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Generalized Renormalization Group Treatment of the Growth Kinetics of Unstable Systems

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We discuss the generalization of a renormalization group technique developed previously for the study of ordering in unstable systems in the context of the ferromagnetic Ising model with spin-flip dynamics. Difficulties encountered in earlier work are eliminated through the use of new recursion relations dependent on a continuous spatial rescaling factor $b \geqslant 1$. A more careful analysis and implementation of the approximation scheme is carried out. Our improved method allows the study of the anisotropy of the time-dependent structure factor and the pre-scaling behavior of the shape function.

KEY WORDS: Renormalization group; growth kinetics.

1. INTRODUCTION

Renormalization group (RG) methods developed previously[1,2] for treating the growth kinetics of a system subjected to a rapid temperature quench have led to a very good understanding of the basic physics in these problems, including the origins of scaling behavior and the degree of universality. Quantitative agreement with Monte Carlo (MC) simulations has been obtained in those regions where reliable MC results are available. In this paper we demonstrate how our previous calculations can be extended by including higher orders in the approximation schemes developed earlier for treating the short time and distance behavior. Of more general interest, we deal with the problem of unphysical oscillations which result from the assumption that the spatial rescaling parameter b is a fixed

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integer. We discuss this point in more detail below. Our basic conclusions are that our previous calculations were quite accurate in the regions of greatest physical interest, such as the scaling regime, although important corrections are found elsewhere.

Use of renormalization group methods for treating problems which show scaling behavior is now a standard procedure. Typically, however, the calculations have been restricted to the extraction of critical indices and universal amplitudes for problems near a critical point.[3] Our own previous work has involved the development of RG methods capable of treating a wide range of properties of systems under a variety of physical situations.[4,1,2] In particular we have been interested in the time evolution of Ising-like systems subjected to a rapid and strong external force. Much of our attention has been directed toward systems subjected to temperature quenches from an initial state in thermal equilibrium at temperature T_I to a final state in thermal contact with a heat bath at temperature T_F, where $T_I > T_c > T_F$ and T_c is the critical temperature. It is, by now, well understood that the growth of order in these circumstances leads to scaling behavior in the quasistatic structure factor near those wave numbers, $\mathbf{q}$, associated with Bragg peaks in the ordered state. It should be appreciated that this scaling behavior is not related to critical phenomena, unless T_F is near T_c. In Refs. 1, 2, 5, and 6 we have developed RG methods for treating this problem. These involve techniques for calculating correlations over a wide range of temperatures, distances and times, in both equilibrium and nonequilibrium situations. The results were, for the most part, very accurate. We obtained excellent results for the time-dependent structure factor $C(\mathbf{q}, t)$ in comparison with results from Monte Carlo simulations, and those for the equilibrium structure factor $C(\mathbf{q}, T)$ were in agreement with the most sophisticated analysis in this well-researched field.[3,7] There were, however, certain technical problems which limited the accuracy of the method in some time and distance regimes. These difficulties were associated with unphysical oscillations[8] in space or time which developed as part of the iterative solution of our RG recursion relations. These oscillations can be traced back to our use of an integral spatial rescaling factor b ($b = 2$). This choice is natural as long as one is thinking in terms of breaking the system up into a set of cells with b^d spins in a cell (d is the dimensionality) and associating a new block spin with each cell. Clearly the spacing on the new lattice is b times the original, and all wave numbers must be rescaled by a factor of b if one compares properties associated with the two lattices:

$$\mathbf{r}' = \mathbf{r}/b \tag{1.1}$$

$$\mathbf{q}' = b\mathbf{q} \tag{1.2}$$

Unfortunately the process of dividing the system into cells breaks the translational symmetry of the lattice, introduces unphysical quasiperiodicities and leads eventually to the oscillations mentioned above.

For most of the problems we have studied, these oscillations are not quantitatively important, and since one can calculate the period of these oscillations they can be averaged over when they do occur.[2,5] However, they are an unphysical artifact, and for certain purposes they are a limitation. A relevant example is the determination of the anisotropy of the scaling function $F(\mathbf{x})$ associated with the structure factor $C(\mathbf{q}, t)$. Any anisotropy occurs in the wings of $F(\mathbf{x})$ and this is the region where these oscillations, which appear to be more pronounced in certain directions than in others, begin to play a role.

From a renormalization group point of view the question of the oscillations and quasiperiodicity is related to the RG flows of the parameters characterizing the problem. Thus we have for the quench problem the variables T_I, T_F, $\mathbf{q}$, and t and associated recursion relations characterizing their flows under rescaling. As usual, T_I $(>T_c)$ scales to infinity and T_F $(<T_c)$ scales to zero and the three fixed points correspond to a completely disordered state, a critical point and a completely ordered state. The rescaling of time, $t' = \Delta(b)t$, is such that the system flows to earlier times $(\Delta < 1)$. The wave vector rescaling, $\mathbf{q}' = b\mathbf{q}\ (\mathrm{Mod}\ 2\pi)$, however, is qualitatively different from the other rescalings. For any $\mathbf{q} \neq \mathbf{0}$ one does not scale to a fixed point, but instead one eventually generates a sequence of values of $\mathbf{q}$ which depend on whether or not the original wave number is a rational multiple of π, and which can generate a chaotic sequence in the first Brillouin zone. This also allows the mapping of antiferromagnetic degrees of freedom ($\mathbf{q} = \boldsymbol{\pi}$, where $\boldsymbol{\pi} = (\pi, \pi)$ for the square lattice) onto the ferromagnetic point ($\mathbf{q} = \mathbf{0}$). In the next section we discuss how the recursion relation for $\mathbf{q}$ can be put on an equal footing with those for T and t.

There are two additional improvements and generalizations of the methods introduced in Ref. 2 which we want to discuss. First, in treating $C(\mathbf{q}, T)$ only the lowest-order spatial approximation was introduced in Ref. 2. It was mentioned there that the procedure could be generalized to include information from any number of static short-range correlation functions. We will show here how this can be done in a systematic fashion. The second improvement relates to the time dependence. In Refs. 1, 2, and 5 we used a simple relaxation form for the short-range quantities which appear in the recursion relations. We pointed out that the relaxation rate can be determined from the initial derivative of the correlation functions upon quenching, a quantity which is known exactly. Since all the initial derivatives, not only the first, can be calculated exactly, it is obviously

desirable to have a systematic way of bringing in any number of additional derivatives. This is developed in the present paper, and in particular we show, for the case of spin-flip dynamics, how the results for the quasistatic structure factor are improved by the inclusion of second-derivative information. Similar procedures can be used for exchange dynamics.

We want to briefly clarify here the use of the expression "renormalization group" to describe the methods of this paper and of Refs. 2, 5, and 6. This should not be taken in the narrow sense of a Niemeijer–van Leeuwen[3] rigid block-spin type of analysis (as used, for example, in Ref. 4). It is better, for the problem discussed here, to use methods where the system is not subdivided into cells. These alternate implementations of the RG have largely been developed in the context of field theory. The use of the RG term to describe our methods can best be understood by referring to Chap. 8 of Ref. 9. As it is pointed out there, there are a number of different ways of developing the RG which do not involve block-spin transformations. In general, the RG is defined in Ref. 9 as a "group of transformations between different versions of the renormalized theory and one given theory" (Ref. 9, Section 8.1). The recursion relations we derive [Eq. (3.1) and corresponding equations in Refs. 2 and 6] are in fact the appropriate adaptation of Eq. (8.1) of Ref. 9 to the problem of growth kinetics.

This paper is organized as follows. In Section 2 we discuss the new recursion relations and the equilibrium properties. In Section 3 we introduce the nonequilibrium recursion relations for SF dynamics and obtain results for $C(\mathbf{q}, t)$ which are free from the spurious oscillations discussed above. In Section 4 we demonstrate how our approximations can be extended in a systematic fashion.

2. GENERAL DEVELOPMENT AND EQUILIBRIUM CALCULATIONS

Our first objective in this section is to show that equilibrium correlation functions for the Ising model can be calculated using RG techniques similar to those used in Refs. 1 and 2 for the same problem, but with a more physical treatment of short-ranged degrees of freedom under rescaling with an arbitrary, not necessarily integer, spatial rescaling factor b. We will begin by generalizing the work of Refs. 2, 4, 8, and 10, where the fixed value $b=2$ was used. In the next section, we will show how the quasistatic structure factor can also be evaluated, using the same techniques, for the case of growth kinetics generated by spin-flip dynamics. It is important to realize that the use of a fixed, integer b is tied to the division of the system into cells, which is in turn basic to the earliest formulations of

the real space RG.[3] Escape from the constraint of an integer b, therefore, is possible only when one avoids the block spin methods of Refs. 1, 3, 4, and 8 used to derive recursion relations for correlation functions. The procedures developed in Refs. 2, 5, and 6, while free from the necessity of breaking the system into cells, retained a remnant of the block-spin procedure through the use of an integer value of b and a recursion relation for wavenumbers $\mathbf{q}' = b\mathbf{q}$ (Mod 2π). We discuss here how these conditions can be replaced by more physical recursion relations $\mathbf{q}' = \mathbf{q}'(b, \mathbf{q})$.

Throughout this paper, we will focus our attention on the case of a square lattice with nearest-neighbor interactions only, but it will be clear that many of our conclusions and procedures have a more general validity and they are also applicable to the one-dimensional case of Ref. 8 and the cubic lattice of Ref. 10.

Let us first recall that the establishment of a thermal recursion relation poses no difficulties whatsoever. If K is the nearest-neighbor coupling ($K = \beta J$, where J is the nearest-neighbor exchange constant) the relation between K and the renormalized coupling K' after an arbitrary rescaling b is given by

$$\xi' = \xi(K') = \xi(K)/b \tag{2.1}$$

where ξ is the true correlation length which, for the square lattice, is known[7] as a function of K. Equation (2.1) can therefore be shown to be equivalent to

$$\phi' = \phi^b \tag{2.2}$$

$$\phi = e^{2K} \tanh K \tag{2.3}$$

We recall[2] that the recursion relation satisfied by the equilibrium structure factor is

$$C(\mathbf{q}, K) = C_0(\mathbf{q}, K) + P(\mathbf{q}, K)\, C(\mathbf{q}', K') \tag{2.4}$$

where K' is given by (2.2), and the quantities $C_0(\mathbf{q}, K)$ and $P(\mathbf{q}, K)$ are defined by (2.4), once K' and $\mathbf{q}'$ are determined. Physically $C_0(\mathbf{q}, K)$ represents the contribution to $C(\mathbf{q}, K)$ from short-range degrees of freedom (roughly from wave numbers in the shell $\pi > q > \pi/b$), and $P(\mathbf{q}, K)$ represents a normalization factor relating $\sigma_{\mathbf{q}}$ and $\sigma_{\mathbf{q}'}$, where $\sigma_{\mathbf{q}}$ is the Fourier transform of the spin field.[2] In the block-spin picture one is naturally led to the recursion relation

$$q_i' = bq_i \ (\text{Mod } 2\pi) \tag{2.5}$$

where the index i denotes the components of the vector $\mathbf{q}$. This relation is physically sensible only for long wavelengths. However as $\mathbf{q}$ increases away from the center of the first Brillouin zone, (2.5) brings $\mathbf{q}'$ to the zone edge, and then beyond, thereby introducing an artificial connection between unrelated wave vectors in the first Brillouin zone. This is the artificial periodicity discussed in the Introduction, and it is, in turn, the result of a failure to distinguish between those wave numbers which are associated with scaling behavior and those which are not. It is sensible that the short-range degrees of freedom characterized by a wave number in the middle of the Brillouin zone flow away from the unstable fixed point associated with the ordering at the magnetic points at $\mathbf{q}=0$. This implies that under renormalization the wave number flows into attractive fixed points associated with the high symmetry points at the zone boundary.

A more physical relation between $\mathbf{q}'$ and $\mathbf{q}$ as a function of arbitrary b must have the following properties: (i) It must reduce to (2.5) for small q, (ii) it should have the periodicity of the lattice, (iii) it should reduce to the identity at the zone edge, and (iv) also, obviously, in the limit $b=1$. Of course, these conditions do not uniquely determine the transformation. Our task is to choose, among the transformations satisfying the above requirements, one that is convenient to use. Given that transformation, we can then proceed with the determination of P and C_0, along the lines discussed in Ref. 2.

A simple recursion relation which satisfies the above requirements, and which we shall adopt for our calculations is

$$q_i' = 2\tan^{-1} b \tan(q_i/2) \tag{2.6}$$

Equation (2.6) clearly has the properties

$$q_i' = bq_i \qquad (q_i \ll \pi) \tag{2.7a}$$

$$\mathbf{q}'(\mathbf{q}+\mathbf{G}) = \mathbf{q}'(\mathbf{q}) \tag{2.7b}$$

$$q_i'(\pi) = \pi \tag{2.7c}$$

$$\lim_{b\to 1} q_i'(q_i) = q_i \tag{2.7d}$$

where $\mathbf{G}$ is any reciprocal lattice vector. Note that all wave vectors are measured in units of the inverse lattice constant. Equations (2.7) are mathematical restatements of conditions (i)–(iv) above. It is often convenient to rewrite (2.6) as

$$\cos q_i' = \frac{\cos q_i - \alpha}{1 - \alpha \cos q_i}, \qquad \alpha = \frac{b^2-1}{b^2+1} \tag{2.8}$$

We note, for b near 1, that α is small, which may be convenient for calculational purposes.

We can now proceed with the determination of $P(\mathbf{q})$ and $C_0(\mathbf{q})$. As in Ref. 2 (see also Ref. 4), these functions are determined from the behavior of known static correlations. Note, however, that in previous work[1,2,4] the restriction

$$P(\boldsymbol{\pi}) = 0 \tag{2.9}$$

has been imposed on the function $P(\mathbf{q})$ to prevent mapping the antiferromagnetic onto the magnetic susceptibility. Since (2.7c) already precludes this mapping, the restriction (2.9) is no longer necessary.

In the determination of $C_0(\mathbf{q})$ and $P(\mathbf{q})$ [see (2.4)] we are guided by our knowledge of the static correlation function in certain limits. The $\mathbf{q} = 0$ limit of (2.4) gives the recursion relation for the susceptibility:

$$\chi = \chi_0 + b^d \pi_0 \chi' \tag{2.10}$$

where, for convenience, we have defined $P(0) = b^d \pi_0$. In the ordered phase, simple RG arguments[2] show that

$$\pi_0 = (m/m')^2 \qquad (T < T_c) \tag{2.11}$$

where m is the equilibrium spontaneous magnetization. Near the phase transition the critical singularities cancel and π_0 is a smooth function of temperature. Above T_c we can write

$$b^d \pi_0 = \frac{\chi - \chi_l}{\chi' - \chi_l'} \tag{2.12}$$

where χ_l is the local, analytic part of χ.[11,12] Equations (2.10) and (2.12) therefore show that

$$\chi_0 = \chi_l - b^d \pi_0 \chi_l' \tag{2.13}$$

is also a smooth function of temperature. Because of the trade-off between χ_0 and π_0 in (2.10), we have found that their particular form is relatively unimportant. We can, therefore, fix χ_l at its value at the critical temperature, $\chi_l^* = 0.11$[12] in two dimensions, and obtain

$$\chi_0 = \chi_l^*(1 - b^d \pi_0) \qquad (T > T_c) \tag{2.14}$$

The quantity π_0, defined by (2.11) for $T < T_c$ and (2.12) with $\chi_l = \chi_l^*$ for $T > T_c$, is smooth at $T = T_c$. One can then determine χ_0 for $T < T_c$ using low temperature expansions for χ, while π_0 [and χ_0 via (2.14)] is

determined for $T > T_c$ from (2.12) using high-temperature expansions for χ. The results for π_0 are shown in Fig. 1 for several values of b. Notice from (2.11) and (2.12) that as $b \to 1$ and $\chi' \to \chi$, $\pi_0 \to 1$, and $\chi_0 \to 0$ and (2.10) reduces to the identity.

In generalizing (2.10) to nonzero wave vectors, our guiding principle is that (2.4) should always reduce to a trivial equality in the limit $b \to 1$, i.e.,

$$\lim_{b \to 1} C_0(\mathbf{q}) = 0 \tag{2.15}$$

$$\lim_{b \to 1} P(\mathbf{q}) = 1 \tag{2.16}$$

We can choose $P(\mathbf{q})$ in agreement with (2.16) and (2.10) if

$$P(\mathbf{q}) = \pi_0 f(\mathbf{q}) \tag{2.17}$$

where

$$\lim_{b \to 1} f(\mathbf{q}) = 1 \tag{2.18}$$

and

$$\lim_{\mathbf{q} \to 0} f(\mathbf{q}) = b^d \tag{2.19}$$

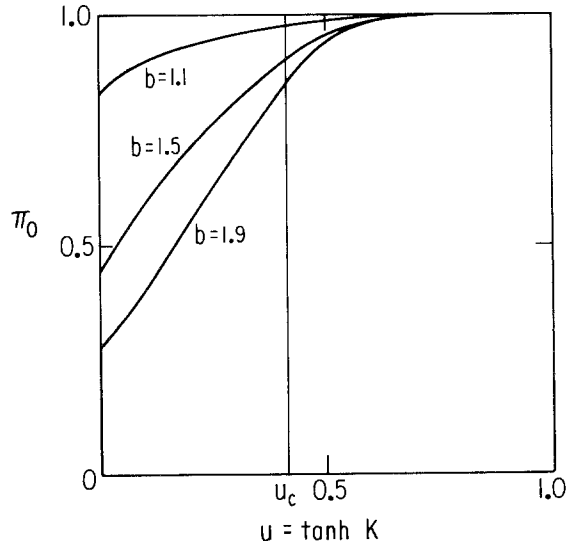

Fig. 1. The parameter π_0 as a function of temperature, for several values of b.

There is an additional constraint since in the Ising model the "fixed-length spin" sum rule must always be satisfied:

$$1 = \int_{BZ} \frac{d^d q}{(2\pi)^d} C(\mathbf{q}) = \int_{BZ'} \frac{d^d q'}{(2\pi)^d} C'(\mathbf{q}') \tag{2.20}$$

where BZ denotes the first Brillouin zone of the lattice. The mapping (2.6) preserves the Brillouin zone. We see, therefore, that $f(\mathbf{q})$ can be taken to be the Jacobian of the transformation (2.6):

$$f(\mathbf{q}) = \prod_{i=1}^{d} \frac{dq_i'}{dq_i} \tag{2.21}$$

This satisfies (2.18) and (2.19) [see (2.7)] and ensures that $P(\mathbf{q})$ is a periodic function of $\mathbf{q}$. We therefore adopt (2.17) and (2.21).

We now turn to the inhomogeneous term $C_0(\mathbf{q})$ which, like χ_0, should be a local, well-behaved function of T and $\mathbf{q}$. As such, it may be expanded in a Fourier series,

$$C_0(\mathbf{q}) = \sum_{\mathbf{m}} \varepsilon_0(\mathbf{m}) \prod_{i=1}^{d} \cos(m_i q_i) \tag{2.22}$$

and approximated by a finite number of terms. In Ref. 2 the coefficients $\varepsilon_0(\mathbf{m})$ were determined from

$$\chi_0 = \sum_{\mathbf{m}} \varepsilon_0(\mathbf{m}) \tag{2.23}$$

and from recursion relations for exactly known short-range spatial correlations which were developed there. However, the recursion relation in momentum space (2.6) suggests that we take a different approach. The flows generated by (2.6) under iteration lead into the antiferromagnetic point of the Brillouin zone. It is therefore important that the recursion relation be as accurate as possible near that point. This can be accomplished by using the known values, from series expansion,[13] for the antiferromagnetic susceptibility, χ_a, to determine the quantity

$$\chi_{0,a} = C_0(\pi) = \chi_a - b^{-d} \pi_0 \chi_a' \tag{2.24}$$

in addition to χ_0. Together with Eqs. (2.23) and (2.20), knowledge of $\chi_{0,a}$ enables us to find the first three coefficients in (2.22):

$$\varepsilon_0(0, 0) = 1 - \pi_0 \tag{2.25a}$$

$$\varepsilon_0(1, 0) = (\chi_0 - \chi_{0,a})/8 \tag{2.25b}$$

$$\varepsilon_0(1, 1) = (\chi_0 + \chi_{0,a} + 2\pi_0 - 2)/8 \tag{2.25c}$$

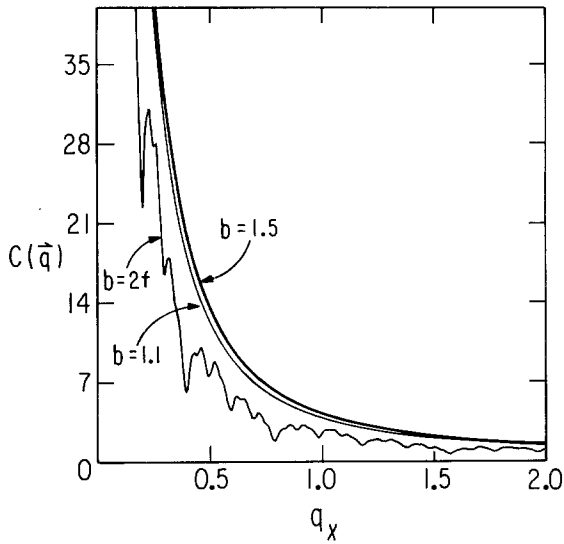

Fig. 2. The static structure factor $C(\mathbf{q})$ as a function of $q_x = q$. The curve labeled $b = 2f$ is from Ref. 2 and $b = 1.1$, 1.5 are from the present calculation. This is in the critical region, $u = \tanh K = 0.41$.

The structure factor $C(\mathbf{q})$ which results from iterating (2.4) within the above approximations is shown in Fig. 2 for several values of b, along with the result of previous work,[2] $b = 2$, which we will refer to as $b = 2f$. Because this is in the critical region, $u = \tanh K = 0.41 \leqslant u_c$, the wiggles in the $b = 2f$ case, which were discussed in the introduction, are very pronounced. The present calculation is only slightly b dependent, and is very smooth: the spurious oscillations have indeed been eliminated.

3. THE QUASISTATIC STRUCTURE FACTOR

We now turn to the calculation of nonequilibrium properties. We will focus our attention on the quasistatic structure factor $C(\mathbf{q}, t)$, whose recursion relation is a generalization of (2.3):

$$C(\mathbf{q}, t) = C_0(\mathbf{q}, t) + P(\mathbf{q}, t)\, C'(\mathbf{q}', t') \tag{3.1}$$

$C(\mathbf{q}, t)$ and the quantities $C_0(\mathbf{q}, t)$ and $P(\mathbf{q}, t)$ depend on both the initial and final temperatures T_I and T_F. The renormalized couplings K'_I, K'_F and wave vector $\mathbf{q}'$ are determined, as for the static case, by (2.2) and (2.6), respectively. The time variable is also renormalized; this is discussed in

detail in Refs. 2 and 6. We consider here spin-flip dynamics in zero field, in which case we have[2]

$$t' = \Delta t \tag{3.2a}$$

$$\Delta = b^{-2} \tag{3.2b}$$

Spin-flip dynamics approximate[5] the behavior of a binary alloy which orders at low temperatures. We use here the same flipping probability as in Ref. 2.

The time dependence of the functions $C_0(\mathbf{q}, t)$ and $P(\mathbf{q}, t)$ is determined in a manner similar to Refs. 2 and 6. They depend on the local quantities $\chi_{0,a}(t)$, $\chi_0(t)$ and $\pi_0(t)$ which will decay rapidly to their final equilibrium values from their initial state. This decay is assumed[2] to be given by the relaxational form

$$\pi_0(t) = \pi_0^F - e^{-\lambda t}(\pi_0^F - \pi_0^I) \tag{3.3a}$$

where

$$\lambda = \dot{\pi}_0(0)/(\pi_0^F - \pi_0^I) \tag{3.3b}$$

and the dot denotes the time derivative taken at $t = 0$. Since λ must be positive, $\dot{\pi}_0(0)$ must have the same sign as $\pi_0^F - \pi_0^I$. One can see in Fig. 1 that π_0 is a monotonic function of the temperature. This is not true for χ_0 which vanishes both at $T = 0$ and $T = \infty$. Since $\Delta < 1$, Eq. (3.2) implies that the recursion relations iterate to $t = 0$. As in Ref. 2 we will deal here with the case where the initial temperature is infinite, so that at $t = 0$, $C(\mathbf{q}, t = 0) \equiv 1$. It is then convenient to perform the iterations in terms of the quantity

$$D(\mathbf{q}, t) = C(\mathbf{q}, t) - 1 = D_0(\mathbf{q}, t) + P(\mathbf{q}, t)\, D'(\mathbf{q}', t') \tag{3.4}$$

and define

$$\psi_0(t) = D_0(0, t) = \chi_0 + b^2\pi_0 - 1 \tag{3.5a}$$

$$\psi_{0,a}(t) = D_0(\boldsymbol{\pi}, t) = \chi_{0,a} + b^{-2}\pi_0 - 1 \tag{3.5b}$$

which have the desired monotonicity. Using the exactly known initial time derivatives[2] $\dot{\chi}(0)$ and $\dot{\chi}_a(0)$ and (2.10), (2.13), and (2.24), we find that

$$\dot{\pi}_0(0) = 4\alpha \frac{ba_F - a'_F}{b^4(1 - \chi_I^*)} \tag{3.6a}$$

$$\dot{\psi}_0(0) = 4\alpha \frac{b^2 a_F - a'_F}{b^2} \tag{3.6b}$$

$$\dot{\psi}_{0,a}(0) = -4\alpha \frac{b^6 a_F - a'_F}{b^6} \tag{3.6c}$$

where $a_F = \tanh(2K_F)$ and α is, as usual, the flip rate at infinite temperature. The quantities $\psi_0(t)$ and $\psi_{0,a}(t)$ are assumed to have a time dependence of the form (3.3a) with decay rate given by expressions analogous to (3.3b).

The recursion relation (3.4) may then be iterated to obtain the time-dependent structure factor. Results corresponding to a quench to zero temperature are shown in Fig. 3 for several values of b, at time $t = 5$ (all times are in units of α^{-1}). For comparison, we include also in Fig. 3 results obtained using the fixed $b = 2$ method of Ref. 2. Note the convergence of these results as b approaches unity. As in the static case (see Fig. 2) the fixed b method introduces spurious oscillations, which disappear when using the present procedure. This is clearly shown in Fig. 4, obtained under the same conditions as Fig. 3, but for very long times and along the (10) wave vector direction. The new results are again very smooth.

The wave vector directions (11) and (10) are compared in Fig. 5, at time $t = 10$. One of the advantages of these renormalization group calculations as compared to Monte Carlo simulations is the detailed wave vector dependence that can be generated; as can be clearly seen in Fig. 5, the structure factor is anisotropic, with a smaller width q_w in the (11) direction. This was also found in the alloy problem of Ref. 6. Since the domain size $L \sim q_w^{-1}$, this shows that the growth is greater in this direction. The degree of anisotropy is significant at 18%.

Figure 6 displays the susceptibility $\chi(t) = C(0, t)$. It is seen that $\chi(t)$ is proportional to t. This is in agreement with the Lifshitz–Cahn–Allen law[14] $[L(t) \sim t^{1/2}]$ combined with scaling. We also see that at least at the relatively early times included in Fig. 6 the results at $b = 1.1$ are in better agreement with MC simulation results (also shown) than the previous theoretical results obtained for $b = 2f$.

For sufficiently long times, $C(\mathbf{q}, t)$ for this model is known[2,5,15] to be of the scaling form,

$$C(\mathbf{q}, t) = \chi(t)\, F(\mathbf{x} = \mathbf{q}/q_w(t)) \tag{3.7}$$

where $q_w(t)$ is the width of $C(\mathbf{q}, t)$. $F(\mathbf{x})$, the scaling function, is plotted as a function of $|\mathbf{x}|$ in Fig. 7. Again, we see wiggles for fixed $b = 2$; while $b = 1.1$ is very smooth. The wiggles prevent F from being a truly scale-invariant function, whereas the $b = 1.1$ result is independent of time and also, as in Refs. 2 and 5, essentially independent of temperature. Of course, the scaling behavior is found only at sufficiently long times, or small $|\mathbf{x}|$, or both. At early times, and large $|\mathbf{x}|$, F is a periodic function. This is clearly seen in Fig. 8. But for times $t \geqslant 10$ and $|\mathbf{x}| \leqslant 10$, $F(\mathbf{x})$ is essentially time independent. In this regime, there is an algebraic decay $F(\mathbf{x}) \sim |\mathbf{x}|^{-\alpha}$, where $\alpha = 2.9$;

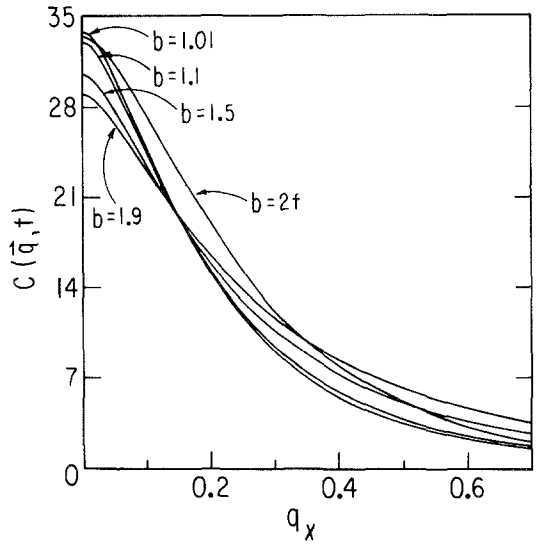

Fig. 3. The time-dependent structure factor $C(\mathbf{q}, t)$ as a function of $q_x = q/\sqrt{2}$. This is for a quench from $T_I = \infty$ to $T_F = 0$, after a time $t = 5$. Again, the curve labeled $b = 2f$ is from Ref. 2, and $b = 1.9$, 1.5, 1.1, and 1.01 are from the present calculation.

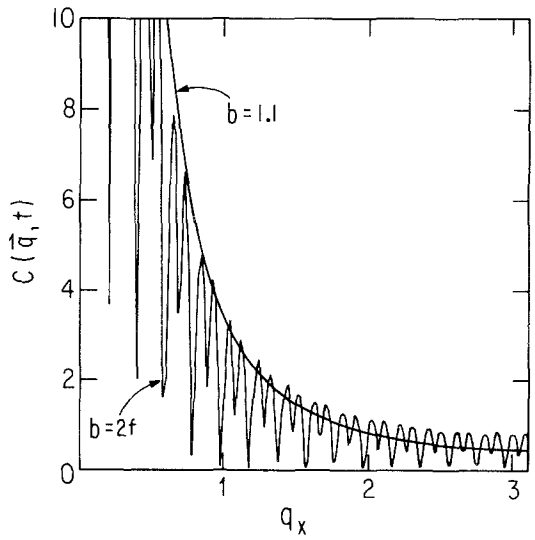

Fig. 4. The time-dependent structure factor $C(\mathbf{q}, t)$ in the (10) direction as a function of $q_x = q$, after a long time $t = 1000$. Again, $T_I = \infty$ and $T_F = 0$, $b = 2f$ is Ref. 2 and $b = 1.1$ is the present calculation.

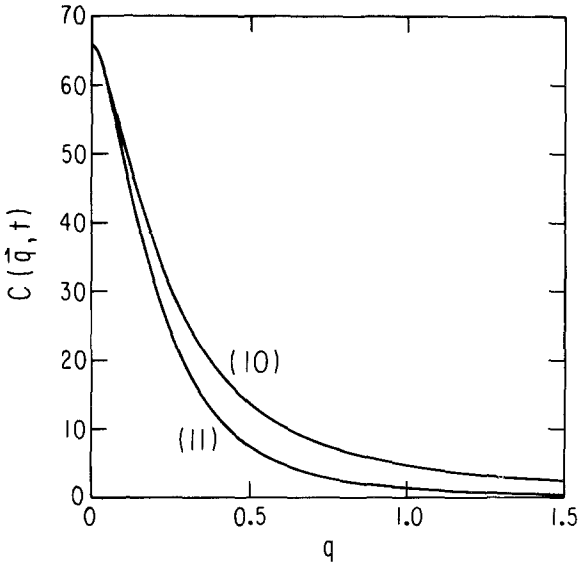

Fig. 5. The time-dependent structure factor in the two wave vector directions (11) and (10). Both are plotted versus q. $T_I = \infty$, $T_F = 0$, and $t = 10$ for all curves.

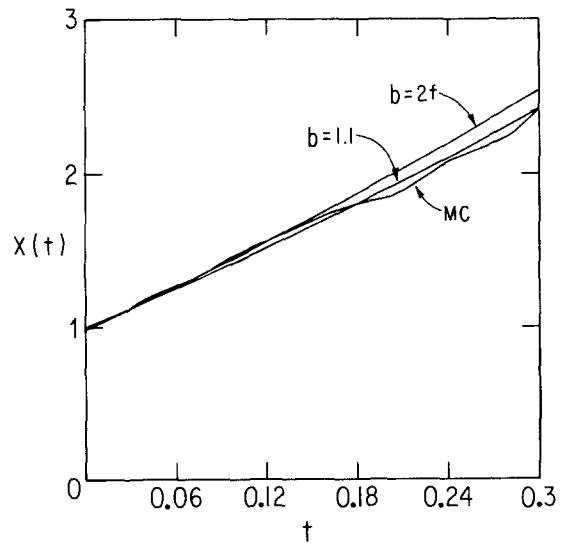

Fig. 6. The susceptibility $\chi(t) = C(0, t)$ for early times. Along with the $b = 2f$ and $b = 1.1$ RG results, a Monte Carlo simulation of $\chi(t)$ is shown (from a 128×128 lattice, averaged over 100 runs).

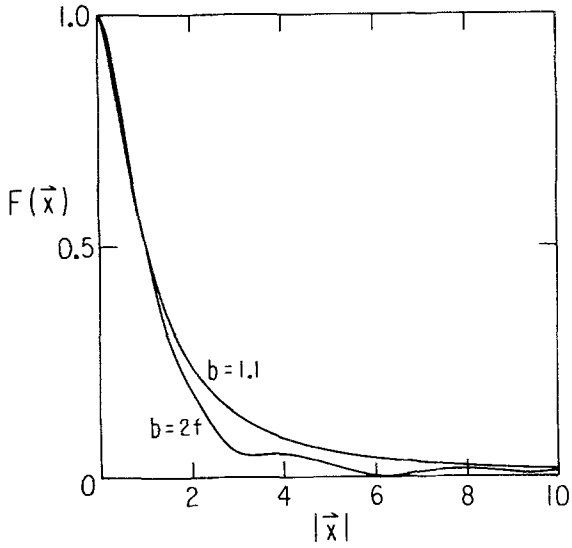

Fig. 7. The shape function $F(\mathbf{x})$ for $\mathbf{x}$ in the (10) direction. $T_I = \infty$, $T_F = 0$, $t = 10$.

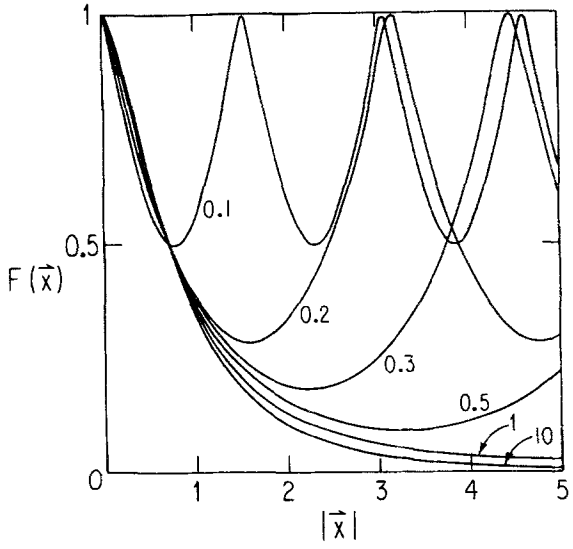

Fig. 8. The shape function $F(\mathbf{x})$ for $\mathbf{x}$ in the (11) direction, at early times which label each curve. $T_I = \infty$, $T_F = 0$.

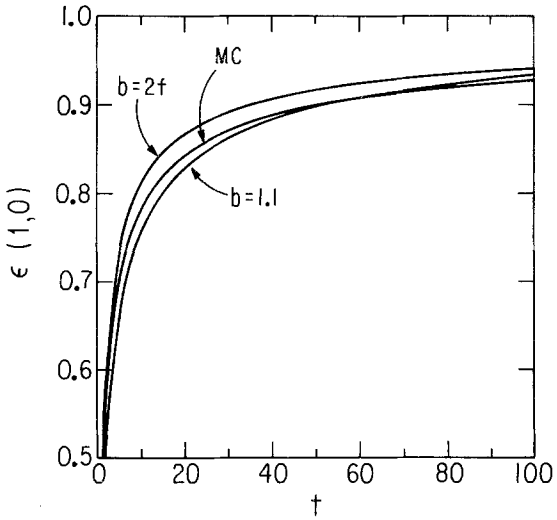

Fig. 9. The nearest-neighbor order parameter $\varepsilon(1, 0)$ as a function of time. Both $b = 1.1$ and Monte Carlo results are shown. $T_I = \infty$, $T_F = 0$; the Monte Carlo calculation is for a 128×128 lattice and 100 runs.

this is in agreement with $\alpha = d + 1$ (Porod's law[16]), and as previously found in Refs. 2 and 17.

Another quantity of interest is the nearest-neighbor correlation function, $\varepsilon(1, 0)$, through which one can monitor the growth of short-range order. The most straightforward way to calculate $\varepsilon(1, 0)$ is to numerically integrate the structure factor $C(\mathbf{q}, t)$ as calculated by iterating Eq. (3.1), and this is the approach we have used since the alternative procedure[2] of Fourier transforming the recursion relation (3.4) first and then iterating is less practical in this case. Figure 9 shows the $b = 1.1$ result, along with a Monte Carlo calculation of $\varepsilon(1, 0)$. We see that there is only a difference of a few percent between the two.

We see that the results obtained are extremely satisfactory: they compare with MC simulation as well or better than the results of Ref. 2, while both equilibrium and nonequilibrium quantities are now free of oscillatory artifacts.

4. EXTENSIONS OF THE BASIC MODEL

In developing our basic model in Sections 2 and 3, we have made two approximations which can be improved upon in a systematic fashion. The first was the truncation of the Fourier series for $C_0(\mathbf{q})$, Eq. (2.22). The only information used to determine $C_0(\mathbf{q})$ was the fixed-length-spin condition

expressed through (2.25a), and information about the ferromagnetic ($\mathbf{q}=0$) and antiferromagnetic ($\mathbf{q}=\pi$) fixed points (2.25b,c). In Fourier space, the latter two are an anisotropic set, and may very well contribute to the anisotropy which is observed in Fig. 5. Therefore, when including more Fourier coefficients in the expansion $C_0(\mathbf{q})$, it is reasonable to choose the next one to be the (1, 0) point in wave vector space:

$$\chi_{10} = C_0(\pi, 0) = C(\pi, 0) - \pi_0 C'(\pi, 0) \tag{4.1}$$

It is straightforward to approximate χ_{10} in a manner similar to $\chi_{0,a}$, since $C(\pi, 0)$ is accurately known from series expansions[7] [both χ_a and $C(\pi, 0)$ are, of course, well-behaved quantities at all temperatures]. This allows an extra term $[\varepsilon_0(2, 0)]$ to be included in the expansion (2.22).

The resulting structure factor shows a small but significant difference from the lower order or "basic" model. The difference is easily seen by plotting the width of the structure factor in Fourier space, as in Fig. 10. The basic model is seen to be much flatter in the (11) direction; including χ_{10} does indeed produce a more isotropic structure factor, with an anisotropy that is still 10%. This indicates that there really is preferential domain growth in the (11) direction as discussed in Section 3 and found in Ref. 5.

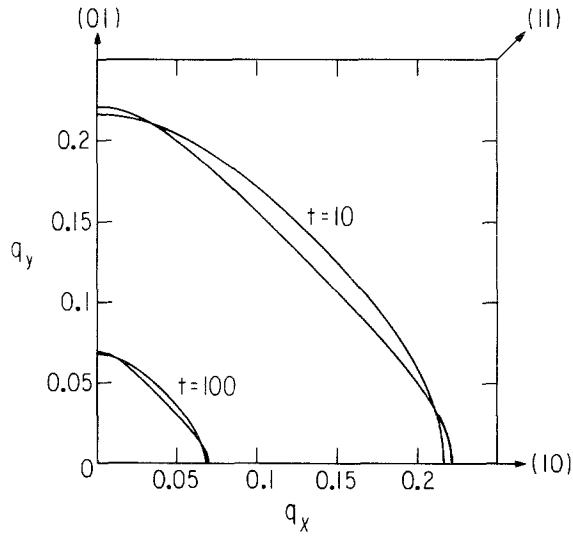

Fig. 10. The structure factor width $q_w(t)$ for the basic and extended Fourier models. The latter is seen to be somewhat more isotropic. $T_I=\infty$, $T_F=0$, $b=1.1$.

If one wishes, it is straightforward to extend this procedure and include more of the "high-symmetry" points of the Brillouin zone. Simple approximants for well-behaved quantities such as χ_0, χ_a, χ_{10} can be formed using information from, for example, Tarko and Fisher.[7] We expect, however, that there will be very little change beyond the inclusion of these first three.

The other approximation involves the time dependence of these local variables. With the simple relaxational form (3.3), there is only one parameter, λ, which is determined by the first time derivative ($D=1$). However, more parameters may be included to systematically incorporate higher-derivative information into the model. For example, to include the second time derivative ($D=2$), we add in the appropriate power of t to (3.3):

$$\pi_0(t) = \pi_0^F - (\pi_0^F - \pi_0^I)(1 + Bt^2)\, e^{-\lambda t} \tag{4.2}$$

Thus

$$\lambda = \dot{\pi}(0)/(\pi_0^F - \pi_0^I) \tag{4.3a}$$

$$B = -\left[\lambda^2 + \frac{\ddot{\pi}_0(0)}{\pi_0^F - \pi_0^I}\right]\Big/2 \tag{4.3b}$$

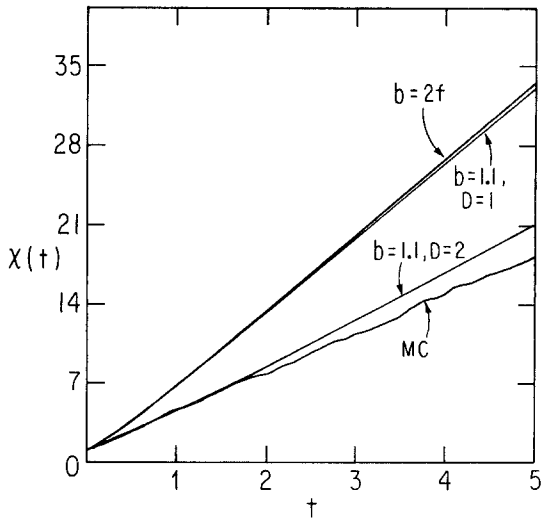

Fig. 11. The susceptibility $\chi(t)$ for $D=1$ ($b=2F$, $b=1.1$), $D=2$ ($b=1.1$), and Monte Carlo (128×128 lattice, 100 runs), for later times than Fig. 6.

The second time derivative $\ddot{\pi}_0(0)$ may be determined in the same way as the first derivatives (Ref. 2 and Section 3). The form (4.2) ensures that the value of λ is unchanged from the $D=1$ case, and it is easy to verify that the value of B derived from (4.3b) ensures that $\pi_0(t)$, as defined by (4.2), is a monotonic function of time. Additional derivatives can be incorporated in the theory by adding higher order terms to the $1+Bt^2$ polynomial in (4.2).

The $D=2$ result for the time-independent susceptibility is shown in Fig. 11, along with the previous $D=1$ results ($b=1.1, 2f$), and a Monte Carlo simulation. This is an extension to later times of Fig. 6, showing that the $D=1$ susceptibilities, while remaining close together, separate from the Monte Carlo. The $D=2$ susceptibility, however, remains close to the Monte Carlo result for much longer times.

5. CONCLUSIONS

We have studied in this paper the extension of previously developed RG methods for the growth kinetics of unstable systems. Three independent questions have been studied. The first, which affects even the calculation of static correlation functions, is the development of spatial recursion relations which properly treat short-distance behavior. We have shown how the introduction of these recursion relations yield smooth results for the correlation functions in Fourier space, eliminating the unphysical nonmonotonicities which had been found in previous work which used the standard form of the recursion relations. This was the major problem that we set out to solve. Elimination of these artificial oscillations permits a more detailed study of the anisotropy of the quenched system as time evolves, as we have seen earlier in the paper.

The two other questions discussed, in Sections 3 and 4, were the procedures used to include known information in the calculation in the form of static correlation functions and initial time derivatives. It is clear that these methods can be extended in a straightforward and systematic way. The results were favorably compared with previous work and MC simulations.

In this paper we have used spin-flip dynamics which, for example, model order–disorder transitions in binary alloys. It was shown in Ref. 5 that results obtained using spin-flip dynamics are very similar to those obtained using antiferromagnetic spin-exchange dynamics, which includes one conserved quantity (not the order parameter) and represents, therefore, a more accurate modeling of the actual dynamics in a binary alloy undergoing an order–disorder transition. However we expect only minor changes in this case from the spin-flip results. A separate question, which we have not directly addressed here, is how to introduce the

methods discussed in the present work in the case of spinodal decomposition, where the order parameter is conserved (see Ref. 6). The conservation law for the order parameter and the fixed-length-spin sum rule, as incorporated into the formalism of Ref. 6, must be considered together with the recursion relation (2.6). Further work is required to carry this out in a convenient manner. On the other hand, the inclusion of additional time derivatives in such models can be handled in the same way as in Section 4 and pose no technical difficulties whatsoever. The same is true of the techniques used in Section 4 to incorporate the information of static correlations.

ACKNOWLEDGMENTS

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REFERENCES

1. G. F. Mazenko and O. T. Valls, *Phys. Rev. B* **27**:6811 (1983).
2. G. F. Mazenko and O. T. Valls, *Phys. Rev. B* **30**:6732 (1984).
3. T. Niemeijer and J. M. J. van Leeuwen, in *Phase Transitions and Critical Phenomena*, Vol. 6, C. Domb and M. S. Green, eds. (Academic Press, New York, 1976).
4. G. F. Mazenko and O. T. Valls, in *Real Space Renormalization*, J. M. J. van Leeuwen and T. W. Burkhardt, eds. (Springer, Berlin, 1982).
5. F. C. Zhang, O. T. Valls, and G. F. Mazenko, *Phys. Rev. B* **31**:1579 (1985).
6. G. F. Mazenko, O. T. Valls, and F. C. Zhang, *Phys. Rev. B* **31**:4453 (1985).
7. M. E. Fisher and R. J. Burford, *Phys. Rev.* **156**:583 (1967); H. Tarko and M. E. Fisher, *Phys. Rev. B* **11**:1217 (1975).
8. G. F. Mazenko and J. Luscombe, *Ann. Phys. (New York)* **132**:121 (1981).
9. D. Amit, *Field Theory, the Renormalization Group and Critical Phenomena* (McGraw-Hill, New York, 1978).
10. S. R. Anderson and G. F. Mazenko, *J. Stat. Phys.* **35**:1 (1984).
11. E. Barouch, B. M. McCoy, and T. T. Wu, *Phys. Rev. Lett.* **31**:1409 (1973).
12. A. J. Guttman, *J. Phys. A* **8**:1236 (1975).
13. C. Domb, in *Phase Transitions and Critical Phenomena*, Vol. 3, C. Domb and M. S. Green, eds. (Academic Press, New York, 1976).
14. I. M. Lifshitz, *Zh. Eksp. Teor. Fiz.* **42**:1354 (1962) [*Sov. Phys. JETP* **15**:939 (1962)]; S. M. Allen and J. W. Cahn, *Acta. Met.* **27**:1085 (1979), J. W. Cahn and S. M. Allen, *J. Phys. (Paris) Colloq.* **C7**:54 (1977).
15. M. K. Phani, J. L. Lebowitz, M. H. Kalos, and O. Penrose, *Phys. Rev. Lett.* **45**:366 (1980).
16. A. Guinier and G. Fournet, in *Small Angle Scattering of X-Rays* (John Wiley, New York, 1955).
17. T. Ohta, D. Jasnow, and K. Kawasaki, *Phys. Rev. Lett.* **49**:1223 (1982).