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Dynamics of order-parameter-conserving Ising models at $T > T_c$

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The dynamics of spin fluctuations in nonequilibrium and equilibrium states is studied in the one-phase region above T_c . The equal-time structure factor is computed after quenching the system from an infinite temperature to $T > T_c$. The result shows growing spatial patterns which can be scaled with temperature-dependent scaling functions. The different-time (dynamic) structure factor is computed by taking time averages while the system is fluctuating in equilibrium states. The equilibrium autocorrelation decays following a diffusive exponential term and a slower but transient term. The relaxation rate due to the diffusion supports the dynamic scaling.

I. INTRODUCTION

The dynamics of concentration fluctuations in binary systems has been studied in the past, both in nonequilibrium states and in equilibrium states. When a system is suddenly quenched from the disordered one-phase region to the stable part of the two-phase coexistence region at $T < T_c$, the displaced system begins to separate into two stable phases. At late times the system enters a scaling regime where the domain structures at different times are statistically similar apart from the scale change due to the growing domain size. This scaling has been the subject of intensive investigation during the last two decades.¹⁻⁴ If the system is quenched to $T = T_c$, a different scaling, and thus a different growth law, applies for the dynamics.^{4,5}

The case of $T > T_c$ has received very little attention. This is probably because there is no asymptotic global phase separation in this temperature regime and, moreover, the equilibrium state is reached in a finite amount of time even in infinite systems and therefore one would not suspect scaling behavior. But Bortz *et al.*⁶ and Marro *et al.*⁷ showed in their early pioneering investigations that there is a peak in the equal-time structure factor which grows with time and that the peak position moves in the direction of decreasing wave vectors as time progresses. Subsequently, Binder and Stauffer⁸ and Binder⁹ proposed a power law for the growth kinetics which suggests scaling. In addition, experiments by Jefferson, Petschek, and Cannell¹⁰ with binary liquids showed that the relaxation time (of the equal-time structure factor) exhibits scaling behavior. All of this is enough motivation to explore the possibility of scaling in the one-phase region. We carry out this effort in Sec. II. We compute the structure factor of an Ising model with a conserved order parameter (IMCOP) and examine whether the structure factor itself exhibits any kind of scaling behavior. The result turns out to be that it does.

Now with regard to the equilibrium dynamics, the IMCOP is believed to belong to the same dynamic universality class as model *B* of Hohenberg and Halperin,¹¹ the critical dynamics of which is well understood. Our pur-

pose in computing the dynamic structure factor of an IMCOP is as follows. One of the current issues in the equilibrium dynamics of phase-separating binary systems is centered on the decay pattern of the intensity-intensity autocorrelation function of binary liquids in porous media.¹²⁻¹⁴ When dilute silica gel is used as the medium, the autocorrelation function shows an extremely slow decay pattern in the one-phase region near the two-phase boundary.¹³ This decay pattern cannot be explained by present theory. Binary liquids in macroporous glasses also show other kinds of puzzling behavior in the decay pattern of the intensity-intensity autocorrelation function.¹⁴ Due to the complex nature of the disordering effects of the porous media, the ultimate theory is unlikely to emerge soon and computer simulations may provide some useful clue. To that end, the IMCOP with an added term for the disordering effects would be a good model, but unfortunately the pure IMCOP itself is notorious for transient behavior which tends to slow down the dynamics. Thus, without an actual study of the pure IMCOP, it may be difficult to sort out the effects of the disorder from those of the pure IMCOP.

The equilibrium dynamics of the pure IMCPO has been investigated by Binder⁹ and by Heilig *et al.*,¹⁵ but the present author has not been able to locate any attempts to data to compute the dynamic structure factor itself as a function of all wave vectors and time. Thus we carry out this computation in Sec. III. We find that the IMCOP is indeed plagued by transient behavior even in the one-phase region. The transient behavior appears in the guise of an activated dynamics, but the relaxation time due to the "activation" is actually shorter than the relaxation time due to the diffusion. Thus the transient part does not affect the late-time behavior and can be removed. The relaxation time obtained from the remaining part supports the dynamic scaling. Some additional discussions follow in Sec. IV.

II. THE NONEQUILIBRIUM DYNAMICS AFTER QUENCHING

A total number of $N = 256 \times 256$ spins are placed on a square lattice with periodic boundary conditions. The

Hamiltonian is given by $H = -\sum_{\langle i,j \rangle} S_i S_j$, where $S_i, S_j = +1$ (species *A*) or -1 (species *B*), and $\langle i,j \rangle$ refers to all nearest-neighbor (NN) pairs. The time evolution is governed by the spin exchange dynamics which allows exchanges of NN pairs only. In one "sweep through the lattice," each NN pair is called (from a prepared table) $\frac{1}{2}$ times on average for an exchange (thus each spin is tried twice on average), and each trial exchange succeeds with probability $\min[1, \exp(-\Delta H/T)]$, where ΔH is the change in energy due to the proposed exchange and T is the temperature.

The system is quenched from a random initial state to $T/T_c = 1.1, 1.01, 0.99$, and 0.676 , where T_c is the transition temperature. As the spins relax, we monitor the spin fluctuation,

$$\rho_q(t) = N^{-1} \sum S_i(t) \exp(ir_i \cdot q), \quad (1)$$

and measure the equal-time structure factor given by

$$S(q,t) = \langle \rho_q(t) \rho_{-q}(t) \rangle, \quad (2)$$

where time t is represented by the number of sweeps through the lattice. The ensemble average is taken over

approximately 70 different initial spin configurations. In what follows, the wave vector q is given in units of $2\pi/L$, where $L = 256$.

When the system is quenched into the one-phase region near T_c , there is no asymptotic global phase separation. But the thermal fluctuations create global patches of local patterns which bear some resemblance to those in the two-phase region. As can be seen in Figs. 1 and 2, these patches actually show a growing spatial pattern. Notice how the results for $T/T_c > 1$ in Fig. 1 are similar to those for $T/T_c < 1$ in Fig. 2. Moreover, as Figs. 3 and 4 show, the growing patterns may be scaled in the form of,

$$S(q,t)/S(q_m,t) = F(q/q_m(t)), \quad (3)$$

where q_m is the wave vector corresponding to the peak.² The scaling functions are different, however, from that of the deep quench shown in the bottom of Fig. 4 and change with the temperature. These temperature-

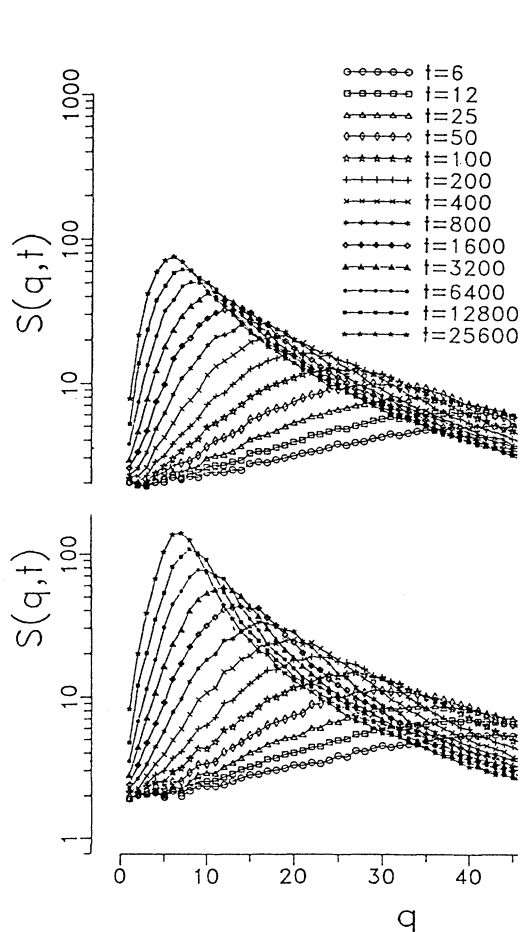


FIG. 1. The equal-time structure factor $S(q,t)$ at $T/T_c = 1.1$ (the top figure) and at $T/T_c = 1.01$ (the bottom figure). Here and in all following figures, the wave vector q is given in units of $2\pi/L$ where $L = 256$.

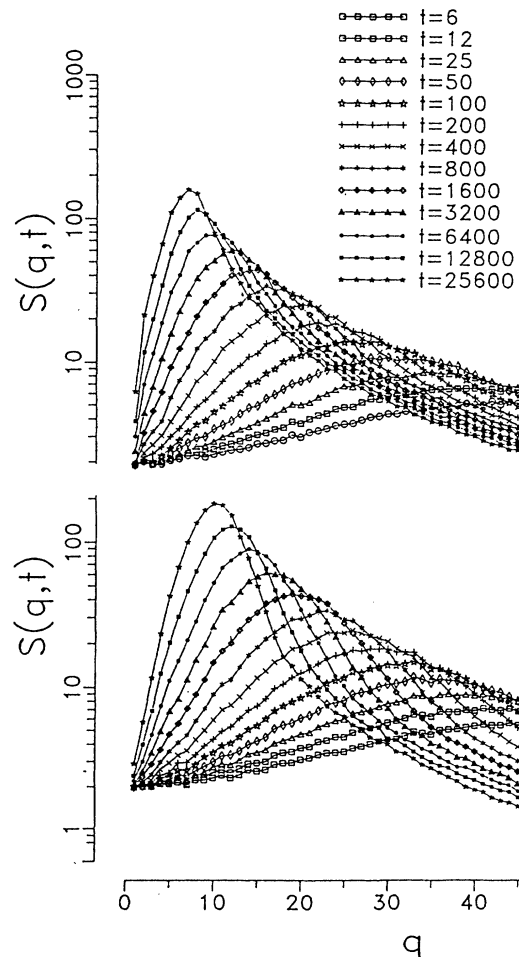


FIG. 2. The equal-time structure factor $S(q,t)$ at $T/T_c = 0.99$ (the top figure) and at $T/T_c = 0.676$ (the bottom figure).

dependent scaling functions are quite similar to those of off-critical quenches to $T < T_c$,² but on closer examination we find that they are different. Thus the scaling does not carry the kind of universality that it has deep in the two-phase region. We will return to this discussion later in Sec. IV.

We now compute the nonequilibrium autocorrelation function¹⁶

$$D(q, t) = \langle \rho_q(t) \rho_{-q}(0) \rangle, \quad (4)$$

where $t=0$ refers to the initial time immediately after the

quench. Figures 5 and 6 show the results which display both relaxation and growth processes. The autocorrelation grows in the regime of small wave vectors and relaxes to zero in the regime of large wave vectors. The growth regime becomes narrower and narrower as time progresses which reflects the distribution of the growing domain sizes. The relaxation regime also becomes narrower and shifts toward smaller wave vectors. This makes the division between the two regimes quite dramatic at late times. Figures 7 and 8 show that $D(q, t)$ may be scaled as

$$D(q, t)/D(q_m, t) = G(q/q_m(t)). \quad (5)$$

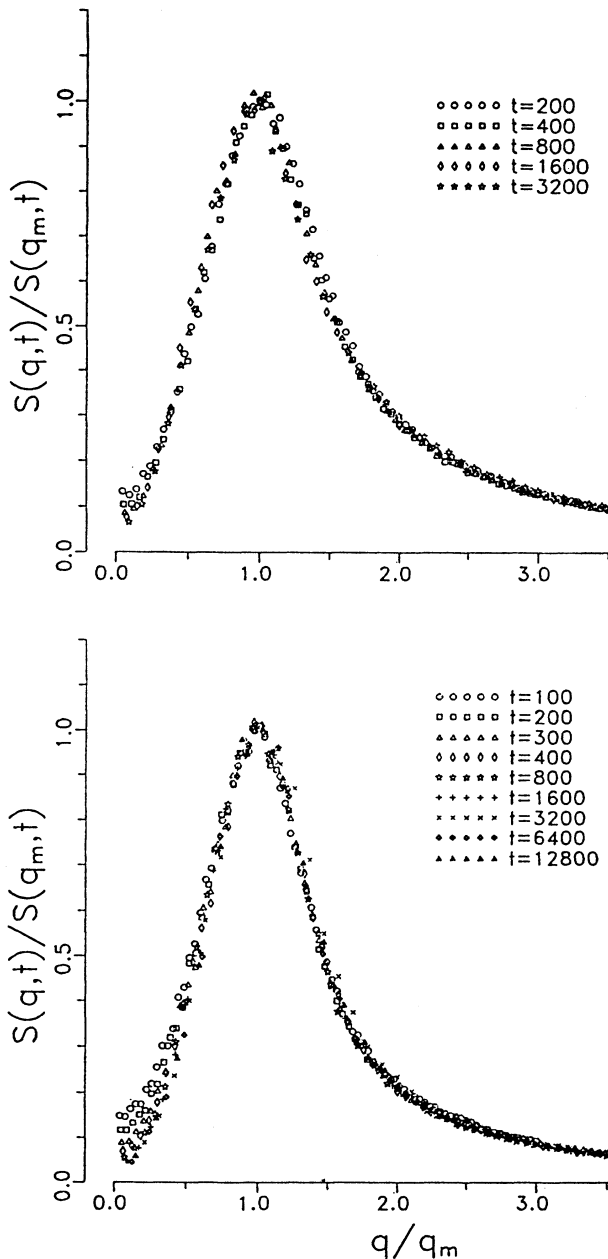


FIG. 3. Scaling plot for $S(q, t)$ at $T/T_c = 1.1$ (the top figure) and at $T/T_c = 1.01$ (the bottom figure).

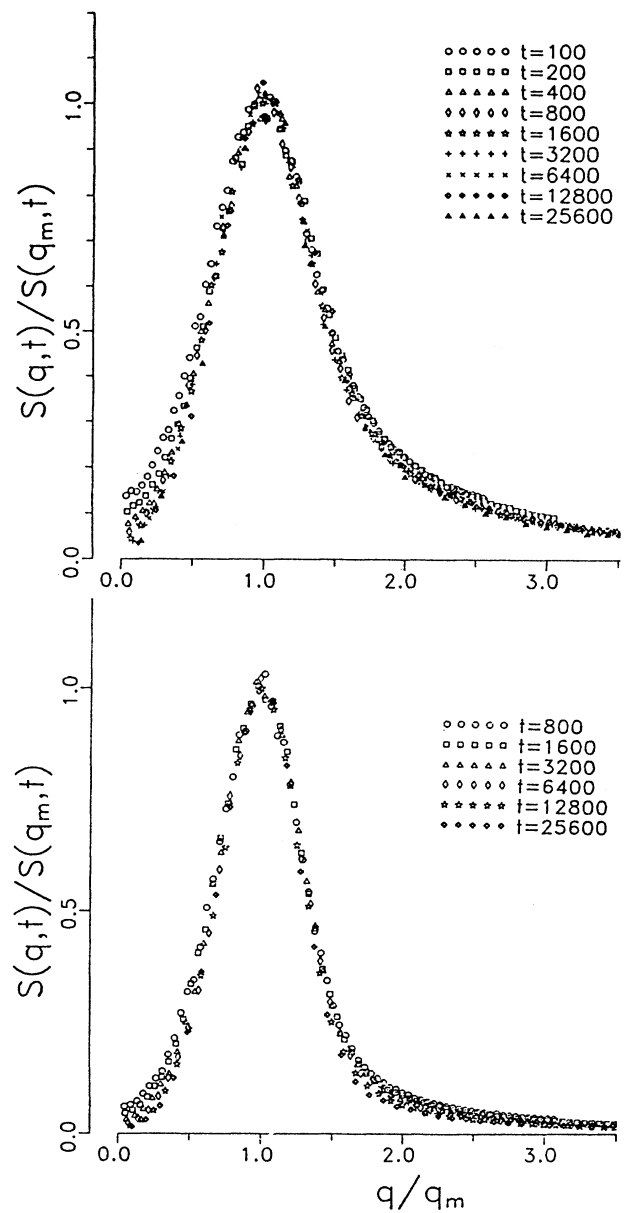


FIG. 4. Scaling plot for $S(q, t)$ at $T/T_c = 0.99$ (the top figure) and at $T/T_c = 0.676$ (the bottom figure).

The same nonequilibrium autocorrelation function has been studied very recently by Alexander, Huse, and Janowsky⁵ in position space and for the quench temperature $T = T_c$.

III. THE EQUILIBRIUM DYNAMICS

To investigate the spin fluctuation at equilibrium, we now thermalize the spins for a long time until the system reaches its equilibrium state and then measure the dynamic structure factor defined by

$$C(q, t) = \langle \rho_q(t + t_0) \rho_{-q}(t_0) \rangle, \quad (6)$$

where the average is taken over different initial times t_0 .

After a sufficient waiting period for equilibration, we take about five averages each over about 70 to 100 different t_0 . This is repeated over five different initial spin configurations. Because of the long waiting period, our computations have been limited to $T/T_c = 1.2, 1.1,$ and 1.05 . The measurements were taken at times given by $t_i = t_1 2^{(i-1)}$ where $i = 1, 2, 3, \dots, n$. For $T/T_c = 1.2$ and 1.1 , $t_1 = 2$, and $n = 10$. For $T/T_c = 1.05$, $t_1 = 6$, and $n = 9$. The results for $T/T_c = 1.1$ are shown in Fig. 9. It appears that there is no long-lasting tail. To examine the decay pattern in more detail, we now plot the data in Fig.

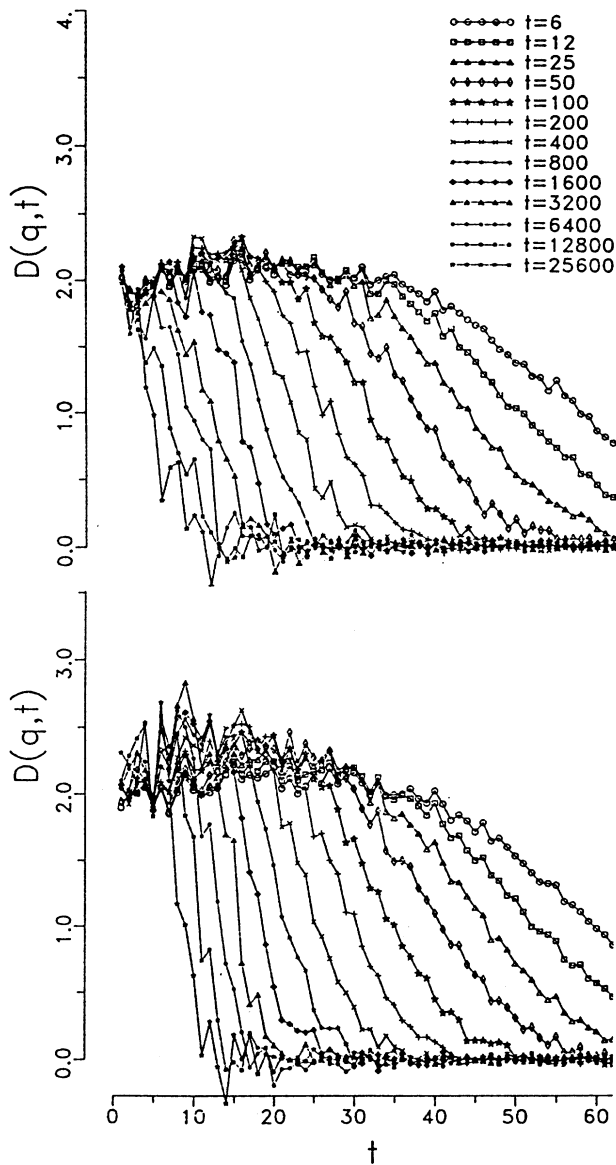


FIG. 5. $D(q, t)$ at $T/T_c = 1.1$ (the top figure) and at $T/T_c = 1.01$ (the bottom figure).

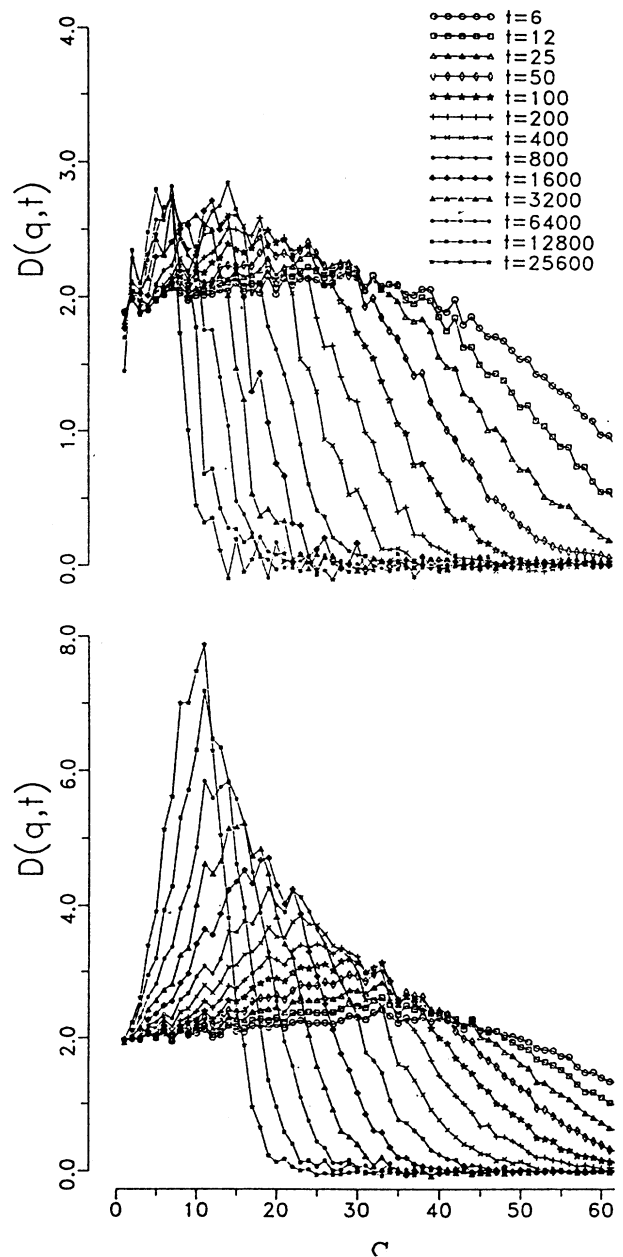


FIG. 6. $D(q, t)$ at $T/T_c = 0.99$ (the top figure) and at $T/T_c = 0.676$ (the bottom figure).

10 as a function of time for several values of q . The auto-correlation decays following the exponential diffusive dynamics at early times. At late times, however, there is a notable deviation from the exponential decay. The deviation may be fitted reasonably well by adding another term, as follows:

$$C(q, t) = A_1 \exp(-\Gamma_q t) + A_2 \exp\{-[\ln(t)/\ln(\tau_A)]^2\}, \quad (7)$$

where the second term implies activation dynamics.¹⁷ This is unfortunate because the quantity of primary interest, Γ_q , now has to be determined alongside as many as three other parameters. Moreover, the second term makes the slow relaxation in the regime of small q even slower. As a result, our measuring time was not long enough for $q < 25$; the measuring stopped long before the effect of the transient behavior died out. In the regime of large q , on the other hand, the exponential term dies out quite rapidly, which requires very frequent measurements for a reliable information on the exponential term. Un-

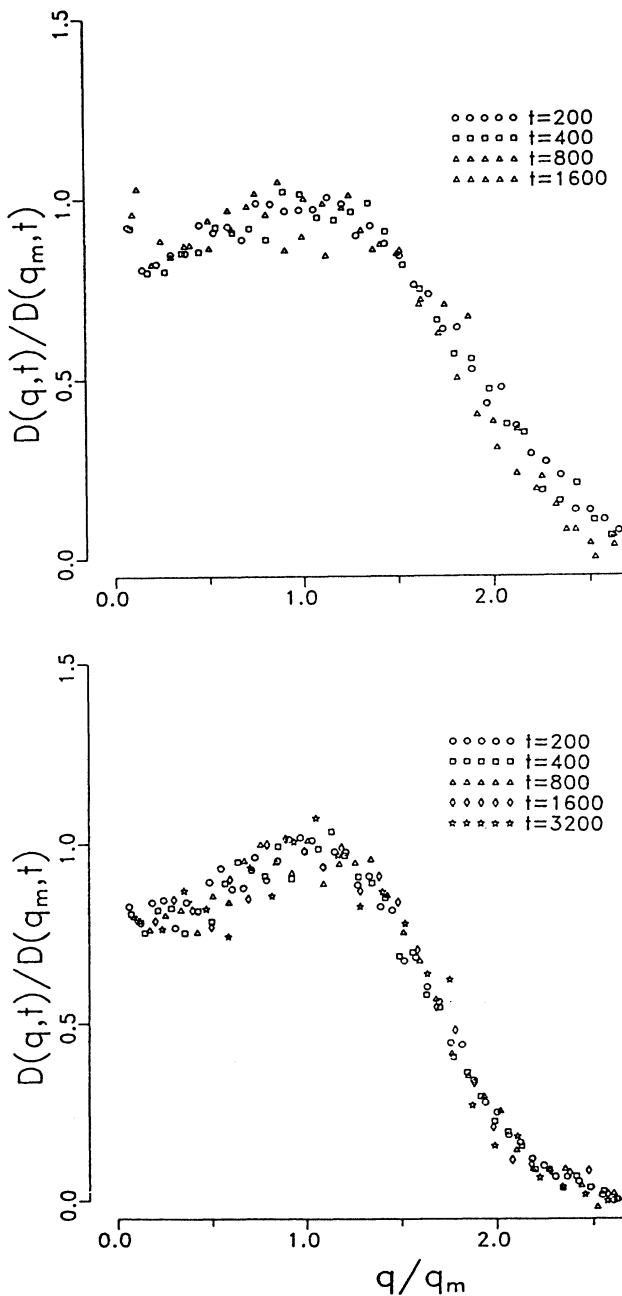


FIG. 7. Scaling plot for $D(q, t)$ at $T/T_c = 1.1$ (the top figure) and at $T/T_c = 1.01$ (the bottom figure).

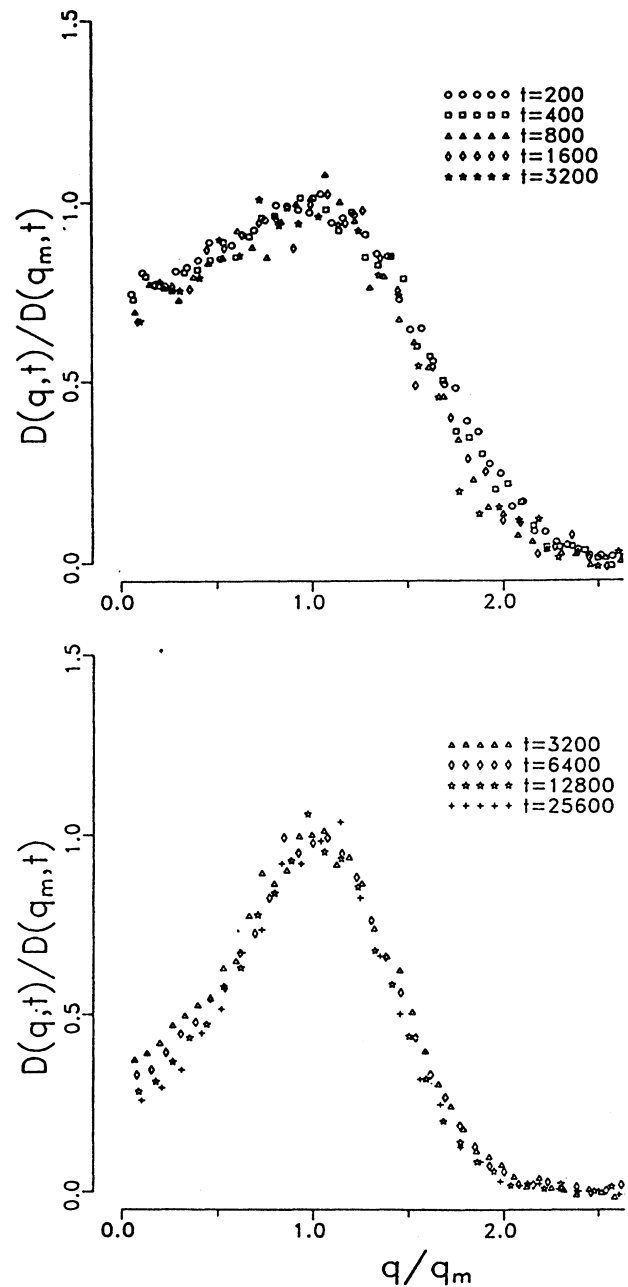


FIG. 8. Scaling plot for $D(q, t)$ at $T/T_c = 0.99$ (the top figure) and at $T/T_c = 0.676$ (the bottom figure).

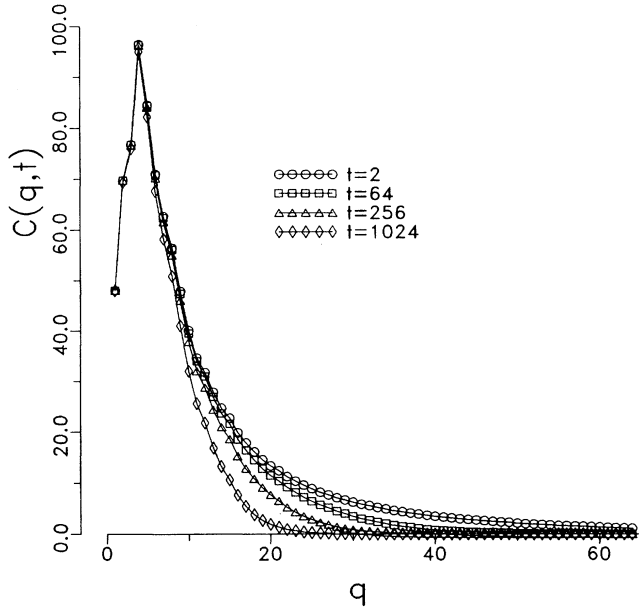


FIG. 9. The dynamic form factor $C(q,t)$ at $T/T_c = 1.1$.

fortunately our measurements were not frequent enough. This leaves only the regime $25 < q < 55$ where our data fit¹⁸ is reliable.

The ratio $A_2/(A_1 + A_2)$ is plotted in Fig. 11(a). The deviation from the exponential decay increases with increasing q . Thus the effect of the second term is more ap-

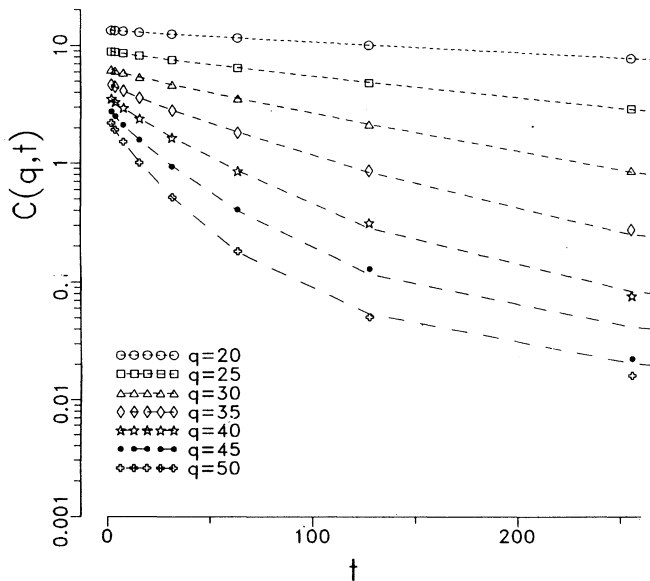


FIG. 10. The relaxation pattern of $C(q,t)$ is highlighted at early times for several values of wave vectors. The fitted area points (not shown in the figure) are connected by straight dotted lines. Ten data points are used for the fit of which the last two are not shown in this figure.

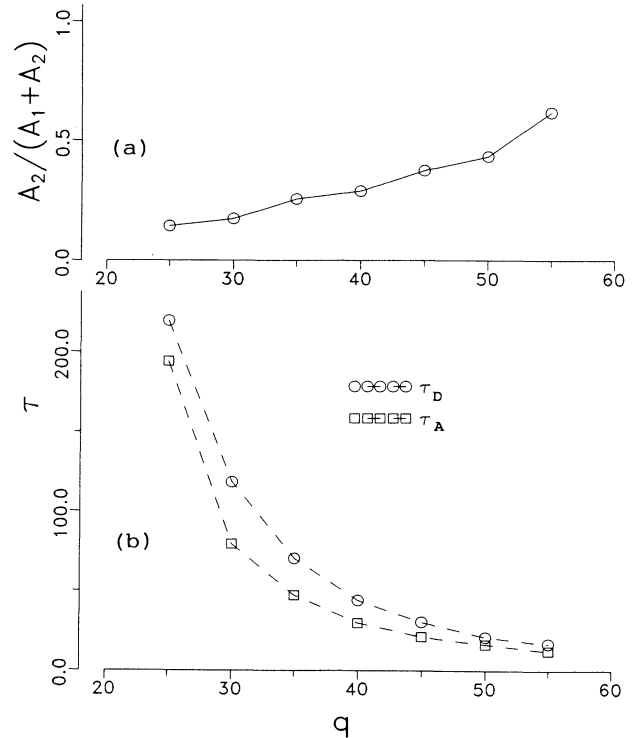


FIG. 11. (a) The q dependence of the relative amplitude of the nonexponential term. (b) Comparison of the two relaxation times.

preciable in small length scales, as is true when there are true energy barriers. In contrast to cases of true energy barriers, however, the activation relaxation time τ_A is actually shorter than the diffusion relaxation time $\tau_D = 1/\Gamma_q$ as Fig. 11 (b) shows. While this seems reasonably certain for large wave vectors, it is less certain for small wave vectors $q \leq 25$ as our data are not reliable in this regime. But the following observation proves helpful. Notice that the difference between τ_A and τ_D increases with decreasing q , but the trend seems to be changing at $q = 25$. To find out how much this is due to the insufficient measuring time, we intentionally decreased the measuring time for $q = 25$ by ignoring the last two late-time data in the fit. This decreased τ_D by less than a factor of 2 but increased τ_A by about 4 orders of magnitude. On the basis of this observation we believe that if the measuring time had been large enough, the data for τ_A at $q = 25$ would have been smaller than shown in the figure and the trend would have continued.

Now we test the dynamic scaling^{11,19} which may be written in the form of

$$\Gamma_q = \xi^{-z} f(q\xi), \tag{8a}$$

or

$$\Gamma_q = q^z g(q\xi), \tag{8b}$$

where ξ is the correlation length and z is the dynamic exponent. We try the scaling with the known value of

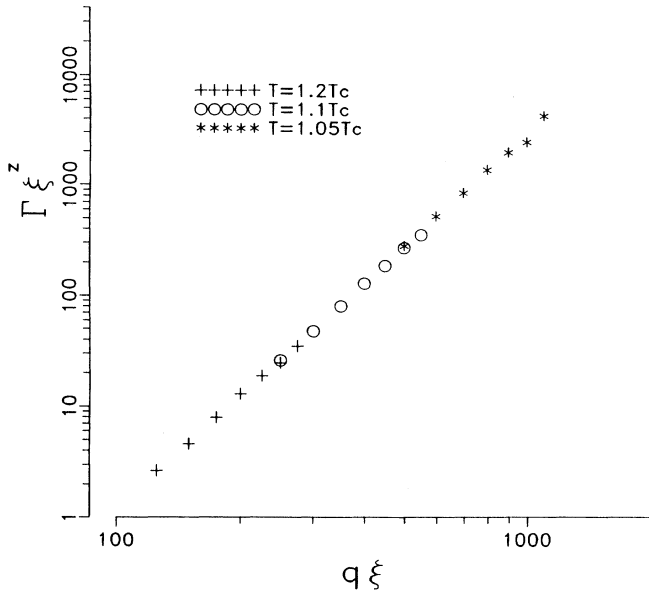


FIG. 12. Scaling plot for the decay rate Γ_q in the form of Eq. 8(a).

$z=4-\eta=3.75$. The results are shown in Fig. 12 for Eq. 8(a) and in Fig. 13 for Eq. 8(b). For the data points in these figures, q ranged from approximately 25 to 55. The temperature differs from T_c by as much as 20%, but with $\nu=1$ the correlation length is not negligible. The resultant scaling variable $q\xi$ covers less than two decades, all within the critical regime $q\xi > 1$ but not within the critical limit $q\xi \gg 1$. With these provisos, the results show

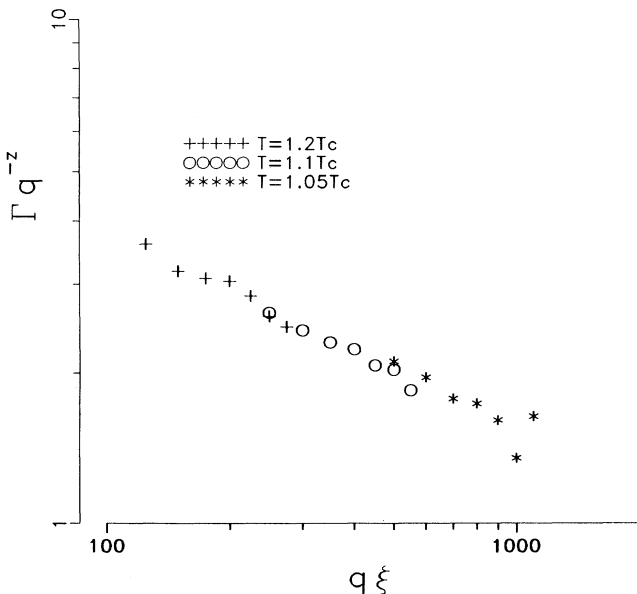


FIG. 13. Scaling plot for the decay rate Γ_q in the form of Eq. 8(b).

reasonably convincing scaling behavior.

The scaling functions show power-law behavior of $f(x) \sim x^{3.26}$ for Eq. 8(a) and $g(x) \sim x^{-0.43}$ for Eq. 8(b). The two values 3.26 and -0.43 are consistent with the chosen value of $z=3.75$ since Eqs. 8(a) and 8(b) together imply $f(x)=x^z g(x)$, which is approximately satisfied in this case. The appearance of power-law behavior is only local in the scaling variable; the value 3.26 would become 2 in the limit of small x and 3.75 in the limit of large x . In the above we tested the scaling with the correct value of z . How sensitive is the scaling to the choice of z ? It is not very sensitive. If the correct value of z were to be determined by the scaling test, it would be deemed to be in the range of $z=3.70 \pm 0.05$.

IV. DISCUSSIONS AND SUMMARY

We have studied two different kinds of dynamics of the pure Ising model with a conserved order parameter (IM-COP). In Sec. II we computed both the equal-time structure factor $S(q,t)$ and the nonequilibrium autocorrelation function $D(q,t)$, after quenching the system from an infinite temperature to a final temperature above T_c . For comparison, we have also performed the same computation for $T < T_c$. Both $S(q,t)$ and $D(q,t)$ exhibit scaling behavior but with temperature-dependent scaling functions. Returning back to Figs. 3 and 4, examine how the scaling function of $S(q,t)$ changes as the quench temperature is raised from $T/T_c=0.676$ to $T/T_c=1.1$. The result for $T/T_c=0.676$ represents the zero-temperature scaling which shows a peak at $y=q/q_m=1$ with more or less symmetric shoulders on its two sides. The result for $T/T_c=0.99$ shows a difference from this pattern as the two shoulders are notably asymmetric. Thus, even in the two-phase region, if the temperature is very close to T_c , the zero-temperature scaling is corrected. The nonequilibrium dynamic renormalization⁴ cannot quite drive the system to $T=0$.

When the temperature is raised from $T/T_c=0.99$ to $T/T_c=1.01$, there is no notable change in the scaling function. When the temperature is further raised to $T/T_c=1.1$, however, the two shoulders become far more asymmetric than before. But the scaling is now limited only to a much shorter period. This is an important difference between $T < T_c$ and $T > T_c$. In an infinite system, this difference would be far more dramatic. The system would take an infinite amount of time to reach its equilibrium state in the two-phase region. In the one-phase region, on the other hand, the infinite system would take a finite amount of time because the phase-separated domains do not grow to an infinite size. Therefore the asymptotic behavior is quite different in the two-phase region and in the one-phase region, but the difference lies mainly in the time scale and the manner in which the displaced systems evolve toward their equilibrium states is remarkably similar. Thus the asymptotic scaling exists only in the two-phase region, but it has a rather remarkable precursor in the one-phase region. Since the scaling is not asymptotic, it is presumably not related to any fixed point behavior.

The results for $D(q, t)$ also show that the initial spin fluctuation actually grows in the regime of small wave vectors while it relaxes to zero in the regime of large wave vectors. But, since the initial spin fluctuation is distributed mainly in the regime of large wave vectors and there is little or no fluctuation in the regime of small wave vectors, the growth in the regime of small wave vectors cannot have a notable effect in the autocorrelation unless the growth is asymptotic. Thus, unlike in the results for $S(q, t)$, there is a dramatic difference between $T/T_c < 1$ and $T/T_c > 1$. The scaling function is also more sensitive to the changing quench temperature. Notice that there is a detectable difference between $T/T_c = 0.99$ and $T/T_c = 1.01$ in the shape of the scaling function. That was not the case for $S(q, t)$.

In Sec. III we computed the dynamic structure factor which reveals how the system fluctuates in equilibrium at $T > T_c$. The computed dynamic structure factor shows an activationlike slow dynamics, but it is only transient and may be removed. The relaxation time due to diffusion supports the dynamic scaling. The presence of

the activationlike term may have been anticipated. According to Bray,⁴ the dynamics can be different depending on whether or not a system freezes when quenched to the zero temperature. Unlike the Langevin type of continuum dynamic model, the IMCOP does freeze and thus the dynamics is strongly activated at $T = 0$. It is not unreasonable to expect that such an effect may remain to some degree even after the system has reached its equilibrium state. Our result suggests that that is indeed the case.

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