -0.28 for larger sizes. Hartmann and Moore[18] find evidence for this crossover in their numerical studies in which a certain prescription was used to generate droplets, though earlier Hartmann and one of us[32], who generated droplets in a different way, did *not* find evidence for an effective exponent close to -0.47. This difference may indicate that the amplitude of the correction term B in Eq. (1) depends significantly on the precise way in which the droplets are generated. In yet another way of generating droplets, Picco et al.[33,34] find θ close to the -0.47 value but with *no* crossover to the domain wall value of around -0.28 for the larger sizes.

Recently, in an interesting paper, Lamarcq et al.[35] have calculated the energy of droplet (cluster)[36] excitations in three dimensions, in a manner very similar to the spirit of the droplet model[1–3]. Interestingly they find that the energy actually *decreases*, although very slightly, with increasing size. They also find that the volume of the droplets has a non trivial fractal dimension less than the space dimension. In Ref. 17, this slow decrease of the droplet energy was taken as a possible evidence of the relevance of the correction to scaling term in Eq. (1). Note however that no sign of a crossover towards the supposedly correct value of the stiffness exponent was reported, even when larger clusters could later be included in the analysis[37].

Here we perform a calculation similar to that of Lamarcq et al. but in two dimensions. The aim is to see if the energies of the droplet energies calculated in this way fit Eq. (1) and give an effective exponent close to -0.47 at small sizes crossing over to about -0.28 at larger sizes as has been proposed by Moore[17] and Hartmann and Moore[18]. Since the way our clusters are generated is directly inspired by the original definition of the droplets, one could expect the prediction (1) to be well suited in our case. Instead, we do not find any crossover in ΔE by applying the definition of Lamarcq et al. in $2d$ for clusters as large as 64 spins, neither do we find a very negative exponent -0.47. We find however an exponent similar to -0.47 at very small sizes if a slight modification of the definition of the clusters is made, namely if the size of the clusters is let free to evolve between n and $2n$, as suggested by the original "scale invariant" definition of the droplets.

II. THE MODEL AND DETAILS OF THE NUMERICS

We take the standard Edwards-Anderson spin glass model

$$\mathcal{H} = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j, \tag{2}$$

where the $S_i = \pm 1$ are Ising spin variables at the sites of a simple cubic lattice, and the J_{ij} are nearest neighbor interactions with a Gaussian distribution with zero mean and standard deviation unity. Periodic boundary conditions are applied on lattices with $N = L^2$ spins. For most of our work we take $L = 64$ but we also did some calculations with smaller sizes down to $L = 16$. We use $N_s = 1000$ realizations of the disorder.

We are interested in the properties of low-energy, droplet-like excitations above the ground state of the Hamiltonian in Eq. (2). In order to determine these, we first find the ground state for each realization of the disorder. This is done using either the Köln spin glass server[38], or, for small sizes, by parallel tempering[39,40].

Following Ref. 35, we then generate a droplet by first choosing randomly a "central" spin in the system and reversing it. We then construct a connected cluster of fixed size n around this central spin by flipping all the spins in this cluster. We then find the new ground state with the following three constraints:

1. The central spin is always flipped with respect to the ground state,

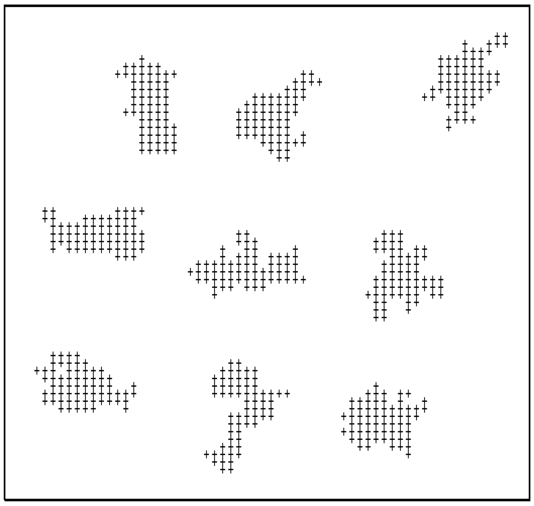

FIG. 1: Randomly chosen clusters of size $n = 64$ obtained by the procedure described in Sec. II.

2. The number of spins in the cluster is always n,
3. The cluster is always connected.

The new ground state is found by a combination of parallel tempering and a Kawasaki-type dynamics for the spins in the cluster, in order to conserve its size n constant. Our algorithm does not satisfy detailed balance, but this is irrelevant since we only want to find the new, constrained ground state. The lowest temperature in the parallel tempering is taken to be sufficiently low, $T = 0.02$, that the system is always in a local minimum with no random noise kicking the system to higher energy states. Our results for ground states in the presence of a droplet are obtained from spin configurations at this lowest temperature. We study cluster sizes up to $n = 64$.

In this procedure, which follows Ref. 35, the size of the cluster is strictly fixed. It is therefore slightly different from the droplets of Fisher and Huse[1–3] which are defined in a "scale-invariant" way, i.e. the size is not strictly fixed but allowed to vary over a certain scale. We have therefore also computed the energies of scale-invariant excitations in which the size of the cluster is allowed to vary by a factor of 2, more precisely to lie between $n/2$ and $n-1$ for $n = 4, 8, \cdots, 64$. Examples of some randomly chosen clusters of size $n = 64$ are shown in Fig. 1.

Our criterion for ensuring that we have found the true ground state in the presence of an overturned cluster is as follows. We first make a few (typically 10) extremely long runs with different bond configurations to estimate the typical time scale to reach the new ground state, $t_{\rm typ}(n)$. We record the energy versus time of the lowest temperature for the two copies, for simulations of at least $10 t_{\rm typ}$ sweeps. From these graphs, we can evaluate $t_{\rm typ}$

as the typical time it takes those 10 realizations of the disorder to give a result that can be confidently taken as the ground state. Then, for each of the N_s samples, we first run two copies of the system with independently drawn initial clusters for $t_{\rm typ}(n)$ Monte Carlo steps. We then require that the two copies have the same energy for a further continuous period of time equal to $t_{\rm typ}(n)$. In this way, we spend more time on the "hard" samples, which need several times $t_{\rm typ}(n)$ to converge, than on the easy samples for which we do not need to run much more than $t_{\rm typ}(n)$ sweeps. Obviously, one can not be absolutely sure that the ground state has really been found since it might happen that both copies stay for a time larger than $t_{\rm typ}(n)$ in the same state which is not the ground state. However, this seems to be fairly unlikely. To be on the safe side we used $t_{\rm typ}(n = 64)$, for *all* sizes, even though, for $n < 64$, one has $t_{\rm typ}(n) \ll t_{\rm typ}(n = 64)$.

For the scale-invariant clusters we start one copy with the minimum-size cluster, $n/2$, and the other with the maximum-size cluster, $n - 1$, to minimize further the probability that the two copies inadvertently spend a long time in the same state which is not the ground state.

We now present our numerical results.

III. RESULTS

A. Clusters of Fixed Size

In this section we present results of the simulations where we fix the droplet size precisely, as was done by Lamarcq et al.[35] on the $3d$ model.

1. *Droplet Energies*

Fig. 2 shows the droplet energy, $\langle \Delta E\rangle$, where the average is over $N_s = 1000$ samples, as a function of n, the number of spins in the droplet, on a log-log scale. For each sample, ΔE is the energy difference between the constrained and unconstrained systems, by definition a positive quantity. If we define the fractal dimension of the volume of the droplets to be d_f, i.e.

$$n \sim R^{d_f}, \tag{3}$$

where R is the mean "radius" of the droplet (to be defined below) then the slope of the data is θ/d_f, since by definition $\langle \Delta E\rangle \sim R^{\theta}$. The expectation of the droplet theory is that d_f is equal to the space dimension, $d_f = d = 2$. The slope of -0.115 for $L = 64$ would lead to $\theta = -0.23$, not quite as negative as the established value of -0.28 from domain wall calculation, but perhaps the difference is not significant given the rather small range of droplet sizes than we can study. Actually, fits to data presented below indicate that d_f is somewhat less than two, which would accentuate the difference between our value of θ and -0.28. However, the apparent difference between d_f and 2 may itself be due to corrections to scaling.

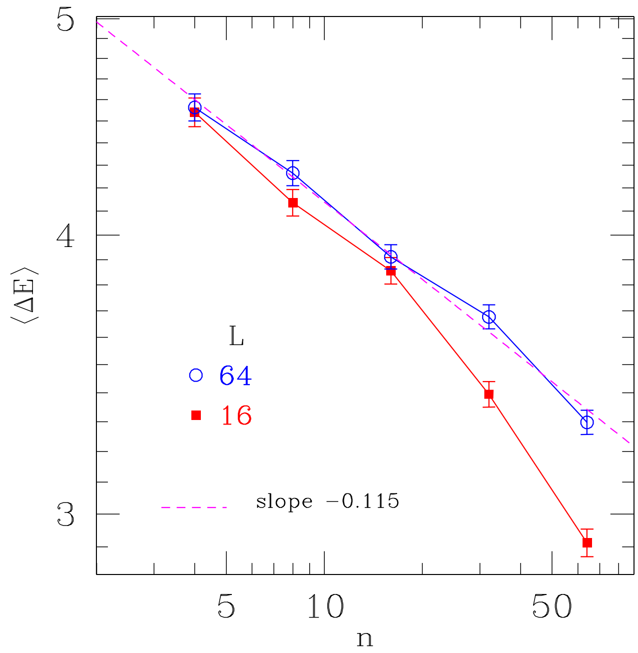

FIG. 2: Mean droplet energy against the number of spins in the droplet for lattice sizes $L = 16$ and 64 for droplets of fixed size. Data for $L = 32$ is very similar to that for $L = 64$ and is not shown for clarity. The slope for $L = 64$, which is equal to θ/d_f, is -0.115. No crossover in the slope can be detected in the $L = 64$ data.

We note also in Fig. 2 that the data for $L = 16$ shows an interesting feature. For small cluster sizes, the relation between $\langle \Delta E\rangle$ and n follows that of the $L = 64$ and the two sets of data start to depart from each other at large cluster sizes, so that the apparent stiffness exponent becomes more negative at large sizes. This crossover is however exactly opposite to the one expected from Eq. (1). A visual inspection reveals that even the clusters with $n = 64$ have a radius smaller than the system size $L = 16$, so that the effect is not trivially due to the fact that boundaries of the clusters interact with each other. Rather, this crossover is most probably due a finite size effect on the initial ground state energy, a smaller size making it too large, resulting then in too small an energy difference ΔE.

An important conclusion drawn from Fig. 2 is that no crossover from a large to a smaller value of the stiffness exponent is visible, although our data cover a reasonably large size window. We are led to the conclusion that the definition of the droplets used here is relatively free of the corrections to scaling expected from Eq. (1), and moreover that it leads, for $d = 2$, to a determination of the stiffness exponent in fair agreement with domain wall calculations.

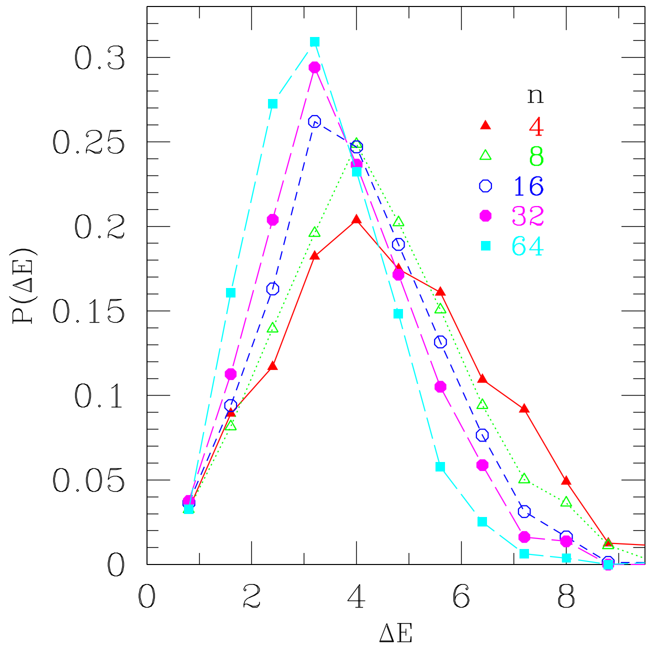

FIG. 3: Distribution of the energy of the droplets of fixed size n, for different n and system size $L = 64$.

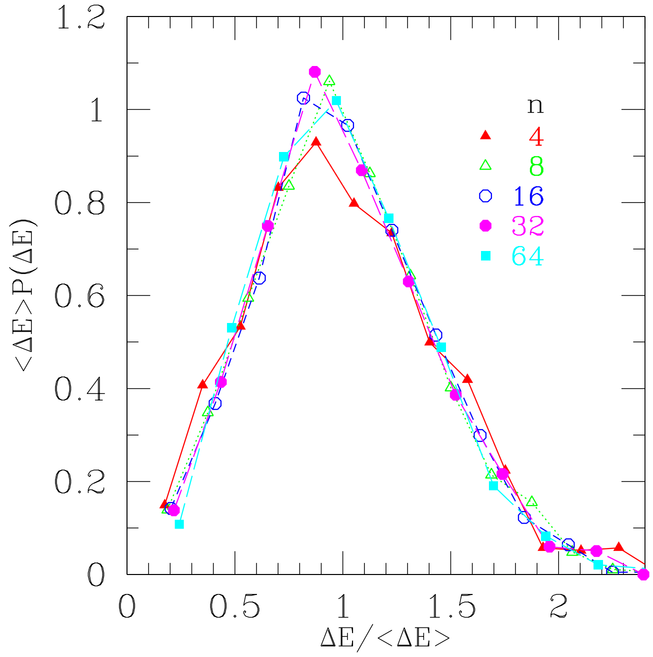

FIG. 4: The data in Fig. 3 scaled by the mean energy $\langle \Delta E \rangle$, according to Eq. (4).

2. Distribution of Droplet Energies

Fig. 3 shows the distribution of the energy, $P(\Delta E)$, of fixed size droplets for different sizes with $L = 64$. In Fig. 4, we show that these distributions can be satisfactorily scaled using the form

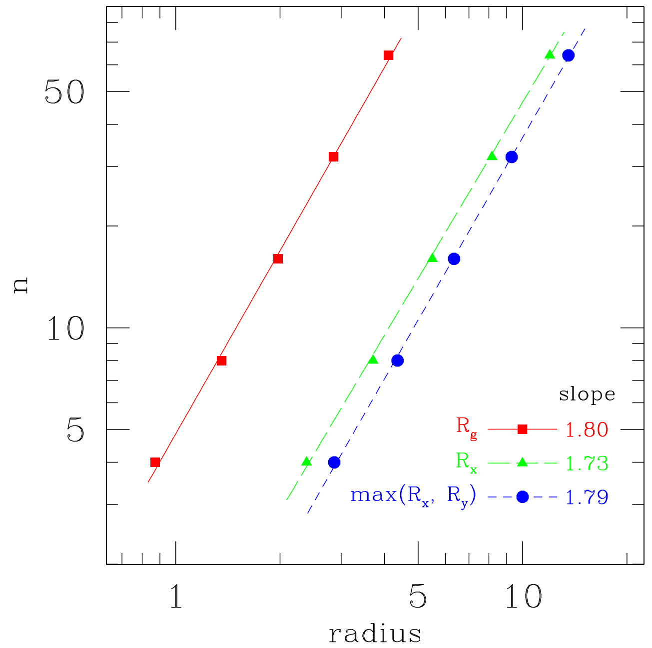

FIG. 5: The number of spins in the droplet, n, as a function of various definitions of the "radius", as described in the text. This is for droplets of a fixed size.

$$P(\Delta E) = \frac{1}{\langle \Delta E \rangle} \mathcal{P}\left(\frac{\Delta E}{\langle \Delta E \rangle}\right), \tag{4}$$

using the mean energy $\langle \Delta E \rangle$ which is plotted in Fig. 2. The data indicates that the scaling function $\mathcal{P}(x)$ varies *linearly* for small x. This result was also obtained in three-dimensions[35], but differs from the usual assumption in droplet theory that the distribution has a finite weight at the origin.

3. Fractal Dimension of the Droplets

To determine the fractal dimension of the volume of the droplets through Eq. (3), we need to give a definition of their "radius". We have done this in different ways and checked that they give consistent results for d_f. We measured R_x and R_y, the maximum extent of the droplets in the x and y direction as well as $\max(R_x, R_y)$. In addition we determined the radius of gyration, R_g, of the droplet defined by:

$$R_g = \sqrt{\frac{1}{n} \sum_{i \in \text{cluster}} |\mathbf{r}_i - \mathbf{r}_{\text{cm}}|^2}, \tag{5}$$

where $\mathbf{r}_{\text{cm}}$ is the position of the center of mass of the cluster.

Figure 5 shows the result of this analysis for $L = 64$, together with power law fits to the data. The agreement

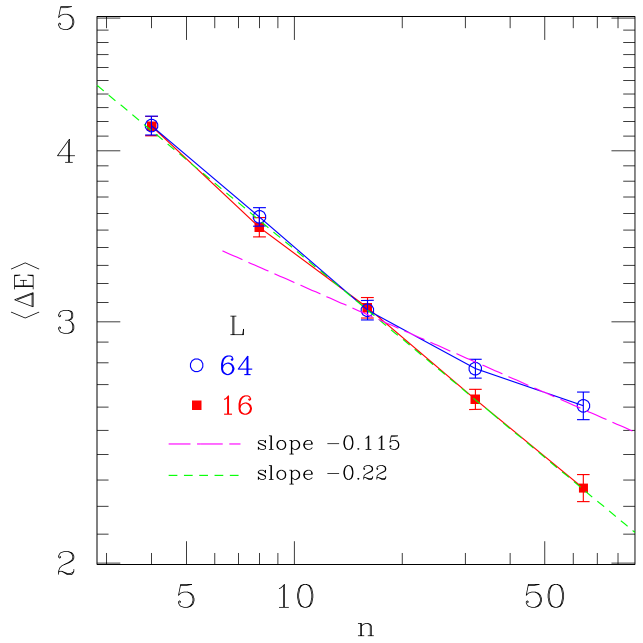

FIG. 6: The mean energy of the scale-invariant droplets and system sizes $L = 16$ and $L = 64$. For the size indicated as n, the droplets are allowed to range in size between $n - 1$ and $n/2$.

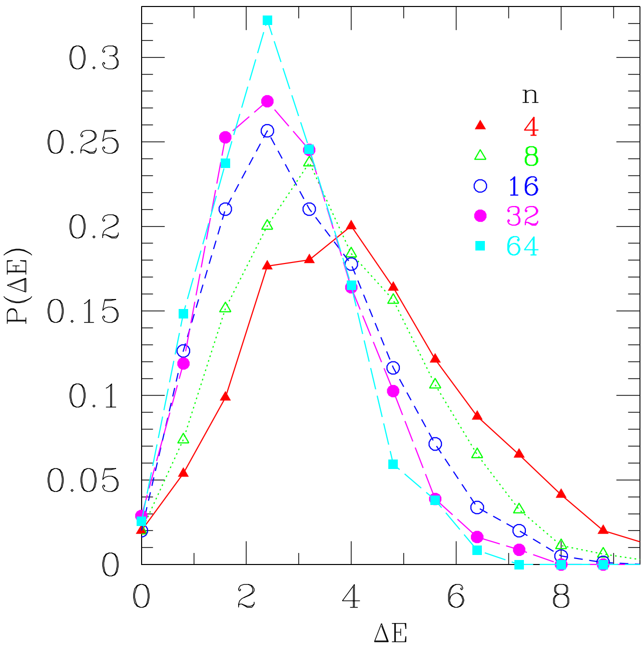

FIG. 7: Distribution of the energy of droplets of variable size, for different ranges of size for $L = 64$. For a size indicated as n, the droplets are allowed to range in size between $n-1$ and $n/2$.

between R_g and $\max(R_x, R_y)$ is excellent. If we exclude the $L = 4$ point, the fits give d_f closer to 2. For example the fit to R_g gives $d_f \simeq 1.88$. Combining these values of d_f with θ/d_f obtained from Fig. 2 we get:

$$\theta \simeq \begin{cases} -0.23 & \text{(assuming } d_f = 2\text{)}, \\ -0.21 & \text{(fit to } R_g\text{)}, \\ -0.22 & \text{(fit to } R_g, \text{ excluding } n = 4\text{)}. \end{cases} \tag{6}$$

We emphasize again that no trace of a more negative exponent of the order of -0.47 can be detected in our data, thus in disagreement with the predictions by Moore[17] that this method should reveal the corrections to scaling included in Eq. (1).

B. Clusters with a Range of Size

In this section we allow the size of the droplets to vary over a factor of two, more precisely between $n/2$ and $n-1$. This is more in the spirit of the droplet picture of Fisher and Huse[1–3], where droplets are defined, in $3d$, as objects with boundaries lying between a cube of linear size ℓ and another one of size 2ℓ. We now perform the same analysis as above for these new clusters.

1. Droplet Energies

The mean droplet energy as a function of size n is shown in Fig. 6. For the size specified as n, the droplets were allowed to vary in size between $n-1$ and $n/2$. For very small sizes, where the data for $L = 16$ and 64 agree, the slope is about -0.22, considerably more negative than the value of -0.115 found for droplets of fixed size in Sec. III A. For larger sizes, where the data for $L = 16$ differs from that for $L = 64$, the slope of the presumably more reliable $L = 64$ data becomes less negative and is compatible with -0.115, though there is not enough range of size to allow for a precise fitted value. If we insert $d_f = 2$, then, according to Eq. (3), this would give a crossover from $\theta \simeq -0.44$ to $\theta \simeq -0.23$, not very different from the crossover proposed in Refs. 17,18.

However, it should be pointed out that no such crossover was found in Sec. III A for fixed size droplets, and, furthermore, the values of the droplet radius R, discussed in Sec. III B 3 are extremely small, of order one or two lattice spacings, in the region where the data of Fig. 6 suggests $\theta \simeq -0.44$, so that the meaning of a power law correction of the type $L^{-\omega}$ for such sizes is not clear. Note finally that the apparent fractal dimension for these very small clusters is quite far from 2 (see below), so that, if we accept this value for d_f the initial apparent stiffness exponent is around -0.35, rather far from the value -0.47 expected by Moore[17,18].

Finally, we have to admit that we do not understand why the crossover in Fig. 6 is absent when the size is exactly fixed, see Fig. 2.

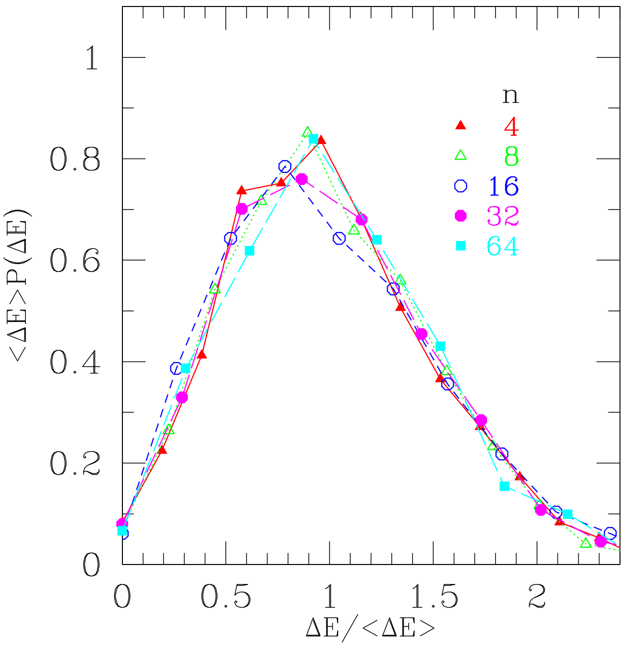

FIG. 8: The data in Fig. 7 scaled by the mean energy $\langle \Delta E \rangle$, according to Eq. (4).

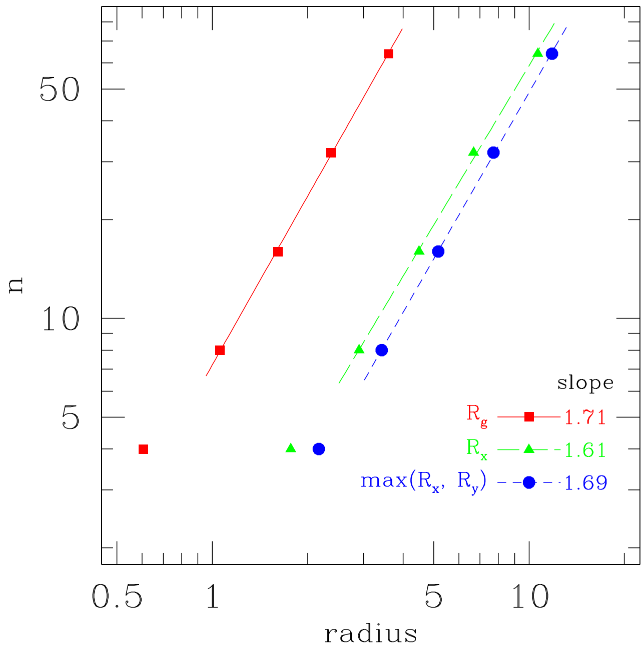

FIG. 9: The number of spins in the droplet, n, as a function of various definitions of the "radius", as described in the text. This is for droplets whose size is allowed to vary between $n-1$ and $n/2$. Data for $n = 4$ has been excluded from the power law fit.

2. Distribution of Droplet Energies

The distribution of droplet energies is shown in Fig. 7 and the scaled data is plotted in Fig. 8, again making use of Eq. (4). As for droplets of fixed size, the distribution is essentially linear for small energy, though in this case there is a very small, but definitely non-zero, intercept.

3. Fractal Dimension of the Droplets

Figure 9 shows the various definitions of the radius of the droplets, discussed in Sec. III A 3, for different values of n. The data does not fit well a straight line if the smallest size is included ($n = 4$, corresponding to droplets with 2 and 3 spins) so this has been omitted in the fits. The values of d_f for R_g and $\max(R_x, R_y)$ agree well, as for droplets of fixed size, though the value of d_f ($\simeq 1.7$) is a little lower than in that case. However, the trend is for the slope to increase with increasing n, this is particularly noticeable for the R_g data, and so it is possible that d_f is actually equal to 2, as we concluded also in the case of the cluster of fixed size.

IV. CONCLUSIONS

The main motivation for our work is to test Moore's proposal[17] that contradictory results of the literature, both in 2 and 3 dimensions, for the determination of the stiffness exponent θ in spin glasses were mainly due to "corrections to scaling" and captured by Eq. (1). We have performed simulations similar to those of Lamarcq et al.[35,37] but in the $2d$ case, where this theoretical conjecture could be checked. From our results, we can draw the following conclusions.

1. Following exactly the procedure of Ref. 35, we do not find any crossover in the behavior of the energy of the cluster as a function of their size, up to $n = 64$, contrary to Moore's prediction;

2. The value of the extracted stiffness exponent, $\theta \simeq -0.23$, is in fair agreement with domain wall calculations, $\theta = -0.28$. This result is clearly different from the $3d$ case, where the droplet and domain wall exponents are found to be very different.

3. For scale invariant clusters, a crossover not inconsistent with (1) is obtained, but only for very small cluster sizes.

As a conclusion, the problems we wanted to tackle in this paper unfortunately remain unsolved. We still do not understand the $3d$ results by Lamarcq et al.[35] and we do not understand the origin of the two different stiffness exponents reported in $2d$. Apart from very small sizes for one of the two methods of generating clusters, we did not find evidence for the crossover implied by Eq. (1). The nature of corrections to scaling in spin glasses therefore remains poorly understood.

Suppose we take the point of view that the differing claims obtained in Refs. 18,32–34 and the present work for the existence, or otherwise, of the proposed crossover in two-dimensions, are evidence for a wide range of values of the amplitude of the correction B in Eq. (1). It is then surprising that, to our knowledge, *all* estimates of θ from Monte Carlo simulations at $T \ll T_c$ give θ (for droplets) close to (and consistent with) zero, and different from θ for domain walls which is positive. This is true for Ising spin glasses in three and four dimensions[8], vector spin glass models[9,10], and a one-dimensional model with long range interactions[19]. In addition, various $T = 0$ calculations[5–7] also find $\theta\,(\text{droplets}) \simeq 0$. If the amplitude of the correction term is highly non-universal, as perhaps implied by the $2d$ results, it is surprising to us that the parameters in Eq. (1) systematically conspire to give a droplet energy for, say, Monte Carlo simulations which is independent of size over the range studied. Note too, that for the $1d$ simulations[19], the range of sizes is very large, up to $L = 512$.

Of course, the usual criticism that the truth lies beyond the reach of numerical simulations may be true. In this case, it is worth discussing the relevance of physics which can only be seen on such astronomically long time scales. From a *mathematical* point of view, understanding this physics is of fundamental importance. However, if the asymptotic behavior would only be seen on time scales which are inaccessible to experiments as well as to simulations, then the *physical* relevance is rather limited. In fact, experimental systems below the spin glass transition temperature T_c are not truly in equilibrium but are only equilibrated up to some coherence length scale, $\ell(t)$, which increases slowly, presumably logarithmically, with the time of the experiment t and also depends on T. One of us and Bouchaud[41] have estimated that $\ell(T) \lesssim 10$ (in units of the spacing between spins) at reasonable experimental time scales at $T \simeq 0.5T_c$. Refs. 42,43 estimate a somewhat larger value (rather more than 20) at this temperature and quite a lot larger[42] closer to T_c. Hence a reasonable estimate of $\ell(t)$ well below T_c in experiments is around 10-20 times the spacing between the spins, not very different from the sizes that can be simulated numerically, and much less than the sizes which appear to be necessary to see droplet behavior.

It is therefore possible that even if the droplet theory is asymptotically correct, the region in which its predictions can be observed quantitatively is not accessible experimentally. Close to T_c the length scales which can be equilibrated in experiments may be much larger[41,42], but in this region critical fluctuations give significant corrections to droplet behavior so *even larger* length scales are needed[44,45] to see droplet behavior than at lower temperatures.

Acknowledgments

APY acknowledges support from the National Science Foundation under grant DMR 0086287 and the EPSRC under grant GR/R37869/01. He also thanks David Sherrington for hospitality during his stay at Oxford when part of this work was performed. LB's work is supported by a European Marie Curie Fellowship No HPMF-CT-2002-01927, CNRS (France) and Worcester College, Oxford. Numerical results were obtained on Oswell at the Oxford Supercomputing Center, Oxford University.

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