Numerical simulation of the critical dynamics of disordered 2D Ising systems

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Critical relaxation of the magnetization has been studied by numerical simulation in the 2D Ising model with nonmagnetic impurity atoms frozen in lattice sites. A square lattice with dimensions of 400^2 was studied at spin concentrations $p=1.0$, 0.95, 0.9, 0.85, 0.8, 0.75, and 0.7. The dynamic critical exponent z was determined by the Monte Carlo method and the dynamic renormalization-group method. The following values were found for $z(p)$: $z(1)=2.24\pm0.07$, $z(0.95)=2.24\pm0.06$, $z(0.9)=2.24\pm0.06$, $z(0.85)=2.38\pm0.05$, $z(0.8)=2.51\pm0.06$, $z(0.75)=2.66\pm0.07$, and $z(0.7)=2.88\pm0.06$. A singular scaling of the exponent was found: $z=A'\cdot|\ln(p-p_c)|+B'$ with the constants $A'=0.56\pm0.07$ and $B'=1.62\pm0.07$.

According to the hypothesis of dynamic scaling,[1] as the temperature T of a system approaches the critical value T_c, such characteristics of the critical behavior as the relaxation time τ and the correlation length of long-lived thermal excitations of the system, ξ_T, are related by

$$\ln \tau=f(\ln \xi_T), \tag{1}$$

where $f(x)$ is a generalized uniform function of its argument x. For most of the critical phenomena which have been studied to date, the relaxation time of the system satisfies Eq. (1) with a function $f(x)=zx$, in which the constant z—the "dynamic critical exponent"—is independent of the temperature. As a result, as $T\to T_c$, the system is characterized by critical slowing of the relaxation time with

$$\tau\sim\xi_T^z\sim|T-T_c|^{-z\nu_T}, \tag{2}$$

where ν_T is the critical exponent of the correlation length, which specifies the divergence of this length at the critical temperature. Studies have shown that the numerical values of the critical exponents, while depending on the spatial dimensionality of the system, d, and on the number of components of the order parameter, are universal for a large number of systems. The classification of systems which exhibit very diverse phase transitions into universality classes of equilibrium[2] and dynamic[1] critical behavior has made it possible to introduce an unusual degree of order in the theory of phase transitions and critical phenomena. Studies of the critical behavior of disordered magnetic systems with randomly distributed nonmagnetic impurity atoms have made it possible to expand our ideas regarding the factors which influence a systematic classification based on universality classes.[3] Studies have shown[4] that frozen impurities alter the properties of magnetic materials whose specific heat in the homogeneous state has a divergence at the critical point with an exponent $\alpha>0$. This condition is satisfied by only those 3D systems whose effective Hamiltonian is isomorphic with the Ising model near the critical point. A renormalization-group analysis making use of an ϵ expansion[5,6] has revealed that the critical behavior of the disordered Ising model is characterized by a new set of critical exponents. The values of these exponents are independent of the concentration of point impurities, c_{imp}, in the region with $c_{imp} \ll 1-p_c$, where p_c is the threshold for spin percolation. The equilibrium critical behavior of dilute magnetic materials was analyzed directly for 3D systems in Refs. 7 and 8; a corresponding analysis for the dynamic critical behavior of such systems was carried out in Ref. 9. The experiments of Ref. 10 confirm that there is a numerical difference between the static critical exponents for impurity systems and those for homogeneous magnetic materials. Those experiments demonstrate a good agreement with theoretical results.

Disordered reduced-dimensionality magnetic materials describable by an Ising model are of particular research interest. Since the specific-heat exponent a of the homogeneous model is zero, the disorder resulting from the presence of an impurity has an uncertain effect. A detailed analysis[11,12] of this case has led to the conclusion that the impurity influences only the behavior of the specific heat; other thermodynamic and correlation functions undergo no change in critical behavior. A field-theory analysis of the relaxation regime of the critical dynamics of disordered 2D Ising-like magnetic materials has shown[9] that this regime is the same as the dynamics of a homogeneous model in the region with $c_{imp} \ll 1-p_c$ and is characterized by an exponent $z=2.277$. One question has remained unresolved, however: Are the critical exponents of disordered systems universal? In other words, are they independent of the impurity concentration up to the percolation threshold, or does there exist a line of fixed points which determines a continuous variation of the critical exponents with the concentration?

Of particular interest in the critical behavior of disordered systems is the region of high impurity concentrations, close to the percolation threshold. It has been suggested in several papers[13–15] that the standard form of the dynamic scaling, (1), with $f(x)=zx$ and with a universal dynamic exponent z, is disrupted at the percolation level of the spin concentration. It has been suggested that there is a singular dynamic scaling behavior in (1) with $f(x)=Ax^2+Bx+C$ at $p=p_c$. In this case one can introduce a temperature-dependent effective dynamic exponent $z(\tau \sim \xi^z)$ of the following form:

$$z=A \cdot \ln \xi_T + B, \tag{3}$$

with $z \to \infty$ as $\xi_T \to \infty$ $(T \to 0,\ p=p_c)$. This form of the exponent z makes it possible to explain the anomalously large value of this exponent which has emerged from neutron-scattering measurements[16] in $Rb_2(Mg_{0.41}Co_{0.59})F_4$. Several numerical simulations of the critical dynamics of disordered systems at $p=p_c$ and near the percolation threshold[17–20] have confirmed a quadratic form for the scaling function $f(x)$ for the logarithm of the relaxation time.

In this letter we are reporting a numerical simulation by the Monte Carlo method of the critical dynamics of the 2D Ising model in the homogeneous case and also in the cases with spin concentrations $p=0.95$, 0.9, 0.85, 0.8, 0.75, and 0.7. This is the first study of the critical dynamics of disordered systems over such a broad range of impurity concentrations. It thus becomes possible to determine just how "universal" the dynamic exponent of the 2D Ising model is in the concentration region in which dynamic effects of the anomalous percolation behavior arise.

The disordered Ising model was specified as a system of spins $S_i = \pm 1$ with a concentration p which are associated with $N = pL^2$ ($L = 400$) sites of a square lattice. As a result, we have $p \cdot 2^N$ possible configurations $\{S\}$ with an energy

$$E = -J \sum_{i,j} p_i p_j S_i S_j, \tag{4}$$

where the summation is over all the nearest pairs of spins, J is a measure of the interaction energy of the spins, and p_i are random variables described by the distribution function

$$P(p_i) = p\,\delta(p_i - 1) + (1-p)\,\delta(p_i). \tag{5}$$

These random variables characterize the frozen nonmagnetic impurity atoms (or vacancies) which are distributed among lattice sites. We consider a ferromagnetic system with $J > 0$. We use the Metropolis algorithm, which consists of the random choice of a spin S_i and a flip of this spin with a probability

$$W(S \to S') = \begin{cases} \exp(-\Delta E_{SS'}/kT), & \Delta E_{SS'} > 0, \\ 1, & \Delta E_{SS'} \leqslant 0, \end{cases} \tag{6}$$

where $W(S,S')$ is the probability for the transition of the system from a microscopic state with a spin configuration $\{S\}$ to a state with a configuration $\{S'\}$. This algorithm makes it possible to realize the dynamics of an Ising model with a magnetization relaxation

$$m_s(t) = \sum_i^N S_i/N$$

to the equilibrium value determined by the temperature of the heat reservoir, T. One can coordinate the time scale t with the scale of $\{S\}$ sequential configurations under the assumption that N random choices of sites of the system are carried out in a unit time. This time unit corresponds to the Monte Carlo step in terms of the spin. In the simulation of the critical dynamics, the initial state of the system is chosen with all spins parallel ($m_s = 1$) and with the temperature of the system equal to the critical value. The critical temperature T_c for disordered systems is a function of the impurity concentration, decreasing with increasing value of this concentration and vanishing at the threshold concentration $c_{\text{imp}} = 1 - p_c$. For a square lattice of Ising spins we would have $p_c \simeq 0.59$, and $T_c(p)$ would have the following values:[21] $T_c(1.0) \simeq 2.2692$, $T_c(0.95) \simeq 2.0883$, $T_c(0.9) \simeq 1.9004$, $T_c(0.85) \simeq 1.7071$, $T_c(0.8) \simeq 1.5079$, $T_c(0.75) \simeq 1.2921$, and $T_c(0.7) \simeq 1.0751$, in units of J/k. To determine the dynamic exponent z in the present study we used the Monte Carlo method along with the dynamic renormalization-group method.[22] For this purpose we carried out a block partitioning of the system, in which a block b^d of neighboring spins was replaced by a single spin with direction determined by the direction of the majority of the spins in the block. The redefined system of spins forms a new lattice with a magnetization m_b. If, in the course of the relaxation, the magnetization of the original lattice reaches a certain value m_1 over a time t_1, and if the

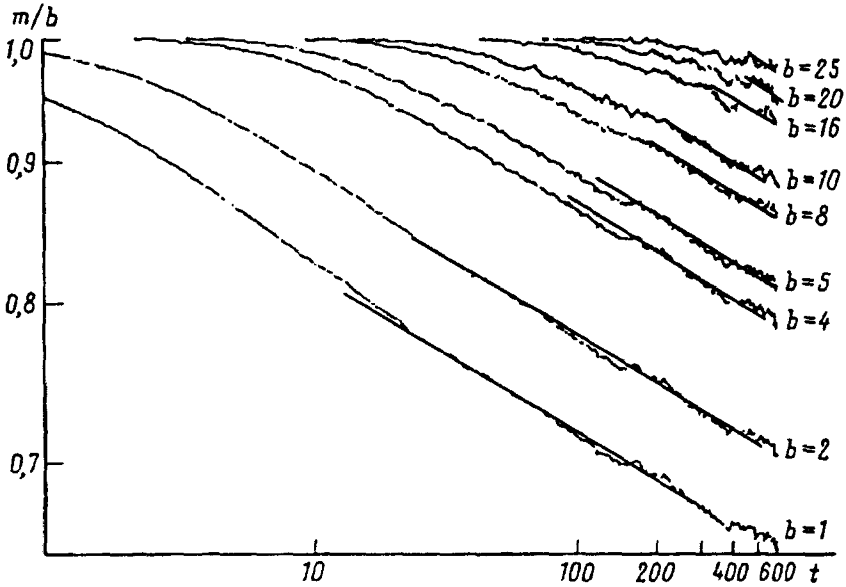

FIG. 1. Time evolution of the initial (m_1) and renormalized (m_b) magnetizations for the homogeneous Ising model (the unit of time corresponds to the Monte Carlo step in terms of the spin). The dark line segments show the intervals Δm_b corresponding to a power-law behavior of the critical relaxation, $m_b(t)$ (Ref. 23). The points of these intervals were used along with (7) to determine mean values of z_b for various values of b with $b'=1$.

redefined system reaches the same value (m_1) over a time t_b, then the use of the two systems after a block partitioning with block dimensions b and b' and a determination of the time intervals t_b and $t_{b'}$, over which their magnetizations m_b and $m_{b'}$ reach the same value m_1, allow us to determine the dynamic exponent z from the relation

$$t_b/t_{b'}=(b/b')^z \quad \text{or} \quad z=\ln(t_b/t_{b'})/\ln(b/b') \tag{7}$$

in the limit of large b and $b'\to\infty$. We have applied this algorithm to homogeneous and impure systems with dimensions of 400^2 and with the spin concentrations specified above. For systems with $p\geqslant 0.9$ we carried out a procedure of simulating the relaxation from 1000 Monte Carlo steps in terms of the spin with 10–15 passes with various impurity configurations. The functional dependence $m_b(t)$ was averaged over these configurations. For the systems with $p=0.85$, 0.8, 0.75, and 0.7 the procedure for simulating the relaxation consisted of respectively 2000, 4000, 8000, and 16 000 Monte Carlo steps per spin with 30 passes with various impurity configurations. The reason for this circumstance is that, as the percolation threshold is approached, the fluctuations in the distribution of impurities over the lattice grow, and this growth requires an increase in the number of impurity configurations for the averaging of $m_b(t)$. The size of the system was consistent with a partitioning into blocks with dimensions $b=2$, 4, 5, 8, 10, 16, 20, 25, and 40. As an example, Fig. 1 shows curves of the behavior of the original and renormalized magnetizations $m_b(t)$ versus the time for a homogeneous system. We used Eqs.

TABLE I. Values of the dynamic exponent z_b found from (7), along with extrapolated values $z_{b=\infty}$ for a system with dimensions of 400^2 with various spin concentrations p.

	p						
b	1.0	0.95	0.9	0.85	0.8	0.75	0.7
4	2.456 ±0.068						
5	2.454 ±0.061	2.439 ±0.053					
8	2.401 ±0.047	2.394 ±0.048	2.433 ±0.042				
10	2.357 ±0.036	2.366 ±0.034	2.417 ±0.034	2.473 ±0.040			
16	2.305 ±0.046	2.334 ±0.026	2.389 ±0.041	2.469 ±0.028	2.565 ±0.048	2.805 ±0.051	
20	2.285 ±0.031	2.291 ±0.032	2.332 ±0.031	2.461 ±0.016	2.557 ±0.042	2.803 ±0.056	2.954 ±0.057
25	2.242 ±0.029	2.252 ±0.023	2.269 ±0.032	2.385 ±0.029	2.547 ±0.035	2.788 ±0.054	2.942 ±0.048
40					2.532 ±0.036	2.703 ±0.035	2.912 ±0.053
$z_{b=\infty}$	2.24 ±0.07	2.24 ±0.06	2.24 ±0.06	2.38 ±0.05	2.51 ±0.06	2.66 ±0.07	2.88 ±0.06

(7) to select values of the exponents z_b corresponding to various values of b (Table I). The trend found in the b dependence of z made it possible to carry out an extrapolation to the case $b \to \infty$ under the assumption of a dependence $z_b = z_{b=\infty} + \text{const}\, b^{-1}$. The reader interested in the details of the procedure for simulating the critical dynamics of disordered systems and for determining the exponent z is referred to Ref. 23. As a result, we found the following values of $z(p)$: $z(1) = 2.24 \pm 0.07$, $z(0.95) = 2.24 \pm 0.06$, $z(0.9) = 2.24 \pm 0.06$, $z(0.85) = 2.38 \pm 0.05$, $z(0.8) = 2.51 \pm 0.06$, $z(0.75) = 2.66 \pm 0.07$, and $z(0.7) = 2.88 \pm 0.06$. The relatively large errors in $z(1)$ and $z(0.95)$ are consequences of the broader sets of z_b used to find the extrapolated exponent $z_{b=\infty}$. The increases in the error for $z(p)$ with $p \leqslant 0.8$ are due to an increase in the fluctuations in the distribution of impurities and a resulting increase in the number of impurity configurations involved in the averaging.

Analysis of the values found for the exponent $z(p)$ shows that at concentrations $p \geqslant 0.9$ the critical dynamics of the disordered 2D Ising model belongs to the same universality class as the critical dynamics of a homogeneous model with an exponent $z = 2.24 \pm 0.07$. The value found for the exponent agrees well with the results of a field-theory analysis[9] with $z = 2.277$ and with the results of several other studies of the dynamics of a homogeneous 2D Ising model: $z = 2.22 \pm 0.13$ (Ref. 24), 2.23 (Ref. 25), 2.22 (Ref. 15), and 2.24 ± 0.04 (Ref. 26). On the other hand, there are some different results: $z = 2.125 \pm 0.010$ (Ref. 27), 2.14 ± 0.02 (Ref. 28), and 2.13 ± 0.03 (Ref. 29).

For systems with spin concentrations $p \leq 0.85$ we found that the dynamic exponent z increases with decreasing p. These changes in $z(p)$ can be interpreted as resulting from crossover effects of the percolation behavior. We found that the p dependence of z for $p=0.7$, 0.75, 0.8, and 0.85 can be described well by the logarithmic function

$$z = A'|\ln(p-p_c)| + B' \tag{8}$$

with $A'=0.56\pm0.07$ and $B'=1.62\pm0.07$. The behavior in (8) can be compared with the anomalous scaling in (3) for an effective dynamic exponent z with $\xi_T \simeq \xi_p = \xi_0(p-p_c)^{-\nu_p}$ and $A' = A\nu_p$ and $B' = B + A\ln\xi_0$, where ν_p is the exponent of the percolation correlation length ξ_p. The equality $\xi_T \simeq \xi_p$ corresponds to the conditions of the numerical simulation at $T=T_c(p)$ and at p values close to p_c, since the use of several known relations for the Ising model led to $\xi_T/\xi_p \simeq \exp[2J\nu_T(T-T_c)/kTT_c]$ as $p \to p_c$ and $T \to T_c(p)$. Comparison with the results of a Monte Carlo study[18] of the temperature dependence of the relaxation time τ with $p=p_c$ ($A=0.62\pm0.12$) and with the results of a study[19] of the concentration (p) dependence of this time at $p<p_c$ ($A=0.48$) shows that the value $A=0.42\pm0.07$ which we found for $\nu_p=4/3$ agrees well with the results of Ref. 19.

In summary, we have found confirmation of a singular dynamic scaling near the percolation threshold, whose effects begin to be seen at spin concentrations $p \leq 0.85$ in the case of the 2D Ising model. This phenomenon reflects a general property of the dynamic behavior of impure systems in the long-wave limit. This dynamic behavior differs from the static behavior in that the local conservation laws in the scattering of spin fluctuations by impurities are different. As a result, the presence of impurities has a stronger effect in the critical dynamics than in a description of the equilibrium properties at the critical point.

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