Numerical simulation of the critical dynamics of dilute magnetic materials

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The critical relaxation of the magnetization in a 3D Ising model with nonmagnetic impurity atoms frozen at lattice sites has been studied by numerical simulation. A system with dimensions of 48^3 with impurity concentrations $p = 0.05, 0.2, 0.4$, and 0.6 was studied. The Monte Carlo method was combined with the dynamic renormalization-group method to determine the dynamic critical exponent z. The following values were found for $z(p)$: $z(0.05) = 2.19 \pm 0.07$, $z(0.2) = 2.20 \pm 0.08$, $z(0.4) = 2.58 \pm 0.09$, and $z(0.6) = 2.65 \pm 0.12$. A power-law universality is suggested for the critical exponents of dilute 3D magnetic materials.

Over the past two decades, many researchers have devoted effort to reaching an understanding of how impurities and other structural defects affect the behavior of various systems in the course of phase transitions. Of particular interest is the effect of frozen impurities, whose presence is manifested as a perturbation of the local temperature and which is of a random nature. Studies have shown[1] that frozen impurities alter

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the properties of magnetic materials whose specific heat in the homogeneous state has a divergence at a critical point with an exponent $\alpha > 0$. This condition is satisfied only by systems whose effective Hamiltonian is isomorphic with respect to the Ising model near the critical point.

A renormalization-group analysis using an ϵ expansion[2,3] has revealed that the critical behavior of impure systems is characterized by a new set of critical exponents, whose values are independent of the concentration of point impurities, p, at $p \ll p_c$, where p_c is the threshold for spin percolation. The asymptotic convergence of the ϵ-expansion series for dilute magnetic materials is even weaker than that for homogeneous materials, however. The equilibrium critical behavior of dilute magnetic materials was analyzed in Refs. 4 and 5, and the dynamic critical behavior was analyzed in Ref. 6, directly for 3D systems. The experiment of Ref. 7 confirms that there is a numerical difference between the static critical exponents for impure systems and the values for homogeneous magnetic materials. That experiment yielded results which agreed well with theoretical predictions. No experimental research has been carried out on the critical dynamics of dilute magnetic materials. Another question which remains unanswered is whether the critical exponents of impure systems are universal, i.e., independent of the impurity concentration up to the percolation threshold, or whether there instead exists a line of fixed points which determines a continuous change in the critical exponents with the concentration.

Numerical simulation of critical phenomena has now emerged as an alternative to a real physical experiment. Experimental studies,[8,9] which were carried out to simulate a dilute Ising model, have shown that the effective critical exponent β for the magnetization varies continuously with the impurity concentration. In Ref. 10, on the other hand, confirmation was found for the concept of a universality of critical exponents, within the errors in certain values of the susceptibility exponent γ and the correlation-length exponent ν, for impurity concentration $p = 0.2$, 0.4, and 0.6.

In this letter we are reporting a numerical simulation by the Monte Carlo method of the critical dynamics of the 3D Ising model, both in the homogeneous case and for impurity concentrations $p = 0.05$, 0.2, 0.4, and 0.6. There is reason to believe that the influence of frozen impurities on the critical dynamics will be seen more clearly than the influence on equilibrium properties, because of the specific conservation laws. The Ising model is specified by a system of spins S_i which are associated with $N = L^d$ sites of a d-dimensional lattice (L is a length scale of the lattice). The spin can take on the values $S_i = \pm 1$. There are accordingly 2^N possible configurations $\{S\}$, with an energy

$$E = -J \sum_{i,j} S_i S_j - h \sum_i S_i. \tag{1}$$

The first sum is over all the nearest spin pairs: J represents their interaction energy, and h is the external field associated with the spins. We consider a ferromagnetic system with $J > 0$. It is customary to describe the dynamics of the Ising model by means of a conditional-probability function $P_s(t) \equiv P(\{S\},t)$, for which a Glauber kinetic equation is given:

$$\frac{dP_s}{dt} = -P_s(t)\sum_{s'} W(S \to S') + \sum_{s'} W(S' \to S)P_{s'}(t). \tag{2}$$

Here $W(S \to S')$ determines the probability for a transition of the system from the microscopic state specified by the spin configuration $\{S\}$ to the state with the configuration $\{S'\}$. If the Markovian process described by Eq. (2) is to have the property of convergence on an equilibrium state of a Gibbs ensemble with $P_s = \exp(-E_s/kT)$, we must impose the condition of detailed balance: $W(S \to S')P_s = W(S' \to S)P_s$. This relation does not determine the function W unambiguously. It is customary to choose W in the form of a Metropolis function,

$$W(S \to S') = \begin{cases} \exp(-\Delta E_{ss'}/kT), & \Delta E_{ss'} > 0, \\ 1, & \Delta E_{ss'} \leq 0, \end{cases} \tag{3}$$

or a Glauber function,

$$W(S \to S') = \exp(-\Delta E_{ss'}/kT)/[1 + \exp(-\Delta E_{ss'}/kT)]. \tag{4}$$

The relation $\langle A(t)\rangle = \Sigma A_s P_s(t)$ specifies the dynamic evolution of the quantity A_s through the $P_s(t)$ dependence, i.e., the solution of Eq. (2).

The use of the Metropolis algorithm, which consists of a random choice of the spin S_i and its flip with a probability specified by the function W in (3), makes it possible to immediately realize the dynamics of the Ising model with a relaxation of the magnetization $m_s(t) = \Sigma_i^N S_i/N$ to the equilibrium value determined by the reservoir temperature T. The scale of the time t can be coordinated with the scale of $\{S\}$ of successive configurations by assuming that N random samplings of the sites of the system are carried out per unit time. This unit of time corresponds to the Monte Carlo spin step. In the simulation of the critical dynamics, we choose an initial state of the system with all the spins parallel ($m_s = 1$) and with a temperature equal to the critical temperature. For dilute magnetic materials, the critical temperature T_c is a function of the impurity concentration p. It decreases with increasing p and vanishes at the threshold concentration p_c. For a cubic lattice of Ising spins we would have $p_c \simeq 0.69$ and $T_c(0) \simeq 4.5108$, $T_c(0.05) \simeq 4.2571$, $T_c(0.2) \simeq 3.4959$, $T_c(0.4) \simeq 2.4178$, and $T_c(0.6) \simeq 1.2066$ (Ref. 10), in units of J/k. To determine the dynamic exponent z, which characterizes the critical slowing of the relaxation time of the system, $t_c \sim |T - T_c|^{-z\nu}$, we use the Monte Carlo method combined with the dynamic renormalization-group method.[11] For this purpose we go through a procedure of a block partitioning of the system. A block b^d of neighboring spins is replaced by one spin, with the direction determined by the direction of the majority of the spins in the block. This redefined system of spins forms a new lattice, with a magnetization m_b. We assume that the magnetization of the original lattice reaches some value m_1 over a time t_1 in the course of the relaxation, while the redefined system reaches the same value, m_1, over a time t_b. The use of two systems, after block partitionings with block sizes 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, then makes it possible to determine the dynamic exponent z, from

$$t_b/t_{b'} = (b/b')^z \quad \text{or} \quad z = \ln(t_b/t_{b'})/\ln(b/b') \tag{5}$$

in the limit of large b, $b' \to \infty$. We have applied this algorithm to homogeneous and impure systems with dimensions of 48^3 and with the frozen-impurity concentrations listed above (the impurities are vacant lattice sites, distributed with a probability p). For each system we went through a procedure of simulating the relaxation from 1000 Monte Carlo spin steps, with 20–30 passes, with various impurity configurations, over which we averaged the functional dependence $m_b(t)$. At the given size of the system, it was possible to carry out partitionings into blocks with sizes $b = 2$, 3, 4, 6, 8, and 12. A block b^d was replaced by a spin if a spin percolation occurred in it; otherwise it was replaced by an impurity. Working from (5), we found sets of values of the exponent z_b corresponding to the various values of b. The trend found in the dependence of z on b made it possible to extrapolate to the case $b \to \infty$ under the assumption $z_b = z_{b=\infty} + \text{const}\, b^{-1}$. As a result, we found the following values: for the homogeneous system, $z(0) = 1.97 \pm 0.08$; for the impure systems, $z(0.05) = 2.19 \pm 0.07$, $z(0.2) = 2.20 \pm 0.08$, $z(0.4) = 2.58 \pm 0.09$, and $z(0.6) = 2.65 \pm 0.12$. We thus see that the values of the dynamic exponent are essentially the same for $p = 0.05$ and 0.2, while those for $p = 0.4$ and 0.6 are comparable within the error of their determination. Making use of the exponent z for the homogeneous system, we can (somewhat arbitrarily) classify the resulting values into three groups, which differ significantly in magnitude.

Let us compare the results of this numerical simulation with the results found by methods of the theory of critical phenomena for homogeneous and impure systems. In Ref. 6 we carried out a field-theory description of the critical dynamics of dilute magnetic materials directly for the 3D case. In the two-loop approximation, we used the Padé–Borel summation technique and found exponent values $z(p) = 2.237$, which are valid for impurity concentrations much lower than the threshold for spin percolation. A corresponding calculation for a homogeneous Ising system in the three-loop approximation yielded the values $z(0) = 2.014$. A comparison of the theoretical results with the results of the numerical simulation reveals a good agreement in the case of the homogeneous system and also in the case of the impure systems with $p = 0.05$ and 0.2. For $p = 0.4$ and 0.6, the results of the simulation reveal a substantial increase in the dynamic exponent z. We explain this result on the basis that the impurities form a binding cluster in the case of a cubic lattice of Ising spins at $p \geqslant p_c^{(\text{imp})} \simeq 0.31$. At $T \leqslant T_c$, this cluster coexists with a spin binding cluster up to the threshold of spin percolation, $p_c^{(s)} = 1 - p_c^{(\text{imp})}$. As a result, in the region $p_c^{(\text{imp})} \leqslant p \leqslant p_c^{(s)}$ the spin correlation length is not the only scale determining the behavior of the system near the critical temperature $T_c(p)$. There is also a change in the nature of the impurity scattering of long-wave fluctuations of the magnetization.

We wish to propose a hypothesis of a power-law universality of the critical exponents for dilute 3D magnetic materials (such effects do not occur for 2D materials, because of the condition $p_c^{(\text{imp})} > 0.5$). According to this hypothesis, in the dilution region $p \leqslant p_c^{(s)}$ one can observe five distinct types of critical behavior: homogeneous; impurity I, at $0 < p < p_c^{(\text{imp})}$, with effects stemming from an influence of point impurities; impurity II, at $p_c^{(\text{imp})} < p < p_c^{(s)}$, with effects stemming from the influence of an

extended impurity structure; a percolation impurity behavior at $p = p_c^{(\mathrm{imp})}$; and a percolation spin behavior at $p = p_c^{(s)}$. For impurity concentrations far from the threshold values, we would expect to see manifestations of these types of critical behavior in dilute magnetic materials at temperatures $|T - T_c(p)|/T_c(p) \leqslant (\Delta J/J_0)^{1/\varphi}$. This temperature region is determined by the value of the corresponding crossover exponent φ and by ΔJ, which is a measure of the randomness in the exchange interaction. For $|p - p_c|/p_c \ll 1$, on the other hand, we would expect these manifestations at $|T - T_c(p)|/T_c(p) \leqslant \{|p - p_c|/p_c\}^{1/\varphi}$. For Ising magnetic materials with $0 < p < p_c^{(\mathrm{imp})}$ we have $\varphi = \alpha_{\mathrm{pure}} \simeq 0.11$, so the impurity behavior with the corresponding universal exponents should be observed in a narrow temperature interval near $T_c(p)$, with crossover effects of a transition to the exponents for homogeneous systems. At $p_c^{(\mathrm{imp})} < p < p_c^{(s)}$, crossover effects can be observed near the percolation thresholds. Far from them, either the crossover is not observed, or it can be seen as a transition between exponents of two types of impurity behavior. As a sort of experimental test of this hypothesis we might look at the results of Ref. 7, in which dilute magnetic materials $Fe_{1-p}Zn_pF_2$ with $p = 0.4$ and 0.5 were studied in specifically the region $p_c^{(\mathrm{imp})} < p < p_c^{(s)}$ with $p_c^{(s)} = 1 - p_c^{(\mathrm{imp})} \simeq 0.75$. The critical exponents found in that study differed from the exponents of a homogeneous system, but no crossover effects of a transition to the exponents of a homogeneous critical behavior were found.

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