Critical Ising Spin Dynamics near the Percolation Threshold

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(Received 13 March 1985)

A low-temperature approach for the critical Ising spin dynamics on percolation clusters is proposed. The average energy barrier to overturning a cluster of s spins is shown to scale as $\ln s$. This basic result is supported by exact numerical calculations of the energy-barrier distribution for two- and three-dimensional percolation clusters, and is argued to be a consequence of scale invariance. The resulting temperature as well as size dependence of the relaxation-time scales agrees very well with the results of our Monte Carlo simulations.

PACS numbers: 05.50.+q, 64.60.Ht, 75.40.Dy

At the percolation threshold, both the infinite cluster and its backbone are self-similar (fractals). This self-similarity also holds at concentrations p near p_c for length scales l which are smaller than the percolation length ξ_p. For $l < \xi_p$, the number of bonds (or sites) on the infinite cluster scales as l^{d_p}, where $d_p = d - \beta_p/\nu_p$ denotes the fractal dimensionality and β_p, ν_p are the percolation-transition critical exponents. In the last few years, the influence of the scale invariance on the physics of fractals has been the object of various studies. For instance, anomalous behavior of physical properties described by linear problems (classical diffusion, spectrum of the discrete Laplacian operator, localization, etc.) has been shown[1,2] to occur on fractals.

In addition to linear problems, the static critical behavior of spin models on dilute lattices is now well established. In the following we consider the Ising spin model, defined by the Hamiltonian $H = -\sum_{\langle ij\rangle} J_{ij}\sigma_i\sigma_j$ on a diluted lattice. Here $\sigma_i = \pm 1$ and $J_{ij} = J$ (if both the nearest-neighbor sites i and j are occupied) or $J_{ij} = 0$ (otherwise). This model is relevant for dilute magnets and is known to have no long-range order at $p < p_c$, and orders at $T_c(p)$ for $p > p_c$, with $T_c(p) \to 0$ as $p \to p_c$.[3] Near the multicritical point $p = p_c$, $T = 0$, the critical line is given by $\exp[-2J/T_c(p)] \sim (p - p_c)^{\phi}$, where the crossover exponent ϕ has been shown to be equal to unity for all dimensions d. Accordingly, at $p = p_c$ ($\xi_p = \infty$), the spin-spin correlation length scales as $\xi_T \sim \exp(2K\nu_p) \sim \xi_1^{\nu_p}$, i.e., $\nu_T = \nu_p$. Here $K = J/T$ and ξ_1 is the correlation length for the one-dimensional (1D) Ising model. The other thermal exponents associated with the zero-temperature [$T_c(p_c) = 0$] ferromagnetic transition on the infinite cluster are given in terms of the percolation exponents ($\beta_T = 0$, $\nu_T = \nu_p$, $\eta_T = 2 - d_p$, etc.).

In this Letter, we report on some new results relative to the critical dynamics of the above model. These results should describe recent neutron-scattering experiments[4] performed on a 2D material. Our approach is based on the stochastic kinetic Ising model on percolation clusters, with a single-spin-flip dynamics satisfying the usual detailed-balance condition. In this framework of Glauber dynamics,[5] the flip rate of a spin at site i is given by $\Gamma_i = \tau_0^{-1}[1 - \sigma_i \times \tanh(K\sum_j \sigma_j)]$, where the sum is taken over neighbors j of i. Critical Glauber dynamics at $p = 1$ has been studied previously[6] and the exact solution for the diluted Ising chain[7] is known. Unusual time behavior of the relaxation functions, close to $p_c = 1$ and $T = 0$, has been shown to take place in that case. As will be shown below, the fractal structure of the percolation clusters leads to unusual critical dynamics in sharp contrast with the Euclidean regime (i.e., at $p = 1$).

Our method is mainly a low-temperature approach, with use of the concept of thermal activation and energy-barrier description. Let us consider first a finite cluster at threshold, containing $s \sim l^{d_p}$ spins. The relaxation problem is, in principle, solvable, involving a diagonalization of a $2^s \times 2^s$ matrix, leading to a spectrum of relaxation times. The size dependence of the relaxation time (actually this is the longest of the spectrum) of a given cluster is the relevant information. On the other hand, the equation of evolution for $\sigma_i(t)$ involves multispin correlation functions, and a rigorous analysis of the problem is difficult.[6] Even in the limit of high temperatures, when higher-order correlations may be neglected, the resulting equations are difficult to solve in the disordered problem. However, it is easy to see that at low temperature ($\xi_T >> l$), the thermal-relaxation rate will be dominated by the (free) energy barrier for single-spin dynamics. Near $T = 0$, entropy can be neglected and the energy barrier for the (dominant) reversal process from the state up ($\sigma_i = +1$, all i) to the state down ($\sigma_i = -1$, all i) will be defined as follows. We reverse the s spins in a given sequence and find the energy barrier (maximum energy) for that sequence. There are $s!$ sequences (paths) between the states up and down and the cluster energy barrier V_s is defined as the smallest energy barrier among the $s!$ paths. The optimal path associated with such a "minimax" sequence is very well defined but not unique in general. With this definition, V_s can be calculated exactly for relatively small clusters, thanks to a fast algorithm to generate permutations by $s!$ successive interchanges

of adjacent elements. The algorithm appears to be optimal for our purpose, up to $s = 10$, and has been used for an exact enumeration calculation[8] (low-p expansion). For large s, up to $s \sim 500$ in 2D and 200 in 3D, we have developed a very efficient new algorithm, giving the exact value of V_s for a given cluster. This new algorithm, based on the phase-space exploration, allows us to investigate the energy-barrier distribution for large clusters (technical details will be given elsewhere[9]). A similar procedure has been used to calculate the domain-wall energy barrier W_s. For a cluster of arbitrary shape, $W_s \geq V_s$ and the equality is reached for Euclidean blocks: $W_s \sim V_s \sim 2Js^{1-1/d}$.

Our results for 2D site-percolation clusters at threshold (square lattice, $p_c = 0.5927$) are shown in Fig. 1. Each point represents the average over ~ 500 clusters. Similar results were obtained for 3D percolation clusters on a simple cubic lattice. Extensive calculations ($s \leq 500$ for W_s, 250 for V_s in 2D, and 200 for V_s in 3D) have been performed in order to extract the asymptotic behavior of V_s. From the best fits of data, we obtained in 2D

$$V_s/2J = A \ln s + B, \quad A = 1.058 \pm 0.05,$$
$$B = 0.024, \quad W_s/2J = A' \ln s + B', \qquad (1)$$
$$A' = 1.16 \pm 0.03, \quad B' = -0.075,$$

and in 3D

$$V_s/2J = A \ln s + B,$$
$$A = 0.97 \pm 0.0, \quad B = 0.065. \qquad (2)$$

As can be seen, V_s and W_s exhibit the same logarithmic behavior in cluster size s; only the numerical factors are different. The logarithmic dependence appears to hold for both 2D and 3D clusters. The numerical coefficient B is very small and A seems to be very close to 1 in the two cases. It is important to notice that Eqs. (1) and (2) refer to the energy barrier for a typical cluster of size s. A more precise analysis would take into account the fact that the individual barrier V and then the relaxation rate depend on the shape of the cluster. Therefore, for a given size s, there is a probability distribution $p_s(V)$ for the energy barriers and then V_s, as calculated here, must be viewed as the average energy barrier.

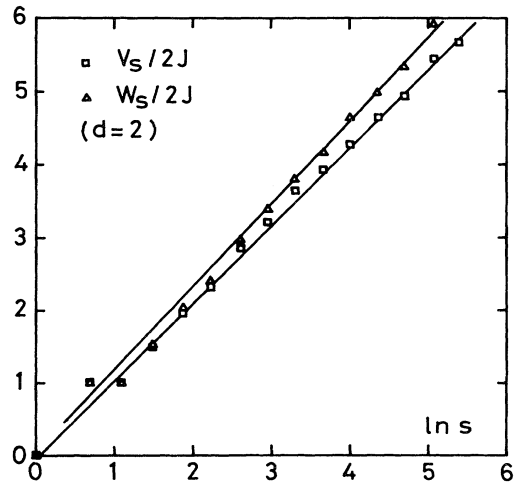

FIG. 1. Size dependence of the energy barrier for overturning 2D site-percolation clusters at threshold (square lattice). V_s and W_s denote the energy barrier and domain-wall energy barrier for clusters of s spins, respectively.

Although the result of Eqs. (1) and (2) can appear at first as suprising,[10] this is actually the most natural behavior of V_s as a function of s. Such a scaling form of barriers is a direct consequence of the scale invariance of the percolation clusters. Following McMillan[11] let us consider a renormalization-group procedure on the infinite percolation cluster ($p = p_c$) which forms a block spin from λ^{d_p} spins with a length scale change of a factor λ. The generic renormalization-group recursion relation can be written as $K^{(n+1)} = K^{(n)} F(K^{(n)})$, where $K^{(0)} = K$. In the strong-coupling limit, $F(K)$ approaches a constant and, to first order in $1/K^{(n)}$, $F(K^{(n)}) = \lambda^x - 1/K^{(n)}$, where x is a real number. According to Ref. 11, one can assume that the average energy barrier $V^{(n)}$ has, near the critical region, the recursion equation $V^{(n+1)} = V^{(n)} + K^{(n)} T$. The iteration equations for $K^{(n)}$ and $V^{(n)}$ can easily be solved leading to coupling and barrier at length scale $l = \lambda^n$. It turns out that only $x = 0$ can describe correctly the thermal critical behavior of percolation clusters, $T_c = 0$ and $\ln \xi_T \sim J/T$. In this case $K_l = K_0 - \ln l / \ln \lambda$ and $V_l \sim J(\ln l / \ln \lambda)$, in agreement with Eqs. (1) and (2). Note that $x > 0$ corresponds to the case where $T_c \neq 0$ exists and the energy barrier at length scale $l < \xi_T$ ($\xi_T \sim |T - T_c|^{-\nu}$) assumes again a logarithmic size dependence near the critical point T_c. Therefore, aside from the case $x < 0$ where V_l becomes independent of l at large l, the logarithmic law $V_l \sim \ln l$ appears as the most general one.

The phenomenological scaling analysis above provides a convenient framework to extract the temperature dependence of equilibration (relaxation) time scale: $\tau(T) \sim \exp[V(T)/T]$. Here $V(T)$ denotes the largest thermal barrier, associated with length scales $l \sim \xi_T$. For instance at $x < 0$, $\tau(T)$ is given by a simple activation (Arrhenius) law with $V(T \sim 0) \sim J$. In contrast, near T_c ($x > 0$), $\tau(T) \sim \xi_T^z$ reproducing the known form of the dynamic-scaling hypothesis.[6,12] Here z denotes the dynamic critical exponent, relating correlation length and relaxation time in the critical regime. In the case of the percolation clusters ($x = 0$), one obtains a temperature-dependent thermal barrier $V(T) \sim J^2/T$ at low temperature. This leads to $\ln \tau(T) \sim T^{-2}$ which can also be cast as $\tau(T) \sim \xi_T^z$ but

with a temperature-dependent dynamical exponent $z = z(T) \sim 1/T$. Such a result can be viewed as a violation of the standard dynamic scaling,[13] if we assume a constant value for z.

In order to check our results, we have performed a Monte Carlo study of finite clusters. Energy and magnetization relaxation were studied on small and large clusters, at different temperatures, and starting from different initial conditions (ordered, disordered, equilibrium). In Fig. 2 are shown some results for the temperature variation of the relaxation time $\tau(s,T)$ of the magnetization of three individual clusters in two dimensions. Here $\tau(s,T)$ is defined by $\tau(s,T) = \int_0^\infty dt\, \Phi(t)$ where $\Phi(t)$ denotes the following nonlinear relaxation function:

$$\Phi(t) = [M(t) - M(\infty)]/[M(0) - M(\infty)].$$

$\tau(s,T)$ was measured according to this definition, starting from a nonequilibrium state [ordered, $M(0) = 1$; disordered, $M(0) = 0$] at each temperature. For the clusters shown here (Fig. 2), a large number ($\sim 10^3$ to 2×10^4) of Monte Carlo steps per spin were done in order to approach equilibrium at each temperature. According to our previous analysis, this typical relaxation time is expected to show a crossover between a low-temperature regime

$$\ln\tau(s,T) \sim V/T \tag{3a}$$

and a singular critical regime

$$\ln\tau(s,T) \sim (A \ln\xi_T^{d_p} + B)/T \sim a/T^2 + b/T, \tag{3b}$$

where $a = 4J^2 d_p \nu_p$ and $b \sim J$. The crossover temperature T^* is defined by $s \sim \xi_T^{d_p}$, i.e., $T^*(s)/2J \simeq \nu_p d_p/\ln s$. Close to $T = T^*(s)$, corrections due to entropy barriers can become important but they have been neglected here. In Fig. 2 the results obtained for $\tau(s,T)$ are shown and are compared with the predictions of Eq. (3) for three typical clusters generated randomly on the square lattice. Similar results for the energy relaxation[9] were also analyzed following the previous scheme, leading to another confirmation of our results for the kinetic Ising model on percolation clusters.[14]

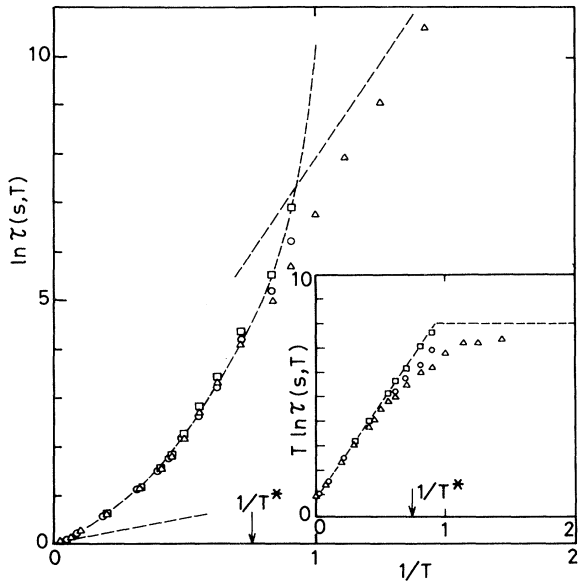

FIG. 2. Temperature variation of the magnetization relaxation times $\ln\tau(s,T)$ vs $1/T$ for three typical clusters (square lattice) with $s = 48$ (triangles), $s = 201$ (circles), and $s = 1471$ (squares). Each point corresponds to an average over 5000 Monte Carlo experiments. T^* denotes the crossover temperature between the singular critical dynamics ($T > T^*$) and the size-dependent regime ($T < T^*$) for $s = 48$ ($V = 8J, 10J$, and $16J$, respectively, for these three clusters). Dashed lines correspond to Eqs. (3), and the inset shows the temperature variation of the "effective" barrier (here $j = 1$).

Let us conclude with two comments. The critical dynamics found here is correct for individual clusters. At $p < p_c$, where $T_c(p) = 0$, the average over the cluster size distribution[15] leads to a nontrivial time dependence of relaxation functions (long-time tail, stretched exponential, etc.) and this will be discussed in a forthcoming paper.[16] Furthermore, the energy-barrier distribution $p_s(V)$ has a tail on the large-barrier side, characteristic of compact clusters. This leads also to a long-time tail of the function $\Phi(t)$, at $\Phi(t) \ll 1$, and can be viewed as the nonequilibrium counterpart of Griffiths singularities. In this respect, the samples shown in Fig. 2 are too small to resolve such dangerous tails. At $p \geqslant p_c$, $T_c(p)$ is finite and a fractal-to-Euclidean crossover is expected to occur. Moreover, accidental compact clusters may prevent $\Phi(t)$ from being described as a simple exponential in time for $T < T_c$ ($p = 1$), but this calls for further numerical investigations.

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[14]Note that for 1D clusters the relaxation is dominated by entropy barriers and does not fit the result of Eq. (3). For this particular case, the rate of flip of a cluster ($s \ll \xi_T$) is given by $\tau(s,T) \sim \xi_T s$, whereas $W_s = V_s = 2J$ (see Ref. 7).

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