Monte Carlo Simulation of a Random-Field Ising Antiferromagnet

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Abstract

Phase transitions in the three-dimensional diluted Ising antiferromagnet in an applied magnetic field are analyzed numerically. It is found that random magnetic field in a system with spin concentration below a certain threshold induces a crossover from second-order phase transition to first-order transition to a new phase characterized by a spin-glass ground state and metastable energy states at finite temperatures.

1 Introduction

Critical behavior of disordered systems with quenched disorder has been the subject of much theoretical and experimental interest, because the presence of quenched defects in most real solids modifies their thermodynamic characteristics, including critical behavior. It is well known that quenched disorder manifests itself by temperature fluctuations in ferro- and antiferromagnetic systems in the absence of external magnetic field or by magnetic field fluctuations in antiferromagnets in uniform magnetic field.

In the former case, quenched disorder affects the properties of only those homogeneous magnetic materials whose specific heat is divergent at the critical point [1]. Otherwise, the presence of defects does not change the critical behavior of magnets. This criterion applies only when the effective Hamiltonian near the critical point is isomorphic to the Ising model Hamiltonian. Disorder-induced critical behavior of the Ising model was analyzed in numerous recent studies [2]. For dilute Ising-like systems, it was found that theoretical calculations are in good agreement with experimental results and Monte Carlo simulations.

Despite extensive theoretical and experimental studies of random-field magnets conducted over the past twenty years [3], very few facts concerning their behavior have been established. In particular, the nature of phase transition in the random-field Ising model

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remains unclear, and the currently available theoretical results in this area disagree with experiment. The only theoretically proved fact is that the upper critical dimension for this phase transition is six (i.e., critical phenomena in systems of higher dimension are described by mean field theory) [3], whereas the critical dimension is four for homogeneous systems. While it had been argued that the lower critical dimension $d_l$ can be both $d_l = 2$ [4] and $d_l = 3$ [5] (i.e., there is long-range order at finite temperatures if the system’s dimension is higher), specialists came to the conclusion that $d_l = 2$ after the publication of [6, 7]. However, the nature of phase transition in the three-dimensional random-field Ising model remains unclear. According to [8, 9], it is a first-order phase transition even at very low random-field strengths; according to [10, 11], it is a second-order transition.

The effect of random fields on the behavior of magnetic systems is described by using two qualitatively equivalent models: the ferromagnetic random-field Ising model (RFIM) [12, 13] and the Ising diluted antiferromagnets in a field (DAFF) [14]. Real random-field magnets are antiferromagnets with quenched nonmagnetic impurities. Their behavior includes manifestations of both antiferromagnetic interaction between nearest neighbor atoms and ferromagnetic interaction between next-nearest neighbor atoms. The structure of an antiferromagnet can be represented as several interpenetrating ferromagnetic sublattices such that the total magnetization of the antiferromagnet is zero even though each ferromagnetic sublattice is magnetically ordered at a temperature below the Neel temperature. Examples of two-sublattice antiferromagnets are the following materials: $NiO$, $MnO$, $Fe_2O_3$, and $MnF_2$. Examples of random-field magnets include the uniaxial Ising-like antiferromagnets $MnF_2$ and $FeF_2$ diluted with zinc atoms in an external magnetic field [15].

2 Model

In this study, a Monte Carlo method is used to simulate the thermodynamic behavior of a diluted antiferromagnetic Ising model in an applied magnetic field on the simple cubic lattice by taking into account next-nearest-neighbor interaction. The Hamiltonian of the model has the form

$$\mathcal{H} = J_1 \sum_{i,j} p_i p_j \sigma_i \sigma_j + J_2 \sum_{i,k} p_i p_k \sigma_i \sigma_k + \mu h \sum_i p_i \sigma_i,$$  \quad (1)
where $\sigma_i = \pm 1$ is the spin located at site $i$; $\mu$ is the Bohr magneton; $J_1 = 1$ and $J_2 = -1/2$ characterize antiferromagnetic nearest-neighbor and ferromagnetic next-nearest-neighbor exchange couplings, respectively; $h$ is the strength of the uniform magnetic field; and $p_i$ and $p_j$ are random variables characterized by the distribution function

$$P(p_i) = p\delta(p_i - 1) + (1 - p)\delta(p_i)$$  \hspace{1cm} (2)

which are introduced to describe quenched nonmagnetic impurity atoms vacancies distributed over the lattice and characterized by the concentration $c_{imp} = 1 - p$, where $p$ is spin concentration. For $p = 1.0$, the model with competing interactions has been studied by Monte Carlo methods for over twenty years \cite{16, 17}. The first study of effects of disorder on critical behavior based on this model was presented in \cite{18}. For the DAFF mentioned above \cite{13}, competition between ferromagnetic order parameters was not taken into account. This model provides the most realistic physical representation. Since the strength of random-field effects is determined by impurity concentration and external field strength both in the model and in real magnets, the parameters of the model can be compared to those of real physical experiments on Ising diluted antiferromagnets. However, an analogous comparison of the random field with the impurity concentration in a sample and the applied field strength is difficult to perform for the ferromagnetic random-field Ising model (RFIM), which is most widely used in numerical simulations. Therefore, random field variation in RFIM cannot be quantitatively compared with structural disorder in real systems, which is shown here to be the key factor that controls phase transitions.

An antiferromagnet is characterized by the staggered magnetization $M_{stg}$ defined as the difference of the magnetizations of the two sublattices, which plays the role of an order parameter. To determine the type of phase transition, we calculate the Binder cumulant

$$U = \frac{1}{2}(3 - \frac{\langle M_{stg}^4 \rangle}{\langle M_{stg}^2 \rangle^2}),$$  \hspace{1cm} (3)

where angle and square brackets denote statistical averaging and averaging over disorder realizations. The calculation of the cumulant is a good test for the order of phase transition: the cumulants plotted versus temperature have a distinct point of intersection in the case of second-order transition, whereas those corresponding to first-order phase transition have a characteristic shape and do not intersect.
We also examine spin-glass states. It is well known that spin glasses are characterized by transition to a phase with an infinite number of metastable states separated by potential barriers in the thermodynamic limit [20]. The complex magnetic ordering in such systems can be described in terms of the spin-glass order parameter

\[ q_s = \frac{1}{pL^3} \langle \sigma_i^\alpha \sigma_i^\beta \rangle \]  

(4)

where \( \alpha \) and \( \beta \) refer to the spin configurations corresponding to replicas of the simulated disordered system characterized by equal temperatures, but different initial disorder realizations.

To obtain correct values of thermodynamic characteristics of critical behavior, both statistical averaging and averaging over disorder realizations must be performed only after the system has thermalized. Critical behavior of disordered systems is characterized by anomalously long relaxation times, which rapidly increase with the size of the simulated system. To reach equilibrium at near-critical temperatures and determine the corresponding thermodynamic characteristics, the system was quenched with a temperature step of \( \Delta T = 0.1 \) starting from a temperature at which no metastable states had been obtained in any sweep. At each temperature step, a relaxation regime was computed in 5000 steps and averaging was performed in 10000 steps by using the spin configuration obtained at the preceding step as an initial condition. This procedure was executed to obtain a stable equilibrium at each temperature and avoid metastable states [18].

For each lattice size \( L \), thermodynamic characteristics were computed for constant \( h \) and \( p \) by ensemble averaging the results of five sweeps executed for different initial spin configurations corresponding to a particular disorder realization and then averaging over 10 to 20 different disorder realizations.

3 Results

We examined the temperature dependence of several thermodynamic characteristics of three-dimensional Ising antiferromagnets in a wide range of impurity concentrations for systems having a size varying from \( L = 8 \) to \( L = 64 \) in applied magnetic fields of a strength between \( h = 1 \) and \( h = 4 \).

Our analysis revealed several intervals of \( p \) corresponding to different behavior for each
Figure 1: Temperature dependence of the Binder cumulant on lattices with $L = 8, 16, 24, 32, 48,$ and 64: (a) $p = 0.5$, $h = 1$; (b) $p = 0.725$, $h = 3$; (c) $p = 0.8$, $h = 4$; (d) $p = 0.5$, $h = 3$.

value of $h$. Second-order transition between paramagnetic and ferromagnetic phases is observed at $T_c(h, p)$ when $p_u < p < 1$ [18], where $p_u$ is the vacancy percolation threshold ($p_u = 0.83$ for the present model).

When $p_c < p < p_u$, where $p_c$ is the magnetic percolation threshold ( $p_c = 0.17$ for the present model ), there exist such $p(L', h)$ that the computed quantities exhibit behavior characteristic of second- and first-order phase transition if $p > p(L', h)$ and $p < p(L', h)$, respectively, on lattices with $L < L'$. The value of $p(L', h)$ increases with $h$ and $L'$, approaching the threshold $p_u = 0.83$.

This size-dependent behavior is explained by the existence of interpenetrating spin and
vacancy clusters whose fractal dimensions vary between 0 and 3, depending on spin concentration. Therefore, the sizedependent parameterization of transition from longrange order to domain structure with characteristic size $L_c$ by

$$\frac{h_r}{J(L)} = \frac{h_r}{J L^{(2-d)/2}}, L_c \approx \left( \frac{J}{h_r} \right)^{2/(2-d)}$$

proposed for Ising-like systems in [21], where $h_r$ is the random-field amplitude, $J$ is the exchange coupling, and $d_f$ is interpreted as the fractal dimension of the spin cluster, can be used to predict that antiferromagnetic long-range order breaks down at $d_f < 2$.

Figures 1-4 illustrate the existence of boundaries separating spin-concentration intervals characterized by different strength of random-field effects for systems with $L \leq 64$ in applied magnetic fields of strength between $h = 1$ and $h = 4$.

Figure 1 shows the temperature-dependent Binder cumulants calculated for several lattices with $p = 0.5$ for $h = 1$, with $p = 0.5$ and 0.725 for $h = 3$, and with $p = 0.8$ for $h = 4$. For spin concentrations close to $p_u$, the Binder cumulants do not intersect only if $L \geq 64$. When $p = 0.5$ and $h = 3$, no intersection of Binder cumulants is observed for lattices of all sizes used in the computations. Comparing Figs. 1a-1c, we see that the sizedependent change in the behavior of Binder cumulants due to the increase in field strength from $h = 1$ to $h = 4$ (increasing random-field effects) corresponds to the spin concentration increasing from $p = 0.5$ to $p = 0.8$. For systems with $p < p(L', h)$, the behavior of $M_{stg}(T)$ (Fig. 2) strongly depends on the lattice size for all values of $h$ used in the computations.

The decrease in staggered magnetization with increasing $L$ points to the absence of an antiferromagnetic ground state. Furthermore, the insignificant increase in total magnetization $M$ with increasing $L$ (Fig. 3a) indicates that the system breaks up into antiferromagnetic domains of size $L < L'$ with nearly compensated magnetizations. As the random-field effects increase with impurity concentration and applied magnetic field, both number and size of antiferromagnetic domains increases (Fig. 2c) and both number and size of ferromagnetic ones increases (Fig. 3b), while it holds that $M_{stg} + M < 1$.

To further elucidate the properties of systems with $p_c < p < p_u$, we examined the temperature dependence of the spin-glass order parameter. The results obtained for several disorder realizations are shown in Fig. 4. The graphs demonstrate that a spin-glass phase with "frozen" configuration of magnetic moments is obtained as temperature
Figure 2: Temperature dependence of staggered magnetization on lattices with $L = 8, 16, 24, 32, 48,$ and $64$: (a) $p = 0.5, h = 1$; (b) $p = 0.725, h = 3$; (c) $p = 0.5, h = 3$.

Figure 3: Temperature dependence of total magnetization on lattices with $L = 8, 16, 24, 32, 48,$ and $64$: (a) $p = 0.725, h = 3$; (b) $p = 0.5, h = 3$. 
Figure 4: Temperature dependence of spin-glass order parameter: \( h = 3; L = 24; p = 0.2 - 0.7, \) and 0.725.

Figure 5: Phase diagram for random-field Ising antiferromagnet at \( h = 3 \): PM = paramagnet; AFM = antiferromagnet; Domains+SG = domain structure and spin glass.

approaches zero. Thus, a random magnetic field induces transition from antiferromagnetic to spin-glass ground state in the Ising model with competing interactions when \( p < p_u \). At finite temperatures, the corresponding change in the state of a disordered system is a first-order transition from a paramagnetic to a mixed phase. When the spin concentration is high, the latter consists of antiferromagnetic domains separated by spin-glass regions. With decreasing spin concentration, the number and size of antiferromagnetic domains decrease and the number and size of ferromagnetic domains increases, while the volume fraction occupied by the spin-glass phase decreases.

We used the temperature and field dependence of magnetization, internal energy, and specific heat to calculate the first-order phase transition lines. The \( T - p \) phase diagram shown in Fig. 5 summarizes the results obtained for \( h = 3 \).

4 Conclusions

The Monte Carlo simulations of thermodynamics of the three-dimensional random-field Ising model performed in this study demonstrate second-order phase transition from paramagnetic to antiferromagnetic state when the spin concentration is higher than \( p_u \) and first order phase transition from paramagnetic to mixed phase consisting of antiferromag-
netic and ferromagnetic domains separated by spin-glass domains when \( p_c < p < p_u \), where \( p_u \) and \( p_c \) are vacancy and magnetic percolation thresholds, respectively. When the spin concentration is high, the system consists of antiferromagnetic domains separated by spin-glass regions. With decreasing spin concentration or increasing applied magnetic field strength, both the number and size of antiferromagnetic domains decrease, both the number and size of ferromagnetic domains increase, and the volume fraction of the spin-glass phase decreases. It is shown that random magnetic field induces a transition from antiferromagnetic to spinglass ground state when \( p_c < p < p_u \) in the three-dimensional random-field Ising model with competing interactions analyzed in this study.

Acknowledgments

This work was supported by the Russian Foundation for Basic Research (project nos. 04-02-17524 and 04-02-39000) and by the Ministry of Education of the Russian Federation (grant no. UR 01.01.230).

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