Comparative Monte Carlo and mean-field studies of random-field Ising systems

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(Received 2 December 1985)

Site-dependent mean-field theory and Monte Carlo (MC) simulations are used to study and compare random-field Ising ferromagnets (RFIM) and Ising diluted antiferromagnets in a field (DAFF). For short-time-scale simulations the two approaches lead to similar results for the various history-dependent magnetizations, and specific heats and for the metastable ground-state spin configurations. The results are also in reasonable qualitative accord with experiment. Mean-field theory which more readily provides information about free energies is used to compute the phase diagram for two- and three-dimensional random-field systems. Since thermal fluctuations are not important in the equilibrium critical behavior a mean-field approach is expected to contain much of the essential physics. At $T=0$, MC simulations corroborate the mean-field results. We distinguish three characteristic field-dependent temperatures which in order of decreasing magnitude are the irreversibility temperature $T_{\rm irr}$, the ordering temperature (T_c or T_N), and the temperature for stability of long-range order (LRO), T_s. $T_{\rm irr}$ corresponds to the temperature at which the free-energy surface first develops multiple minima. At an even lower temperature, T_c or T_N, the metastable LRO minimum first appears. However, the LRO state is not the deepest minimum until the stability temperature T_s is reached. In the two-dimensional (2D) RFIM, the zero-temperature intercept of T_s, called Δ_c, scales to zero with the system size. This result, which is derived in mean-field theory and substantiated in MC, provides strong numerical evidence for the absence of stable LRO in 2D. We find that this 2D behavior is reflected in 3D by the metastability of LRO for a narrow range of T near the ordering temperature. This implies that the LRO state should exhibit time-dependent properties, near T_N as has been reported recently. Furthermore, in equilibrium, the transition to the LRO state may be first order. The effects of $H=0$ disorder in the DAFF lead to different behavior in field hysteresis studies than in the RFIM. This result which is a consequence of the extremely anisotropic Ising limit suggests that theoretical predictions for the time-dependent properties of the RFIM may not be applicable to the experimentally realizable DAFF.

I. INTRODUCTION

Our understanding of random-field systems has greatly increased during the last few years. There is a growing consensus in the experimental and theoretical communities that the lower critical dimension $d_l=2$. Earlier experimental uncertainties[1,2] are attributed to the strong history dependence associated with measurements in these systems. While an appreciation of this history dependence has, in one sense, resolved the controversy concerning d_l, it has also served to underline the complexity of the ordering transition. Even in three dimensions it is clear that the transition to a long-range-ordered state is of a very unusual nature. In the random-field systems, much like the spin glasses, there appears to be a strong interplay between "glassiness" and phase-transition phenomena. In this paper we focus on this interplay by studying the random-field Ising ferromagnet (RFIM) and diluted Ising antiferromagnet in a uniform field (DAFF) using both Monte Carlo simulations and site-dependent mean-field theory. The latter has been previously applied with some success to both spin glasses[3] and random-field systems[4,5] (including both the RFIM and DAFF cases). This paper follows an earlier Rapid Communications[5] on this topic. The key questions we address which pertain to this interplay are as follows:

(i) At what temperatures and fields is the long-range-ordered (LRO) state stable? Closely associated with this are questions concerned with characterizing the order of the (equilibrium) phase transition to the LRO state and the effects of dimensionality.

(ii) How does one characterize the irreversibility phase boundary and how does it relate to the phase boundary for the onset of the ordered state?

(iii) To what extent are the various macroscopic variables such as the magnetization and specific heat dependent on the history? To what extent are microscopic variables such as the configuration of the spins, domain walls, etc. history dependent?

(iv) What are the important differences between random-field ferromagnets and diluted antiferromagnets in a field? In particular, how do these differences manifest themselves in points (i)—(iii)?

These questions all revolve around our ability to distinguish between three characteristic temperatures. In general, T_s below which LRO is stable is distinct from the temperature at which the LRO state first appears (i.e., the Curie T_c or Néel temperature T_N), which is also distinct from the temperature T_{irr} at which irreversibility first sets in.

It is important to realize that the temperature T_s may not be experimentally detectable, except insofar as it relates to the onset of time dependence of the LRO state. It is, however, of central importance in Monte Carlo simulations of equilibrium behavior. The ordering temperature T_c or T_N is the temperature at which, for (finite) experimental times, LRO disappears. Thus in experiments as in the mean-field approach, the LRO state is in effect "superheated" between T_s and T_N. The irreversibility temperature T_{irr} is also readily observed experimentally, although any measurement of it will vary according to the observation time. It can, for example, be detected by determining when the field-cooled (fc) and zero-field-cooled (zfc) magnetizations coalesce.

We view the Monte Carlo simulations and site-dependent mean-field theory as complementary, but not unrelated, approaches which can both be used to address these questions. At $T=0$, the two approaches are equivalent, in principle, since the mean-field equations can be satisfied by Monte Carlo—generated ground states and vice versa. It should parenthetically be noted that for spin glasses the mean-field approach generates[3] better ground states 100 times faster than Monte Carlo (MC) simulations for the Gaussian distribution of random exchange interactions. However, it is considerably less efficient for the δ-function distribution.[6,7] At finite T the results in the two numerical approaches are found to be qualitatively similar although the temperature scales are different. What is important to stress is that the semiquantitative similarity between mean-field and Monte Carlo results is clearly dependent on the Monte Carlo time scale. The longer the MC-simulated state is allowed to evolve the less this state resembles the mean-field results (which ignore relaxation effects). We find the two numerical approaches are rather similar if the simulation involves continuous cooling from above T_c to $T=0$ over a time scale of about 500—1000 Monte Carlo steps (MCS). We find, using both numerical techniques, behavior in reasonable qualitative agreement with experiment. For $T\neq 0$ the mean-field approach has the advantage over Monte Carlo simulations of yielding free energies so that the relative stability of different states may be studied directly rather than inferred indirectly through time-dependent behavior. At the same time, mean-field theory clearly ignores thermal-fluctuation effects so that, on general grounds, one has to be cautious in interpreting the results. It should be stressed, however, that thermal fluctuations are unimportant in determining the equilibrium critical behavior of random-field systems. While our emphasis here is primarily on nonequilibrium phenomena, the present mean-field approach presumably contains more of the essential physics for the RFIM than, say, for spin glasses.

To address point (i) we calculated the phase diagrams in the field- (H) temperature (T) plane for the onset of stable LRO. Our phase diagram is derived by comparing the free energies of canonical FC and ZFC states. The latter, in general, leads to an ordered state, whereas the former consists of randomly ordered domains within which there is short-range order. A stable LRO state is said to occur when its free energy is lower than that of a mean-field-generated FC state. Since *all* domain states are not compared with the LRO state, this procedure *overestimates* the region of stability of the LRO state. While Monte Carlo results at zero T qualitatively confirm the mean-field stability phase diagrams, they suggest that, as expected, the mean-field results yield an upper bound to this region of stability. Above this stability line the LRO state exists but is not the most stable state. Because of the high-temperature metastability of LRO, it is argued that upon cooling in equilibrium the phase transition to the ordered state may be first order. By studying finite-size scaling at $T=0$ it is demonstrated that in two-dimensional systems the region of stable LRO scales to zero as the system size increases. These calculations are among the strongest numerical support thus far obtained for the instability of LRO in two-dimensional random-field systems.

To address point (ii), we use both short-time Monte Carlo and mean-field approaches to create the two canonical FC and ZFC states. We monitor the differences between these two states by comparing macroscopic variables such as the magnetization and specific heat. The locus of points in the H-T plane at which the two states are macroscopically indistinguishable is said to correspond to the irreversibility phase boundary. The phase boundary for the onset of the ordered state T_N or T_c is obtained by heating the ZFC state and observing when the order parameter vanishes. In the course of these studies, we obtain the temperature and field dependence of the various history-dependent magnetizations and specific heats and thus address point (iii). These calculations all compare favorably with their experimental counterparts. Our calculations involve parallel studies based on both the RFIM and DAFF. In general, we find the differences to be quantitative rather than qualitative, with one exception. Studies of field hysteresis show that a domain state in the RFIM relaxes to the LRO state when the random field is turned off. By contrast, in the diluted antiferromagnet the presence of randomness even in zero field prevents a domain state from relaxing to the LRO state when the field is subsequently removed. This rigidity of the domain walls has implications for the difference in dynamics in the two systems.

Our calculations should be compared with previous work on three main topics which are currently of considerable interest and the subject of controversy: (A) The lower critical dimension, (B) history-dependent properties, and (C) first-order transitions.

A. The lower critical dimension in the RFIM

The most conclusive analytical work on the lower critical dimension is that of Imbrie, who has rigorously shown[8] that $d_l \leq 2$. While this contradicts earlier claims[9] that $d_l=3$, it does not conclusively prove that there is no long-range order in two dimensions (2D) at $T=0$. Rather strong evidence on the basis of an interface model for

$d_l = 2$ is presented in Ref. 10. This approach reinforces the original Imry-Ma[11] claim which was deduced using simple domain-wall arguments.

Numerical evidence concerning the lower critical dimension is somewhat divided. Andelman, Orland, and Wijewardhana[12] conclude from their Monte Carlo simulations that LRO is not stable in two dimensions. They find different types of behavior in $d = 2$, after cooling 2000 spins in a field. Either they find domain states, or they find ordered states with equal probability that the magnetization is parallel or antiparallel to a small symmetry-breaking field. This behavior is to be contrasted with what is observed in three dimensions (3D) where LRO is always obtained in the direction of the symmetry-breaking field.

Using Monte Carlo techniques Stauffer, Hartzstein, Binder, and Aharony[13] monitored the time dependence of the magnetization produced upon field-cooling and zero-field-cooling systems containing up to $(150)^3$ spins in 3D and $(225)^2$ spins in 2D. In contrast to the results of Ref. 12, Stauffer *et al.*[13] found no evidence in their Monte Carlo studies for distinguishing between two- and three-dimensional systems. Because the fields Δ applied are all large ($\Delta > \Delta_c$ in our notation), it may be that these fields were sufficiently strong so that, even in 3D, LRO is not stable.[14]

Transfer-matrix calculations of Pytte and Fernandez[15] have provided rather convincing evidence for $d_l = 2$. In 2D the field dependence of the domain size or correlation length is expected to be exponential if $d_l = 2$ and to vary as a power law if $d_l = 3$. The observation of an exponential dependence reported in Ref. 15 supports the claim that $d_l = 2$.

Our own zero-temperature 2D Monte Carlo and mean-field studies address the lower critical dimension by using energetic arguments to demonstrate that, for a fixed number of spins $N = L^2$, there exists a critical (random) field Δ_c above which the LRO state has higher energy than a domain state. We generated this fiducial domain state by slow cooling in mean-field theory. An event slower cooling by Monte Carlo techniques produces a somewhat better domain state so that the $\Delta_c(L)$ we compute is clearly an upper bound. As the size of the system L increases, $\Delta_c(L)$ is found to approach zero. Most importantly, we find Δ_c is related to L as $\ln L \propto 1/\Delta_c^2$ with the coefficient of proportionality close to that obtained[15] from the Δ dependence of the characteristic domain size or correlation length ξ. In all cases ξ is slightly less than L so that we are in a situation where the occurrence of domains is not limited by the size of the system.

This scaling of Δ_c to zero as $L \to \infty$ is strong numerical support for the absence of stable LRO in two-dimensional systems. These conclusions (at $T = 0$) are not based solely on the use of mean-field theory. Nevertheless, it is of some interest that site-dependent mean-field theory does lead to the breakdown of LRO in two dimensions. In this respect it is clear that this mean-field theory includes fluctuation effects to some degree. Furthermore, these finite-size scaling calculations suggest that in 3D LRO is clearly stable.

Experimentally, the evidence for the lack of stable LRO in two dimensions is reasonably strong, although from the perspective of neutron-scattering measurements two- and three-dimensional systems do not appear to be very different.[1] By contrast, birefringence measurements[2] show clearly that a magnetic field induces rounding of the transition in 2D, whereas in 3D, the transition appears to be sharper at finite than at zero field.

B. History-dependent properties

Significant insight into the nature of metastability in random-field systems has been provided by the work of Villain, Bruinsma, and Aeppli and by Grinstein and Fernandez.[16] These authors showed that once domain states were formed (e.g., by rapid quenches), relaxation to the (presumably stable) LRO state proceeds by surmounting energy barriers. This occurs slowly so that infinite-size systems can reach thermal equilibrium only after infinitely long time. This class of papers[16] did not address the question of how the metastable domain states were initially formed, but rather focused on the time dependence of the decay of a given metastable state.

Yoshizawa and Belanger[4] used site-dependent mean-field theory applied to diluted antiferromagnets to illustrate how domains are formed. They determined that field cooling will lead to a domain state, whereas zero-field cooling leads to a long-range-ordered state as is observed experimentally. The physical picture that emerges from this approach is similar to that of Ref. 16. At low temperatures there are many distinct minima in random-field systems which are presumably separated by large energy barriers. Among these are the LRO state and a large number of different domain states. If the system is initially prepared in one of these many metastable states it will only very slowly decay to the stable minimum. While mean-field theory does not address the process of the decay, it does establish the connection between the various experimental procedures and the character of the low-temperature state which is thereby accessed.

There are relatively few Monte Carlo studies which probe the history dependence of random-field systems. Instead, the focus in Monte Carlo studies has been on establishing the nature of the equilibrium states.[12,13,17,18] The work of Stauffer *et al.*[13] clearly indicates that FC and ZFC processes for short-time scales lead to distinct low-temperature states. Bekker and co-workers[17] studied field cooling in a DAFF system with $(40)^2$ and $(14)^3$ sites. They found using rather long running times (10 000 MCS) that for high fields the system enters a domain state upon field cooling, whereas for low H the LRO state is accessed in both 2D and 3D. This latter effect is presumably a consequence of the finite system size (which is less than the domain size at low fields) and may not be indicative of true LRO. As in Ref. 13, these authors claim that there is no significant difference between 2D and 3D. It is somewhat surprising that random-field systems appear in numerical simulations to "equilibrate" (i.e., establish LRO) much more rapidly than, for example, spin glasses equilibrate. This is presumably a consequence of finite-size effects which make it impossible to distinguish between the LRO state and the very large number of domain states whose size is larger than the size of the system.

The MC simulations presented here are among the most detailed studies in the literature of the history-dependent properties. Using intentionally short Monte Carlo times, we plot the two history-dependent FC and ZFC magnetizations and specific heats for both the RFIM and DAFF cases, as well as the staggered magnetization for the diluted antiferromagnet. Using the results of Ref. 16 it is seen that the domain size easily exceeds the system size for rather short Monte Carlo running times (e.g., several thousand MCS) and for small to moderate values of the field. For this reason in Monte Carlo simulations many properties appear to be reversible upon, for example, temperature cycling. Field-cooled and zero-field-cooled measurements frequently cannot be distinguished. This result, because it underestimates irreversibility, is somewhat misleading. It is clearly a consequence of finite-size effects and the indistinguishability of all metastable states whose domain size exceeds that of the system. By contrast, in mean-field theory these finite-size effects are less apparent. Because no relaxation is allowed, the mean-field results on small systems simulate more accurately irreversibility effects observed experimentally than do all but very short Monte Carlo simulations.

It should be stressed that because it is *not* our intention to focus on equilibrium effects (which are not, for the most part, observable experimentally), we consider rather short MC running times. However, longer-time Monte Carlo simulations are clearly useful for other purposes; for, example, to study the critical behavior when T_c is approached from above. Qualitatively, our MC results are quite similar to what is found in mean-field theory and reported here and elsewhere.[4,5] More importantly, for these "short"-time MC studies these results are in reasonable qualitative accord with experiment.

Experimentally, the difference between the FC and ZFC states has been thoroughly studied in neutron measurements,[19] and despite some initial controversy,[20,21] is now observed in specific-heat experiments.[22] Earlier dilation measurements[23] also indicated that the specific heat would exhibit some history dependence. Direct magnetization studies are not as extensive and we are aware only of the measurements of Ikeda and Kikuta[24] on nearly isotropic diluted antiferromagnets.[25]

C. First-order transitions

Using standard mean-field theory for the RFIM, Aharony[26] pointed out that the δ-function distribution of random fields has a tricritical point. Above the tricritical point $H^t(T_c)$ the transition to the LRO state is necessarily first order, whereas below it is second order. For a Gaussian distribution of random fields mean-field calculations do not find a tricritical point. Recently, however, Houghton, Khurana, and Seco[27] used a high-temperature-series expansion of the susceptibility to deduce that such a tricritical point also exists for a Gaussian distribution of random fields.

There have been several claims in the literature,[5,18] based on numerical calculations, that the transition to the ordered state may be first order even at arbitrarily small random-field strengths. Young and Nauenberg[18] performed Monte Carlo simulations on a RFIM lattice of $(64)^3$ spins. Using evidence based on their measured critical exponents as well on a direct observation of abrupt and hysteretic magnetization jumps, they claimed that the transition to the LRO state was first order.

Even earlier, it was suggested,[5] on the basis of site-dependent mean-field theory, that the RFIM and DAFF systems may exhibit first-order transitions. This conjecture arises from observed behavior of the free energies of the domain and LRO states. In Fig. 1 is plotted the mean-field free-energy surface $F\{m_i\}$ for a diluted antiferromagnet as it evolves upon cooling from high temperature at fixed fields. The same picture applies to the random-field ferromagnet. The configuration space which is represented by the abscissa corresponds to the N-dimensional space of the $\{m_i\}$. Here, m_i is the thermally averaged spin at the ith site. At high temperatures there is a single paramagnetic minimum. As T is lowered, upon field cooling this paramagnetic minimum evolves into a FC state, consisting of randomly oriented domains within which there is a short-range order. This FC state has no LRO.

At the Néel temperature T_N, the LRO-state minimum first appears. In the RFIM and, to a lesser extent, the DAFF, there are domain states other than the FC state at and above T_N (which are not shown in the figure, for simplicity). Near T_N and slightly below it is found[5] that the FC domain state has lower energy than the LRO state. Thus LRO is initially metastable, as shown by the middle figure which depicts a rather shallow LRO minimum. At lower temperatures, $T < T_N$, the LRO minimum is found to be deeper than that of the FC state, as is indicated in the last sketch in the figure.

Figure 1 makes it clear that within mean-field theory the LRO state will not be accessed upon cooling at constant field. The state which evolves directly out of the paramagnetic state upon field cooling is a domain state

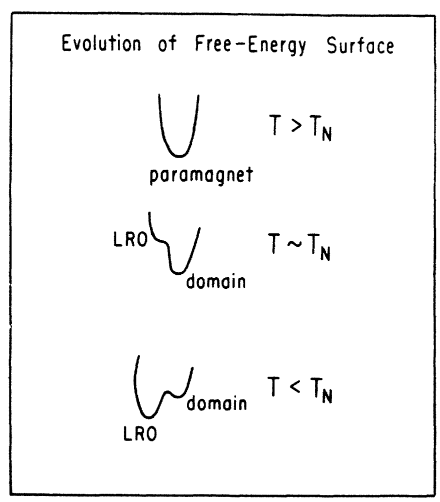

FIG. 1. Schematic free-energy surface in the vicinity of Néel temperature T_N. Paramagnetic minimum evolves into domain state as T is lowered; it is separated by barrier from long-range-ordered (LRO) state.

which is separated from the LRO state by a free-energy barrier. It should be noted that this mean-field picture is consistent with the experimental observation that LRO is not obtained upon field cooling but only upon zero-field cooling. As stated in Ref. 28, "field cooling must of necessity trap the system into some non-equilibrium metastable domain configuration before the expected transition to long range order would otherwise occur upon further cooling." If an ordered system is warmed to temperatures above T_N and subsequently cooled, it always falls out of the long-range-ordered state and into a domain state.

The free-energy surface plotted in Fig. 1 is suggestive of a first-order equilibrium phase transition as in a canonical Landau-Ginzburg theory. The transition to the LRO state only occurs after LRO is well established, i.e., for finite values of the order parameter. It is interesting to note that the occurrence of a first-order phase transition and the inaccessibility of LRO upon cooling are both consequences of the same physics within a mean-field description.

Based on Fig. 1, we have sketched the behavior of the magnetization in the RFIM as a function of temperature for three different time scales. In equilibrium the magnetization exhibits a first-order transition as shown in Fig. 2(a). The magnitude of the discontinuity scales with the separation between the ordering temperature T_c and the temperature at which the LRO state has the lower energy, T_s. For long but not infinite times the magnetization will exhibit abrupt hysteretic jumps as shown in Fig. 2(b). The separation of the two discontinuities is a reflection of supercooling and superheating. This behavior is similar to what was observed by Young and Nauenberg.[18] Finally for shorter, but presumably typical experimental, time scales the magnetization shows no discontinuities, but rather a variety of different behaviors depending on how the system is prepared. On these time scales the system is "frozen" in a given minimum over the time scale of the experiment. The behavior in Fig. 2(c) reflects what is observed in mean-field theory where no "minima hopping" takes place. It is clear that Figs. 2(a)–2(c) correspond to progressively greater degrees of "broken ergodicity."

It should be stressed, however, that *the existence of a first-order transition cannot be definitely established even within mean-field theory* simply because all free-energy minima have not been explored. While the (paramagnetic) FC state clearly represents a better minimum than the LRO state above T_s, it is, however, possible that there is a whole sequence of states with intermediate values of the order parameter through which, in equilibrium, the system passes as T is raised. In this second scenario, it is not possible to rule out a continuous transition between the LRO and paramagnetic state.

Experimentally,[29] neutron-scattering measurements in $Mn_{0.75}Zn_{0.25}F_2$ give some indication of an abrupt transition upon warming from history-dependent to history-independent behavior. Furthermore, upon field cooling there appears to be a break in slope of the correlation length as a function of temperature. It is by no means clear that these experiments are evidence for a first-order equilibrium transition, but they do suggest that the loss of LRO occurs surprisingly abruptly even at low random fields. It should be noted that claims based on these neutron measurements appear to be inconsistent with those of Belanger, King, and Jaccarino,[30] who argue that neutron experiments on $Fe_{0.6}Zn_{0.4}F_2$ are indicative of a "sharp, second order phase transition."

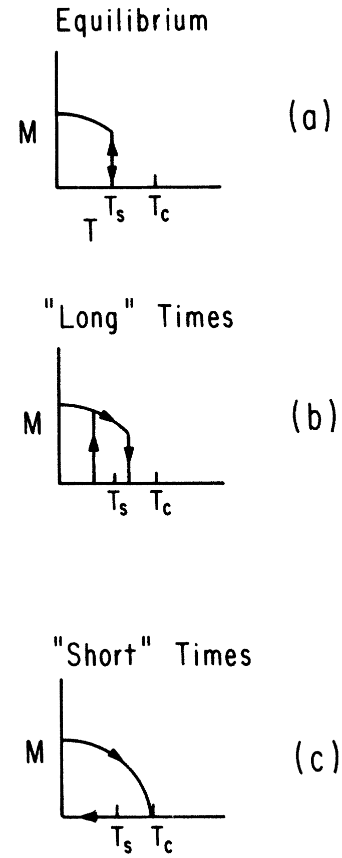

FIG. 2. Schematic representation of temperature dependence of magnetization M. For infinite times (a) M exhibits a first-order jump at the stability temperature T_s. For "long" times (b) supercooling and superheating around T_s is observed, whereas for "shorter"-time scales (c) M behaves very differently upon heating ordered state and cooling from high T.

II. NUMERICAL TECHNIQUES

In order to study the properties of the random-field system, we applied two different numerical techniques: site-dependent mean-field theory and standard Monte Carlo simulations. The Ising Hamiltonian describing these systems is given by

$$\mathscr{H} = -\sum_{i,j} J_{ij} S_i S_j - \sum_i (H + H_i) S_i \ , \tag{2.1}$$

where $S_i = \pm\frac{1}{2}$. H_i is a site random field with probability distribution $P(H_i)$. This field is nonzero for the RFIM and zero in the DAFF. In Eq. (2.1) H is the applied field and J_{ij} the near-neighbor exchange interaction. For random-field ferromagnets $J_{ij} = J$, whereas in the DAFF $J_{ij} = -J\epsilon_j\epsilon_i$. Here, $\epsilon_j = 1$ if the jth site has a spin and is equal to zero otherwise. In the DAFF a fraction c of the sites are occupied by a spin. Our 3D systems consisted of up to $N = (50)^3$ sites on a simple-cubic lattice, while in

2D we considered systems up to $N=(200)^2$ sites on a square lattice. In all our studies we applied periodic boundary conditions. For the RFIM we studied both the Gaussian and δ-function probability distributions corresponding, respectively, to

$$P(h_i)=\frac{1}{\sqrt{2\pi}}\frac{1}{\Delta}\exp[-(h_i/\sqrt{2}\Delta)^2] \tag{2.2}$$

and

$$P(h_i)=\tfrac{1}{2}[\delta(h_i-\Delta)+\delta(h_i+\Delta)] \ . \tag{2.3}$$

The parameter J sets the energy scale for magnetic fields and temperatures. Henceforth T, H, and Δ are always measured in these dimensionless units.

Our Monte Carlo studies, for the δ-function RFIM and the DAFF, used the more efficient continuous-time algorithm discussed in Ref. 31. (Note, however, that because we chose the spin value to be $\frac{1}{2}$, the temperature and magnetic fields H or Δ here are effectively rescaled by multiplicative factors of $\frac{1}{4}$ and $\frac{1}{2}$, respectively.) Because we are interested in history-dependent effects, all the simulations were done at a fixed cooling rate. The temperature changes were in units of $\Delta T=\pm 0.005$ or 0.0025 and the simulations were run for a fixed number of steps at each T. All results shown below are averaged over the last half of the run at each T.

In the mean-field studies the N coupled equations

$$\langle S_i\rangle \equiv m_i=\tfrac{1}{2}\tanh\left[\frac{\beta}{2}\left[H+H_i+\sum_j J_{ij}m_j\right]\right] \tag{2.4}$$

were solved iteratively following Ref. 3. The equations were assumed to have converged when

$$\frac{\sum_i[(m_i)_n-(m_i)_{n-1}]^2}{\sum_i[(m_i)_n]^2}\le 10^{-6} \ , \tag{2.5}$$

where n indexes the iteration number. Within mean-field theory the free energy $F\{m_i\}$ is readily calculated so that the relative stability of the various states can be directly discussed. In the DAFF it follows that

$$\begin{aligned} F=(J/2)\sum \epsilon_i\epsilon_j m_i m_j - H\sum_i \epsilon_i m_i \\ +k_B T\sum_i \epsilon_i[(\tfrac{1}{2}+m_i)\ln(\tfrac{1}{2}+m_i) \\ +(\tfrac{1}{2}-m_i)\ln(\tfrac{1}{2}-m_i)] \ , \end{aligned} \tag{2.6}$$

whereas for the RFIM

$$\begin{aligned} F=-(J/2)\sum_{i,j} m_i m_j - \sum_i H_i m_i \\ +k_B T\sum_i [(\tfrac{1}{2}+m_i)\ln(\tfrac{1}{2}+m_i) \\ +(\tfrac{1}{2}-m_i)\ln(\tfrac{1}{2}-m_i)] \ . \end{aligned} \tag{2.7}$$

In both numerical procedures the field-cooled and zero-field-cooled states were generated according to the appropriate experimental prescription. For example, in mean-field theory, the FC state was obtained by first preparing the system in the unique high-T paramagnetic state at the field in question. The system is then slowly cooled by iteratively solving the mean-field equations with small temperature decrements. The LRO state is generally obtained by cooling slowly to zero field and then applying the random or external field. However, in some instances in the DAFF, the ZFC procedure did not[32] generate LRO and the system was frozen in a domain state due to the presence of disorder even in $H=0$. In those cases we created the ordered state directly, verified which of the two staggered magnetization (or magnetization) directions was favored, and then reheated to obtain thereby the ZFC properties. The temperature changes in mean-field theory were generally ± 0.1 in units of J.

III. THE PHASE DIAGRAMS

In this section we discuss the field dependence of the three characteristic temperatures in random-field systems: the irreversibility temperature $T_{\rm irr}$, the temperature corresponding to the onset of (metastable) LRO, T_c or T_N, and the temperature at which LRO is stable, T_s. We use primarily a mean-field approach to establish our phase diagrams on the basis of free-energy comparisons. Nevertheless, it is important to note that the zero-temperature behavior is qualitatively confirmed by Monte Carlo simulations, which, however, cannot readily provide us with the free energies at finite T. The phase diagrams represent in a compact form a number of key features of random-field systems. They are the basis for our discussion of the lower critical dimension and the occurrence of first-order phase transitions.

In Fig. 3(a) are shown the spin configurations in the ZFC and FC ground states for three values of H (in units of J) in a $N=(60)^2$ 2D diluted antiferromagnet with vacancy concentration $c=0.75$. The top (and bottom) panels correspond to the ZFC and FC states, respectively. The open and solid circles represent the two directions of the staggered magnetization. As expected, the FC state consists of domains with no net antiferromagnetic LRO. The larger the H the smaller the domain size. As first noted in Ref. 4, the domain boundaries lie preferentially along the vacancy sites, which are denoted by blanks in the figure. For sufficiently large H, the FC and ZFC states are indistinguishable and the system is then totally reversible. By $H=1.5$ the similarity between the two states is apparent.

In Fig. 3(b) the mean-field-generated FC ground states are shown in the RFIM for three values of the random-field Δ with a Gaussian field distribution and a 2D lattice of $(100)^2$ spins. The ZFC states are not shown since the system is completely ordered for the two lowest values of Δ. The FC behavior is qualitatively similar to that shown in Fig. 3(a) for the diluted antiferromagnet. There is no substantial difference between the Gaussian and δ-function models. The FC domain state of the latter is shown in Fig. 3(c) for comparison. Some comparisons of the FC domain states in Monte Carlo and mean-field theory will be addressed in Sec. V for the DAFF. In gen-

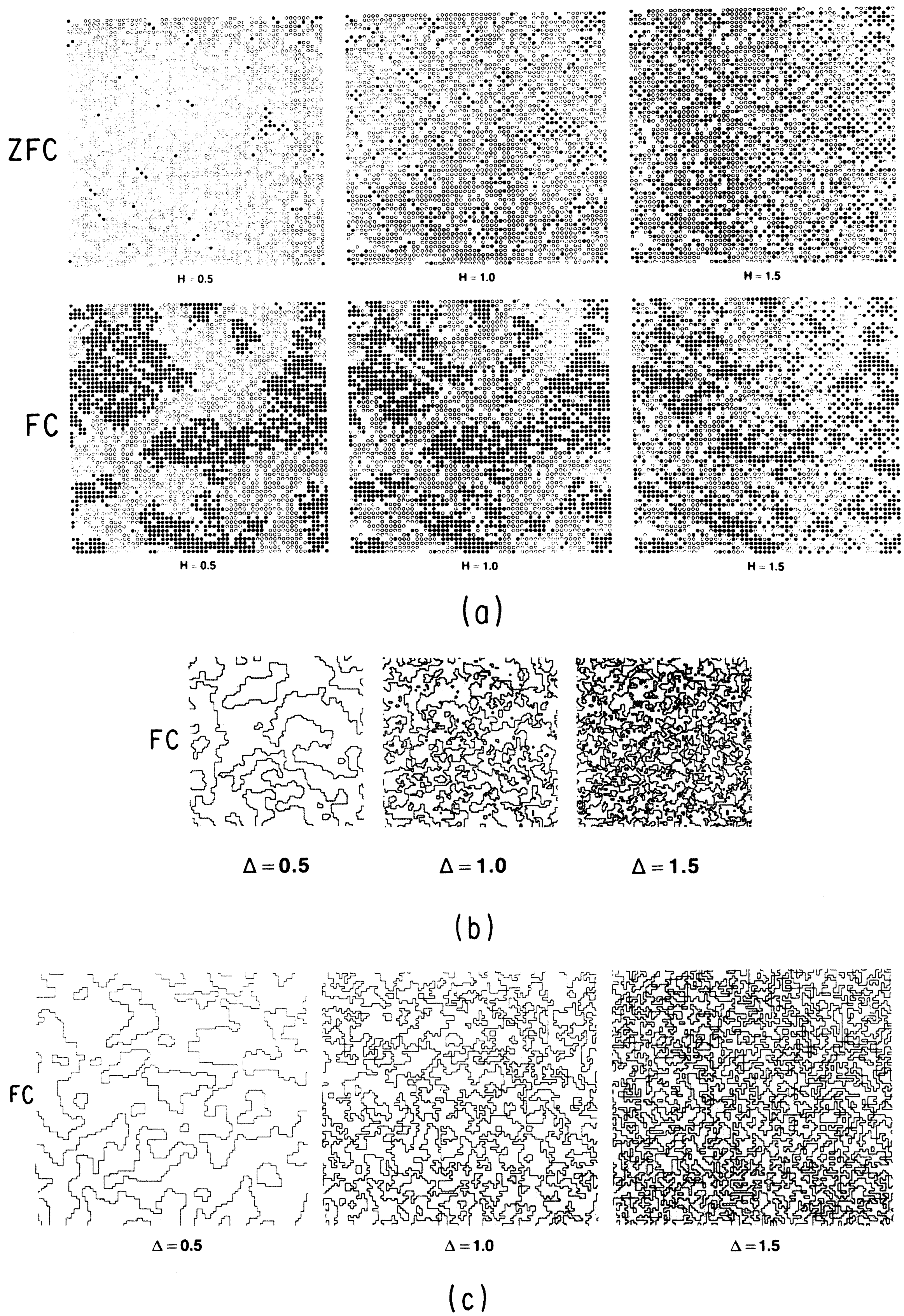

FIG. 3. Ground-state spin configuration in various fields for (a) field-cooled (FC) and zero-field-cooled (ZFC) states in the diluted antiferromagnet (DAFF), (b) FC states in the RFIM with Gaussian, and with (c) δ-function field distributions. The two staggered magnetization [panel (a)] directions are represented by open and solid symbols. In this and all subsequent figures, field and temperature variables are in units of J.

eral, for short Monte Carlo time scales, the domain configurations in the two numerical approaches are rather similar.

To produce phase diagrams we compared the free energies of the FC and ZFC states as a function of H and T. We also monitored the characteristic order parameter for the ZFC state to determine where LRO disappears upon heating. Our results for the δ-function distribution in the RFIM are shown in Fig. 4(a). For definiteness we chose $N=(30)^3$ on a 3D simple-cubic lattice. The solid line in the figure, which represents the highest characteristic temperature, corresponds to that below which the FC and ZFC states are distinct. While this temperature, called $T_{\rm irr}$, is obtained by comparing only two states, it appears to give a reliable estimate of the temperature at which general irreversibility first occurs. The solid line is thus the random-field counterpart of the so-called de Alemeida—Thouless[33] line in spin glasses.

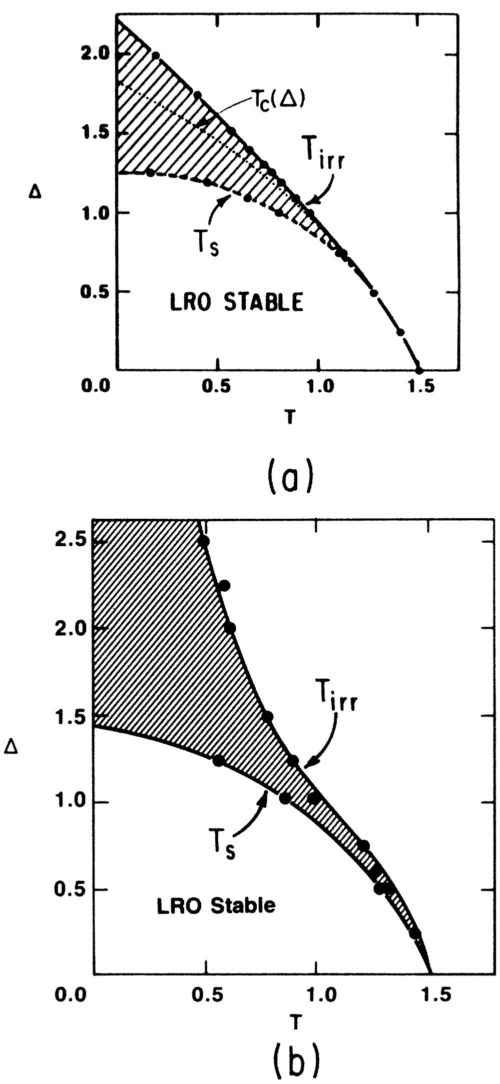

FIG. 4. Phase diagram in the RFIM in 3D for (a) the δ-function and (b) Gaussian random-field distributions. $T_{\rm irr}$ corresponds to the onset of irreversibility and T_s to the onset of stable LRO. $T_c(\Delta)$ is the (metastable) Curie temperature. The shaded region indicates where LRO is only metastable.

It is important to note that for the RFIM, at and slightly below the irreversibility line, the state obtained upon ZFC and subsequent warming does not have LRO. In fact, upon warming the ZFC state, LRO disappears at a lower temperature, $T_c(\Delta)$, shown in 4(a) by the dotted line. For $T_c=0$, this line corresponds to $\Delta \cong 1.7$, which compares favorably with the Aharony[26] estimate of 1.5. Above $T_c(\Delta)$, the ZFC state is a domain state which is nevertheless distinct from the FC domain state. Thus between $T_c(\Delta)$ and the $T_{\rm irr}$, the system has many metastable states which have no LRO, much as one sees in spin glasses. Irreversibility of the ZFC state occurs at $T_c(\Delta)$.[34] The loss of LRO at $T_c(\Delta)$ occurs rather abruptly whenever $T_c(\Delta)$ and $T_{\rm irr}$ are well separated. For larger Δ, one sees a sharp drop in the magnetization at $T_c(\Delta)$. This suggests that even in a nonequilibrium situation (i.e., on these short-time scales) there are features in the magnetization which are suggestive of a first-order transition. However, for the DAFF we find that the counterpart of $T_c(\Delta)$, called the Néel line $T_N(H)$, is indistinguishable from the irreversibility line and that the loss of LRO at $T_N(H)$ does not appear to be abrupt. Our observations, on sudden nonequilibrium transitions in the RFIM (which have no counterpart in the DAFF), can probably *not* be related to the abrupt transition reported in Ref. 29 for the DAFF. The latter may be an effect which involves larger time scales than considered in mean-field theory.

The lowest characteristic temperature indicated in Fig. 4(a) corresponds to the temperature T_s at which in the δ-function model the ZFC state has a lower free energy than the FC state. As shown in Fig. 1, this occurs below the onset temperature for LRO, $T_c(\Delta)$. Thus over a fairly wide range of Δ and T indicated by the shaded region in the figure the LRO state is only metastable. A time dependence associated with this state is expected at sufficiently large fields. Some experimental indications for time dependence of the ZFC state near $T_N(H)$ were reported in Ref. 24. Clearly, further experiments along these lines are needed to verify these interesting results. It should be stressed that this prediction for the metastability of LRO is corroborated at $T=0$ by our Monte Carlo studies. Other $T=0$ Monte Carlo studies[35] based on rapid quenches to $T=0$ followed by relaxation find $\Delta_c=1.35$, which is, as expected, above the site-dependent mean-field value ($\Delta_c=1.25$). Not surprisingly, the mean-field theory generates a better ground state than rapid quenching to $T=0$, but not better than that obtained by slow Monte Carlo cooling.

In Fig. 4(b) is plotted the phase diagram for a 3D RFIM with a Gaussian distribution of random fields. Here, $N=(30)^3$. The $T_c(\Delta)$ line is not shown for the Gaussian case because the magnetization-versus-T curves are rather broad, thus making it difficult to extract $T_c(\Delta)$. We estimate that by $\Delta=2.8$, T_c is zero. This, together with the results shown in Fig. 4(b), imply that as in the δ-function case for sufficiently large Δ, there is a clear separation between the irreversibility line $T_{\rm irr}$ and $T_c(\Delta)$. An important difference between the Gaussian and δ-function probability distributions is the behavior of the irreversibility temperature, which rises nearly vertically at low T in the Gaussian case. This indicates that even at large Δ there is irreversibility at sufficiently low T, corresponding to the existence of many metastable domain states. In contrast to the δ-function distribution, in the Gaussian case large Δ does not force the system into a unique paramagnetic state. Two $T=0$ intercepts in our phase diagram can be compared with previously obtained results. Andelman *et al.*[12] found that LRO disappeared by $\Delta=1.37$ (in our units). These authors noted their result was in disagreement with the mean-field prediction[26] of $\Delta=2.4$. Presumably most of this disagreement arises from the fact that Monte Carlo simulations are sensitive to the stability transition temperature T_s rather than the onset transition temperature T_c. Our own estimate of the latter is 2.8, which compares favorably with the mean-field result of 2.4. Similarly, we find the value of Δ at $T=0$ above which LRO is no longer stable is $\Delta_c=1.45$, which is in reasonable agreement with the value of 1.37 in Ref. 12.

In Fig. 5 is plotted a phase diagram for the diluted antiferromagnet. Here, $N=(40)^3$ and the spin concentration $c=0.7$. The effects of varying the concentration are discussed in Ref. 5, in which the phase diagram for three concentrations on a bcc lattice are presented. These phase diagrams are rather similar to that of the RFIM [see especially Fig. 4(a)]. Note, however, that for the DAFF there is no resolvable difference between the temperature for the onset of LRO, $T_N(H)$, and the irreversibility temperature T_{irr}. Experimentally, the distinction between these two temperatures is somewhat ambiguous.[29,30] It should be stressed that our phase diagram must necessarily be inaccurate at the lowest field values, since then the characteristic domain size exceeds the system size. Thus we cannot state unambiguously that the shaded region always intercedes between the paramagnetic and stable LRO regions. Our figures, however, suggest that in 3D for arbitrarily low field values LRO is not the most stable state, sufficiently close to T_N.

IV. METASTABILITY OF LRO IN 2D

In the preceding section it has been emphasized that even at $T=0$ LRO is not stable for sufficiently high Δ. More importantly, this occurs even for Δ well below the maximum value of the field which can support LRO. These results are observed in Monte Carlo simulations as well as mean-field theory. The goal of this section is to study how this zero-temperature stability field Δ_c depends on the size of the system as well as on the sample dimensionality. If indeed, $d_l=2$, it must follow that in $d=2$ Δ_c approaches zero for infinitely large systems.

In Fig. 6(a) are plotted the values of $\Delta_c(T)$ for which in mean-field theory the FC-generated domain states have the same energy as the LRO state for various two-dimensional systems. Each curve corresponds to a different sample length L. The $T=0$ intercept on each curve is the parameter Δ_c. The random-field distribution

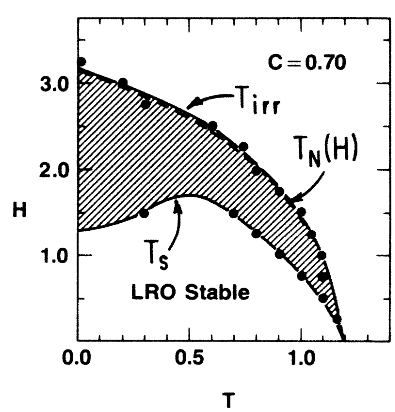

FIG. 5. Phase diagram for the DAFF with characteristic temperatures as defined in Fig. 4.

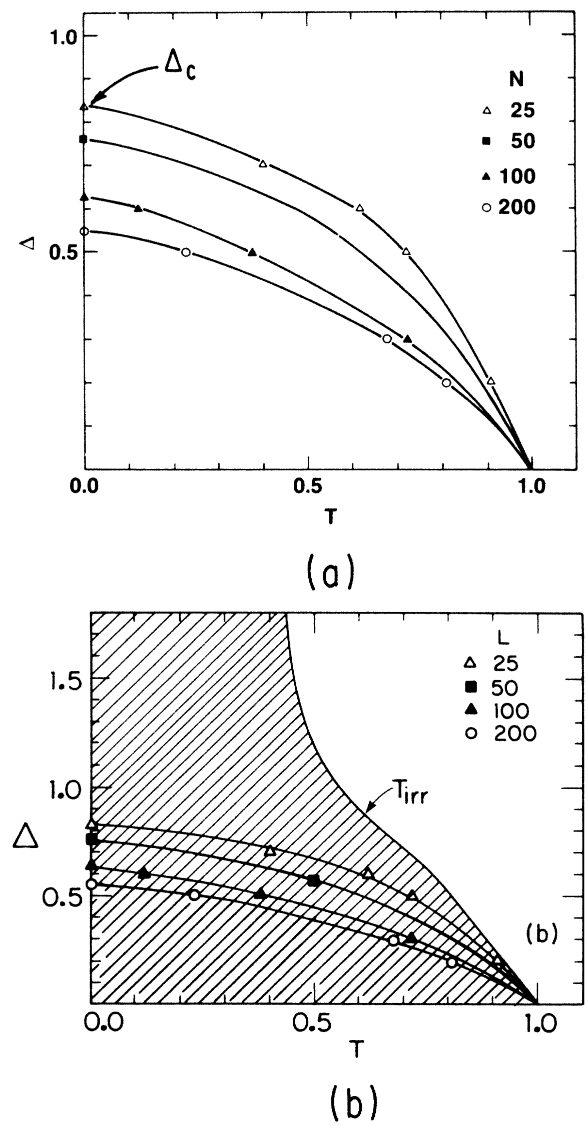

FIG. 6. (a) Temperature-dependent values of the random field below which the LRO state is more stable than the FC state for various-size $N=L^2$ 2D systems. Each line intercepts $T=0$ at the value $\Delta_c(L)$. (b) The full 2D phase diagram for the same system as in (a). By extrapolation to $L\to\infty$, the entire region below T_{irr} is shown shaded to correspond to unstable LRO. This should be compared with Fig. 4(b).

is chosen to be a Gaussian. Figure 6(a) shows clearly that for two-dimensional systems Δ_c approaches zero as L increases to ∞. The implications of this result for the 2D phase diagram are shown in Fig. 6(b). To firmly establish the lower critical dimension, our results for the $L\to\infty$ behavior of Δ_c must be compared with the characteristic domain size ξ, which also depends on Δ_c.

In Ref. 15 it was shown that the domain size

$$\xi(\Delta_c)\sim\exp(\alpha J^2/4\Delta_c^2)\ , \tag{4.1}$$

where $\alpha\simeq3.4$. In order for energetic comparisons to be reasonable at $\Delta=\Delta_c$, it must follow that the size of the system exceeds the correlation length ξ. It is, however, extremely unlikely that $\xi(\Delta_c)$ can be considerably smaller than the system size L, for this would suggest that a state with many small domains has the same energy as a monodomain state. Therefore for our estimates of Δ_c to be reasonable we require

$$L(\Delta_c)\gtrsim\xi(\Delta_c)\ . \tag{4.2}$$

In Fig. 7 is plotted $\ln L$ versus Δ_c^{-2} for the same system as in Fig. 6. The results fall close to a straight line, except for the smallest system size (which might be inaccurate due to configuration-fluctuation effects). We find the line can be described by

$$L(\Delta_c)\sim\exp(\beta J^2/4\Delta_c^2)\ , \tag{4.3}$$

with $\beta=3.52\pm0.1$. This result is thus consistent with Eq. (4.2).

The close agreement between $L(\Delta_c)$ and $\xi(\Delta_c)$ suggests that Δ_c describes the field at which the LRO and FC domain states have the same energy as well as the field for which a given size sample contains slightly more than one domain. Figures 6 and 7 can then be interpreted as strong evidence for the absence of stable LRO in 2D systems.

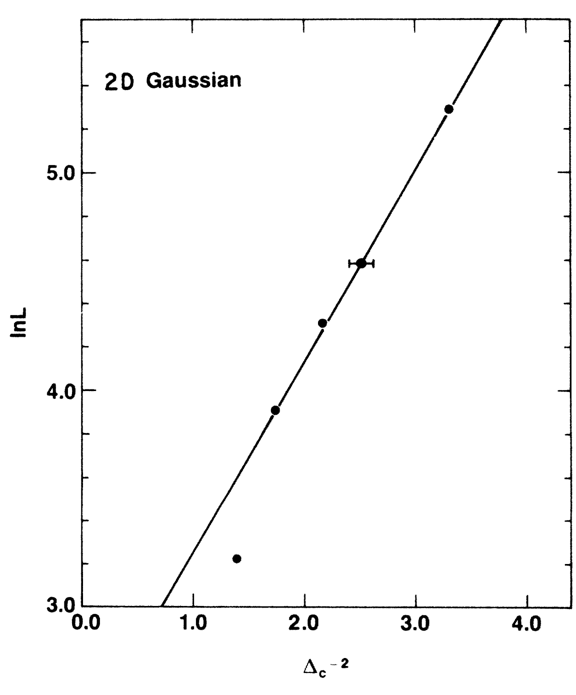

FIG. 7. Size dependence of Δ_c (defined in Fig. 6) for 2D Gaussian RFIM.

At this point it is important to compare and contrast the two phase diagrams shown in Figs. 4(b) and 6(b), which correspond to 3D and 2D systems, respectively (for a Gaussian distribution of exchange interactions). The lack of stability of LRO in 2D is mirrored in 3D systems by the existence of a region of unstable LRO over a narrow portion of the phase diagram. This narrow shaded region which remains in 3D is a remnant of the more extended shaded region found in 2D systems. Thus it is perhaps not surprising in view of the 2D results that in 3D LRO is not fully stable over the entire region of the phase diagram (below T_c or T_N).

We have studied the size dependence of Δ_c for 3D systems, for sample lengths $L=10$, 20, 30, and 40. The results for different-size Gaussian random-field 3D systems are shown in Table I. Here we find the changes in Δ_c for the 3D RFIM to be size independent, in contrast to the exponential dependence found in 2D.

V. COMPARATIVE MONTE CARLO AND MEAN-FIELD THEORY IN THE RFIM

In this section we discuss the behavior of the magnetization in the RFIM as a function of both temperature and random-field strength Δ. We emphasize particularly the comparison of Monte Carlo and mean-field results, as well as the effects of varying the random-field distribution.

In Fig. 8 is plotted the magnetization in the ordered state (obtained upon warming) as a function of temperature. Figures 8(a) and 8(b) correspond, respectively, to mean-field and Monte Carlo results (1000 MCS for $\Delta T=0.05$) for the same $(30)^3$ sample with a δ-function distribution. The value of $M_0=\frac{1}{2}$ and the random-field strength Δ assumes the values 0.5, 1.0, and 1.5. As can be seen, the two approaches lead to rather similar results, although the temperature scales are, as expected, different.

As noted above, for the larger values of Δ the magnetization decreases rather abruptly at the Curie temperature $T_c(\Delta)$. This Curie temperature is also clearly depressed as the random field is increased, as was indicated in Fig. 4(a). Note that the curve for $T_c(\Delta)$ in Fig. 4(a) coincides with the three values for $T_c(\Delta)$ which can be obtained from Fig. 8(a).

In Fig. 9 the mean-field results for a Gaussian field distribution are illustrated. In Fig. 9(a) is plotted the magnetization obtained upon warming as a function of temperature. Figure 9(b) compares the Δ dependence of the low-temperature ($T=0.1J$) magnetization in the Gaussian model with that of the δ-function random-field distri-

TABLE I. Size dependence of Δ_c for Gaussian random-field 3D systems.

Δ_c	N
1.5	$(10)^3$
1.4	$(20)^3$
1.4	$(30)^3$
1.4	$(40)^3$

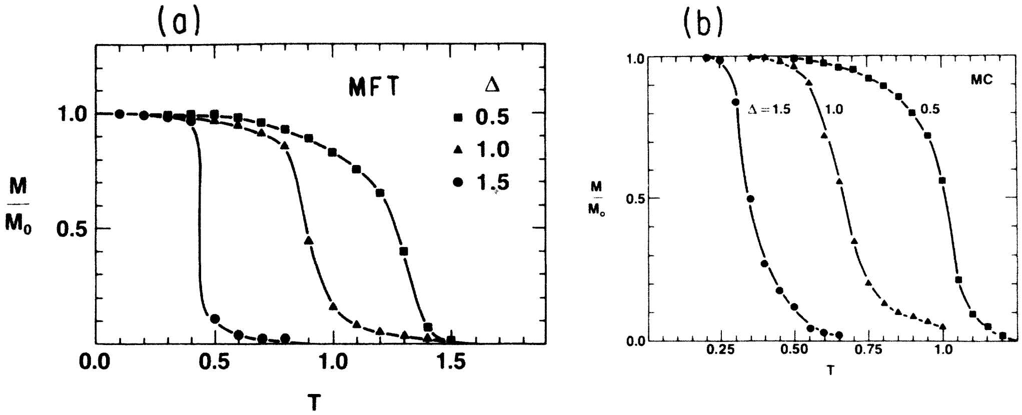

FIG. 8. Temperature dependence of the magnetization for various Δ in the $N=(30)^3$, δ-function-distribution RFIM model. Panel (a) is from mean-field theory (MFT) and panel (b) from Monte Carlo (MC) simulations.

bution. Because they represent low temperatures, these last results reflect the behavior that would be observed in Monte Carlo simulations as well. As can be seen by contrasting Figs. 9(a) and 8(a) the drop in the M at T_c in the Gaussian case is considerably more gradual than for the δ-function distribution. This makes it difficult to obtain reliable estimates of $T_c(\Delta)$ in the former case. Similarly, it can be seen from Fig. 9(b) that the drop in low-temperature magnetization with increasing Δ is sharp in the δ-function and smooth in the Gaussian model. The two arrows in Fig. 9(b) indicate the mean-field predictions of T_c obtained in Ref. 26. These lie a small but consistent amount below our numerical values presumably because of finite-size rounding of the transition observed in the present calculations. Earlier Monte Carlo studies[12] in the Gaussian case found that the magnetization at low but finite T vanished by $\Delta = 1.37$. This is considerably lower than our estimate of $T_c(\Delta)$ which is close to that of Ref. 26. However, as noted earlier we find that, for $\Delta > \Delta_c \sim 1.45$, LRO is not the most stable phase, so that in longer-time Monte Carlo simulations the LRO state should not be observed for values of Δ exceeding this lower critical value. This may thus explain the observed discrepancy between Refs. 12 and 26.

It is of particular interest to study the behavior of a given domain state, say the FC state upon field cycling. Such studies highlight a significant difference between the RFIM and DAFF systems. Figure 10 shows the domain orientations as a field-cooled state (for a 2D Gaussian distribution) is cycled in a magnetic field. The solid lines indicate boundaries of the domains of a given orientation. Initially, the system is in the FC state at $\Delta = 1.0$. As the field is reduced to $\Delta = 0.1$, the domains clearly grow. When the field is then increased to its initial value $\Delta = 1.0$, the domains do not shrink to their smaller size. This magnetization hysteresis is sometimes observed in the laboratory and figures prominently in the work of Ref. 16. However, we will see in Sec. VI that analogous numerical studies in diluted Ising antiferromagnets do not show appreciable hysteresis upon field cycling. This is in contrast to the behavior obtained in anisotropic *Heisenberg* diluted antiferromagnets which more closely resemble the (Ising) RFIM system discussed above.

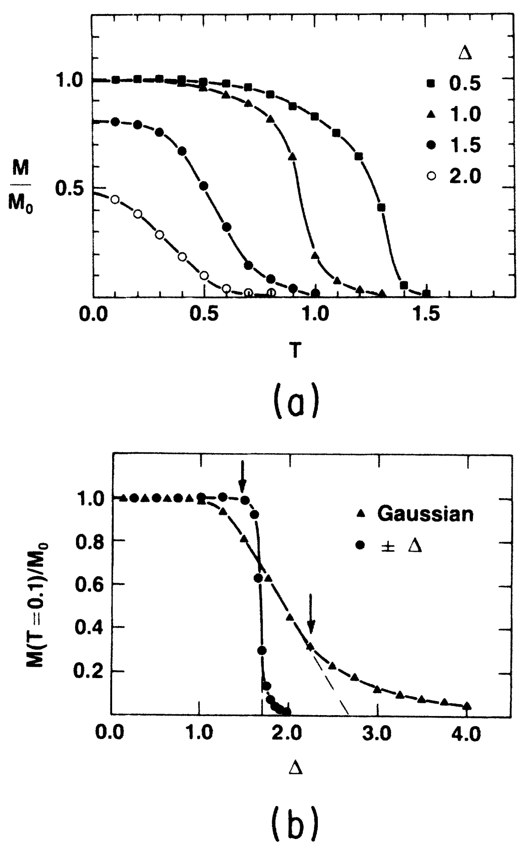

FIG. 9. (a) Temperature dependence of the RFIM magnetization obtained in MFT for the Gaussian distribution. (b) Comparison of field dependence of the low-temperature magnetization in Gaussian and δ-function distributions. Arrows indicate values obtained in Ref. 26.

VI. COMPARATIVE MONTE CARLO AND MEAN-FIELD THEORY IN DILUTED ANTIFERROMAGNETS

In this section we compare and contrast a variety of properties of diluted antiferromagnets using both Monte

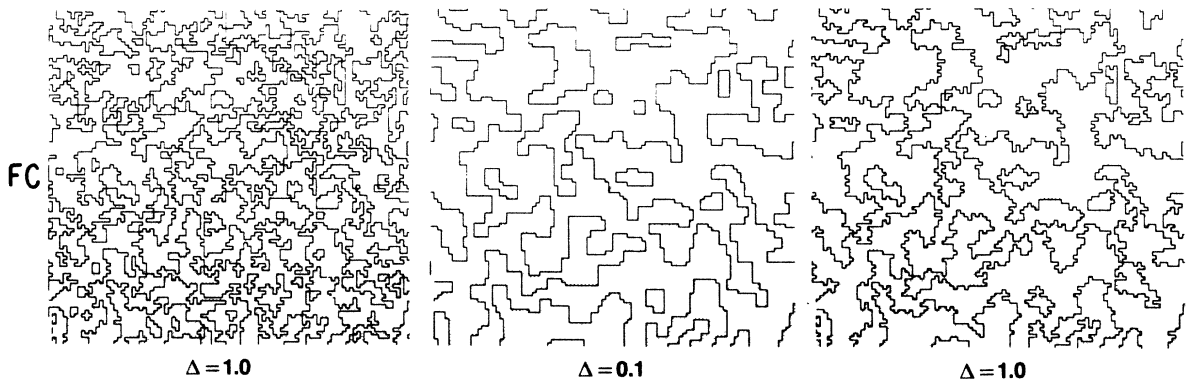

FIG. 10. Ground-state domain configurations in RFIM obtained upon (a) field cooling followed by (b) field reduction and (c) subsequent increase in field.

Carlo and mean-field theory. These results represent among the first detailed MC studies of history-dependent properties in diluted antiferromagnets.

For a given sample, with a fixed distribution of vacancies, various metastable ground-state spin configurations can be directly compared. Figure 11 shows the spin configuration in one layer of a 3D $N=(50)^3$ simple-cubic lattice for a field-cooled state (with $H=0.5$) generated by mean-field theory [Fig. 11(a)] and Monte Carlo simulations [Fig. 11(b)]. The spin concentration $c=0.70$. The Monte Carlo study involved rather rapid cooling with 100 MCS for each temperature, starting at $T=0.8$ and decreasing in units of 0.1. As the cooling rate decreases the ground-state domain size increases appreciably. The ground-state energy was slightly better in the Monte Carlo simulation ($E_G=-0.4334$) than in the mean-field theory ($E_G=-0.4376$) even for this rapid cooling.

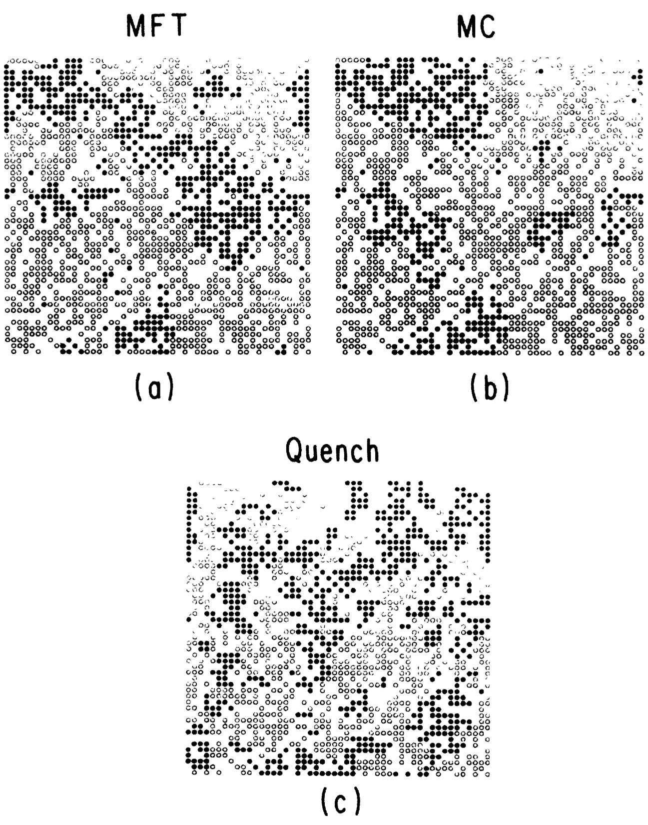

FIG. 11. Comparison of field-cooled domain configurations generated in (a) mean-field theory and (b) Monte Carlo cooling. Panel (c) shows the results of a rapid quench.

The two spin configurations in Figs. 11(a) and 11(b) are, on the whole, rather similar. The domain-wall boundaries clearly overlap, although in the mean-field state the system has managed to incorporate several smaller domains into larger clusters. The similarity between these two FC states is more striking when they are compared with a metastable state generated by a rapid quench to $T=0$. The latter, which is shown in Fig. 11(c), shows no clear correspondence with the domain configurations generated by slower field cooling.

In Fig. 12 the temperature dependent ZFC and FC magnetizations are plotted for several field values. Figure 12(a) corresponds to the mean-field results on a $(40)^3$ lattice and Fig. 12(b) to those obtained in Monte Carlo simulations with $N=(30)^3$ and spin concentration $c=0.7$. The MC simulation corresponds to 1000 MCS per temperature for $\Delta T=\pm 0.05$. While the two approaches give qualitatively similar results, it is clear that in the MC studies irreversibility is less apparent for all but intermediate field values. At low H this lack of irreversibility is related to the fact that the FC domain size is larger than the sample size. This shows up more readily in the MC simulations since relaxation can occur. At high H the two states approach the unique high field limit. This leads to a negligible history dependence at high H.

Figure 12 may be directly compared with experiments by Ikeda and Kikuta,[24] who measured the susceptibility of a more isotropic system, $Mn_xZn_{1-x}F_2$. Direct susceptibility measurements at 50, 500, and 2500 Oe show sharper maxima in the ZFC χ than was observed in our numerical studies (where considerably larger field values were examined). The values of χ^{ZFC} are always less than or equal to χ^{FC}, as in Fig. 12. However, by 2500 Oe the splitting of the two susceptibilities was apparent only over a narrow range of temperatures near the maximum. It would be useful to perform similar dc measurements on more anisotropic systems so that a wider range of field values could

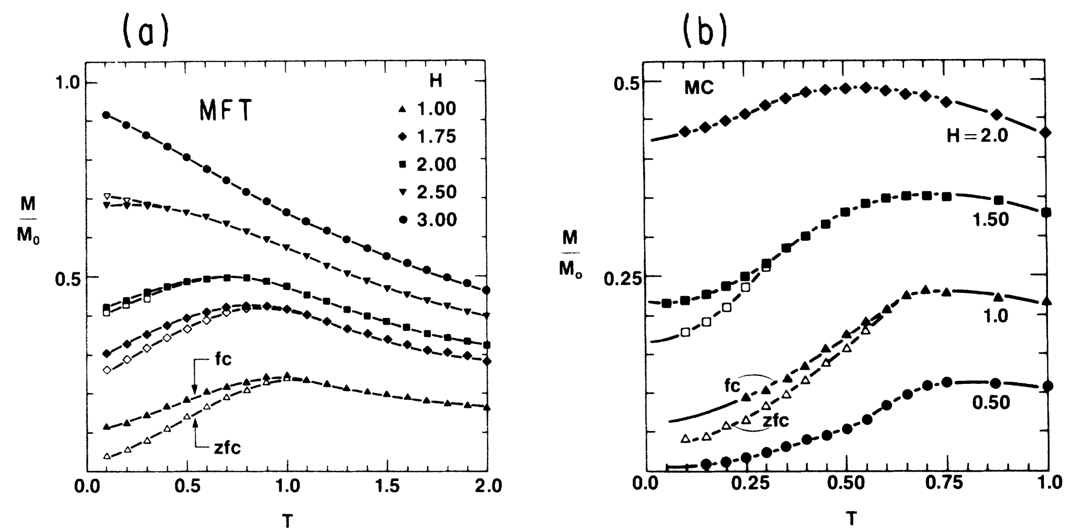

FIG. 12. Comparison of FC (solid symbols) and ZFC (open symbols) magnetization for various fields H in the diluted antiferromagnet obtained in (a) mean-field theory and (b) Monte Carlo simulations.

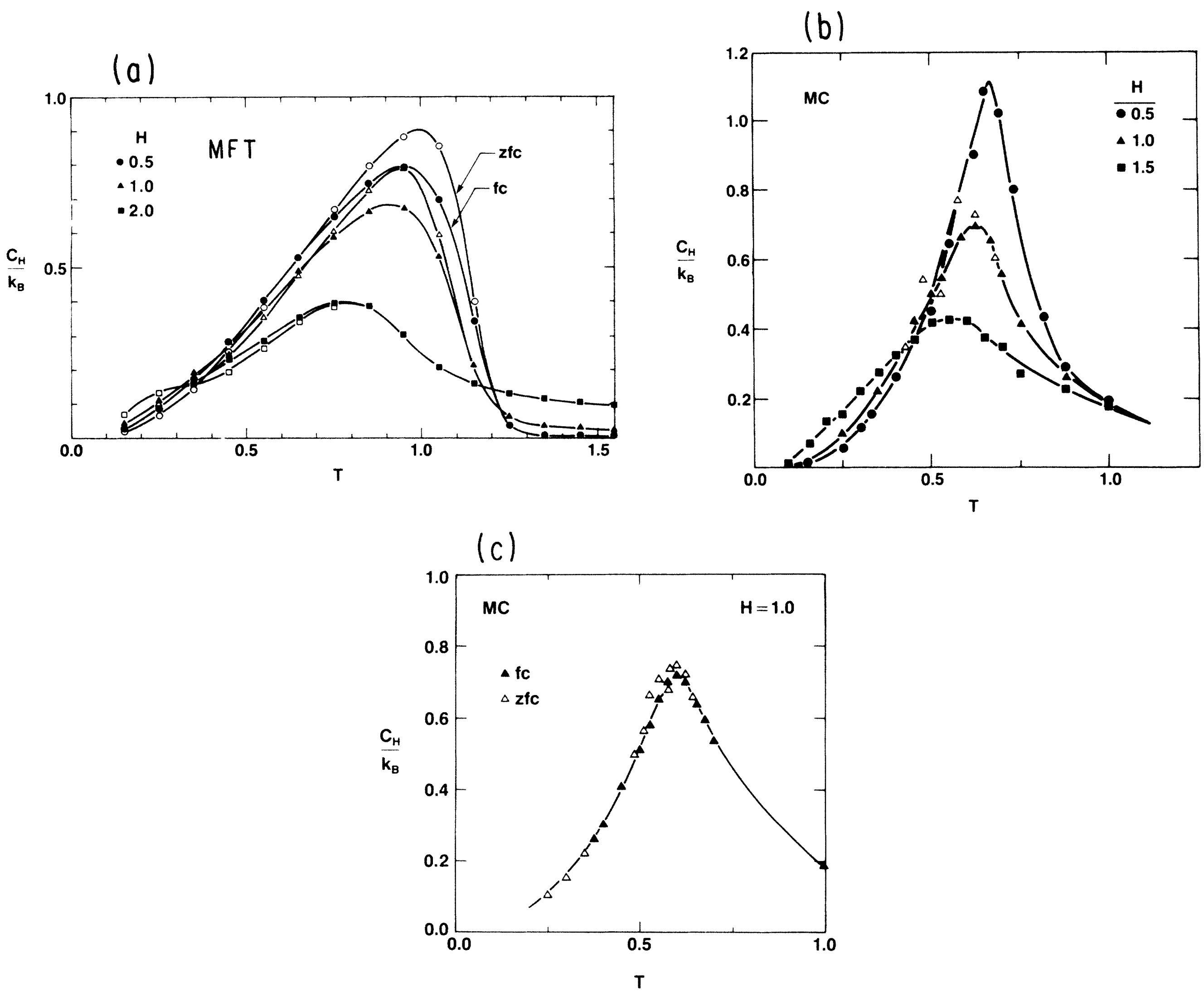

FIG. 13. Comparison of the history-dependent specific heat obtained in MFT and MC. Solid and open symbols are as defined in Fig. 12. Panel (c) corresponds to MC results for a larger $N=(50)^3$ system.

be examined without the added complication of spin-flop effects.

In Fig. 13 are plotted the two temperature-dependent specific heats for three values of the magnetic field for the two systems in Fig. 12. The mean-field results lead to a slightly more asymmetric peak in C_H with more irreversibility than seen in the Monte Carlo results of Fig. 13(b). These MC simulations involved 1000 MCS per temperature with temperature intervals of 0.05. As in the MC magnetization studies, irreversibility in C_H appears to be absent except for intermediate field values. By contrast, in the field-field results, there is no relaxation, so that irreversibility is more apparent.

In an attempt to increase the splitting of the FC and ZFC specific heats, and thereby obtain better agreement with experiments, we performed a MC simulation on a Cray-1S computer. We chose a $N=(50)^3$ with $c=0.7$ sample using 3000 MCS per temperature with $\Delta T=\pm 0.025$ in the vicinity of T_c and ± 0.05 below $0.7T_c$. The results, presented in Fig. 13(c), show somewhat more splitting due to the larger sample size. This study emphasizes that to obtain the experimentally observed splitting of the ZFC and FC heat capacity, one must use larger systems than presently available. In the low-H limit irreversibility is negligible in the simulation because the domain sizes quickly exceed the system size. In the high-H limit the peak in the specific heat is rounded and the splitting again diminished.

Recent specific-heat measurements by King and Belanger[22] have reported direct observation of hysteresis in the specific heat. The results shown in Fig. 13 are also qualitatively in agreement with much earlier dilation measurements reported by Shapiro and Olivera.[23] It should be noted that even earlier Wong and co-workers[20] claimed to see hysteresis in the specific heat which was not in accord with initial claims based on birefringence studies.[21]

In Fig. 14 are shown the staggered magnetizations as functions of T for several values of the field in both mean-field theory [Fig. 14(a)] and MC simulations (with 1000 MCS) [Fig. 14(b)] on the same sample. These results which were obtained upon warming are qualitatively similar in the two approaches. As expected, mean-field theory tends to overestimate the Néel temperature. In both numerical approaches the latter is systematically depressed as the field is increased. It is not possible because of numerical inaccuracies to deduce the field-dependent power-law exponents to compare directly with experiment.

Finally, in Fig. 15 we have repeated the field-cycling studies on the DAFF which were discussed in the context of Fig. 10 for the RFIM. As noted earlier, these calculations highlight an important difference between the RFIM and DAFF systems: the DAFF appears to exhibit little or no field hysteresis as compared with the RFIM. In Fig. 15(a) is shown the ground-state spin configuration for a 2D alloy with $c=0.75$ which has been cooled in a constant field $H=1.0$. The same results were obtained in 3D. In Fig. 15(b) the resulting spin configuration is shown after the field is reduced to $H=0.1$. As can be seen, the spins are virtually unaffected by this reduction in H; nor are they changed significantly when the field is then increased to its initial value of $H=1.0$. These results are a reflection of the rigidity of the domain walls which are effectively pinned to the vacancy sites even when the field is switched off. This is in contrast to the RFIM, where the system has no intrinsic disorder at $H=0$. It might be expected that the presence or absence of field hysteresis in the DAFF is intimately connected with the degree of spin anisotropy. Experimentally, it is observed[36] for weakly anisotropic systems like $MnZnF_2$ that the FC state acquires LRO when the field is turned off. By contrast, in the Ising case, for example, for $FeZnF_2$, no LRO is obtained when H is subsequently reduced to zero.[37] Our numerical mean-field studies on more isotropic DAFF systems show similar results.[38]

VII. CONCLUSIONS

This paper represents a rather detailed comparison of Monte Carlo and mean-field studies of random-field systems. The focus has been on history-dependent properties in both Ising diluted antiferromagnets in a field and Ising ferromagnets in a random field. On short-time scales the Monte Carlo simulations are found to be qualitatively similar to the results of mean-field theory. More importantly, for these time scales both approaches are in quali-

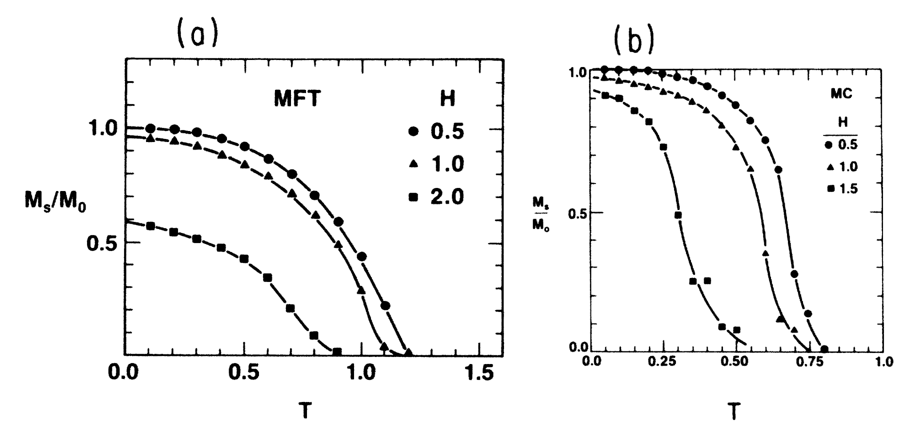

FIG. 14. Comparison of the staggered magnetizations obtained in mean-field theory and Monte Carlo simulations for diluted antiferromagnets in various fields H.

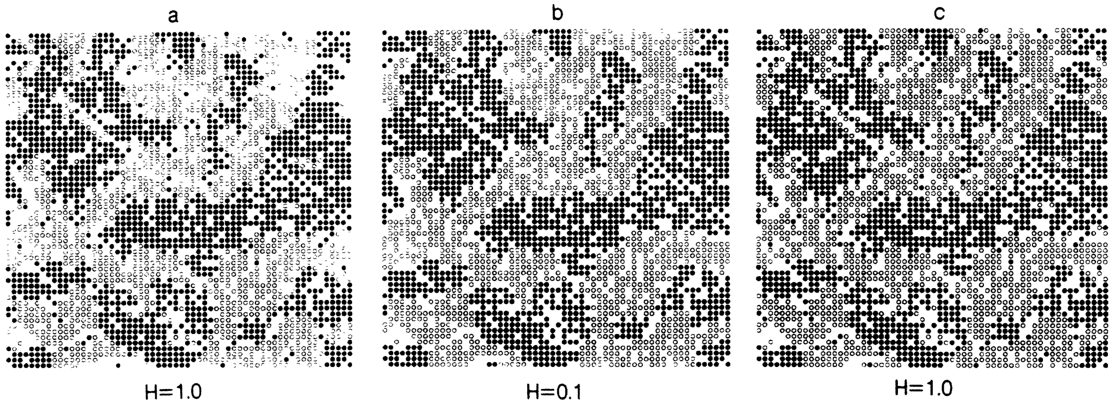

FIG. 15. Ground-state domain configurations in DAFF obtained upon (a) field cooling followed by (b) field reduction and (c) subsequent increase in field. This figure should be compared with Fig. 10 for the RFIM.

tative agreement with experiment. Monte Carlo simulations tend to underestimate the degree of irreversibility. This is due to the fact that in finite-size systems domain states of larger than sample size obtained upon, for example, field cooling and subsequent relaxation, are indistinguishable from the ZFC state which has true long-range order.

We emphasize that there are three characteristic temperatures which are distinguishable at all but very low fields. These are in order of decreasing magnitude: the irreversibility temperature $T_{\rm irr}$, the ordering temperature T_c (or T_N), and the temperature for stability of LRO, T_s. These field-dependent temperatures lead to a complex phase diagram. The fact that T_s lies significantly below T_c (or T_N) implies that LRO is metastable for a narrow range of temperatures near the onset temperature. Preliminary experimental indications which support this picture are presented in Ref. 24. As a consequence of the separation of the two temperatures, it follows from a mean-field description that in equilibrium the transition to the ordered state may be first order. In 2D systems the distinction between T_c (or T_N) and T_s is also essential. We find that T_c is relatively insensitive to the system size, whereas T_s scales to zero with increasing size. This is in accord with the generally accepted picture that in 2D LRO is a metastable as distinct from a globally stable minimum.

We find little qualitative difference between the RFIM and DAFF cases. The only significant effect of the intrinsic disorder in the DAFF comes in field-hysteresis studies. In an Ising DAFF a domain state will not establish LRO when the field is subsequently removed. This is in contrast to behavior in the RFIM and presumably arises because of impurity pinning. Furthermore, in more isotropic DAFF systems[38] the effects of impurity pinning are considerably reduced. These results, which are corroborated experimentally, suggest that a general appreciation of impurity-pinning effects may be important in understanding the dynamics of experimentally realizable random-field systems. Predictions based solely on the RFIM model may not be wholly applicable to experiment.

The interplay of intrinsic disorder and Ising spins is related to our observation that the state obtained upon field lowering (at fixed T) will not be the same as the field-cooled state. This appears to be in contrast to experiment,[39] although it may be an artifact of the extreme anisotropy of the Ising case. A more serious contradiction with experiment is the observation that the FC state is not reversible upon subsequent warming,[39] as our results would imply. (It should be noted, parenthetically, that from an experimental point of view this lack of reversibility essentially eliminates the FC state from consideration as the "true equilibrium" state.) Within the mean-field approach this irreversibility of the FC state can only be understood if there is some degree of relaxation out of the FC state, which is evidently not directly observed.[39] Examinations of thermodynamic identities like Maxwell's relations provide further tests of the present picture. Our mean-field studies indicate that Maxwell's relations will hold for both the ZFC and FC states, but that in the ZFC state this relation should break down at the ordering temperature above which in the RFIM the ZFC state represents a domain state which is nevertheless distinct from the FC state.

In summary, our mean-field and Monte Carlo studies combine to give a fairly consistent picture of the static properties of random-field systems. While agreement with existing experiments is generally satisfactory, further and more direct measurements of the various magnetizations and specific heats are clearly needed in systems with varying degrees of anisotropy. We view studies of the time-dependent FC and ZFC magnetizations over a range of temperatures and fields as essential in helping to unravel the underlying physics in the random-field systems.

After this manuscript was completed, we received copies of analytical[40] and numerical[41] studies of the equilibrium RFIM and DAFF which conclude that in the vicinity of the ordering temperature there exist exponentially-long-time scales. In addition in Ref. 41, evidence is presented for a continuous equilibrium transition to the ordered state. As discussed in Sec. I C, we cannot rule out the possibility of a second-order transition. The present work does not directly address equilibrium or dynamical properties. However, it follows from our free-energy surface picture (see Fig. 1) that in the vicinity of T_N the system will equilibrate extremely slowly as it finds its way over energy barriers to the new equilibrium state. In the present language the existence of exponentially long relaxation times is a consequence of two (or more) metastable states, separated by an energy barrier, each of which corresponds to the equilibrium state over different regimes of temperature. This is, clearly, what we have observed in both the DAFF and RFIM.

ACKNOWLEDGMENTS

This work was partially supported by the National Science Foundation (Grant No. DMR-81-15618), the Materials Research Laboratory (Grant No. NSF-DMR-16892), and the U.S. Department of Energy (Grant No. W-7405-Eng-82). We are grateful to R. Birgineau, M. Nauenberg, and V. Jaccarino for their various comments. One of us (K.L.) acknowledges the hospitality of Argonne National Laboratory. Another of us (C.M.S.) was partially supported by a Northwest Area Foundation Grant and by the Research Corporation (New York, NY). We thank A. T. Ogielski for his helpful comments on the manuscript.

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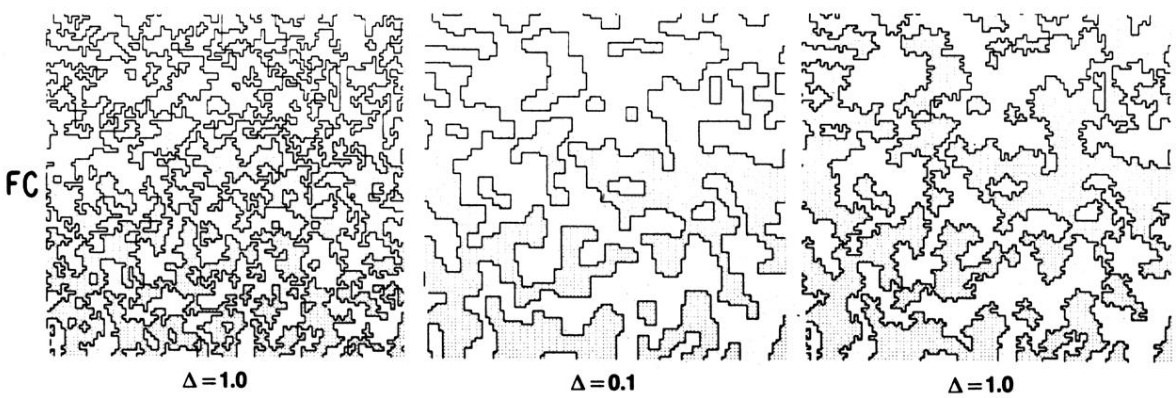

FIG. 10. Ground-state domain configurations in RFIM obtained upon (a) field cooling followed by (b) field reduction and (c) subsequent increase in field.

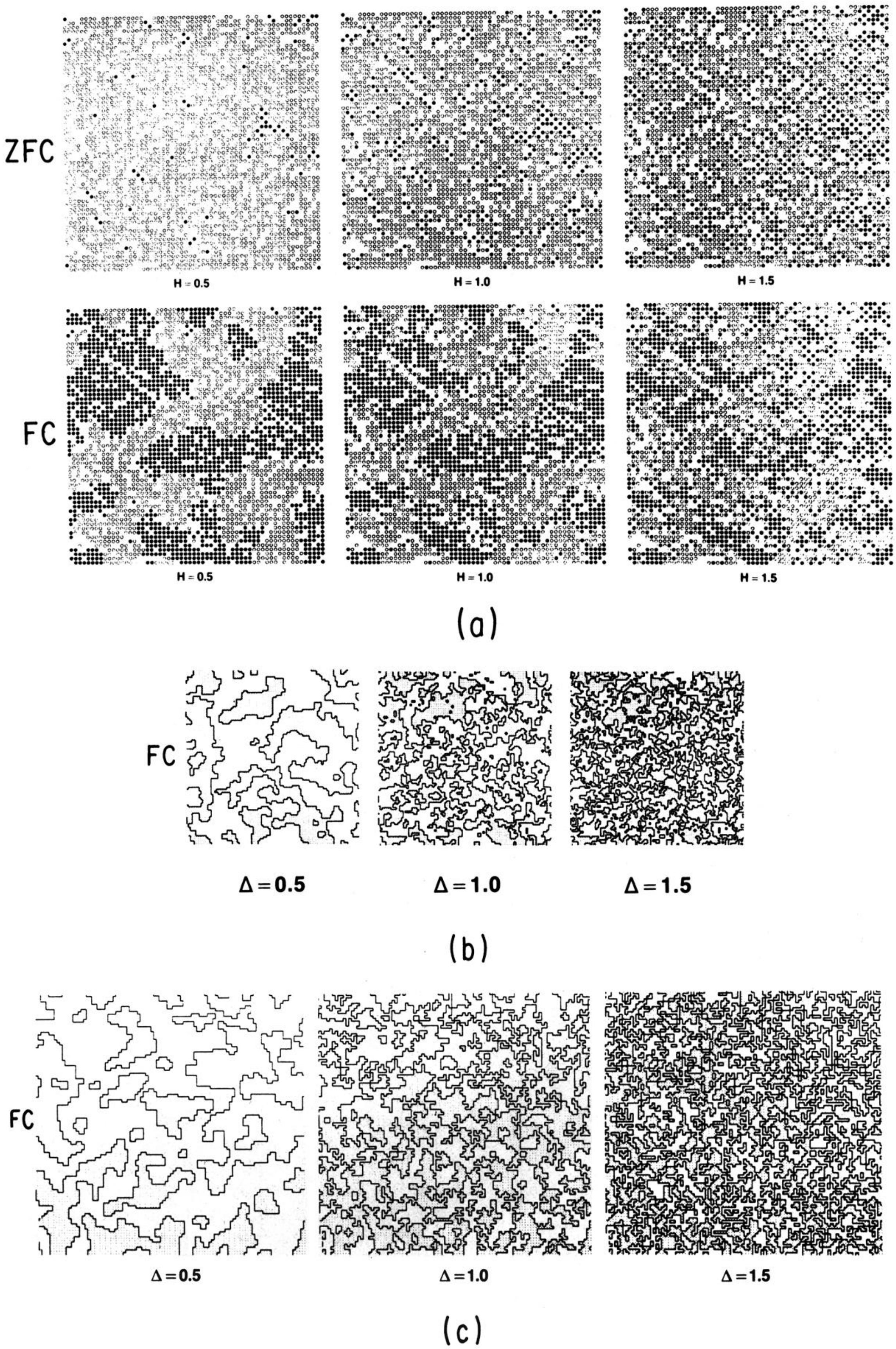

FIG. 3. Ground-state spin configuration in various fields for (a) field-cooled (FC) and zero-field-cooled (ZFC) states in the diluted antiferromagnet (DAFF), (b) FC states in the RFIM with Gaussian, and with (c) δ-function field distributions. The two staggered magnetization [panel (a)] directions are represented by open and solid symbols. In this and all subsequent figures, field and temperature variables are in units of J.