Critical Behavior of the Three-Dimensional Dilute Ising Antiferromagnet in a Field

Andrew T. Ogielski and David A. Huse
AT&T Bell Laboratories, Murray Hill, New Jersey 07974
(Received 4 November 1985)

We report results of large Monte Carlo simulations of an experimentally realizable random-field system: the three-dimensional dilute Ising antiferromagnetic in a field. We find that the correlation time diverges dramatically as $T \to T_c$; the results are consistent with a proposed new type of activated dynamic scaling. The transition appears to be continuous, with effective critical exponents $\eta = 0.5 \pm 0.1$ and $\bar{\eta} = -1.0 \pm 0.3$ for strong fields, away from the weak-field regime where crossover effects distort exponent estimates. These strong-field exponents satisfy recently derived inequalities.

PACS numbers: 75.40.Dy, 05.50.+q, 64.60.Cn, 64.60.Ht

The nature of the phase transition in random-field Ising systems is a problem that has been challenging both theorists and experimentalists for a decade now.[1] Thanks to recent rigorous work[2] the existence of a finite-temperature phase transition in three dimensions is now well established. The equilibration time, τ, for experimental random-field Ising magnets appears to increase very rapidly as this transition is approached from above, as seen in ac susceptibility measurements,[3] and can exceed experimental time scales (hours or days) when the correlation length, ξ, is on the order of 100 lattice spacings.[4]

We have simulated the dilute antiferromagnetic Ising model in a field on a simple cubic lattice, which is a random-field system[5] closely modeling the magnetic systems studied experimentally.[3,4,6] We find that the correlation time does indeed increase very rapidly. In addition, we find that conventional dynamic scaling, in which correlations between measurements separated by a time interval t scale as functions of t/τ, does not hold for this system. This is in agreement with a recent suggestion[7] that the appropriate scaling variable is instead $\ln t/\ln\tau$. Our results are consistent with the prediction[7]

$$\ln\tau \sim \xi^{\theta}, \tag{1}$$

although to really test such a law requires looking at a range of $\ln\tau >> 1$, which is not possible without having a few orders of magnitude more computer time available.

Here we report results obtained at temperatures and fields where it could be verified that our samples reached thermal equilibrium. Because τ diverges so rapidly, equilibrium could not be obtained very close to the transition in strong fields. Therefore we must caution that, as usual, all critical exponents we report must be viewed as effective exponents, since they are extracted from data taken at fairly small correlation lengths.

The staggered susceptibility, χ, scales as $\chi \sim \xi^{2-\eta}$. We find

$$\eta = 0.5 \pm 0.1, \tag{2}$$

which is significantly larger than the $\eta = 0.25 \pm 0.03$ measured by Young and Nauenberg[8] for the random-field Ising model, and is large enough to satisfy the recently derived inequality[9] $\eta \geq \frac{1}{2}$. The data in Ref. 8 (as well as the experimental data in Ref. 6) are taken at a fairly weak random field and temperatures where crossover from non-random-field ($\eta \simeq 0$) to random-field ($\eta \geq \frac{1}{2}$) critical behavior should be occurring. This is presumably why a smaller value of η was measured. Our result (2) for η, on the other hand, is obtained from measurements at strong fields, away from this crossover regime, and so should be more representative of the random-field Ising universality class. We have also performed simulations in a weak field comparable to that used in Ref. 8, where we find an effective exponent $\eta \simeq 0.3$, which we again attribute to crossover.

For the disconnected part of the staggered susceptibility, $\chi^{\mathrm{dis}} \sim \xi^{2-\bar{\eta}}$, we find $\bar{\eta} = -1.0 \pm 0.3$, which satisfies, within errors, the inequalities $2(\eta - 1) \geq \bar{\eta} \geq -1$ and is in reasonable agreement with the experimental measurement[4] $\bar{\eta} = -1.15 \pm 0.1$. The correlation-length exponent that we measure is $\nu = 1.3 \pm 0.3$, which has large enough uncertainties to be consistent with the various recent numerical and experimental measurements.[4,6,8] An expansion[10] to first order in $\epsilon = d - 2$ yields $\eta = \frac{1}{2}$, $\bar{\eta} = -1$, and $\nu = 1$, which are also in reasonable agreement with our results. For the exponent in (1) we find an effective exponent $\theta \simeq 0.9$, which is less than expected from the proposed scaling relation[7] $\theta = \eta - \bar{\eta} = 1.5 \pm 0.4$. This discrepancy is probably not significant because of the uncertainties involved in extracting the estimate of θ from our data and the narrow range of $\ln\tau$ and ξ that we have been able to study.

Finally, we do not see any evidence for a first-order transition. Any hysteretic behavior that we have seen can be attributed to the very long equilibration times of even a finite system near the critical temperature.

The model that we have studied has the Hamiltonian

$$H = \sum_{ij} s_i s_j - h \sum_i s_i, \tag{3}$$

where the sums run over all nearest-neighbor pairs and all sites, respectively, on an $L \times L \times L$ simple cubic lattice with periodic boundary conditions. Each spin is present with probability p, independent of the other spins. Those spins that are present take on values $s_i = \pm 1$, while those that are absent have $s_i = 0$. Note that the antiferromagnetic nearest-neighbor coupling has strength unity $(J=1)$. For each size lattice, temperature, and field strength, we have looked at a number of different realizations (distributions of vacant sites) sufficient to reduce sampling errors to an acceptable level. The variation of measured quantities can be substantial from realization to realization, particularly when the correlation length is large. The simulations were performed on a special purpose computer that executes the heat-bath algorithm.[11]

The bulk of our data are taken above the transition temperature with $p = 70\%$ along the path $h/T = 1.5$. Other fields and concentrations that we studied were the path $h/T = 0.6$ and constant fields $h = 1.5$ and $h = 0$ for $p = 70\%$, and the paths $h/T = 1.0$, $h/T = 0.4$, and $h = 0$ for $p = 50\%$. We concentrated on $p = 70\%$ in order to be well away from both the percolation threshold $(p \simeq 31\%)$ and the pure case $(p = 100\%)$. We chose the path $h/T = 1.5$ in order to be well away from the crossover to zero-field behavior and so we would not approach the phase transition line in the h-T plane in a highly oblique fashion, as would occur if we kept h fixed at a value where $dT_c(h)/dh$ is large. Along this path we studied 64 lattices with $L = 16$, 22 with $L = 32$, and 4 with $L = 64$. For $p = 70\%$ and $h = 0$ we estimate the critical temperature to be $T_c(0) \simeq 2.9$ in agreement with earlier results of Landau[12]; along the path $h/T = 1.5$ we find $T_c(h) = 1.50 \pm 0.15$. That the critical temperature is roughly cut in half shows that we are used a strong field. This contrasts with the rather weak field chosen in Ref. 8, which only reduced T_c by approximately 13% from its $h = 0$ value. In Fig. 1 we show the inverse correlation length, ξ^{-1}, and the inverse square root of the staggered susceptibility, $\chi^{-1/2}$, as functions of temperature for $p = 70\%$ and $h/T = 1.5$. We obtain the correlation length by fitting the momentum dependence of the staggered susceptibility $\chi(q)$ by a Lorentzian form for $q\xi \lesssim 1$, as is described in Ref. 8. The data presented in this paper do not exhibit visible finite-size effects: This is secured by comparing results from different lattice sizes and presenting only data for L large enough. For measurements of ξ and the susceptibilities, $L > 2\pi\xi$ suffices, but the long-time portion of the

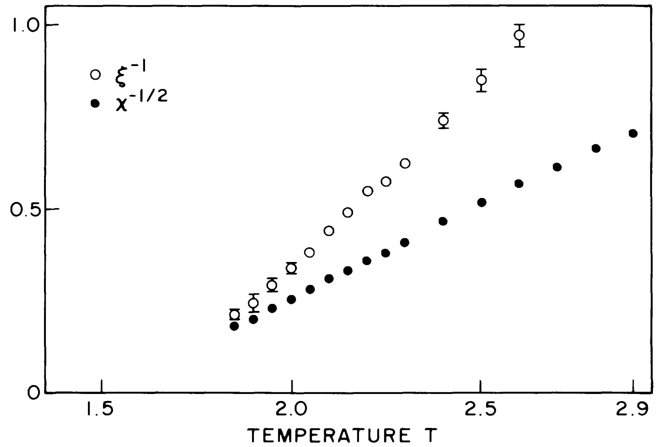

FIG. 1. Inverse correlation length ξ^{-1} and the square root of the inverse staggered susceptibility $\chi^{-1/2}$, for $p = 70\%$ and $h/T = 1.5$. The critical temperature here is estimated to be $T_c(h) = 1.50 \pm 0.15$ from a fitting of these data by the usual power-law form.

time correlation functions (see below) is somewhat more sensitive to finite-size effects.

We must discuss the dynamics first in order to establish that the static measurements that we report represent equilibrium properties. The dynamic scaling behavior is also of interest in its own right, especially because of the unconventional scaling, Eq. (1), predicted.[7] The order parameter and slowest mode in this dilute simple-cubic antiferromagnet is the total staggered magnetization, $M^\dagger$. Therefore we have studied its normalized time correlation function:

$$C(t) = \langle\langle [M^\dagger(0) - \langle M^\dagger\rangle_t] \times [M^\dagger(t) - \langle M^\dagger\rangle_t]\rangle_t\rangle_R / L^3\chi, \tag{4}$$

where the staggered susceptibility is

$$\chi = \langle\langle (M^\dagger - \langle M^\dagger\rangle_t)^2\rangle_t\rangle_R / L^3, \tag{5}$$

$\langle\ldots\rangle_t$ denotes thermal averaging, and $\langle\ldots\rangle_R$ denotes an averaging over different realizations. Note that we have normalized so that $C(t=0) = 1$.

Our results for $C(t)$ at $p = 70\%$, $h/T = 1.5$, and various temperatures are presented in Fig. 2. The unit of time is one Monte Carlo update per spin (MCS). The conventional dynamic scaling *Ansatz* says that $C(t)$ should scale as some function of t/τ, where τ is the correlation time. When plotted versus time on a logarithmic scale, as in Fig. 2, the change in τ from one temperature to the next would then just shift the $C(t)$ curve without changing its shape. That such a scaling *Ansatz* does not describe our data is apparent from Fig. 2, where the decay occurs over larger and larger intervals of $\ln t$ as T decreases and τ increases. The conventional scaling hypothesis also says $\tau \sim \xi^z$, where z is the dynamic critical exponent. Here, how-

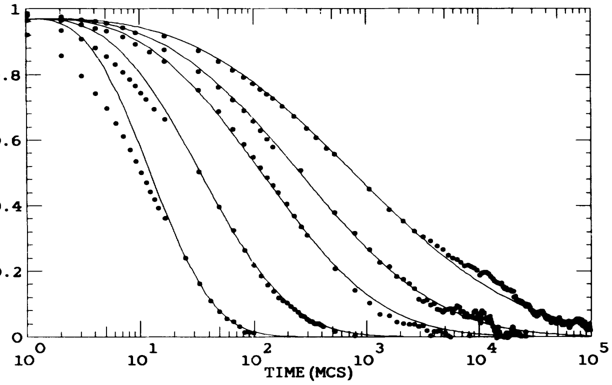

FIG. 2. Time correlation function $C(t)$ for the total staggered magnetization, Eq. (4), recorded with $p=70\%$ along the path $h/T=1.5$ for $T=2.30$, 2.10, 1.95, 1.90, and 1.85 from left to right. Solid lines are fits with the empirical form given by Eq. (6).

ever, we find that the measured average correlation time grows faster than a power of ξ.

The critical behavior of the random-field Ising model is thought to be governed by a zero-temperature fixed point, where the dynamics of fluctuations at long lengths ξ is dominated by thermal activation over free-energy barriers, scaling as ξ^{θ}, with $\theta=\eta-\tilde{\eta}$.[7] In this picture a new dynamic scaling hypothesis has been suggested,[7] according to which the appropriate scaling variable is $\ln t/\ln\tau$ rather than the usual t/τ, and the correlation time should diverge exponentially as in Eq. (1).

Our results are quite consistent with this new scaling *Ansatz.* We find that the measured correlation functions (4) indeed scale well as functions of $\ln t/\ln\tau$, except at very short times and higher temperatures, where scaling need not hold. An empirical function that fits the data reasonably well for $t>20$ MCS is

$$C(t)\approx C_0\exp\{-(\ln t/\ln\tau)^3\}. \tag{6}$$

Correlation functions for several values of temperature are shown in Fig. 2 together with fits by this function. The constant C_0 is temperature independent and close to unity; we have chosen $C_0=0.97$. We do not claim that (6) is the correct form of the scaling function, but merely that it describes the data well in the regime that we are studying. The logarithm of the correlation time, $\ln\tau$, has been estimated along the path $h/T=1.5$ for a range of temperatures in two ways: (1) We have found the temperature dependence of $\ln\tau(T)$ that allows us to scale the correlation functions at the different temperatures to a single curve, and (2) we have have obtained a $\ln\tau$ at each temperature by fitting with (6). The measured values of $\ln\tau$ are shown in Fig. 3. These two procedures give the same temperature dependence of $\ln\tau$, except at the very highest temperature $T=2.3$ which is not fitted well, as do various oth-

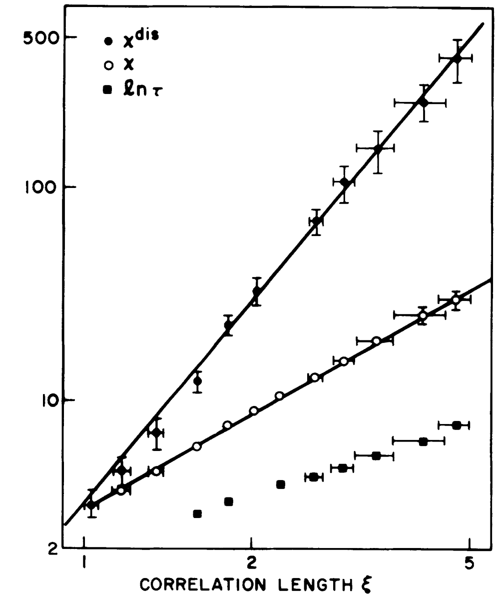

FIG. 3. Log-log plot of the connected and disconnected staggered susceptibilities, χ and χ^{dis}, and of the natural logarithm of the correlation time, $\ln\tau$, showing their dependence on the correlation length ξ. Data are for $p=70\%$ along the path $h/T=1.5$.

er reasonable ways of estimating $\ln\tau$ that we have tried. The results are consistent with Eq. (1) with an effective exponent $\theta\simeq0.9$, lower than the value of about 1.5 estimated from the static measurements and the proposed scaling relation[7] $\theta=\eta-\tilde{\eta}$. However, there is a hint of an increase in the effective θ at lower temperatures, and estimated lower bounds on correlation times closer to $T_c(h)$ which are not presented here suggest that this trend continues and we may not yet be in the asymptotic dynamic scaling regime. We do not quote an error on our estimate of θ because we do not know how to estimate the possible systematic errors due to our fitting scheme and because of the rather narrow range of $\ln\tau$ and ξ studied.

Let us now return to the static critical behavior. Three-parameter fits of the usual form, $\chi\approx A[T-T_c(h)]^{-\gamma}$, for the susceptibility and correlation length yield exponent estimates $\gamma=2.0\pm0.5$ and $\nu=1.3\pm0.3$, respectively. The exponent η in $\chi\sim\xi^{2-\eta}$ can be estimated much more accurately because we need not estimate $T_c(h)$. Fitting a straight line to the data in Fig. 3 yields $\eta=0.5\pm0.1$. The exponent for the disconnected staggered susceptibility

$$\chi^{\text{dis}}=\langle\langle M^{\dagger}\rangle_t^2\rangle_R/L^3\sim\xi^{2-\tilde{\eta}} \tag{7}$$

is estimated to be $\tilde{\eta}=-1.0\pm0.3$; see Fig. 3. These exponents satisfy, within errors, the recently derived[9] inequalities $2(\eta-1)\geqslant\tilde{\eta}\geqslant-1$. That $\tilde{\eta}$ is so near -1 means that the order-parameter exponent[7] $\beta=(1+\tilde{\eta})\nu/2$ is very near zero, which, when combined with the long equilibration times, may make the behavior of the order parameter as a function of temperature look like a first-order transition.[8] We feel that all the numerical, experimental, and theoretical evidence reported here and elsewhere is consistent with a phase transition that is continuous in equilibrium, but has an exponentially divergent correlation time, Eq. (1), as $T \rightarrow T_c(h)$.

We have also measured specific heats; along the path $h/T = 1.5$ at $p = 70\%$ the specific heat saturates around $T = 2.05$ where $\xi \simeq 2.5$, and for lower temperatures is constant within our $\pm 3\%$ errors, showing absolutely no tendency to diverge at T_c. (Of course, the specific heat decreases again below T_c.) This result suggests that the specific-heat exponent α is negative, and contrasts with the interpretation of the birefringence data,[6] which proposes a divergent specific heat at T_c.

We also examined lattices with $p = 70\%$ in uniform field $h = 1.5$, where $T_c(h) \simeq 2.5$. We found an effective $\eta \simeq 0.3$ in the range $2.7 \leqslant T \leqslant 3.5$. This is in the region where crossover to random-field behavior is expected. Note that T_c is suppressed approximately 13% from its $h = 0$ value just as in Ref. 8, where they found $\eta = 0.25 \pm 0.03$. Therefore the random-field strengths are quite comparable and it is not surprising that similar values of η are measured. For $h = 0$ we expect and find an effective $\eta \simeq 0.05$; as the field increases the effective exponent must change to $\eta \simeq 0.5$ for strong fields. Thus the $\eta \simeq 0.3$ measured at intermediate fields is quite consistent with a simple crossover and should definitely not be viewed as a candidate for the asymptotic $T \rightarrow T_c(h)$ exponent. The field $h/T = 1.5$ is, we believe, sufficiently strong that the effective exponent $\eta = 0.5 \pm 0.1$ measured there might be a good estimate of the asymptotic equilibrium η. We have also looked at the more disordered case $p = 50\%$ in strong fields $h/T = 1.0$, and again find $\eta \simeq 0.5$.

We made some preliminary measurements in the ordered phase, $T < T_c(h)$, for $p = 70\%$ and $h/T = 1.5$, starting from the fully antiferromagnetically ordered state at $T = 0$, $h = 0$ and warming up. We found that this ordered state remained stable for $T < T_c(h)$ on the time scales examined ($\lesssim 10^6$ MCS). However, we cannot verify that we reached thermal equilibrium, especially close to the transition where equilibriation times certainly exceeded 10^6 MCS. In this work we did not attempt to study the "domain states" obtained for $T < T_c(h)$ by field cooling,[4,6] which are presumably not in full equilibrium.

We thank D. S. Fisher for many useful discussions.

Note added.—Recent zero-temperature scaling analysis of the *ferromagnetic* random-field Ising model confirms that $\tilde{\eta}$ is very close to -1.[13]

[1]Y. Imry and S.-k. Ma, Phys. Rev. Lett. **35**, 1399 (1975).

[2]J. Imbrie, Phys. Rev. Lett. **53**, 1747 (1984).

[3]J. A. Mydosh, A. R. King, and V. Jaccarino, J. Magn. Magn. Mater. **54–57**, 47 (1986); A. R, King, J. A. Mydosh, and V. Jaccarino, to be published.

[4]R. J. Birgeneau *et al.*, Phys. Rev. Lett. **54**, 2147 (1985), and Physica (Amsterdam) (to be published).

[5]S. Fishman and A. Aharony, J. Phys. C **12**, L729 (1979).

[6]D. P. Belanger, A. R. King, and V. Jaccarino, Phys. Rev. B **31**, 4538 (1985).

[7]D. S. Fisher, Phys. Rev. Lett. **56**, 416 (1986); see also J. Villain, J. Phys. (Paris) (to be published), for some of the same results obtained in a very different manner.

[8]A. P. Young and M. Nauenberg, Phys. Rev. Lett. **54**, 2429 (1985).

[9]M. Schwartz and A. Soffer, Phys. Rev. Lett. **55**, 2499 (1985); see Fisher, Ref. 7, for more discussion of the inequalities.

[10]A. J. Bray and M. A. Moore, J. Phys. C **18**, L927 (1985).

[11]J. H. Condon and A. T. Ogielski, Rev. Sci. Instrum. **56**, 1691 (1985).

[12]D. P. Landau, Phys. Rev. B **22**, 2450 (1980).

[13]A. T. Ogielski, to be published.