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Glassy dynamics and aging in an exactly solvable spin model

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We introduce a simple two-dimensional spin model with short-range interactions which shows glassy behavior despite a Hamiltonian which is completely homogeneous and possesses no randomness. We solve exactly for both the static partition function of the model and the distribution of energy barriers, giving us the equilibration time scales at low temperature. Simulations of instantaneous quenches and of annealing of the model are in good agreement with the analytic calculations. We also measure the two-time spin correlation as a function of waiting time, and show that the model has aging behavior consistent with the distribution of barrier heights. The model appears to have no sharp glass transition. Instead, it falls out of equilibrium at a temperature which decreases logarithmically as a function of the cooling time. [S1063-651X(99)04311-1]

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I. INTRODUCTION

A great deal of effort has been devoted in the last twenty years or so to understanding the behavior of spin glasses and other glassy models [1–3]. In spin glasses, one introduces randomness into the Hamiltonian of some otherwise well-behaved system, creating a hierarchical distribution of energy barriers over state space which prevents the system from reaching thermal equilibrium on reasonable time scales below a certain temperature. The slow dynamics displayed by these systems has made their computer simulation very difficult despite the recent appearance of a number of new and promising algorithms [4,5], and the presence of randomness in the Hamiltonian has, except in a few special cases [6–8], prevented their exact solution. As a result, our understanding of their behavior is, even after many years of effort, still very far from complete. It is, for example, still an open question whether, in the limit of infinitely slow cooling, spin glasses with short-range interactions display a sharp transition from ergodicity to glassy behavior, or whether the transition is a gradual one [2].

However, it is not necessary to have randomness in the Hamiltonian in order for a system to be glassy. Glassiness has its origin in the dynamics by which the system is updated rather than the energy landscape. In fact, no landscape even exists until we specify the dynamics, since the set of elementary moves by which the system moves from one state to another defines which states are neighbors. Given an appropriate choice of dynamics, any system can be ergodic on short time-scales, regardless of the energies of particular states. Conversely, it should be possible to find systems which display glassy behavior without randomness in the Hamiltonian.

One such system is the molecular or configurational glass—window glass, for example—but this is a notoriously difficult system to study mathematically [1]. Recently therefore, a number of authors have investigated spin models which are non-random but show glassy behavior either because of competition between different types of interactions [9] or because of the presence of higher-order interactions [10,11]. For some models with infinite-range interactions, the statics, though not the dynamics, can be solved exactly [12–14].

In this paper we introduce a *p*-spin model in two dimensions which, under a dynamics which flips single spins, displays the classic features of a glassy system. This model possesses the considerable advantage over previously studied models that both its statics and its low-temperature dynamics are exactly solvable, even though it has only short-range interactions.

The structure of the paper is as follows. In Sec. II we define our model. In Sec. III we give an analytic solution for the partition function and internal energy of the model in equilibrium. In Sec. IV we solve for the distribution of energy barriers between the ground state and the lowest-lying excitations of the model and hence argue that it should display glassy behavior. We compare our predictions with extensive Monte Carlo simulations and find excellent agreement between the two. In Sec. V we study the aging properties of our model, and in Sec. VI we give our conclusions.

II. THE MODEL

Our model is a *p*-spin model composed of Ising spins $\sigma_1 = \pm 1$ on a triangular lattice with short-range interactions and a single-spin-flip dynamics. The Hamiltonian is

$$H = \frac{1}{2} J \sum_{i,j,k \text{ in } \triangledown} \sigma_i \sigma_j \sigma_k . \tag{1}$$

The sum here runs over all sets of three nearest-neighbor spins i,j,k which lie at the three vertices of one of the downward-pointing triangles on the lattice. Except for this restriction to downward-pointing triangles, our model is the same as the Baxter-Wu model [15], although its behavior is

entirely different. It is also similar to a model used by Barkema *et al.* [16] to study the formation of adatom islands on (111) surfaces of metals.

For most of our presentation we will find it more convenient to rewrite this Hamiltonian in the form

$$H = J \sum_{i,j,k \text{ in } \triangledown} (s_i + s_j + s_k) \text{mod } 2, \tag{2}$$

which is identical to Eq. (1) except for an additive constant if we map the Ising spins σ_i onto the variables $s_i = \frac{1}{2}(\sigma_i + 1)$, which take the values 0 (down) or 1 (up).

One could also construct a disordered version of the model in which the three-spin interactions were chosen randomly to have strengths $\pm J$. However, this disordered version can be mapped onto the homogeneous one above via a simple gauge transformation, and so the two have identical behavior. (This transformation is particularly obvious when viewed in terms of the defect variables introduced below.)

The dynamics of the model consists of moves which flip single spins. We have chosen to investigate the behavior of the model under the standard Metropolis dynamics [17] in which moves with energy cost ΔE take place with rate 1 if $\Delta E \leqslant 0$, and with rate $e^{-\beta \Delta E}$ if $\Delta E > 0$. However, except for differences in the short-time correlations and a possible overall rescaling of time, we would expect the fundamental properties of the model to be the same for any other single-spin-flip dynamics which respects both ergodicity and detailed balance.

III. EQUILIBRIUM SOLUTION OF THE MODEL

In the following sections we discuss the glassy behavior of our model. First, however, we give an exact solution of its equilibrium properties. An alternative representation of the state of the model is as a triangular lattice of defects: the downward-pointing triangles of the Hamiltonian themselves form a triangular lattice, and for each site on this lattice which corresponds to a trio of spins of which either one or three are up, there is an energy contribution of J to the Hamiltonian. Thus we can represent each state of the lattice by a set of defect variables

$$d_i = (s_i + s_j + s_k) \text{mod } 2, \tag{3}$$

which take the value 1 when a defect is present and 0 otherwise. In terms of these defect variables, the Hamiltonian takes the form of a set of non-interacting Ising spins in an external field J:

$$H = J \sum_i d_i . \tag{4}$$

This simple form for the Hamiltonian allows us to solve for the model's equilibrium behavior exactly. However, there is a price to be paid for this simplicity in terms of an increased complexity in the dynamics. In the defect representation of the model, a single spin-flip corresponds to flipping the states of three defects at the vertices of an *upward*-pointing triangle. Thus our model displays clearly the duality between dynamics and interactions which is present in all systems; we can think of it either as a system of interacting spins with single-spin-flip dynamics, or as noninteracting spins with a constrained dynamics in which we flip three spins at once. In the remainder of the paper, we will for the most part adopt the latter description.

The first step in solving for the equilibrium partition function of the model is to find the set of allowed configurations of the defect variables d_i, so that we can perform the sum over them. Clearly the number of sites on the defect lattice is the same as that on the spin lattice and hence the maximum possible number of defect configurations is the same as the number of spin configurations of our original spin variables. We now show that, for certain boundary conditions, there is a one-to-one correspondence between spin configurations and defect configurations.

Consider three spin configurations $\{s^{(0)}\}$, $\{s^{(1)}\}$, and $\{s^{(2)}\}$, related as follows:

$$s_i^{(2)} = (s_i^{(1)} + s_i^{(0)}) \text{mod } 2. \tag{5}$$

The corresponding defect configurations are similarly related:

$$d_i^{(2)} = (d_i^{(1)} + d_i^{(0)}) \text{mod } 2. \tag{6}$$

If spin configurations 1 and 2 are to have the same defect configuration $d_i^{(1)} = d_i^{(2)}$ for all i, it follows that the defect variables corresponding to configuration 0 must all be zero, i.e., that configuration 0 must be a ground state of the system. If we can show that there is only one such ground state—the trivial one in which all spins are zero—then it follows that $\{s^{(1)}\}$ and $\{s^{(2)}\}$ are identical and the mapping of spin states to defect states is one-to-one. We can indeed show this in the case of a lattice which has length $L = 2^k$ for integer k along one dimension and periodic boundary conditions. The argument runs as follows.

Suppose we have a lattice in the form of a rhombic strip of width $L = 2^k$. If the configuration is to be a ground state, then there can be no defects at any site on the lattice. This allows us to calculate the values of the spins in one row given those in the preceding row since, by Eq. (3), each one must be the sum mod 2 of the two above it. If s_{ij} is the jth spin of the ith row, then

$$s_{i+1,j} = (s_{ij} + s_{i,j+1}) \text{mod } 2, \tag{7}$$

where $s_{i+1,j}$ is the site below s_{ij} and $s_{i,j+1}$. The spins in the next row after this are then

$$\begin{aligned} s_{i+2,j} &= (s_{ij} + 2s_{i,j+1} + s_{i,j+2}) \text{mod } 2 \\ &= (s_{ij} + s_{i,j+2}) \text{mod } 2. \end{aligned} \tag{8}$$

By iterating this argument it can now be shown that a similar result applies for each row which is a power of 2 away from the initial one. For L a power of 2, we then have

$$s_{i+L,j} = (s_{ij} + s_{i,j+L}) \text{mod } 2 = (2s_{ij}) \text{mod } 2 = 0, \tag{9}$$

since $s_{i,j+L} = s_{ij}$ because of the boundary conditions. Given that both i and j are arbitrary, it immediately follows that every spin on the lattice is zero.

Thus we have demonstrated that, for lattices of length a power of two along at least one dimension, there is a unique

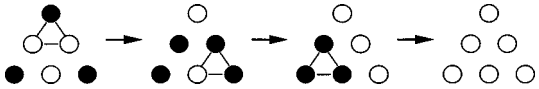

FIG. 1. A triangle of side 2^k can be flipped by flipping three triangles of side 2^{k-1}. The solid circles represent the defects and the lines indicate the triangles to be flipped at each step.

ground state in which all spins have value zero, which in turn implies a one-to-one mapping of defect states to spin states. Given the Hamiltonian (4), the partition function of the model is then simply

$$Z=\sum_{n=0}^{N}\binom{N}{n}e^{-\beta Jn}=[1+e^{-\beta J}]^N. \tag{10}$$

The equilibrium internal energy per site is then

$$E_{\rm eq}=-\frac{1}{Z}\frac{\partial Z}{\partial\beta}=\frac{J}{1+e^{\beta J}}. \tag{11}$$

For lattice sizes which are not a power of 2, the proof above no longer applies and more than one ground state may exist [18]. In that case, not all defect configurations can occur. However, the ones that do exist all correspond to the same multiplicity of spin configurations, one for each ground state. Since the states of the spins in a particular ground state are determined by the spins on any one row of the lattice, the number of ground states can increase at most as $N_{\rm ground}\sim e^L\simeq e^{\sqrt{N}}$ with lattice size. In addition, all of the defect states can be chosen independently except for those on one row, which may be restricted to some extent by the requirement that the spin configuration to be consistent with the periodic boundary conditions. This means that the partition function can be written as a sum

$$Z=N_{\rm ground}\sum_{n=0}^{N-L}\binom{N-L}{n}e^{-\beta J(n+\delta n)}, \tag{12}$$

where δn is the number of additional defects in that row determined by our $N-L$ choices in the other rows. Since $\delta n\leqslant L\simeq\sqrt{N}$, logarithmic derivatives of Z, and therefore bulk properties of the system, converge to those of Eq. (10) for large N.

In Fig. 1 we show our solution for the internal energy as a function of temperature (solid line), along with Monte Carlo results from the simulation of the model (dashed lines). The simulations were performed on a 128×128 rhombic system with $J=1$ using a Bortz-Kalos-Lebowitz continuous time algorithm [19]. Each curve represents the internal energy as a function of temperature during an annealing experiment using an exponential cooling schedule $T=T_0e^{-\gamma t}$ with $T_0=1$ and cooling rates (top to bottom) of $\gamma=10^{-2},10^{-3},10^{-4},10^{-5}$, and 10^{-6} in units of inverse Monte Carlo steps per spin. As the figure shows, the model's behavior is in good agreement with the equilibrium solution at high temperatures, but falls out of equilibrium at lower and lower temperatures as the cooling rate is decreased, in a manner characteristic of glassy systems.

In the inset, we show the results of numerical experiments in which the same system is quenched from $T=\infty$ to a fixed finite temperature. Each point represents the final average internal energy of the system after 10^9 Metropolis Monte Carlo steps per site (i.e., more than 10^{13} steps total). As we can see, the exact solution is again in good agreement with the simulations for high temperatures, but fails badly as $T\to0$.

IV. THE ORIGIN OF GLASSINESS IN THE MODEL

We can gain some insight into the model's loss of ergodicity if we recall that the flipping of a single spin corresponds to flipping the states of three defects in an upward-pointing triangle. In the limit of low temperature only those moves which flip the defects in triangles containing either two or three defects are energetically possible. Triangles with one defect only will be exponentially unlikely to change, and become local minima at $T=0$. Hence there will be a finite energy, and entropy, at $T=0$ [20].

In order to demonstrate that our model is truly glassy in the conventional sense, however, we need to treat the finite temperature case and investigate the distribution of energy barriers. As we have demonstrated above, the model has only one ground state, in which there are no defects and all spins are zero. We now show that the elementary excitations of the model—those states lying closest to the ground state—are trios of defects at the vertices of an upward-pointing equilateral triangle of length $\ell=2^k$ on a side with integer k.

Equation (7) tells us that the spins below an isolated defect form a Pascal's triangle mod 2. If we take a finite region of the lattice in the form of an upward-pointing equilateral triangle, each defect in it produces such a Pascal triangle. Then if the spins along the top sides of the triangle are zero, the bottom row is the sum mod 2 of the corresponding rows of each of the triangles. We call this row of spins the *shadow* of the region's defects. The sum of the Pascal triangles of an upward-pointing triangle of three adjacent defects is zero; thus a move that flips all three conserves the shadow, and one defect configuration can be reached from another by a series of local moves if and only if they have the same shadow. In particular, only configurations with a zero shadow can be local excitations of the ground state. It is then straightforward to show that no configurations with one or two defects can have a zero shadow, and that the only such configurations with three defects are those arranged in an upward-pointing triangle of side 2^k.

Next, we ask what the energy barrier is for flipping a triangular excitation of a given size. The minimum-energy path for flipping a triangle of side 2^k involves flipping three triangles of side 2^{k-1} in series, as shown in Fig. 1. Since the intermediate state on this path has four defects rather than three, the total energy barrier for the process is J higher than that for flipping a triangle of half the size. This in turn is J higher than the barrier for flipping triangles of half *that* size, and so on, down to triangles of side 1 which have barrier zero. Thus the total height of the barrier which must be crossed in order to create or remove a triangular excitation of side $\ell=2^k$ is $J\log_2\ell=kJ$, increasing logarithmically with size [21].

In a system of linear dimension $L<2^{k+1}$, the largest possible excitation is a triangle of side 2^k, and $kJ\simeq J\log_2L$ is the largest energy barrier the system must cross to achieve

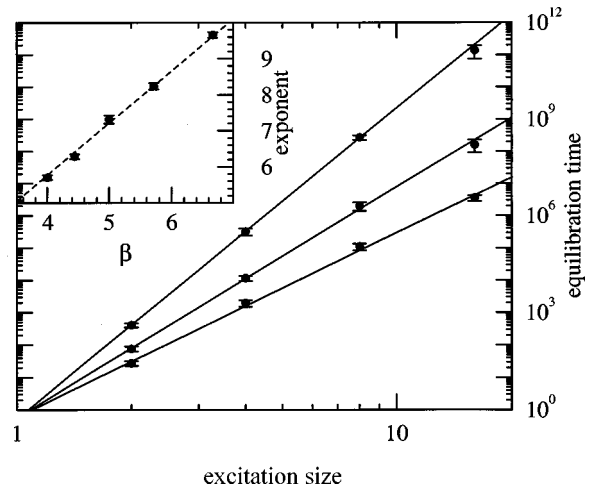

FIG. 2. The time it takes the system to eliminate a single triangular excitation of size $\ell=2,4,8,16$ for temperatures $T=0.15,0.20,0.25$. Each set of points follows the expected power law. Inset: the exponent of the power law as a function of inverse temperature β. The predicted value of $\beta J/\ln 2$, Eq. (13), is shown as the dotted line.

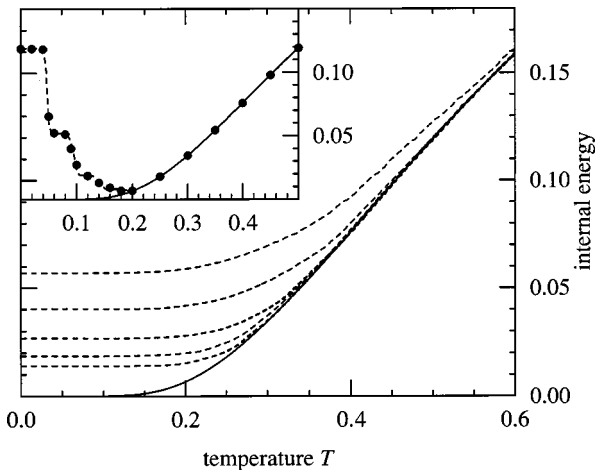

FIG. 3. The internal energy per site as a function of temperature in a series of annealing simulations using an exponential cooling schedule (dashed lines) compared to the exact solution at equilibrium (solid line). Inset: the internal energy following a quench from $T=\infty$ to a finite temperature. The points are data from Monte Carlo simulations, the solid line is the equilibrium solution, and the dashed line is a fit of the form (15). The steps in the fitted function correspond to the time scales τ_k, Eq. (14). Their heights are set by the fit parameters A_k, but their positions are absolute.

ergodicity. The conventional view is that a glassy system should have energy barriers which scale as a power of L. Since $\ln L$ is a limiting case of the power law when the exponent tends to zero, our model can be considered marginally glassy. At low temperatures, assuming an Arrhenius law $\tau\propto e^{\beta\Delta E}$, the correlation time goes as

$$\tau\sim e^{\beta J\log_2 L}=L^{\beta J/\ln 2} \tag{13}$$

i.e., as a power-law in the system size, with the exponent increasing linearly with β. At high temperature, the fact that there are several pathways for annealing away a triangular excitation reduces the free energy barrier somewhat, but we believe that there is no sharp glass transition.

We have confirmed these results in simulations of our model. In Fig. 2 we show the time taken to equilibrate the system starting from a state consisting of a single triangular excitation of a given size for three different temperatures with $J=1$. The expected power-law is obeyed closely. The lines should cross at the origin, since the time to get rid of an excitation of size $\ell=1$ is unity, and to a reasonable approximation they do this. The exponent of the power law is shown as a function of β for five different temperatures in the inset. The expected value of $\beta J/\ln 2$ is shown as the dotted line and agrees well with our measurements.

We are now also in a position to explain the form taken by the Monte Carlo results in Fig. 3. Writing the time scale for equilibration on length-scales up to $\ell=2^k$ as

$$\tau_k=e^{\beta Jk}, \tag{14}$$

we can write the energy of the system after time t as

$$E(t)=E_{\rm eq}+\sum_k A_k e^{-t/\tau_k}, \tag{15}$$

where the quantities A_k are temperature-independent constants. The dashed line in the inset of Figure 3 is of this form with $E_{\rm eq}$ taken from Eq. (11), $t=10^9$ as in the simulations, and the A_k assigned by a least squares fit to the data. Of particular interest are the ''steps'' visible in this fit. The temperatures T_k at which these occur are solutions of $\tau_k=t$:

$$T_k=Jk/\ln t, \tag{16}$$

with k taking integer values up to $\log_2 L$. Thus the temperature at which the system fails to equilibrate is inversely proportional to the logarithm of the cooling time t. This goes to zero more slowly than any power law as t goes to infinity.

V. AGING

We have also looked at the aging behavior of the model by examining the behavior of the two-time spin-spin connected correlation function $C(t_w,t)$ as a function of waiting time t_w. This function is defined by

$$C(t_w,t)=\overline{s_i(t_w)s_i(t)}-\overline{s_i(t_w)s_i(t)}, \tag{17}$$

where the bar indicates an average over the lattice. If a system relaxes to equilibrium exponentially fast, C is a function only of $t-t_w$. In our model, however, as is typical in systems with slow relaxation, C depends on t_w. In Fig. 4 we show C as a function of the ratio t/t_w for a variety of values of t_w. The figure has a number of notable features. The ''steps'' in the correlation function arise because all barriers in the model are multiples of J. This is true in some other glassy models as well, such as the Edwards-Anderson Ising spin glass [2,4] with random bonds $\pm J$. However, in that model, the height of the highest barrier, and hence the density of steps per unit volume, increases as a power of the size of the system, so that for a system of moderate size, the steps in $C(t_w,t)$ are small enough to be indistinguishable to the eye. In our model the height of the highest barrier in the

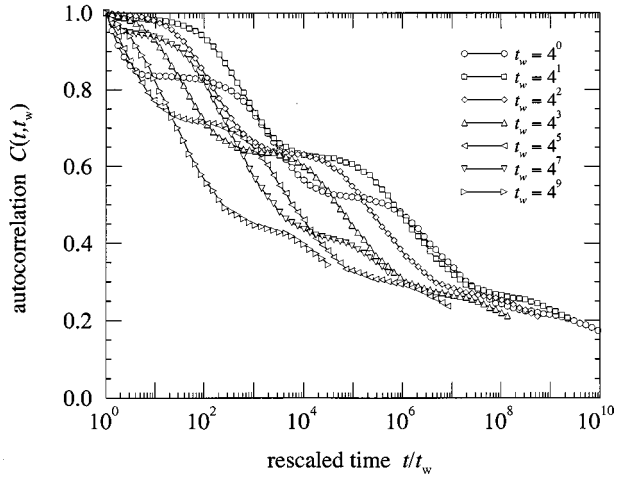

FIG. 4. The two-time correlation function $C(t_w,t)$ plotted as a function of t/t_w for $t_w=4^n$ with $n=0,1,2,3,5,7,9$. Note that the horizontal (time) axis is logarithmic.

system increases only logarithmically with system size, so that the steps are still visible even for quite large lattices.

Ignoring the steps in the correlation function, the figure shows that the rate of decline of the correlation function as a function of t/t_w is roughly independent of t_w, although there is no actual collapse of the curves onto one another as there is in some other models [11]. This is precisely the type of behavior which one would expect to see in this system, since the energy barriers we need to cross at each succeeding length scale $\ell=2^k$ are a constant amount J higher than those at the previous one, so that the corresponding time-scales increase by a constant factor [see Eq. (14)]. (By contrast, a plot in which the time is not scaled by the factor t_w gives no collapse of the correlation function, whereas in a nonglassy system such a plot should collapse perfectly.) Our model is instructive in this respect, since it makes the origins of the aging behavior particularly clear.

VI. CONCLUSIONS

To conclude, we have introduced a two-dimensional spin model with no randomness and only short-range interactions. Under single-spin-flip dynamics it displays glassy behavior, with barrier heights growing logarithmically with system size. We have given an exact solution for both the equilibrium properties of the model and the distribution of energy barriers. We have performed numerical simulations which confirm our analytic results to within the available precision. The model seems to have no sharp glass transition, and falls out of equilibrium at a temperature which decreases logarithmically as a function of the cooling time. It also displays clear aging behavior consistent with our understanding of the distribution of energy barriers.

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[21] We can generalize this to higher dimensions. For example, in $d=3$ the excitations of a model with four-spin interactions on tetrahedra of one orientation on a fcc lattice will be tetrahedra of size 2^k with energy barriers $2kJ$. A model with interactions on both kinds of tetrahedra is discussed in Ref. [10].