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Domain growth in the three-dimensional random-field Ising model

Enis Oğuz
Physics Department, Boğaziçi University, 80815 Istanbul, Turkey

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Abstract. Domain growth in the three-dimensional random-field Ising model is investigated by Monte Carlo simulation. The time dependence of the average domain size is monitored following a quench to a low temperature. The logarithmic growth predicted by the theories of Villain and of Grinstein and Fernandez is observed. The dynamical scaling of the structure factor is also studied and found to be well satisfied. The field strength dependence of the scaling function is found to be weak.

1. Introduction

In recent years there has been a great interest in random-field Ising (RFIM) systems both theoretically and experimentally (for reviews, see [1]). It is now well established that in three dimensions the RFIM is ordered at low temperatures for small field strengths, while in two dimensions there is no long-range order for any finite field strength [1–3]. Thus, the lower critical dimension of this model is now known to be 2.

Non-equilibrium properties of the RFIM have also been a focus of interest [1]. The presence of a random field strongly affects the dynamics of growing domains which are formed when the system is quenched from a disordered state to a low temperature state. In the pure (zero-field) system, the average domain size R obeys the well known Lifshitz–Allen–Cahn (LAC) growth law [4]:

$$R(t) \sim t^{1/2} \tag{1.1}$$

where t is the time. In the RFIM, the curvature-driven growth mechanism that leads to (1.1) is impeded by the random field induced roughening of the domain walls. In a late-time regime, the domains tend to get pinned in favourable locations and further growth relies on thermal fluctuations to surmount the energy barriers introduced by local fluctuations of the random field [1].

Several theories have been developed to analyse the time dependence of R. Grant and Gunton [5] investigated the growth using a generalized LAC analysis. Their theory, which is expected to apply in the early stages of growth [5, 7], predicts that in three dimensions the growth law is unchanged from the zero-field result (1.1) except for a field-dependent reduction in the amplitude:

$$R(t) \sim [A - Bh^2]t^{1/2} \tag{1.2}$$

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where h is the field strength and A and B are field-independent constants. In two dimensions, the Grant and Gunton prediction for $R(t)$ differs from (1.2) by a time-dependent term in the amplitude and yields a maximum size for the domains in equilibrium.

Villain [6] considered a continuum version of the RFIM and investigated the kinetics of the interfaces in a late-time regime where pinning is effective. By estimating the maximum height of the scale-dependent energy barriers encountered by the domain walls and using the Arrhenius law, he deduced a logarithmic dependence for R, independent of dimensionality,

$$R(t) \sim \frac{T}{h^{\nu_1}} \ln t \tag{1.3}$$

where $\nu_1 = 2$ and T is the temperature.

Grinstein and Fernandez [7] used a discrete-lattice RFIM and studied the domain growth in the framework of a solid on solid model. They argued that at low temperatures three-dimensional domain walls decay through peeling of two-dimensional layers. They estimated the typical decay time of such layers using an analysis similar to that of Villain's in the continuum case. Their result coincided with (1.3) apart from a factor of 2. For shorter times when the decay of two-dimensional layers is dominated by the diffusion of isolated kinks on their boundaries, they predicted a logarithm-square time dependence for R:

$$R(t) \sim \frac{T^2}{4h^{\nu_2}} \ln^2 t \tag{1.4}$$

where $\nu_2 = 2$.

In contrast to the above predictions, experiments on dilute antiferromagnets in uniform fields, which are physical realizations of the RFIM, have shown that the average size of the domains does not change with time when the system is cooled to a low temperature in the presence of an external field [1, 8]. The discrepancy is believed to be due to the pinning effect of the vacancies that are present in dilute antiferromagnets but not in the RFIM [1, 9].

Domain growth in the RFIM has been the subject of several numerical simulations as well. The two-dimensional case has been studied extensively and the predictions of the above theories have been tested. Equation (1.4) was verified by Pytte and Fernandez [10], Chowdury and Stauffer [11], and Anderson [12]. The logarithmic growth (1.3) was observed by Anderson [12], Oğuz *et al* [13] and recently by Puri and Parekh [14]. The dynamical scaling behaviour of the structure factor was also studied. For high field strengths, evidence for a breakdown of scaling was obtained [13–15]. For smaller fields, the scaling was found to be well satisfied with a scaling function that is independent of the field strength [14]. There have been fewer studies in the three-dimensional case. Stauffer *et al* [16] qualitatively pointed out the slowness of the growth. Pytte and Fernandez [10] studied the decay times of small domains by Monte Carlo simulation and observed a logarithm-square growth (1.4). Chowdury and Stauffer [11] investigated the growth by measuring the relaxation time of magnetization and tested the various theories. Their results were consistent with a power law growth at short times and a logarithm-square growth (1.4) at later times.

A logarithmic dependence of R on time as in (1.3) has not been observed in the above three-dimensional simulations. Thus, the prediction in (1.3) has been left unverified. As well the scaling behaviour of the structure factor in three dimensions has not been studied. In order to investigate these features and to study the various growth regimes in more detail we have here carried out further Monte Carlo simulations of the three-dimensional kinetic RFIM. (We have only considered the case with a non-conserved order parameter.) To be able to investigate various stages of the growth within the duration of our simulations we have considered a wide range of field strengths from zero to large values close to the phase boundary. Our main results are as follows. For some large field strengths, we have obtained fairly extended intervals of time in which our data are consistent with a logarithmic growth (1.3). We have also observed intervals of logarithmic-square growth (1.4) for several intermediate fields. The short-time growth is consistent with the modified LAC formula (1.2) only for small field strengths. Finally, we have found that the dynamical scaling of the structure factor is well satisfied with a scaling function that is weakly dependent on the field strength.

In section 2 we describe the model and the method of numerical calculations. In section 3 we present our results. We conclude with a brief summary in section 4.

2. Model and the method of calculation

The Hamiltonian for the RFIM is given by

$$\mathscr{H}/J = -\sum_{\langle ij\rangle} \sigma_i\sigma_j - \sum_i h_i\sigma_i \tag{2.1}$$

where $\sigma_i = \pm 1$, J is the coupling constant and the interaction sum runs over nearest-neighbour pairs of N spins. The dimensionless random magnetic fields h_i are assumed to take on the values $\pm h$ randomly at each site and the values at different sites are uncorrelated. Thus,

$$\langle h_i\rangle = 0 \tag{2.2a}$$

and

$$\langle h_i h_j\rangle = h^2\delta_{ij}. \tag{2.2b}$$

The dynamics is generated by the standard Monte Carlo spin–flip algorithm [17] with Glauber flip probabilities:

$$W_i = \tfrac{1}{2}[1 - \tanh(\Delta E_i/2kT)] \tag{2.3}$$

where k is the Boltzmann constant, T is the temperature and ΔE_i is the energy change that would result from flipping the spin σ_i. Time is measured in Monte Carlo steps per spin (MCS), which involves N attempts to flip randomly selected spins. We used a simple cubic lattice of linear size $L = N^{1/3} = 64$ with periodic boundary conditions and employed the multispin coding technique. The random field variables were generated at the beginning of each run according to the distribution (2.2), and this configuration remained fixed for the duration of the run. We used a random initial distribution for the spins, corresponding to an infinite initial temperature. For the final temperature of the quench we chose $T = 1.5J/k$, which is roughly one-third of the critical temperature of the pure model. To find the approximate location of the phase boundary at this temperature, we computed the equilibrium magnetization by making runs with 250 000 MCS, discarding the first 100 000 MCS for equilibrium. (We used a completely ordered

Table 1. Equilibrium magnetization for several field strengths near the phase boundary.

h	M
2.20	0.89 ± 0.01
2.25	0.66 ± 0.04
2.30	0.39 ± 0.06
2.35	0.23 ± 0.05
2.40	0.04 ± 0.01

initial state for these particular runs.) The data are averaged over five independent runs. Our results summarized in table 1 suggest that the critical field is approximately located at $h_c = 2.3$.

We monitored the time dependence of the domain size R for a variety of field strengths and for times up to 20 000 MCS. The averages were calculated over an ensemble of at least 200 runs for each field strength we considered. (The statistical error in R based on sample to sample variations was less than 5%.) Our simulations were entirely carried out on PC microcomputers over the course of many months. (The time-critical parts of the computer program were written in assembly code. The program produced about 9×10^5 spin updates per second on a 50 MHz machine).

We have determined the average domain size by the relation [18]

$$R(t) = \frac{1}{L}\left\langle\left(\sum_i \sigma_i\right)^2\right\rangle^{1/3} \tag{2.4}$$

which corresponds to the structure factor evaluated at zero wavevector. (R is measured in units of the lattice spacing.) We have also computed other length scales derived from the perimeter area density and the moments of the structure factor with respect to wavenumber. We have found that the known results in the zero-field case, i.e. the LAC growth and the dynamical scaling of the structure factor were best reproduced by using the length scale given in (2.4). Thus, we will discuss our results here in terms of this length scale only.

To investigate the scaling behaviour we have also computed the non-equilibrium structure factor

$$s(\mathbf{k}, t) = \frac{1}{N}\left\langle |\sigma_{\mathbf{k}}|^2 \right\rangle \tag{2.5}$$

where $\sigma_{\mathbf{k}}$ is the Fourier transform of σ_i:

$$\sigma_{\mathbf{k}} = \sum_{i=1}^{N} \sigma_i \exp(i\mathbf{k} \cdot \mathbf{r}_i). \tag{2.6}$$

Here $\mathbf{r}_i$ and $\mathbf{k}$ denote positions on the space and wavevector lattices, respectively. We have performed a circular average on the $s(\mathbf{k}, t)$.The circularly averaged quantity will be denoted by $S(k, t)$. Here, the wavenumber $k = 2\pi j/L$ with $j = 0, 1, 2, \ldots, j_{\max}$, where $j_{\max}$ is the integer fraction of $\sqrt{3}L/2$. Let us recall that in d dimensions the dynamical scaling condition states that [19]

$$S(k, t) = R^d(t)F(kR(t)) \tag{2.7}$$

where $F(x)$ is the scaling function. Thus, here we have computed the scaling function in the form

$$F(x)=\frac{S(k,t)}{R^3(t)} \tag{2.8}$$

where $x=kR(t)$. We discuss our results in the next section.

3. Results

We first present our zero-field ($h=0$) result for $R(t)$, which we have included here as a check on our method against known results. As seen in figure 1, a clear LAC growth

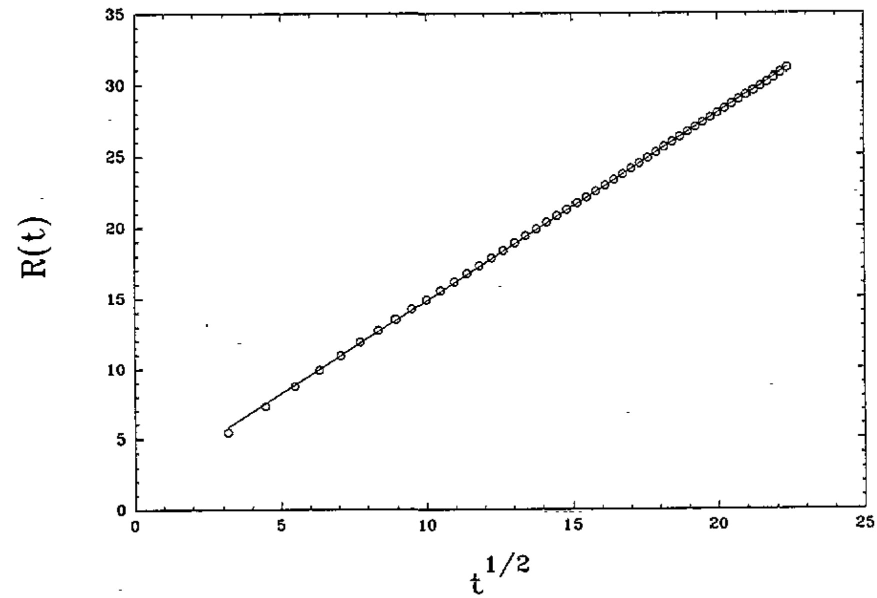

Figure 1. $R(t)$ versus $t^{1/2}$ in the absence of a random field. The full line shows the linear best fit to the data.

is obtained. ($R(t)$ starts deviating from the LAC growth for $R \gtrsim 35$ (not shown) due to finite-size effects. Thus, to avoid these effects we have studied the growth only up to times such that $R \lesssim 35$, here and in the case of finite fields as well.) In the absence of a field, it is also known that the structure factor satisfies dynamical scaling (2.7) [19] and the scaling function is well approximated by the theory of Ohta, Jasnow and Kawasaki (OJK) [20]. Figure 2 shows our scaling function data in comparison with the prediction of OJK. (The OJK scaling function was normalized (such that $F(0)=1$) and the proportionality constant between the OJK scaling variable $x_{\rm OJK}$ and ours x was adjusted as $x_{\rm OJK}/x=1.2$.) We obtain good scaling and the scaling function is fairly well described by the OJK theory.

We not turn to the case of finite fields and first consider the growth in the short-time regime. As mentioned previously, the Grant and Gunton theory [5] predicts a modified LAC growth (1.2) with an amplitude that decreases with the field strength. To check the $t^{1/2}$ dependence, we plot $R(t)$ versus $t^{1/2}$ in figure 3 for times up to $t=$

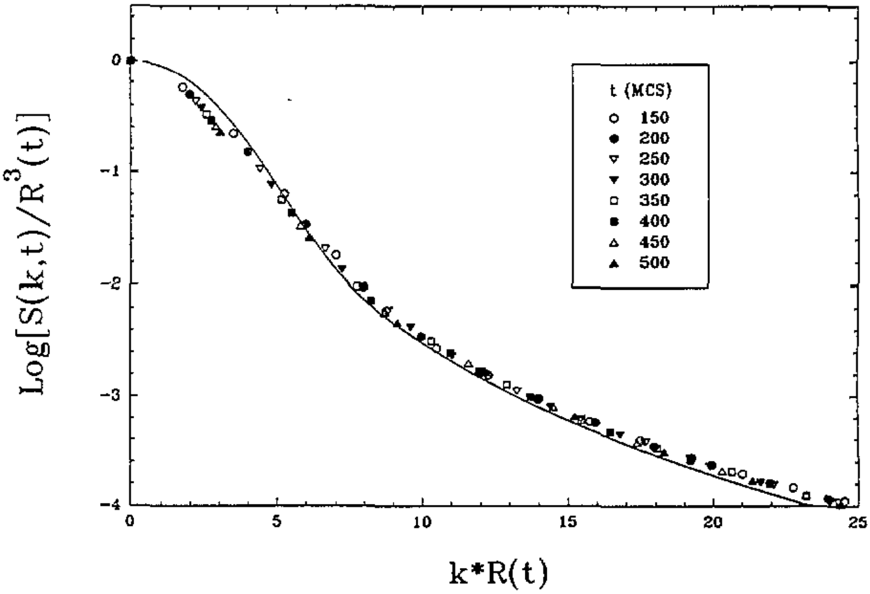

Figure 2. Zero-field scaling function. The full line is the theoretical prediction of OJK [20].

500 MCS and for some relatively small field strengths ($h \leqslant 1.0$). We obtain a fairly straight curve for $h=0.2$ and to a lesser extent for $h=0.4$. As h is increased to higher values, the curvatures of the plots rapidly increase, confining the $t^{1/2}$ growth regime to extremely early times, as can be seen from figure 3. Thus, (1.2) appears to be a reasonable description of the short-time growth only for field strengths $h \leqslant 0.4$. We have not been able to quantitatively investigate the amplitude in (1.2). We have found that a somewhat

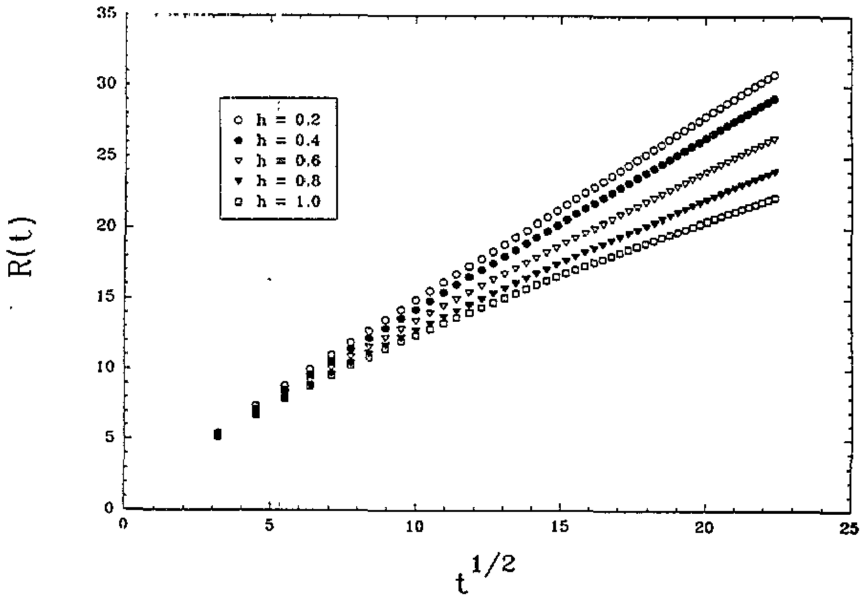

Figure 3. $R(t)$ versus $t^{1/2}$ for several field strengths h.

better approximation for $R(t)$ in the regime $t \lesssim 500$ MCS and $h \lesssim 1.0$ is a power law growth with an exponent which uniformly decreases from its initial value of 0.5 as the field strength is increased from zero. This power law regime may represent a cross-over behaviour between the initial LAC growth and the activated growth regime which is expected to apply at later times.

We now consider the growth for longer times up to $t=5000$ MCS and investigate the validity of (1.4). Figure 4 shows $R(t)$ as a function of $\ln^2 t$ for several field strengths

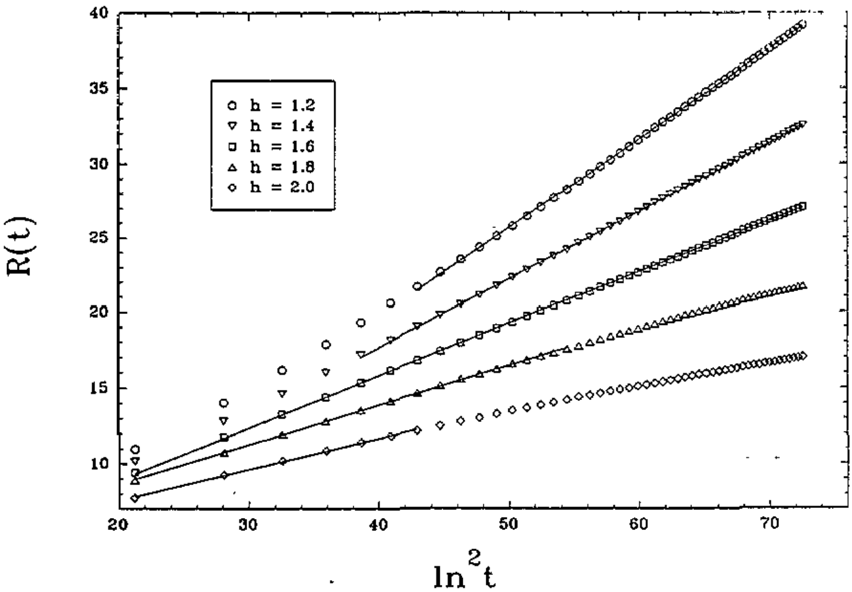

Figure 4. $R(t)$ versus $\ln^2 t$ for several field strengths h. Intervals in which the growth is approximately $\ln^2 t$ are indicated by full lines.

in the range $1.2 \leqslant h \leqslant 2.0$. It is seen that for each field strength an interval can be obtained in which the data are consistent with a $\ln^2 t$ growth, as indicated by the full lines. (The criterion for determining the fitting intervals is inevitably somewhat arbitrary. We sought to maximize the size of the interval while still maintaining a good fit.) We note that the observed $\ln^2 t$ growth interval shifts towards earlier times as the field strength is increased. This behaviour can be qualitatively understood by considering the fact that as h is increased, the retarding effects of the random field on the curvature-driven growth are expected to become appreciable at smaller domain sizes and thus at earlier times.

As can be clearly seen in figure 4 for $h=1.8$ and $h=2.0$, the $\ln^2 t$ growth eventually crosses over to a slower growth regime. We have investigated the validity of the logarithmic growth (1.3) in this regime for times up to $t=20\,000$ MCS and for field strengths in the range $1.6 \leqslant h \leqslant 2.4$. As shown in figure 5, we do obtain intervals in which the data are consistent with a logarithmic growth. As h is increased from 1.6, the lower boundary of the $\ln t$ growth interval rapidly shifts towards earlier times, resulting in a fairly extended $\ln t$ growth regime for $h=2.0$. For $h=2.2$, our data indicate an even slower growth than $\ln t$ for late times. This further slowing of the growth may be due to the effects of critical fluctuations in view of the fact that $h=2.2$ lies in close vicinity to the phase boundary $h_c \simeq 2.3$ according to our equilibrium results mentioned earlier.

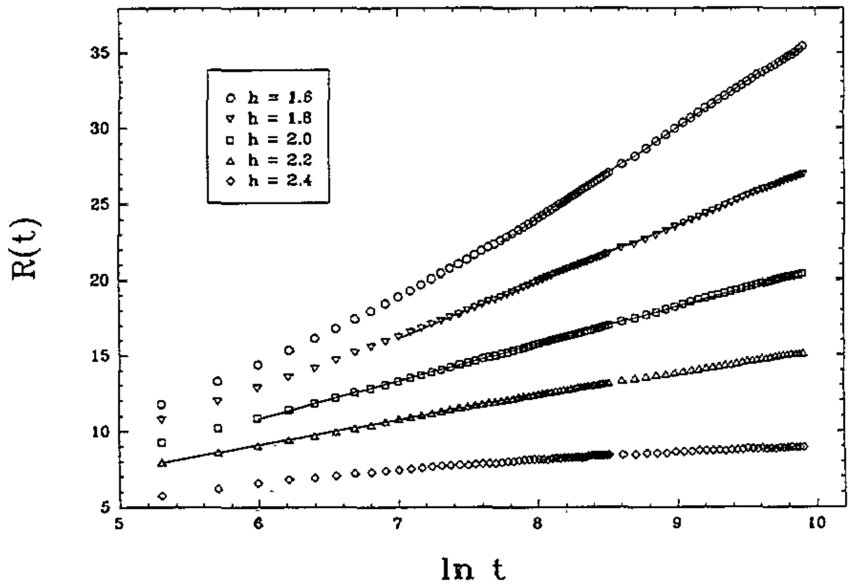

Figure 5. $R(t)$ versus $\ln t$ for several field strengths h. Intervals in which the growth is approximately $\ln t$ are indicated by full lines.

At $h=2.4$, which is on the disordered side of the phase boundary, $R(t)$ indeed grows extremely slowly after initial times, displaying a final approach to equilibrium with a rather small equilibrium value.

We have not been able to investigate the validity of (1.3) or (1.4) for small field strengths ($h \lesssim 1.0$), since this would require much longer simulation times and also much larger lattices to avoid the finite-size effects. Due to the relatively small number of h-values for which we obtained a $\ln^2 t$ or $\ln t$ growth interval and to the difficulty in judging the precise locations of such intervals, we have also not been able to make an accurate analysis of the exponents ν_1 and ν_2 in (1.3) and (1.4). An inspection of the slopes in figures 4 and 5 nevertheless gives the rough estimates $\nu_1=3.9$ and $\nu_2=2.1$, to be compared with the Villain and Grinstein and Fernandez prediction of $\nu_1=\nu_2=2$. We note that the exponents ν_1 and ν_2 determine the location of the cross-over regime between (1.3) and (1.4), as can be seen from the characteristic cross-over time $\tau \sim \exp(4h^{\nu_2-\nu_1}/T)$, which one can derive from (1.3) and (1.4). A higher value for ν_1 compared to ν_2, as we obtain here, thus means that the cross-over time should decrease with increasing field strength. We note that this property of the cross-over time is clearly implied by our results contained in figures 4 and 5, in view of the shift of the observed $\ln^2 t$ and $\ln t$ growth intervals towards earlier times as the field strength is increased. The displacement of the various growth regimes towards earlier times with increasing field strength has also been observed in simulations of the two-dimensional RFIM [12, 13].

We now turn to the scaling behaviour of the structure factor. Our scaling function data indicate that the scaling persists for non-zero field strengths. We have observed fairly good scaling for all the field strengths we have considered above. The onset of the scaling regime rapidly shifts to later times as h is increased from zero. In figures 6(a) and 6(b), we show our scaling function data for $h=1.6$ and $h=2.2$. We have included the zero-field scaling function curve in these figures for comparison. (We

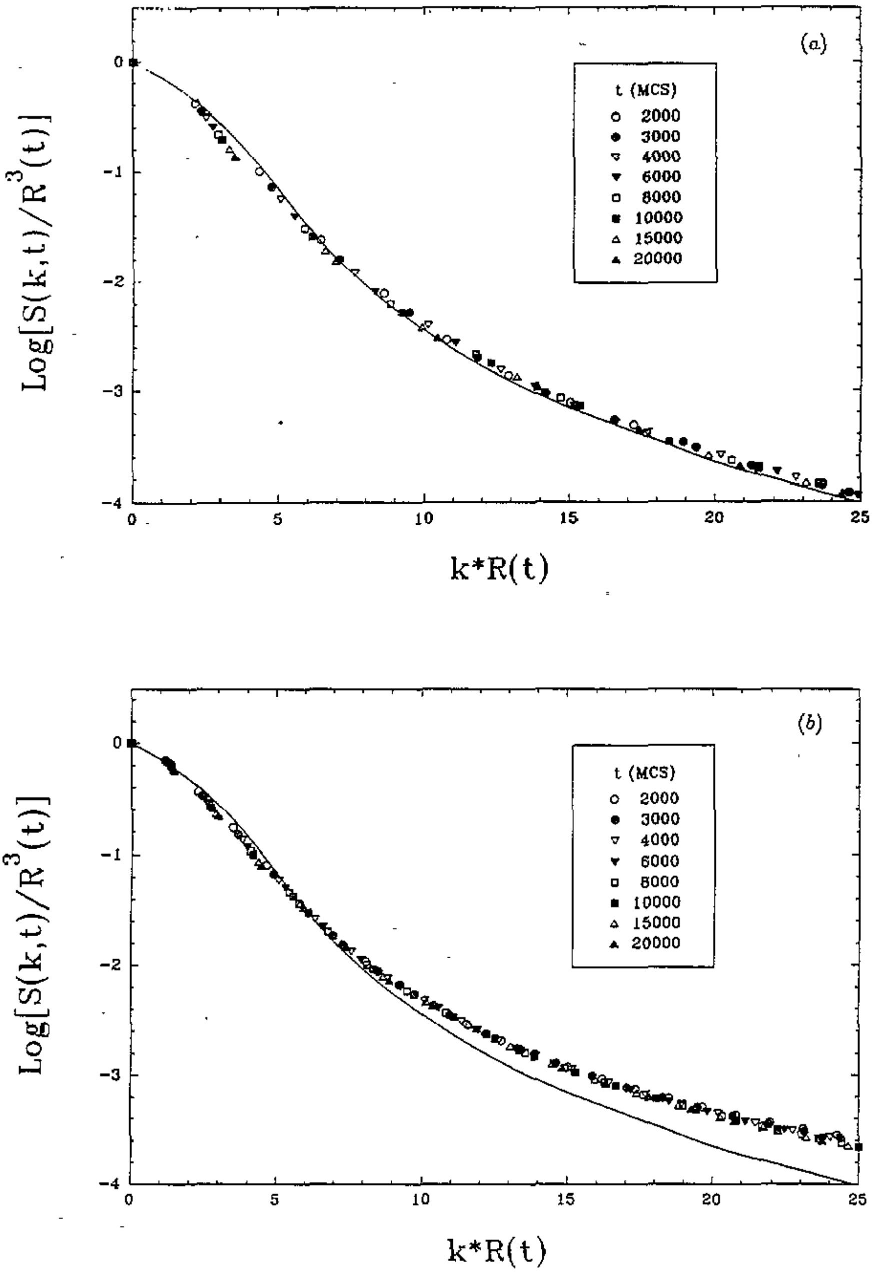

Figure 6. Scaling function for (*a*) $h=1.6$ and (*b*) $h=2.2$. The full line shows the zero-field scaling function, which is included for comparison.

present our scaling function data on a semi-logarithmic scale so as to display the large-x region more clearly.) We recall that in two-dimensions Puri and Parekh [14] found (in a continuum version of the RFIM) no field dependence for the scaling function for the field strengths they considered. Here we obtain a similar behaviour for $h \lesssim 1.6$, i.e. the scaling function does not show any appreciable deviation from the zero-field result for field strengths up to $h \simeq 1.6$. As h is increased to higher values, the scaling function does deviate from the zero-field curve. However, the deviation is very gradual and even for large field strengths the differences are only appreciable in the tail (large x) region, as can be seen in figure 6*b* for $h=2.2$. Thus, the field strength of the scaling function appears to be fairly weak, in sharp contrast with the drastic field dependence of the average domain size discussed above.

4. Conclusions

We have studied the domain growth in the three-dimensional RFIM through Monte Carlo simulation. Our results are in general consistent with theories of Villain [6] and of Grinstein and Fernandez [7]. In particular, the predicted logarithmic growth of the average domain size is observed. We have also studied the scaling of the structure factor and found that the scaling is well satisfied as in the case of the pure model. The field strength dependence of the scaling function is observed to be weak. Further theoretical and numerical work is necessary for a more accurate investigation of the prefactors in (1.3) and (1.4) and also for a quantitative analysis of the cross-over behaviour between different growth regimes as well as for an investigation of the temperature dependence of the growth.

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