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Critical dynamics of disordered two-dimensional Ising systems: a Monte Carlo study

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Abstract. The critical relaxation of the magnetization in a two-dimensional Ising model with quenched random non-magnetic impurities has been studied by numerical simulation. A squared lattice of size 400^2 with spin concentrations $p = 1.0$; 0.95, 0.9, 0.85, 0.8, 0.75 and 0.7 was considered. The dynamical critical exponent z was determined by the Monte Carlo method combined with the dynamical renormalization group method. The following values were received for $z(p)$: $z(1) = 2.24 \pm 0.07$, $z(0.95) = 2.24 \pm 0.06$, $z(0.9) = 2.24 \pm 0.06$, $z(0.85) = 2.38 \pm 0.05$, $z(0.8) = 2.51 \bullet 0.06$, $z(0.75) = 2.66 \pm 0.07$ and $z(0.7) = 2.88 \pm 0.06$. A singular dynamic scaling behaviour with $z = A'|\ln(p - p_c)| + B'$ was found for systems with spin concentrations $p \leqslant 0.85$ near the percolation threshold p_c, where $A' = 0.56 \pm 0.07$ and $B' = 1.62 \pm 0.07$ are temperature-independent constants.

1. Introduction

The dynamic scaling hypothesis states [1] that as the temperature T of a system approaches the critical temperature T_c the relaxation time τ and the corresponding thermal correlation length ξ_T are related through the generalized dynamical scaling relation

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

where $f(x)$ is a generalized homogeneous function of its argument x. In most of the critical phenomena studied so far τ follows the relation (1) with $f(x) \equiv zx$, where the temperature-independent constant z is called the dynamic exponent. As a result as $T \to T_c$ the system is characterized by a 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 for the correlation length. The numerical value of z depends not only on the space dimensionality d of the system and on the symmetry of the order parameter but also on its dynamics. The dynamic universality class to which a system belongs depends crucially on the conservation laws of the order parameter and other slow modes [1]. Non-dissipative couplings between the order parameter and slow modes can determine the critical dynamics of such a system and, consequently, the numerical value of z. In this paper we are concerned with the nature of dynamic universality in a particular critical phenomenon in a class of random magnetic systems.

Investigations [2] have shown that quenched random impurities change the properties of magnetic systems, in which the heat capacity in the 'pure' state diverges at the critical point with exponent $\alpha_{pure} > 0$. Only systems with an effective Hamiltonian which is isomorphic to

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the Ising model near the critical point satisfy this criterion. Renormalization group analysis using the ε-expansion [3, 4] has revealed that the critical behaviour of the disordered Ising model is characterized by a new set of critical exponents, with values which do not depend on the concentration of point impurities in the region $c_{\text{imp}} \ll 1 - p_c$, where p_c is the spin-percolation threshold. The equilibrium critical behaviour of dilute magnetic materials was analysed in [5, 6], and the dynamic critical behaviour was analysed in the work of one of us [7], directly for three-dimensional systems. The experiment in [8] confirms the fact that the static critical exponents for impurity systems are different from their values for pure magnets and the experimental results agree well with theoretical predictions.

Of particular interest to researchers are dilute low-dimensional magnetic materials which can be described by the two-dimensional Ising model. Since the exponent for the specific heat in the pure model is zero, the effect of disorder caused by an impurity becomes a secondary factor. A detailed inspection of this case [9, 10] has led to the conclusion that the impurity affects only the behaviour of the specific heat and that the other thermodynamic and correlation functions undergo no change in critical behaviour. A field-theoretical consideration [7] showed that the critical relaxational dynamics of dilute two-dimensional Ising-like magnets in the region of impurity concentrations $c_{\text{imp}} \ll 1 - p_c$ is the same as the dynamics of the pure model and is characterized by the exponent $z = 2.277$. However, the question which remains unanswered is whether the critical exponents of disordered systems are universal, i.e. independent of impurity concentration up to the percolation threshold, or whether there exists a line of fixed points that determines a continuous change in the critical exponents with concentration.

The critical behaviour of disordered systems in the region of high-impurity concentrations approaching the percolation threshold is particularly noteworthy. It has been suggested in several works [11–13] that the standard form of dynamical scaling relation (1) with $f(x) \equiv zx$ and universal exponent z is violated when there is an impurity concentration in the percolation region. It has been suggested that a singular dynamic behaviour is realized for a percolation concentration of impurities with a scaling relation of the form (1) with $f(x) = Ax^2 + Bx + C$. Then a temperature-dependent effective dynamic exponent z can be introduced:

$$\tau \sim \xi_T^z \qquad z = A \ln \xi_T + B \tag{3}$$

with $z \to \infty$ as $\xi_T \to \infty$ ($T \to 0, p = p_c$). This form of the exponent z leads to an explanation for the anomalously large value which has been measured for this exponent in $Rb_2(Mg_{0.41}Co_{0.59})F_4$ during neutron scattering [14]. At the present time there is evidence from Monte Carlo simulations [15–18] supporting the quadratic form of the scaling function $f(x)$ instead of the linear form.

In this work we report on a numerical simulation by the Monte Carlo method of the critical dynamics of the two-dimensional Ising model, both in the 'pure' case and for spin concentrations $p = 0.95$, 0.9, 0.85, 0.8, 0.75 and 0.7. This investigation of the critical dynamics of disordered systems for a wide range of impurity concentrations might possibly provide an answer to the question about the range of impurity concentrations where the dynamic exponent z is universal and where the dynamic effects of the singular percolation behaviour begin to develop.

2. The model and Monte Carlo simulation

The disordered Ising model is specified by a system of spins $S_i = \pm 1$ with concentration p, which are associated with $N = pL^2$ ($L = 400$) sites of a squared lattice. This gives

$p2^N$ possible configurations $\{S\}$ with energy

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

where the sum runs over nearest neighbours only, J characterizes the spin interaction energy and the p_i are quenched site disorder variables with probability distribution

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

We consider a ferromagnetic system with $J > 0$. Ising model dynamics is customarily described by the conditional probability function $P_S \equiv P(\{S\}, t)$, which satisfies Glauber's kinetic equation

$$\frac{\mathrm{d}P_S}{\mathrm{d}t} = -P_S(t) \sum_{S'} W(S \to S') + \sum W(S' \to S) P_{S'}(t) \tag{6}$$

where $W(S \to S')$ is the probability of a transition of the system from a microscopic state given by the spin configuration $\{S\}$ to a state with the configuration $\{S'\}$. In order for the Markov process described by equation (6) to converge to the equilibrium state of a Gibbs ensemble with $P_S = \exp(-E_S/kT)$, the detailed balancing condition must be satisfied: $W(S \to S')P_S = W(S' \to S)P_{S'}$. This relation does not determine the function W unambiguously. The function W is usually chosen in the form of Metropolis's function

$$W(S \to S') = \begin{cases} \exp(-\Delta E_{SS'}/kT) & \text{for } \Delta E_{SS'} > 0 \\ 1 & \text{for } \Delta E_{SS'} \leqslant 0 \end{cases} \tag{7}$$

or Glauber's function

$$W(S \to S') = \exp(-\Delta E_{SS'}/kT)/[1 + \exp(-\Delta E_{SS'}/kT)]. \tag{8}$$

The relation $\langle A(t) \rangle = \sum_S A_S P_S(t)$ determines the dynamical evolution of the quantity A_S by means of the function $P_S(t)$—the solution of equation (6).

The use of the Metropolis algorithm, which consist of a random choice for the spin S_i and its flip with a probability specified by the function W in (7), makes it possible to immediately realize the dynamics of the Ising model with a relaxation of the magnetization $m_S(t) = \sum_i^N S_i/N$ to the equilibrium value determined by the thermostat temperature T. The time scale t can be associated with the scale $\{S\}$ of successive configurations by assuming that N system sites are chosen randomly per unit time. This unit of time corresponds to the Monte Carlo spin step. In the simulation of the critical dynamics the initial state of the system is chosen with all spins parallel ($m_S = 1$) and with a temperature equal to the critical temperature. The critical temperature T_c for dilute magnetic materials is a function of the impurity concentration $c_{imp} = 1 - p$. It decreases with increasing c_{imp} and vanishes at the threshold concentration $c_{imp} = 1 - p_c$. For a squared lattice of Ising spins $p_c \simeq 0.59$ and the $T_c(p)$ are equal to: $T_c(1) \simeq 2.2692$, $T_c(0.95) \simeq 2.0883$, $T_c(0.9) \simeq 1.9004$, $T_c(0.85) \simeq 1.7071$, $T_c(0.8) \simeq 1.5079$, $T_c(0.75) \simeq 1.2921$ and $T_c(0.7) \simeq 1.0751$ in units of J/k [19].

3. The dynamical renormalization group method and its realization

We have used here the Monte Carlo method, combined with the dynamical-renormalization-group method [20], to determine the dynamic exponent z. For this, the system was partitioned into blocks, where a block b^d of neighbouring spins was replaced by a single spin with its direction determined by the direction of most spins in the block. The redefined spin system forms a new lattice with magnetization m_b. Let the magnetization of the initial lattice relax to some value m_1 over a time t_1, and let the redefined system reach the same value m_1 over the time t_b. Then by using two systems with block sizes b and b' and determining the relaxation times t_b and $t_{b'}$ of the block magnetizations m_b and $m_{b'}$ to the same value m_1, the dynamic exponent z can be determined from the relation

$$t_b/t_{b'} = (b/b')^z$$

or

$$z = \ln(t_b/t_{b'})/\ln(b/b') \tag{9}$$

in the limit of sufficiently large b and $b' \to \infty$.

We applied this algorithm to pure and impure systems with dimensions 400^2 and the impurity concentrations presented above. The size of the system made it possible to partition it into blocks with sizes $b = 2$, 4, 5, 8, 10, 16, 20, 25 and 40. The procedure for block partitioning the initial spin and impurity configurations was implemented on the basis of the criterion of spin connectivity. Thus a b^d-dimensional block was considered to be a spin block and replaced by an effective spin oriented in a direction determined by the direction of most spins in the block if the block contained a spin cluster connecting opposite faces of the block. Otherwise, the block was considered to be an impurity block and replaced by an empty site in the renormalized lattice. For systems with $p \geqslant 0.9$ a relaxation simulating procedure consisting of 1000 Monte Carlo steps per spin was performed for each system with 15–20 runs with different impurity configurations over which the function $m_b(t)$ was averaged. For systems with $p = 0.85$, 0.8, 0.75 and 0.7 the relaxational simulating procedure consisted of 2000, 4000, 8000 and 16000 Monte Carlo steps per spin, accordingly, with 30 runs for each system with different impurity configurations. Figures 1(*a*)–(*c*) show plots of the initial and renormalized magnetizations $m_b(t)$, averaged over impurity configurations, with spin concentrations $p = 1$, 0.9 and 0.75, respectively, as functions of time.

The computer modelling of the relaxation properties of a two-dimensional homogeneous Ising model, performed in [21], showed that near the critical temperature the change in the magnetization is characterized by an effective exponential dependence. Our analysis of the relaxation curves $m_1(t)$ at the critical temperature $T_c(p)$ revealed a power-law dependence $m_1(t) \sim t^{-a}$. The following values were obtained for the exponent $a(p)$ with m_1 ranging from 0.8 to 0.67: $a(1) = a(0.95) = 0.056 \pm 0.006$; $a(0.9) = 0.055 \pm 0.006$; $a(0.85) = 0.050 \pm 0.008$; $a(0.8) = 0.043 \pm 0.008$; $a(0.75) = 0.037 \pm 0.008$; $a(0.7) = 0.031 \pm 0.010$. The well-known scaling relation for the magnetization

$$m(h, \theta) = \theta^\beta \tilde{m}(h/\theta^\Delta) \tag{10}$$

where $\theta = (T_c - T)/T_c$ is the reduced temperature, h is the external magnetic field, and β and Δ are the critical exponents, can be generalized for the time-dependent case in the form

$$m(h, \theta, t) = \theta^\beta M(h/\theta^\Delta, t/\tau) = \theta^\beta M(h/\theta^\Delta, t/\theta^{-z\nu}) = t^{-\beta/z\nu}\tilde{M}(ht^{\Delta/z\nu}, \theta t^{1/z\nu}) \tag{11}$$

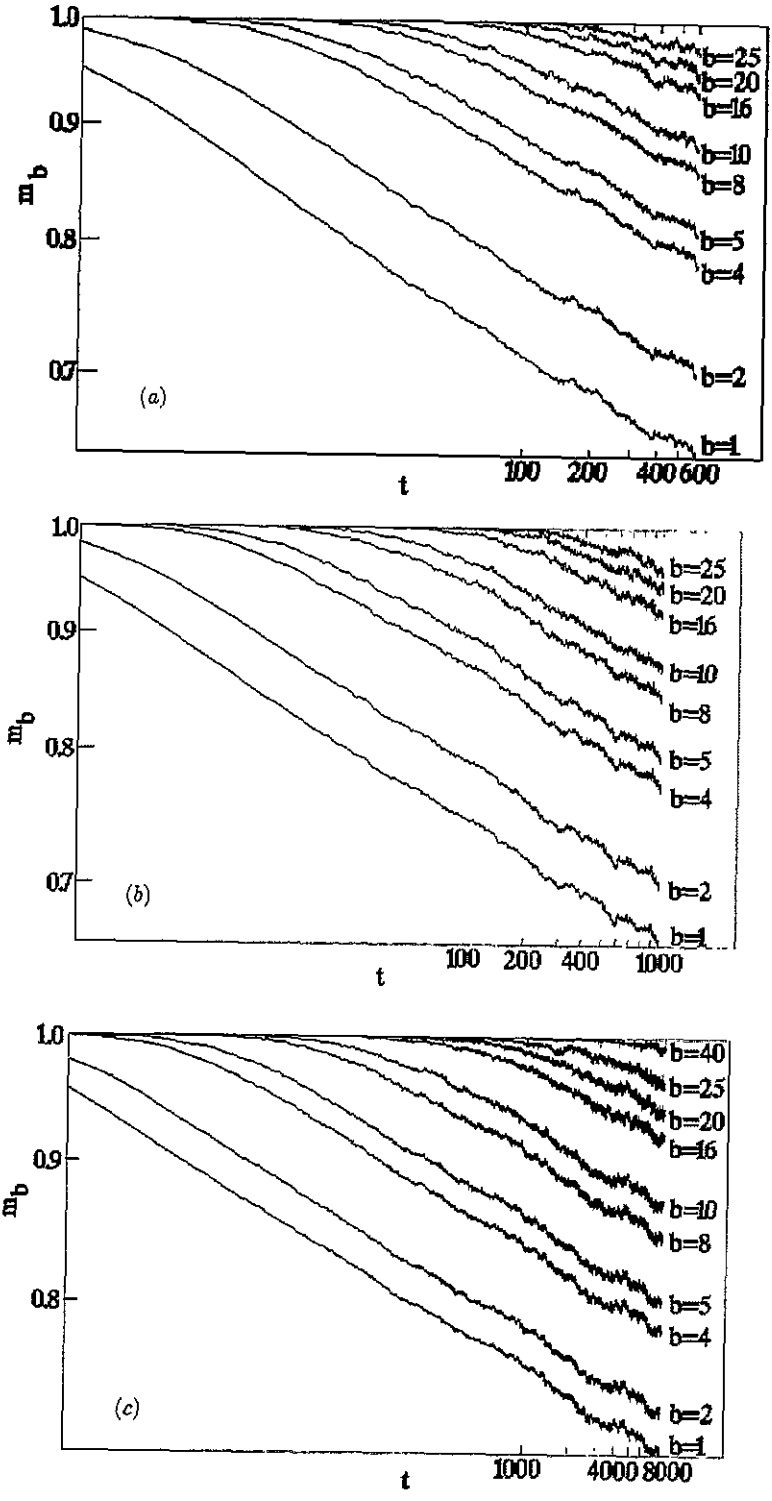

Figure 1. Initial m_1 and renormalized m_b magnetizations as functions of time for the pure Ising model (*a*) and for a disordered Ising model with spin concentrations $p = 0.9$ (*b*) and 0.75 (*c*).

using the asymptotic time dependence of the relaxation $\tau \sim |\theta|^{-z\nu}$. Hence, for $h = 0$ and $\theta = 0$, the power-law character of the relaxation is reflected in the form of the following equation

$$m(t) \sim t^{-\beta/z\nu}. \tag{12}$$

According to Monte Carlo simulation results [19] for the disordered two-dimensional Ising model $\beta/\nu = 0.125 \pm 0.005$ ($p = 1.0, 0.95, 0.9$); 0.120 ± 0.010 ($p = 0.85$); 0.110 ± 0.010 ($p = 0.8$); 0.100 ± 0.020 ($p = 0.75$). We used these values of β/ν and exponents $a(p) = \beta/z\nu$ and determined the next values of the dynamic exponent $z(p)$: $z = 2.23 \pm 0.33$ ($p = 1.0$; 0.95); 2.27 ± 0.34 ($p = 0.9$); 2.40 ± 0.58 ($p = 0.85$); 2.56 ± 0.72 ($p = 0.8$); 2.70 ± 1.13 ($p = 0.75$). Although the typical errors for a Monte Carlo study of disordered systems were made, when determining the exponents $a(p)$ the small mean values of $a(p)$ led to a low accuracy in their relative values and therefore to low accuracy in values of the exponent z.

In order to determine the values of the exponent z independently it is better to employ relation (9). However, the power-law character found for the relaxation of the magnetization at the critical temperature enabled us to employ, in contrast to [20, 21], a different and, we believe, better-founded procedure for processing the curves for the renormalized magnetizations $m_b(t)$ [22]. Thus the $m_b(t)$ curves plotted in a double logarithmic scale were approximated by the straight lines $\ln m_b = k_b \ln t + n_b$ by the least-squares method in intervals Δm_b corresponding best to a power-law variation of m_b. Next, the coefficients k_b were averaged and an average value k_{av} was determined, after which the parameters n_b of the straight lines $\ln m_b = k_{av} \ln t + n_b$ were determined by extending the lines through the point of intersection with $\ln m_b = k_b \ln t + n_b$ at the centre of the intervals Δm_b. As a result, the formula for z becomes

$$z = (n_{b'} - n_b)/[k_{av} \ln(b/b')]. \tag{13}$$

Sets of values of the exponent z_b corresponding to different values of b with $b' = 1$ were obtained using relation (13) (table 1). For impurity systems the renormalization-group-transformation procedure reaches the proven asymptote of m_b as a function of the block-partition parameter b at larger values of b than in the case of a pure system. For this reason we selected for the analysis the values of the exponent z_b corresponding to $b \geqslant 4$ for the pure system and $b \geqslant 5$ ($p = 0.95$), $b \geqslant 8$ ($p = 0.9$), $b \geqslant 10$ ($p = 0.85$), $b \geqslant 16$ ($p = 0.8$; 0.75) and $b \geqslant 20$ ($p = 0.7$) for the impurity systems. The obtained dependence of z on b made extrapolation to the case $b \to \infty$ possible, assuming that $z_b = z_{b=\infty} + \text{constant} \times b^{-1}$. The following results were obtained: for the homogeneous system $z(1) = 2.24 \pm 0.07$ and for the impurity systems $z(0.95) = 2.24 \pm 0.06$, $z(0.9) = 2.24 \pm 0.06$, $z(0.85) = 2.38 \pm 0.05$, $z(0.8) = 2.51 \pm 0.06$, $z(0.75) = 2.66 \pm 0.07$, and $z(0.7) = 2.88 \pm 0.06$. The lower accuracy in the values of the exponents $z(1)$ and $z(0.95)$ is conditioned by the wider set of z_b, which we used for calculating the extrapolated values $z_{b=\infty}$. However, the increase in errors for $z(p)$ with $p \leqslant 0.8$ is connected to the increase in disorder in systems and a resulting increase in the number of impurity configurations involved in the averaging. Comparing the two sets of dynamic exponents calculated by different methods shows that they are in sufficiently good agreement with each other. However, the Monte Carlo method combined with the dynamical-renormalization-group method is preferable as it is characterized by a higher accuracy in the received values of the dynamic exponent z and independence of the static critical exponents β and ν.

Table 1. Values of the dynamic exponent z_b obtained using formula (9) and the extrapolated values $z_{b=\infty}$ for systems with different 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

4. Analysis of results and conclusions

An analysis of the obtained values $z(p)$ shows that the critical dynamics of a disordered two-dimensional Ising model with spin concentrations $p \geqslant 0.9$ and pure model are concerned with one class of dynamic universality characterized by the exponent $z = 2.24 \pm 0.07$. We note that this value agrees well with value $z = 2.277$ obtained by the field-theoretical method [7] and with results on critical dynamics of the pure two-dimensional Ising model of several other works: $z = 2.22 \pm 0.13$ [23], $\simeq 2.23$ [24], 2.22 [13], 2.24 ± 0.04 [25]. However, there are also other results with $z = 2.125 \pm 0.010$ [26], 2.14 ± 0.02 [21], 2.13 ± 0.03 [27].

For systems with spin concentrations $p \leqslant 0.85$ an increase in the values of the dynamic exponent z with decrease in p was discovered. These changes in $z(p)$ can be interpreted as the result of the crossover from pure and weak-disorder-type behaviour to percolation-type critical behaviour. It was found that the dependence of the dynamic exponent z on p for $p = 0.7$, 0.75, 0.8 and 0.85 is described well by a logarithm law

$$z = A' |\ln(p - p_c)| + B' \tag{14}$$

with $A' = 0.56 \pm 0.07$ and $B' = 1.62 \pm 0.07$ (figure 2). The received dependence (14) can be compared with singular scaling dependence (3) for the effective dynamic exponent z at $\xi_T \simeq \xi_p = \xi_0(p - p_c)^{-\nu_p}$ and $A' = A\nu_p$, $B' = B + A \ln \xi_0$, where ν_p is the critical exponent for percolation correlation length ξ_p. The use of known relations for the Ising model gives $\xi_T/\xi_p \simeq \exp[2J\nu_T(T - T_c)/kTT_c]$ as $p \to p_c$ and $T \to T_c(p)$, therefore the equality $\xi_T \simeq \xi_p$ corresponds to the conditions of our computer simulations at $T = T_c(p)$ and p near p_c. A comparison with the results from Monte Carlo simulations of the temperature dependence of the relaxation time τ at $p = p_c$ ($A = 0.62 \pm 0.12$) [16] and the spin concentration dependence of τ at $p < p_c$ ($A = 0.48$) [17] shows that the calculated numerical value of $A = A'/\nu_p = 0.42 \pm 0.07$ at $\nu_p = 4/3$ agrees well with the results in [17].

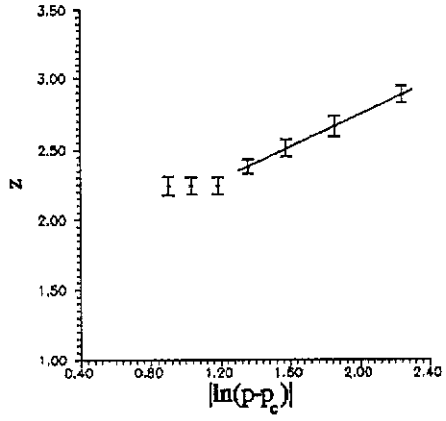

Figure 2. The dynamic critical exponent z plotted against $|\ln(p - p_c)|$. The straight line is the best quadratic fit for $z(p)$ with the expression $A'|\ln(p - p_c)| + B'$.

Thus, in the present paper the singular dynamic scaling behaviour for disordered systems near the percolation threshold was confirmed. It was shown that the percolation behaviour effects begin to be displayed in the dynamics of the two-dimensional Ising model at spin concentrations $p \leqslant 0.85$. In this phenomenon a common property of the disordered system dynamics is exhibited. In contrast to the static behaviour the disordered system dynamics characterized by other local conservation laws for impurity scattering of long-wavelength fluctations of the magnetization. In consequence, the impurities affect the critical dynamics more strongly than the static critical behaviour.

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