

Finite-size-scaling analysis of domain growth in the kinetic Ising model with conserved and nonconserved order parameters

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Standard finite-size-scaling techniques are introduced to obtain domain growth exponents during a first-order phase transition. A scaling ansatz for the nonequilibrium structure factor in a finite lattice is presented. It explicitly includes a time rescaling exponent x , related to the domain growth exponent n ($n = 1/x$). We first analyze domain growth in the kinetic Ising model with a nonconserved order parameter. The method correctly gives the expected exponent $n = \frac{1}{2}$. We have also studied the kinetic Ising model with a conserved order parameter at a critical value of the order parameter. The scaling behavior of the peak of the structure factor is consistent with $n \approx 0.27$. The analysis of higher wave numbers is more consistent, however, with $n \approx 0.33$.

I. INTRODUCTION

When a system is rapidly quenched from a high-temperature, disordered equilibrium state to a low temperature below its transition point, domains of the new equilibrium phases appear and grow to macroscopic size as time passes.¹ Theoretical studies, computer simulations, and experimental evidence indicate that there is a regime in time after the quench in which the characteristic length scale in the system $\bar{R}(t)$ (related to the average size of the growing domains) follows a power law behavior in time

$$\bar{R}(t) \simeq At^n. \quad (1)$$

The nonequilibrium structure factor $S(q, t)$ (which is the spatial Fourier transform of the nonequilibrium average of the equal-time order-parameter-order-parameter correlation function) satisfies, to a very good approximation, a dynamic scaling relation

$$S(q, t) = [\bar{R}(t)]^d \mathcal{F}(q\bar{R}(t)), \quad t > t_0, \quad (2)$$

where $\mathcal{F}(x)$ is a universal function, independent of time. This scaling has been observed in a variety of systems,¹ in both $d=2$ and $d=3$ dimensions, for times longer than some transient time t_0 (t_0 is different for different systems). As in critical phenomena, there appears to be a certain degree of universality in the growth exponent and scaling function of different systems, although its origin and extent is not yet completely understood.

It is now reasonably well established that in systems with only two low-temperature phases which are described by a nonconserved, scalar order parameter, the growth exponent is $n = \frac{1}{2}$. Examples of these systems include the kinetic Ising model,²⁻⁶ the Langevin equation for model A,⁷ ordering processes in (2×1) -type structures,^{8,9} etc.

If, instead, the order parameter is conserved, the late time behavior is expected to follow the Lifshitz-Slyozov law ($n = \frac{1}{3}$) (Ref. 10) for quenches close to the coexistence curve. The situation for critical concentrations, however, is much more controversial. Early computer simulations of the kinetic Ising model with a conserved order parameter (Kawasaki dynamics) showed the existence of approximate dynamical scaling and obtained an estimate for the growth exponent: $n \sim 0.20-0.25$.¹¹ More recently, it has been argued that if the growth process is statistically self-similar, the asymptotic behavior for a quench at a critical value of the concentration also follows the Lifshitz-Slyozov law.¹² Correction terms have also been estimated which incorporate the effects of surface diffusion along the interfaces of the highly interconnected structures.¹³ The inclusion of such a correction term leads to an effective exponent $n_{\text{eff}}(t) \equiv \partial \ln \bar{R}(t) / \partial \ln t$, which in the present case would be given by

$$n_{\text{eff}}(t) = \frac{1}{3} - \frac{A}{\bar{R}(t)}, \quad (3)$$

where A is a constant which could depend, in principle, on the temperature and relative volumes of the two phases. Recent extensive Monte Carlo studies of the kinetic Ising model with a conserved order parameter^{14,15} and the continuum Langevin model with conserved order parameter (model B) (Refs. 16 and 17) show evidence for a power law with an exponent close to $n = \frac{1}{3}$, once a correction term like Eq. (3) has been taken into account. However, if the correction term is not included, effective exponents in the range $n \sim 0.27-0.29$ are obtained in the case of the kinetic Ising.

On the other hand, numerical simulations together with renormalization-group ideas have been used to study both the kinetic Ising model with a conserved order parameter⁵ and the continuum Langevin model¹⁸ in two dimensions. Concerning a critical quench, a logarithmic

growth has been predicted in the case of the kinetic Ising model¹⁹ and a power law with an exponent $n = \frac{1}{4}$ for the Langevin model. This, in turn, would imply that the two models belong to different universality classes.

Most of the analyses that have been used to calculate exponents from computer calculations involve power law fits of the form given in Eq. (1) to the calculated average domain size $\bar{R}(t)$. Two techniques have been recently introduced that explicitly exploit the temporal-spatial scaling invariance of the system to calculate both the exponent n and the scaling function. They include real space Monte Carlo renormalization-group methods using standard blocking transformations⁶ and a direct analysis of the scaling properties using subsystems of different sizes embedded in a larger system.^{4,5,18,20} Both methods yield $n = \frac{1}{2}$ in the case of the kinetic Ising model with nonconserved order parameter. They disagree, however, in the conserved case (the value given by the Monte Carlo renormalization-group technique is $n = \frac{1}{3}$).²¹

Another technique which makes use of the scale invariance explicitly and has been successfully used in critical phenomena to determine critical exponents is finite-size scaling.²² The divergent length at the critical point (the bulk correlation length ξ) becomes finite in a lattice (of size L) and of the same order of the lattice size. It is then assumed that, in the vicinity of the bulk critical temperature, the behavior of the system, for large enough L , is determined by the scaled variable ξ/L . Such an assumption was later justified by using renormalization-group methods. Domain growth during a first-order phase transition also involves a divergent length (the average size of the domains would diverge at infinite times in an infinite system) that becomes bounded in a finite lattice. It can be assumed here that, for late enough times and large enough lattices, the behavior of the system is determined by the time-dependent scaled variable $\bar{R}(t)/L$. A finite-size-scaling theory for domain growth during a first-order phase transition has been developed recently,²³ but it has not been yet tested with actual computer simulations or used to determine growth exponents directly.

We show in this paper that finite-size-scaling methods can be used to obtain the domain growth exponent n . The details of the scaling ansatz are given in Sec. II. We test the method in the case of the kinetic Ising model with a nonconserved order parameter. The results obtained are presented and discussed in Sec. III. We have also analyzed (Sec. IV) the kinetic Ising model with a conserved order parameter.

II. FINITE-SIZE-SCALING ANSATZ

Let us denote by $S(\mathbf{q}, t, \xi, L)$ the time-dependent structure factor calculated in a finite lattice with $N = L^d$ spins (in d dimensions). The system has been quenched to a final temperature T which determines the bulk equilibrium correlation length ξ . Since we will be only concerned with isotropic systems, it is useful to introduce the circularly averaged structure factor

$$S'_c(q_\alpha, t, \xi, L) = \frac{1}{N_q} \sum_{\mathbf{q}} S(\mathbf{q}, t, \xi, L), \quad (4)$$

where the average for a given q_α includes all the N_q wave vectors such that

$$q_\alpha - \frac{\Delta q}{2} \leq |\mathbf{q}| < q_\alpha + \frac{\Delta q}{2}$$

with $\Delta q = 2\pi/L$.

In the case of a nonconserved order parameter, the pattern formation process is manifest in a developing Bragg peak ($q_{\text{Bragg}} = 0$ in the case which we will consider), the amplitude of which would diverge in an infinite system at infinite times. In a finite lattice and at temperatures well below the critical temperature, $S'_c(q_{\text{Bragg}}, t, \xi, L)$ is bounded by L^d . We assume the following scaling behavior for the structure factor, valid for late times [when $S'_c(q_{\text{Bragg}}, t, \xi, L) \sim L^d$]

$$S'_c(q, t, \xi, L) = L^d \mathcal{F}_1(qL, t^{1/x}/L, \xi/L), \quad (5)$$

where wave numbers are measured with respect to the Bragg peak and $n = 1/x$ is the growth exponent. Since the quench temperature is well below the critical region,²⁴ $\xi/L \ll 1$. We simply write

$$S_c(q, t, L) = L^d \mathcal{F}(qL, t^{1/x}/L). \quad (6)$$

We consider next a system with a conserved order parameter. In this case, the length scale of the developing structure is contained in the peak of the structure factor $S_c(q_{\text{max}}, t, L)$; $q_{\text{max}} \rightarrow 0$ and $S_c(q_{\text{max}}, t, L) \rightarrow \infty$ as $t \rightarrow \infty$. If we assume the same scaling behavior as in the case of a nonconserved order parameter, the position of the maximum of the structure factor satisfies

$$\begin{aligned} 0 &= \left. \frac{\partial S_c(q, t, L)}{\partial q} \right|_{q=q_{\text{max}}} \\ &= L^d f_1(qL, t^{1/x}/L) \Big|_{q=q_{\text{max}}} L, \end{aligned} \quad (7)$$

where $f_1(x, y)$ denotes the partial derivative $\partial f(x, y)/\partial x$. Consequently, $q_{\text{max}}(t, L)$ satisfies the following scaling relation:

$$q_{\text{max}}(t, L) = \frac{1}{L} Q(t^{1/x}/L). \quad (8)$$

Substituting Eq. (8) in Eq. (6), we obtain

$$S_c(q_{\text{max}}, t, L) = L^d \mathcal{G}(t^{1/x}/L). \quad (9)$$

III. KINETIC ISING MODEL WITH A NONCONSERVED ORDER PARAMETER

We have considered a system of N spins $\sigma_i = \pm 1$ on a two-dimensional square lattice with periodic boundary conditions. The system sizes used in this case are $N = 32^2, 64^2, 128^2$, and 192^2 . The Hamiltonian of the system is taken to be

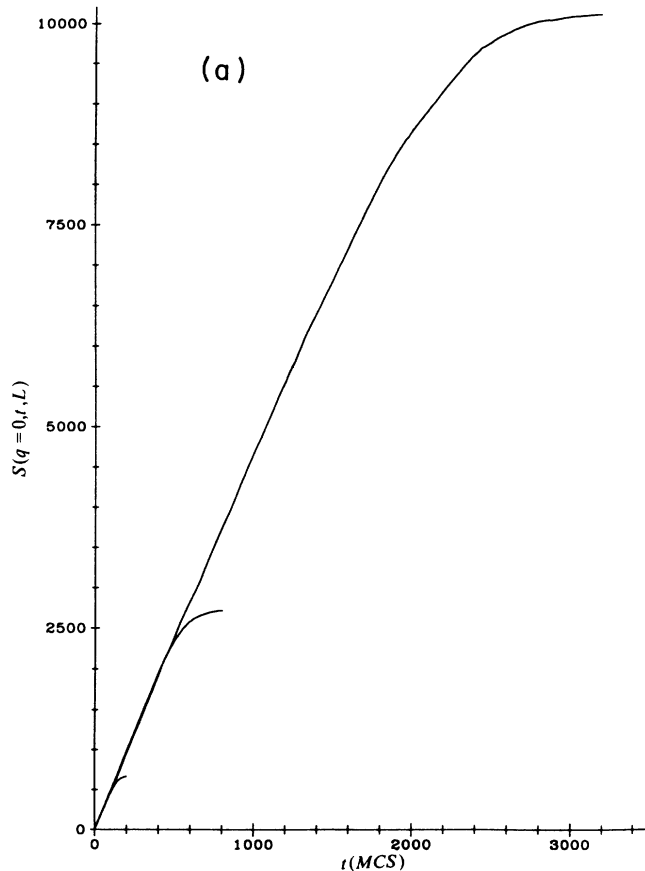
$$H = J \sum_{\langle i, j \rangle} \sigma_i \sigma_j, \quad (10)$$

where the sum runs over nearest neighbors. We have chosen as initial equilibrium configuration a totally ran-

dom distribution of spins ($T = \infty$). The dynamical evolution is defined in this case by the standard spin-flip algorithm: A spin is chosen at random and its sign reversed according to a probability distribution p given by $p = \min[1, e^{\Delta H/k_B T}]$. ΔH is the configurational energy difference in flipping the spin. The unit of time is one Monte Carlo step (MCS) per spin defined as N attempts to flip individual spins. The system evolves in this manner until the final equilibrium state is reached. Such a procedure is then repeated a number of times ("runs") to average over both initial configurations and dynamical evolutions.

The four systems have been quenched to the same final temperature, $k_B T/J = 1.0$ ($T \simeq 0.5 T_c$). Their evolution has been monitored for 200 MCS's ($L=32$), 800 MCS's ($L=64$), 3200 MCS's ($L=128$), and 7200 MCS's ($L=192$). The results presented for $S_c(q=0, t, L)$ are averages over 950 runs for the $L=32$ lattice, 480 runs for $L=64$, and 150 runs for $L=128$. Figure 2 also includes 14 runs for $L=192$. We have formed the time-dependent structure factor,

$$S(\mathbf{q}, t, \xi, L) = \frac{1}{N} \sum_{i,j} e^{-i\mathbf{q} \cdot (\mathbf{x}_i - \mathbf{x}_j)} \langle \sigma_i \sigma_j \rangle, \quad (11)$$



and circularly averaged it according to Eq. (4). The results which will be presented for $S_c(q, t, L)$ are averages over 300, 250, and 160 runs for $L=32, 64$, and 128, respectively.

We show in Fig. 1(a), $S_c(q=0, t, L)$ as a function of time for three of the lattices analyzed ($L=32, 64$, and 128). Figure 1(b) shows the same data scaled with Eq. (6), $x = 2(n = \frac{1}{2})$. The scaling ansatz described in the preceding section is expected to hold only for relatively long times, such that $S_c(q=0, t, L)$ becomes comparable to L^d . Nevertheless, good scaling is observed in this case over the entire range of times studied.

Two additional remarks should be made on Fig. 1(b). Firstly, the quality of the scaling, especially at long times, appears to be very sensitive to the number of runs included in the averages. Secondly, the saturation value for

$$S_c(0, t, L)/L^2 = \langle m^2 \rangle(t)$$

as $t \rightarrow \infty$ is not 1, as it should be at low temperatures. We attribute both facts to the appearance of a significant fraction of runs which evolve into very long-lived metastable configurations.^{3,25} These metastable configurations are mostly one strip of one equilibrium phase surrounded

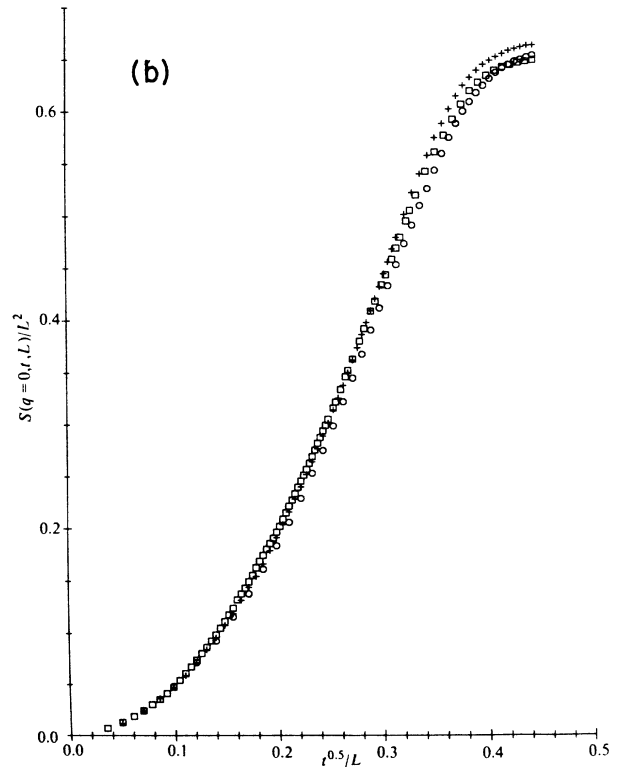


FIG. 1. (a) Peak of the structure factor, $S_c(q=0, t, L)$, as a function of time for the kinetic Ising model with nonconserved order parameter for three different lattice sizes. From top to bottom they correspond to $L=128, L=64$, and $L=32$. (b) The same data scaled with Eq. (6). The exponent used is $n = 1/x = \frac{1}{2}$; (\circ), $L=32$; (\times), $L=64$; and (\square), $L=128$.

by the other phase in such a way that $m(t) \simeq 0$ for long times after the quench. Since the value of $\langle m^2 \rangle(t)$ for $t \rightarrow \infty$ is very sensitive to the fraction of such configurations present in the sample, we conclude that a large number of runs is essential in order to obtain the correct scaling behavior.²⁶

A possible way to overcome this difficulty would appear to be to discard from the analysis all the runs which do not reach equilibrium in observable times. We show in Fig. 2 $S_c(q=0, t, L)$ averaged over only those runs in which $m^2(t \rightarrow \infty) \geq 0.95$. We do not observe a good scaling in this case.²⁶

We have finally analyzed the scaling form for the circularly averaged structure factor at finite q [Eq. (6)]. Figures 3(a) and 3(b) show the scaled structure factor at $qL = 6\pi$ and $qL = 10\pi$, respectively. The scaling exponent used in this figure is again $x = 2$. The data follow Eq. (6) quite accurately even though a significantly smaller number of runs have been included in our calculation of the structure factor at finite q . In fact, $S_c(q, t, L)$ at finite values of q is seen to be less sensitive to the addition of new runs than $S_c(q=0, t, L)$. There are two possible

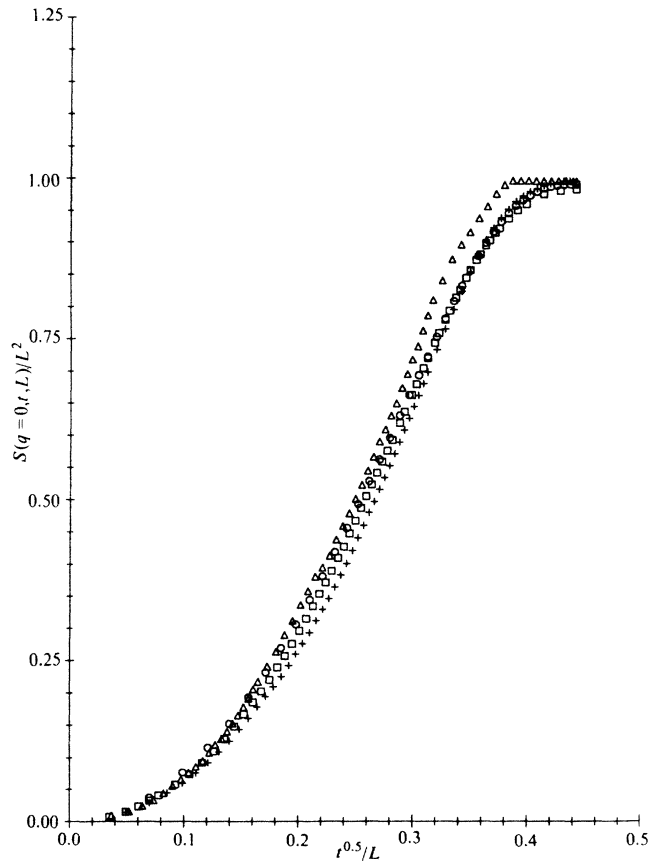


FIG. 2. Scaled amplitude of the peak of the structure factor, $S_c(q=0, t, L)/L^2$, vs $t^{1/2}/L$. Only those runs in which $m^2(t \rightarrow \infty) \geq 0.95$ have been included. (\circ), $L=32$; (\times), $L=64$; (\square), $L=128$; and (\triangle), $L=192$. Compare the quality of the scaling observed here with Fig. 1(b).

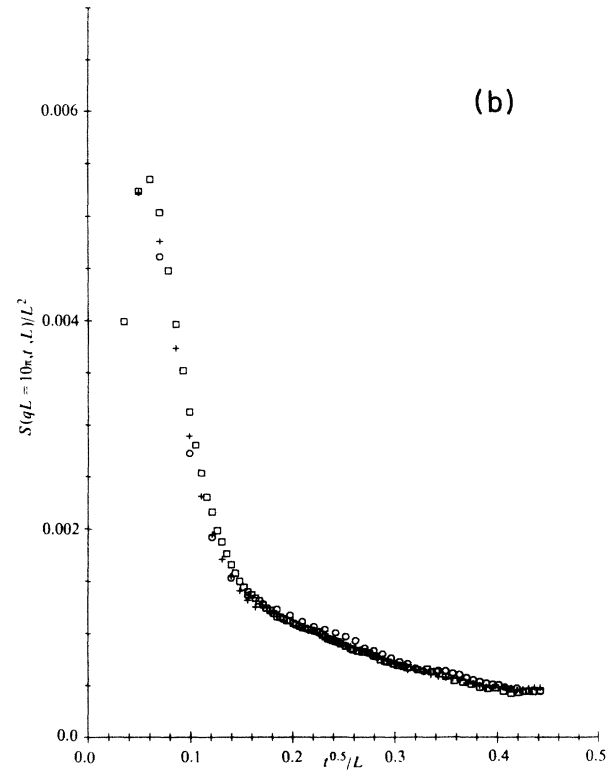
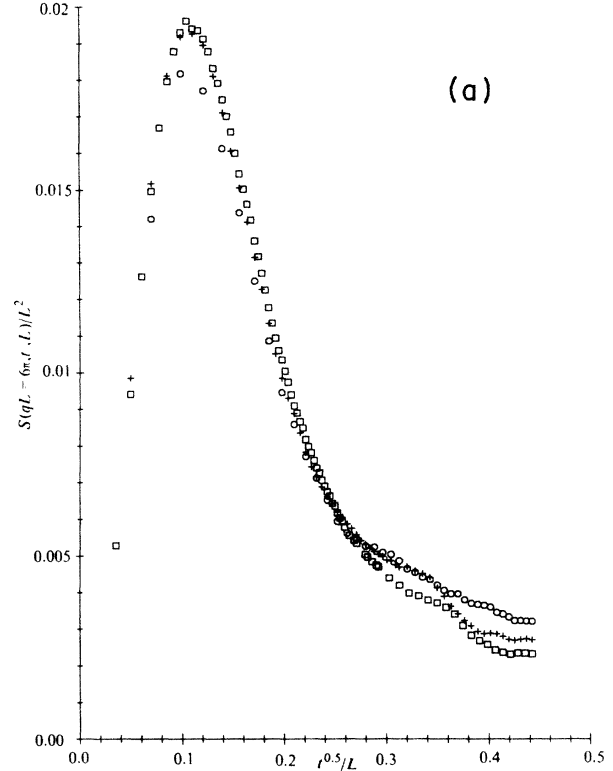


FIG. 3. Scaled structure factor at finite wave numbers, $S_c(qL, t, L)/L^2$, as a function of $t^{1/2}/L$. (\circ), $L=32$; (\times), $L=64$; and (\square), $L=128$. (a) $qL = 6\pi$ and (b) $qL = 10\pi$.

explanations for this observation. On one hand, the fact that averages over large samples are necessary to obtain the scaling behavior of $S_c(q=0, t, L)$ seems related to the appearance of a significant number very long-lived metastable configurations. Such runs are likely to contribute more strongly to $S_c(q=0, t, L)$ than to $S_c(q, t, L)$ for finite q . On the other hand, $S_c(q=0, t, \xi, L)$ has been shown to be a non-self-averaging quantity.²³ There is, however, some self-averaging of initial conditions at finite q .

IV. KINETIC ISING MODEL WITH CONSERVED ORDER PARAMETER

We have also analyzed the kinetic Ising model defined by the Hamiltonian [Eq. (10)] with a conserved order parameter. We have considered here a system of N spins ($N=16^2$, 24^2 , and 32^2) on a two-dimensional square lattice with periodic boundary conditions. The initial configuration has also been chosen at random; i.e., $\langle m \rangle(t=0)=0$. The dynamical evolution of the system is defined by a spin-exchange algorithm: A pair of nearest-neighbor spins is chosen at random and their location on

the lattice is interchanged (provided they have a different sign) with a probability

$$p = \frac{1}{2} \left[1 - \tanh \frac{\Delta H}{2k_B T} \right].$$

ΔH is the difference in energy between the configuration after and before the attempted exchange. N attempted exchanges is the unit of time (1 MCS).

The three systems analyzed have been quenched to $k_B T/J=1.5$ ($T \simeq 0.7T_c$) and their evolution followed for 50 000 MCS's ($L=32$), 140 000 MCS's ($L=24$), and 400 000 MCS's ($L=32$). All of our results have been averaged over 160 runs ($L=16$), 110 runs ($L=24$), and 100 runs ($L=32$). We have calculated the structure factor defined in Eq. (11) and circularly averaged it [Eq. (4)].

We show in Fig. 4(a) $S_c(q_{\max}, t, L)$ for the three system sizes studied. Figure 4(b) shows the best scaling according to Eq. (9) obtained with $n=0.27$. This value is in agreement with other Monte Carlo simulations of the same model.¹³ It disagrees, however, with the value of $n=1/3$ given in Refs. 14 and 15, where an extrapolation to $\bar{R}(t) \rightarrow \infty$ was used (our result agrees, however, with the exponent obtained from their Monte Carlo data without

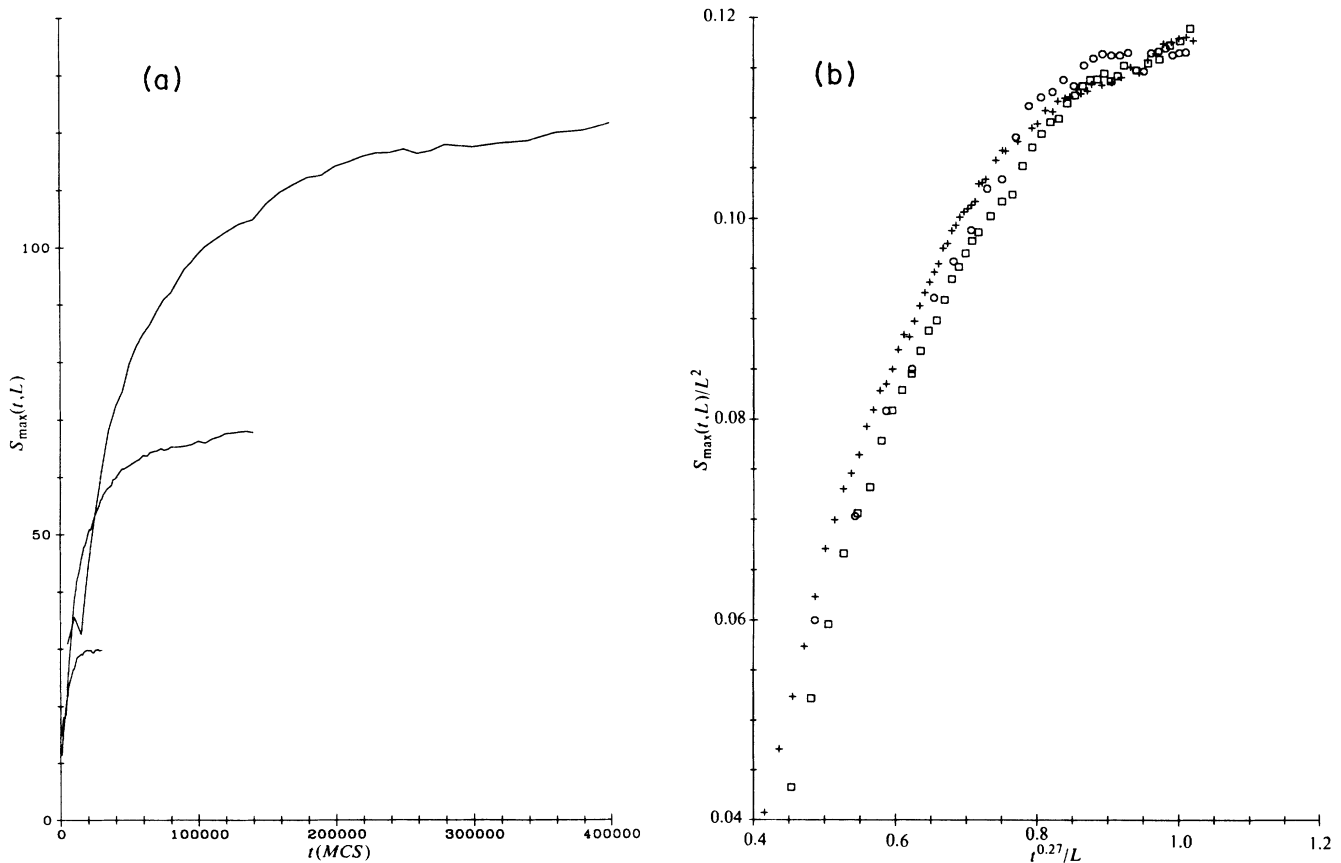


FIG. 4. (a) Amplitude of the maximum of the structure factor $S_c(q_{\max}, t, L)$ for the kinetic Ising model with a conserved order parameter as a function of time for three different lattice sizes. (b) $S_c(q_{\max}, t, L)/L^2$ as a function of $t^{1/x}$, with $1/x=0.27$; (\circ), $L=16$; (\times), $L=24$; and (\square), $L=32$.

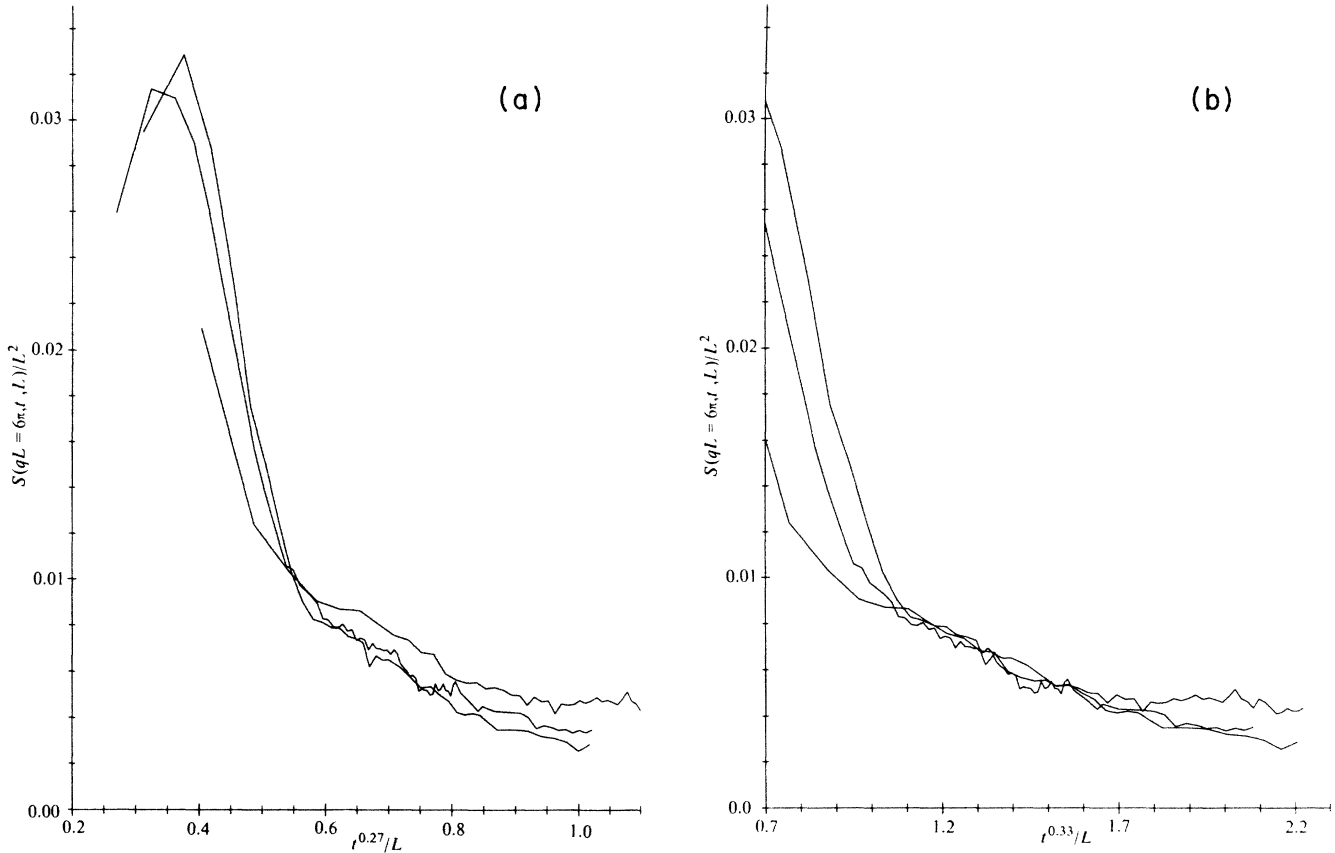


FIG. 5. Scaled structure factor at finite wave numbers, $S_c(qL, t, L)/L^2$, as a function of $t^{1/x}/L$ for the kinetic Ising model with a conserved order parameter with $qL = 6\pi$. (a) $1/x = 0.25$ and (b) $1/x = 0.33$.

the extrapolation). We have also analyzed the scaling behavior at larger q . We show the scaled structure factor for finite q ($qL = 6\pi$ and $qL = 10\pi$) in Figs. 5 and 6 with both $n = 0.27$ and $n = \frac{1}{3}$. Somewhat better scaling is observed in this case with $n = \frac{1}{3}$ as opposed to the previous case [the smallest lattice markedly deviates in all the cases; note that there are only nine independent momentum components for $L = 16$, so high q values of $S_c(q, t, L)$ are very distorted].

The exponent $n = \frac{1}{3}$ for quenches close to the coexistence curve follows from growth by an evaporation-condensation mechanism.¹⁰ Large domains of the minority phase grow at the expense of small ones; the growth process is limited by long-range diffusion inside the majority phase. For quenches near critical values of the order parameter, it has been argued that other mechanisms, such as diffusion along or across the interfaces separating domains,¹³ may be relevant even at moderate times after the quench. It is quite possible that we have not reached in our analysis domain sizes large enough to see an asymptotic behavior in which only one mechanism dominates. As a consequence, it is not clear whether the exponent that we have obtained should be considered only as an effective exponent.

To conclude, we remark that finite-size-scaling techniques can be used to determine growth exponents during a first-order phase transition, even with relatively small lattices. In the case of the kinetic Ising model with a nonconserved order parameter, the method gives $n = \frac{1}{2}$ quite accurately. Unfortunately, our results for the kinetic Ising model with a conserved order parameter are not conclusive, possibly because the lattice sizes used are not large enough. We note that $q_{\max}(t)$ becomes equal to $\Delta q = 2\pi/L$ for very early times in all the lattices studied. This is the minimum value that $q_{\max}(t)$ can ever reach due to the conservation law and the discretization in q space. Consequently, $q_{\max}(t)$ already saturates at early times, although the system is not yet in equilibrium. However, long-range diffusion could presumably still be observed over smaller length scales. If this is the case, such processes could account for the exponent $n = \frac{1}{3}$ obtained from the scaling at finite q . Although the scaling of the maximum of the structure factor gives an exponent $n = 0.27$, we find it encouraging that the scaling for higher q is more consistent with $n = \frac{1}{3}$, even with lattices as small as $L = 24$ and 32 . Further work, especially on larger lattices, seems necessary in order to elucidate this point.

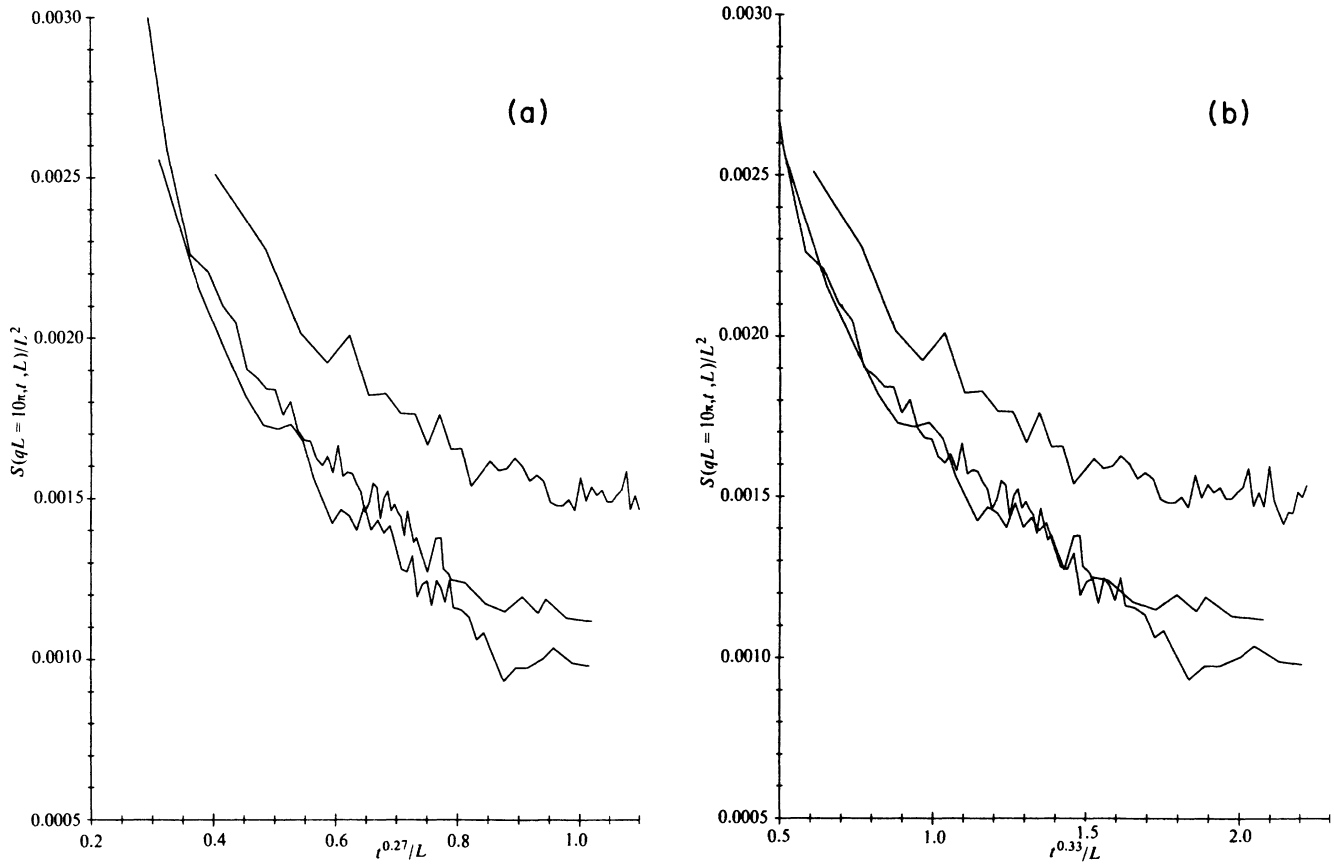


FIG. 6. Scaled structure factor at finite wave numbers, $S_c(qL, t, L)/L^2$, as a function of $t^{1/x}/L$ for the kinetic Ising model with conserved order parameter with $qL = 10\pi$. (a) $1/x = 0.25$ and (b) $1/x = 0.33$.

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