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LETTER TO THE EDITOR

Scaling of energy barriers in Ising spin glasses

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Abstract. An exact algorithm of search for energy barriers against inversion of ground states is presented. For the case when each spin is allowed to flip only once, the barriers in ferromagnetic and spin glassy 2D systems are found to scale linearly with the linear size of the system.

Dynamics of Ising systems are of a purely relaxational nature [1]. In the absence of an external driving force each time-dependent quantity is a superposition of exponentially decaying processes which can be characterized by their corresponding relaxation times. Studies of various spin clusters [2] indicate that the spectrum of relaxation contains, in general, a portion of very long times and a portion related to rapid processes. The number of long relaxation times is equal to the number of local energy minima in the system (without counting the mirror images of the spin configurations as different).

In uniform ferromagnets all but one of the microscopic processes are rapid. In spin glasses (SG) there are many long times. In paramagnets there are none. In each case the longest relaxation time is given by the Arrhenius law

$$\tau = A\,\mathrm{e}^{B/kT} \tag{1}$$

where A is of order of the microscopic Glauber time for uncoupled spins. For uniform systems, the energy barrier, B, is equal to the energy required to invert the ground state configuration. For random systems B turns out to be of order of this reversal energy. The same result has been also obtained by McMillan [3] in Monte Carlo simulations.

How does B depend on the linear size, L, of the system? We have studied this problem for various 2D models on a square lattice with free boundary conditions. The ground state spin configurations were obtained by the transfer matrix method and the barriers were then calculated using an exact algorithm which is described further on. This algorithm is related to the idea of the 'landscape exploration' used by Rammal and Benoit [4] to study ferromagnets on percolation clusters. The barrier calculation explores possible phase space trajectories in which spins are flipped once (in [4] mixed dynamics in which simultaneous two spin flips were also allowed was studied). Finally we discuss ways to generalize our algorithm for trajectories in which spins are flipped one at a time but not necessarily only once.

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Our results for ferromagnets and SGs are shown in figure 1. System sizes are up to $L=5$ (i.e. up to 6 spins in a row). In the case of random system we averaged over between 2000 and 5000 samples except for $L=5$ when only 50 samples were taken into account. We considered Gaussian (GSG) and bimodal (BSG) spin glasses. For GSG the dispersion in the couplings, J_{ij}, was equal to 1 while in the case of BSG the distribution is given by $P(J_{ij})=\frac{1}{2}[\delta(J_{ij}-1)+\delta(J_{ij}+1)]$.

The uniform ferromagnet (FM) had a unit coupling. In the case of disordered ferromagnets (DFM) the J_{ij}'s were equal to the absolute values of numbers generated from the Gaussian probability distribution. Our results suggest that for each of the models considered the average barriers scale linearly with L

$$\langle B\rangle = b_0 + b_1 L \tag{2}$$

implying some basic similarity in the dynamics involved. The values of b_0 are 4, 2.39 ± 0.10, 2.67 ± 0.10, and 2.28 ± 0.10 for FM, DFM, GSG, and BSG respectively. The corresponding values of b_1 are 2, 1.63 ± 0.02, 0.87 ± 0.02, and 0.82 ± 0.02. The distribution of B in each of the four cases in Gaussian with dispersion which weakly depends on L and on the distribution of couplings. In the best trajectory the region with spins already inverted grew substantially in a compact fashion with only occasional jumps to more distant sites (there were no such jumps in FM).

In the Fisher–Huse [5] theory of the dynamics of Ising SG an elementary excitation in the system consists of a droplet of linear extension L. The creation of a droplet results in the formation of a domain wall. The corresponding energy cost scales as L^y which is the basic tenet of the $T=0$ scaling theory of SGs [3, 6, 7]. For the $D=3$ Ising SG $y>0$, indicating a phase transition at a non-zero T, whereas for $D=2$ SG $y<0$, suggesting no spin glass order at non-zero T. The dynamics are controlled by the rate of creation of such droplets. Fisher and Huse postulate that the barrier against this relaxation scales as L^{ψ} where $y\leqslant\psi\leqslant(D-1)$. The argument for these inequalities goes as follows: the barrier must be at least as large as the energy required to create the

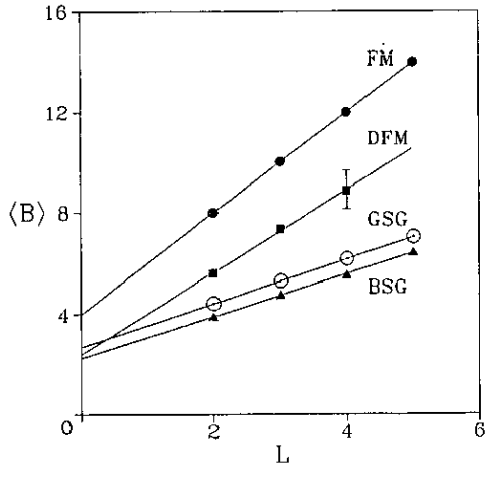

Figure 1. Scaling of average energy barriers for 2D uniform ferromagnets (FM), disordered ferromagnets (DFM), Gaussian (GSG), and bimodal (BSG) Ising spin glasses. L is the linear size or the system. Free boundary conditions are used. A typical dispersion of the distribution of the barriers is indicated for the DFM case.

domain, hence $y \leqslant \psi$; on the other hand, the barrier should be no larger than the barrier found in uniform ferromagnets because a SG should be able to take advantage of the frustration during relaxation, thus ψ must not exceed $(D-1)$.

Our calculation of B should also be valid—as far as the scaling law is concerned—for the case of the Fisher-Huse droplet. There are only two differences: different boundary conditions (free as opposed to those imposed by a background) and the compact shape of our geometry. None of these should matter because reversing a spin cluster requires flipping spins in the bulk of the droplet. The flips on the fractal surface and in the presence of the background constitute merely small corrections. Our results suggest therefore that ψ is actually equal to $(D-1)$, the upper limit postulated by Fisher and Huse.

It should be pointed out that in simple Migdal-Kadanoff approaches to scaling of the energy barriers, one would get $\psi = y$, if $y > 0$, or zero otherwise. In those schemes various relaxation time scales are related to specific length scales of the system and thus barriers behave as the exchange couplings at those scales. Our results suggest that relaxation processes are global in nature and not restricted to particular length scales.

We now proceed to the description of our calculations. For free boundary conditions we consider systems of $N = L_1 * L_1$ spins, where $L_1 = L - 1$ (L is the linear size of the system). The ground state was found by means of the transfer matrix method as used by Bray and Moore [6] ($T = 0$) and Morgenstern and Binder [8] and in our studies of the Potts SGs [9].

We define the barrier to be the energy required to invert all spins in the ground state within the context of single spin flip dynamics. The task here is to search through all trajectories (TR) of reversal. Consider, first, TRs in which spins can change their state only once. Each TR is characterized by an energy $\delta E_{\max}$, in excess of the ground state energy, corresponding to the highest point on the trajectory. Thus $B = \min(\delta E_{\max})$. In order to find B we first compose a table of all single-site energies, r_i, required to invert individual spins in the background of all other spins remaining frozen. This table is updated whenever a spin reversal is made. The initial values of r_i correspond to the ground state. We select first a tentative value, B_1, of the barrier against the reversal of the whole system. In practice, it is convenient to take $B_1 = \max(r_i)$. We select a resolution, R, within which the true barrier, B, will be determined. In practice, we take $R = 0.01$. We then check whether one can find TRs of reversals that do not required a supply of more than B_1 of energy.

The scanning through the TRs proceeds in the following way. First we label the spins 1 through N. Then we start the scan in the forward direction by attempting to flip spin number 1 without exceeding B_1. If this cannot be done we turn directly to the second spin, and so on, until a flip is successful. Each time we succeed we seek a new candidate for flipping in the subset of the still unflipped spins by considering them always from the origin.

Suppose that we arrive at the last spin in this way and that could not be flipped. We then go back to the last successful flip, undo it, and perform a forward search 'to the right' of that spin. If we fail to find another flippable spin we undo still earlier successful flips and search to the right of them. Whenever we manage to flip we scan again from the origin. Note that the search automatically allows for TRs which start from each of the spins. A successful TR is found if the number of flipped spins is equal to N. Should no TR be allowed, one can often learn about it in a search shorter than $N!$ long. The reason is that the constraint placed on the states not to exceed a given energy restricts the class of TRs to be considered.

If no allowed TR is found we conclude that B_1 is too small an estimate of δE and we update B_1 to

$$B_2 = B_1 + R. \tag{3}$$

If at least one allowed TR is found we take note of δE_{max} of the last such TR considered and update B_1 to

$$B_2 = \delta E_{max} - R. \tag{4}$$

We repeat the search with B_1 replaced by B_2. We continue in this way until after one successful choice of B_ν we get to $B_{\nu+1}$ which fails to produce an allowed inversion. The barrier B is then given by B_ν within the resolution R. (We checked that our algorithm gave the correct barrier for TRs generated by 'brute force' in small clusters.)

Within the class of TRs in which spins are inverted only once and within the resolution R, our numerical procedure is exact even though one does not explore in full and the possible TRs. Note also that TRs which have been scanned through are automatically remembered by the selection of regions of search for spins to flip.

The algorithm described above explores TRs on which each spin is inverted once. Consider now a broader class of TRs such that each spin can be inverted up to n times. The inversions should still take place one at a time because the Glauber dynamics is of a single spin nature. The number n must be odd since the ground state needs to be fully inverted. The barriers should be studied as functions of increasing n to extrapolate to infinitely large n.

Our algorithm can be readily generalized to the $n > 1$ case. For simplicity we will consider $n = 3$. In addition to the original N-spin system A we create two replicas B and C and generate TRs in the combined system. Spins with labels $N+i$, $2N+i$ are identical to spins i, $i = 1, \ldots, N$. Each of the $3N$ spins is allowed to flip only once. First reversals of spins will be counted in A, second in B, and third in C. Our algorithm in this case becomes subject to the following restrictions: turn a given spin from B (spin with number $N+i$) only if spin i is already inverted in A and turn spin in C provided its image in B was inverted. A spin in A can always be inverted. During the search for the optional TR described earlier we attempted to redirect a failed search by inverting back the last successfully flipped spin and trying again. That spin was counted as inverted only temporarily. In the generalized algorithm we can reinvert any flipped spin from C but spins in B can be reinverted if the corresponding spin in C did not turn. Similarly, spins in A can be reinverted if their images in B were not flipped. The search for TR is successful if the number of spins inverted in A equals N provided all those spins which are flipped in B are also flipped in C (their number is $\leqslant N$).

We have studied 100 $L = 2$ BSG systems and the $n = 3$ barriers were not found to be lower than when the trajectories were restricted to $n = 1$ for any of them. These results suggest that the $n = 1$ trajectories give the dominant if not the only contribution to $\langle B \rangle$.

That the barrier scaling exponent at short length scales, studied here, is positive does not necessarily imply that there is an equilibrium SG-paramagnet phase transition at a non-zero temperature. For example, there is no non-zero T ordering when arbitrarily large domains can be overturned with finite cost in energy. However, the single spin-flip barriers to overturning each domain can still scale with a positive exponent. For instance, in the case of a percolating FM cluster, $\langle B \rangle$ diverges logarithmically [4, 10] even though it has no long range order at any non-zero T.

It is interesting to observe that our short length scale value of ψ is compatible with experimental findings: recent studies [11] of $Rb_2Cu_{1-x}Co_xF_4$, which is a model compound for the 2D Ising BSG, have revealed an extremely wide distribution of relaxation times. In the limit of $T \to 0$ the median relaxation time τ_c was found to scale across 16 frequency decades according to $\ln(\tau_c/\tau_0) \approx T^{-1-\psi\nu}$ with $\nu = 2.3 \pm 0.4$ and $\psi = 0.9 \pm 0.2$.

In conclusion, we have studied the scaling behaviour of energy barriers in frustrated and unfrustrated 2D systems in the context of single spin flip dynamics. We have found that the barrier scaling exponents in these systems are the same and equal to the upper limit postulated by Fisher and Huse.

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