Corrections to Scaling are Large for Droplets in Two-Dimensional Spin Glasses

A. K. Hartmann
Institut für Theoretische Physik, Universität Göttingen, Bunsenstraße 9, 37037 Göttingen, Germany

M. A. Moore
Department of Physics and Astronomy, University of Manchester, Manchester, M13 9PL, United Kingdom

(Dated: October 25, 2002)

The energy of a droplet of linear extent l in the droplet theory of spin glasses goes as l^{θ} for large l. It is shown by numerical studies of large droplets in two dimensional systems that this formula needs to be modified by the addition of a scaling correction $l^{-\omega}$ in order to accurately describe droplet energies at the length scales currently probed in numerical simulations. Using this simple modification it is now possible to explain many results which have been found in simulations of *three* dimensional Ising spin glasses with the droplet model.

PACS numbers: 75.50.Lk, 02.60.Pn, 75.40.Mg, 75.10.Nr

There are two rival theories to describe the ordered state of spin glasses: the droplet theory [1–3] and the replica symmetry breaking (RSB) theory of Parisi [4, 5]. The droplet picture assumes that the low-temperature behavior is governed by droplet-like excitations, where excitations of linear spatial extent l typically cost an energy of order l^{θ}. Thus in the thermodynamic limit the excitations which flip a finite fraction of the spins cost an infinite amount of energy if $\theta > 0$. These excitations are expected to be compact and their surface has a fractal dimension $d_s < d$, where d is the space dimension. Furthermore it is usually assumed that the energy of different types of excitations, e.g. droplets and domain walls, induced by changing the boundary conditions, are described by the same exponent θ. On the other hand the RSB theory assumes that there are low-energy droplet excitations in which a finite fraction of the spins in the system are reversed but which only cost a finite amount of energy in the thermodynamic limit. The surface of these excitations is space-filling so that the fractal dimension of their surface $d_s = d$ [6].

Many numerical studies have been done in an attempt to resolve the controversy, but studies in three [7] and four dimensional systems [8] are limited in the range of systems sizes which can be studied. In two dimensions, however, much larger systems can be studied. For this dimension, no spin-glass order exists at any finite temperature [9], but there are still puzzling results concerning droplet excitation energies about the groundstate. The energies of cross-system domain walls [10, 11] and droplet-like excitations [12, 13] are apparently descibed by different exponents, which is not compatible with the (usual) droplet picture and might be regarded as a vestige of RSB type behavior.

In this letter we study numerically droplets in two-dimensional spin glasses similar to the droplets studied in Ref. 12, but up to even larger sizes. We show that the numerical results mentioned above can be explained by a simple scaling correction. For larger droplets we find a behavior which is compatible with the droplet prediction, i.e. the exponent θ is the same for droplets and cross-system domain-walls. Smaller droplets appear to be described by an effective exponent θ'. We also study how the volume of an average droplet behaves with system size. We find that when considering just smaller system sizes, droplets appear non-compact, but for larger systems, crossover to a compact behavior looks likely. Thus in two-dimensions the droplet picture seems to be entirely valid. Finally, we discuss also some recent numerical results [14–16] in three dimensions, which also may be explained within the droplet picture using the correction to scaling for droplet energies introduced here.

We consider the Hamiltonian which is usually studied in numerical work of the Ising spin glass model:

$$\mathcal{H} = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j, \tag{1}$$

where the sites i lie on the sites of a cubic lattice with $N = L^d$ sites, $S_i = \pm 1$, the J_{ij} have a Gaussian distribution of zero mean and unit variance and couple nearest-neighbor sites on the lattice.

It is important to realize what the low-energy excitations look like in spin glasses. Consider a domain wall crossing a system $M \times M \times L$. The energy cost of this domain on the droplet picture will be of order M^{θ} and the domain wall will be fractal with dimension d_s and with an area of order M^{d_s}. In three or more dimensions the interface may have holes through it. Because it is fractal the extent of this wandering is of order M. The wandering of the interface by an amount of order M affects the determination of θ, see Ref. 17, where it was found that the best results were obtained when $L \gg M$ as then the interface is not affected by its interactions with the ends of the system. Suppose now we have two domain walls across the system. Then if their separation is large compared to M they will be unaffected by the presence of the other. However, if they are closer together they interfere with each other and their overall energy will be greater than if the other one were absent. This is because domain walls wander to take advantage of weak bonds and since the domain walls cannot cross, the presence of the second domain wall will preclude the first domain wall from cutting through bonds it would have cut in the absence of the second wall. As a consequence of this, domain walls effectively repel each other. If they have a separation of order l, then the repulsive energy between them would be expected to vary with their separation as a power law, $l^{-\omega'}$. No investigations of ω' seem to exist in the literature.

Consider now a droplet of linear extent l. It too will have a fractal surface described by d_s. Pictures of large droplets have now appeared [15], and a systematic investigation of them is in [18]. Their fractal nature ensures that in three or more dimensions that they have holes through them, giving them a sponge-like appearance. However, because the surface of the droplet may wander by a distance of order l the energy of the droplet E will be modified by its wandering and "collisions" with itself to a form which we suppose by analogy with the above is

$$E = Al^{\theta} + Bl^{-\omega}. \tag{2}$$

The term $Bl^{-\omega}$ is a scaling correction to the form of the droplet energy at large l and A and B are positive constants. We will show that the scaling correction is very significant in two dimensions.

In this dimension θ is very accurately determined as systems of 480^2 can be studied [11]. The exponent associated with a single domain wall, that is θ, is approximately -0.29 [11, 17]. However, studies where, say, θ is determined from the effects of thermally excited droplets (such as Monte Carlo simulations of the spin-glass susceptibility) yield an apparent θ' close to -0.47 [12, 13]. This discrepancy has long been a puzzle, and has prompted suggestions that perhaps different exponents describe domain wall energies and droplet energies [12]. However, Eq. (2) offers a way of resolving the discrepancy. For small values of l, droplets would apparently have energies decreasing as $l^{-|\theta'|}$ when their energies are affected by the correction to scaling term, but at large values of l the decrease with l will be slower and be as $l^{-|\theta|}$, as expected from the conventional droplet approach.

We have tested this explicitly by studying larger sizes than before using an exact ground-state (GS) algorithm [19]. For the special case of a planar system without magnetic field, e.g. a square lattice with periodic boundary conditions in at most one direction, there are efficient polynomial-time "matching" algorithms [20]. The basic idea is to represent each realization of the disorder by its frustrated plaquettes [21]. Pairs of frustrated plaquettes are connected by paths in the lattice and the weight of a path is defined by the sum of the absolute values of the coupling constants which are crossed by the path. A ground state corresponds to the set of paths with minimum total weight, such that each frustrated plaquette is connected to exactly one other frustrated plaquette. This is called a minimum-weight perfect matching. The bonds which are crossed by paths connecting the frustrated plaquettes are unsatisfied in the ground state, and all other bonds are satisfied.

We want to mimic the droplet generation used in Ref. 12, where a center spin was forced to reverse its orientation with respect to its orientation in the GS, the boundary spins were fixed, and a new GS under these constraints was calculated. Note that fixing the absolute orientation of a spin does not allow for a fast polynomial algorithm. Hence, a different approach must be used to study large systems.

Our generation of the droplets works in the following way. For each realization, first a ground state is calculated with free boundary conditions in both directions. Then several "hard" bonds are introduced, i.e. bonds with a high value of the absolute strength (e.g. $|J_{ij}| = 2N \times \max_{\langle i,j\rangle}\{J_{ij}\}$). If the subsystem of hard bonds does not exhibit frustration, no hard bond will be broken, if a new GS is calculated. First, all boundary spins are fixed relative to each other by hard bonds around the border chosen to be compatible with their GS orientations, i.e. the bonds between pairs of boundary spins are replaced. Second, a line of hard bonds is created which runs from the middle of (say) the left border to a pre-chosen center spin, again fixing the pair's spins in their relative GS orientations. Next, the sign of exactly one hard bond on this line is inverted. Finally, a GS of the modified realization is calculated. With respect to the original GS, the result is a minimum energy droplet fulfilling the constraints that it contains the center spin, does not run beyond the boundary and that it has a surface which runs through the hard bond which has been inverted. The energy of the droplet is defined as the energy of the resulting configuration calculated using the original bond configuration. For each realization, this procedure is iterated over all the bonds which are located on the line from the boundary to the center, when in each case exactly one hard bond is inverted. Among all generated droplets, the one exhibiting the lowest energy is selected.

This procedure is similar, but not equivalent to the method used in Ref. 12. The difference is that the surface of our droplets crosses the line from the boundary to the center spin exactly once. This means, it cannot cross this line more than once, i.e. it cannot "meander" across this line. But it may meander in all other directions. To reduce the influence of this constraint, we have iterated over all four lines of bonds running from the left, right, top and bottom boundary to the center spin, and selected the minimum energy droplet among all the $2L-2$ droplets generated in this way. Hence, we have obtained droplets which may meander in any direction, but not in all four directions at the same time.

We have tested explicitly the influence of this constraint by measuring in how many directions each of the lowest energy droplets meanders. For small systems meandering does not occur, but meandering increases with system size. For the largest systems we have considered, about half the droplets do not meander at all, about 33 % meander in one direction, 14 % meander in two directions and three percent in three directions. Hence, for the system sizes studied, four-way meandering droplets probably would occur rarely, if it were allowed by the method. Hence, we believe that our results are not strongly influenced by the constraint imposed by our algorithm. Furthermore, we have also tested droplets generated in a different way, which allow for full meandering, but this approach is restricted to small sizes, see below.

We have generated droplets for system sizes in the range $6 \le L \le 160$, each time 5000 independent realizations. The average droplet energy as a function of system size is shown in Fig. 1. For small sizes up to $L = 40$, the energy can be fitted by an algebraic function $\sim L^{\theta'}$ with $\theta' = -0.45(1)$, which is compatible with the earlier result [12] which had been interpreted in favor of the droplet exponent being different from the domain-wall exponent. For larger sizes, a clear crossover can be observed, the data is compatible with an exponent $\theta = -0.29$. A fit of the exponent in $[80, 160]$ yields $\theta = -0.32(1)$, which indicates that the thermodynamic limit may not been fully reached. We have also tested the scaling ansatz Eq. (2) by fixing $\theta = -0.29$, resulting in $\omega = 0.97(5)$ and a very good quality [22] $Q = 0.81$ of the fit. Curiously, the value for ω is close to the value which θ takes in one dimension, -1.

To estimate the influence of the slightly restricted meandering, we have also studied droplets, where in addition to the hard bonds around the boundary, only one additional inverted hard bond was introduced. For each system, this inverted hard bond was iterated over *all* bonds connecting at least one non-boundary spin. The minimum energy droplet was selected among all droplets containing the pre-selected central spin. Due to the large numerical effort, only sizes up to $L = 30$ could be studied. When considering up to 1000 realizations, the data was compatible with an algebraic decay with $\theta' = -0.47(1)$. We have increased the statistics, such that we have treated 80000 realizations for small sizes down to 20000 realizations for $L = 30$. Now the straight algebraic fit has a very low quality ($Q = 10^{-26}$) compared to the fit including the correction to scaling ($\omega = -2, \theta = -0.29, Q = 0.61$).

For further comparison with Ref. 12, we show in Fig. 2 the average droplet volume and surface as a function of the system size. By fitting to algebraic laws, we find a volume fractal dimension of $D_v = 1.80(1)$ and a surface fractal dimension of $d_s = 1.10(1)$, which are both compatible with the results obtained before. Hence, the crossover observed in the energy is not obvious when considering volume and surface and the droplets seem to be non-compact (i.e. $D_v < 2$). We have tested, whether this result may be a consequence of a correction to scaling, by fitting $V(L)$ to a function of the form $EL^2 + FL^{D'_v}$ resulting in $D'_v = 1.52(5)$ and a much better quality of the fit; $Q = 0.59$ as opposed to $Q = 0.002$ for the pure algebraic fit. Hence a crossover to compact droplets seems

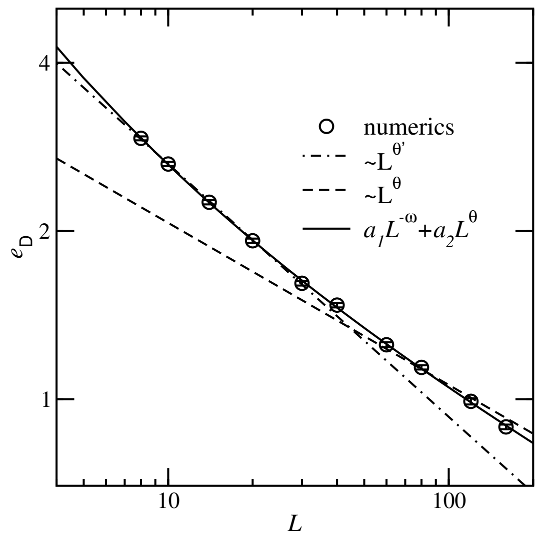

FIG. 1: Average droplet energy E as a function of the system size. The dashed straight lines represent algebraic functions with exponents $\theta' = -0.47$ and $\theta = -0.29$, while the full curved line represents the function from Eq. (2) with $\omega = 1$, $\theta = -0.29$).

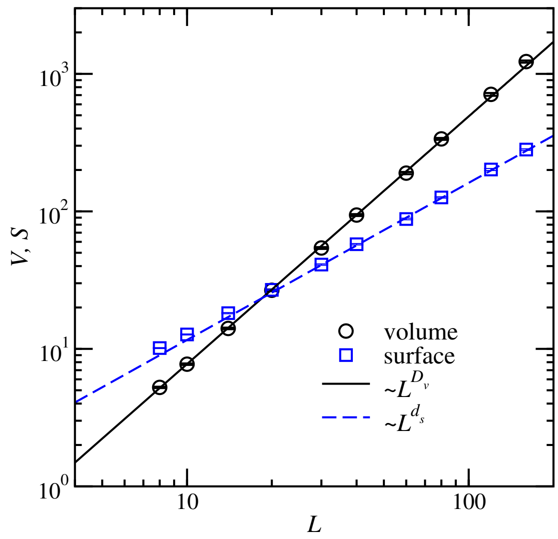

FIG. 2: Average droplet volume V and average droplet surface S as a function of the system size. The straight lines represent algebraic functions with exponents $D_v = 1.8$ respectively $d_s = 1.1$.

likely. In the figure, both functions would be hard to distinguish, hence we have omitted including the correction to scaling fit. We have also tried a correction to scaling for the surface, since d_s around 1.3 in other studies [10], but using the correction to scaling we could change d_s in a wide range without affecting the quality of the fit.

A crossover between large and small L dependencies was seen in the work of Middleton [23]. He studied the scaling of ground-state link overlaps and observed a gradual evolution of the finite-size behavior. Middleton himself attributed this gradual evolution to averages over droplets of all sizes up to the system size L. This kind of behavior is an additional mechanism, independent of our scaling correction for the droplet energies themselves, to explain why certain averages might be slow to converge to the expected behavior for large L.

We have seen that in two dimensions that the corrections to scaling are large, so that for medium-size systems they can mask the true asymptotic behavior. A similar effect would be expected to occur in higher dimensions and indeed might already have been observed by Lamarcq et al. [14] in their study of droplets in three dimensions. They first computed the ground state for both $N = 6^3$ and $N = 10^3$ spins. They then chose an arbitrary reference spin and flipped it along with a cluster containing $V - 1$ other spins connected to it. They next minimized the energy of this cluster by exchange Monte Carlo, but with the constraint that the reference spin is held fixed and the cluster was always connected and of size V. They found the largest extension (mean end-to-end distance) l of the cluster and found that for $V \leq 33$ its energy $E(l)$ varied as $l^{\theta'}$, where the exponent θ' was -0.13 ± 0.02. For larger V values they found that $E(l)$ was increasing rather than decreasing with l but they were unsure whether this might not be an artifact of insufficient numbers of Monte Carlo steps. Note that according to Eq. (2), when both θ and ω are small and positive, $E(l)$ will have a shallow minimum at some value l_0, similar to the behavior actually seen in Ref. 14.

Furthermore, for droplets whose linear dimensions are similar to the minimum at l_0, the apparent value of θ would appear to be close to zero. This may be the origin of the behavior in Refs. 15, 16, where simulations of Parisi's spin overlap distribution function and the link overlap function were only consistent with the droplet picture if θ was taken to be about zero rather than its domain wall value of order 0.20 in three dimensions [7] and 0.70 in four dimensions [8].

To summarize: there exists a natural correction to the usual scaling formula for the energy of a droplet. We have explicitly verified its validity by numerical studies of large systems in two dimensions. If a similar correction is valid in three dimensions, it can explain a number of puzzling features which have been seen in simulations. A direct check of the validity of this scaling correction needs numerical studies of larger three-dimensional systems than those currently studied.

We would like to thank Alan Bray for many discussions. AKH obtained financial support from the DFG (Deutsche Forschungsgemeinschaft) under grants Ha 3169/1-1 and Zi 209/6-1. The simulations were performed at the "Paderborn Center for Parallel Computing" and the "Gesellschaft f—r Wissenschaftliche Datenverarbeitung" in Gvttingen, both in Germany.

[1] W. L. McMillan, J. Phys. C **17**, 3179 (1984).
[2] A. J. Bray and M. A. Moore, in *Glassy Dynamics and Optimization*, edited by J. L. van Hemmen and I. Morgenstern, (Springer, Berlin, 1986).
[3] D. S. Fisher and D. A. Huse, Phys. Rev. Lett. **56**, 1601 (1986); Phys. Rev. B **38**, 386 (1988).
[4] G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979); J. Phys. A **13**, 1101 (1980); Phys. Rev. Lett. **50**, 1946 (1983).
[5] M. Mézard, G. Parisi and M. A. Virasoro, *Spin Glass Theory and Beyond* (World Scientific, Singapore, 1987).
[6] E. Marinari, G. Parisi, F. Ricci-Tersenghi, J. Ruiz-Lorenzo and F. Zuliani, J. Stat. Phys. **98**, 973 (2000).
[7] A. J. Bray and M. A. Moore, J. Phys. C **17**, L463 (1984); W. L. McMillan, Phys. Rev. B **30**, 476 (1984); A. K. Hartmann, Phys. Rev. E **59**, 84 (1999).
[8] A. K. Hartmann, Phys. Rev. E **60**, 5135 (1999); K. Hukushima, Phys. Rev. E **60**, 3606 (1999).
[9] N. Kawashima and H. Rieger, *Europhys. Lett.* **39**, 85 (1997)
[10] A. K. Hartmann and A. P. Young, Phys. Rev. B **66**, 094419 (2002)
[11] A. K. Hartmann and A. P. Young, Phys. Rev. B **64**, 180404 (2001). of order 0.20
[12] A very extensive review of the 2D spin glass problem has been given by N. Kawashima and T. Aoki, J. Phys. Soc. Jpn., **69**, Suppl. A, 169 (2000). See also N. Kawashima , preprint cond-mat/9910366 (1999)
[13] M. Picco, F. Ritort and M. Sales, preprint cond-mat/0106554.
[14] J. Lamarcq, J.-P. Bouchaud, O. C. Martin and M. Mézard, EuroPhys. Lett. **58**, 321 (2002).
[15] F. Krzakala and O. C. Martin, Phys. Rev. Lett. **85**, 3013 (2000).
[16] M. Palassini and A. P. Young, Phys. Rev. Lett. **85**, 3017 (2000).
[17] A. C. Carter, A. J. Bray and M. A. Moore, Phys. Rev. Lett. **88**, 077201 (2002).
[18] J. Houdayer, F. Krzakala, and O. C. Martin, Eur. Phys. J. B **18**, 467 (2000).
[19] A. K. Hartmann and H. Rieger, *Optimization Algorithms in Physics*, Wiley-VCH, Berlin, to be published 2001.
[20] I. Bieche, R. Maynard, R. Rammal, and J.P. Uhry, J. Phys. A **13**, 2553 (1980).
[21] G. Toulouse, Commun. Phys. **2**, 115 (1977).
[22] Q is the probability that the value of χ^2 is worse than in the current fit. See W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery, *Numerical Recipes in C*, Cambridge University Press, Cambridge (1995).
[23] A. A. Middleton Phys. Rev. B **63**, 060202 (2001).