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Phase Ordering Dynamics in a Gravitational Field

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We study the dynamics of phase ordering in the presence of an external "gravitational" field, namely a field that varies linearly with distance in one direction. Starting from microscopic considerations, we motivate reasonable phenomenological models for cases with nonconserved and conserved order parameter. We present detailed numerical results from our model for the case with conserved order parameter.

KEY WORDS: Phase ordering dynamics; gravitational field; master equation approach.

1. INTRODUCTION

Much attention has focused on the dynamics of ordering of a homogeneous mixture of two phases which has been rendered thermodynamically unstable by quenching below the bulk critical temperature T_c (for reviews see refs. 1). It is now well accepted that the growing domains are characterized by a unique, time-dependent length scale $L(t) \sim t^{\phi}$ (where t is the time) and the growth exponent ϕ depends on whether or not the order parameter is conserved. The determination of ϕ for pure isotropic systems has been so demanding computationally[1] that considerably less attention has been paid to more realistic situations. One of the realistic problems that has been studied is the effect of a gravitational field on phase ordering dynamics for the case with conserved order parameter but with no hydrodynamic effects.[2,3] However, for reasons which we describe shortly, previous studies suffer from certain inadequacies. In this paper, we use a master equation approach[4] to motivate reasonable phenomenological models for phase ordering dynamics in a field which varies linearly in one direction (e.g., gravity). We study both the cases with nonconserved and

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conserved order parameter, and the resultant model for the conserved case hasd the same static solution as the nonconserved case—an important check on the reasonableness of our model. At the outset, we should emphasize that it is not our intention to propose the master equation approach as a rigorous means of deriving coarse-grained models from microscopic considerations. The approximations involved are too drastic to support any such contention. However, we do believe that, if properly used, the master equation approach can serve as a good guide to obtain a reasonable phenomenological model in physical situations when such a model is not immediately obvious, e.g., a binary mixture in contact with a surface which has a preferential attraction for one of the components.[5]

Existing phenomenological models[2] for the dynamics of segregation of a binary alloy in a gravitational field (and for the closely related problem of driven, diffusive systems[6]) lead to a rate equation for the order parameter which is usually of the form (in terms of dimensionless quantities)

$$\frac{\partial \phi(\mathbf{r}, t)}{\partial t} = -\nabla \cdot \left[M(\phi) \nabla \left(\frac{\delta F\{\phi\}}{\delta \phi(\mathbf{r}, t)} \right) \right] \tag{1}$$

where $\phi(\mathbf{r}, t)$ is the order parameter at point $\mathbf{r}$ and time t; $M(\phi)$ is an order-parameter-dependent mobility; and $F\{\phi\}$ is a coarse-grained free-energy functional, usually of the form

$$F\{\phi(\mathbf{r}, t)\} = \int d\mathbf{r} \left(\frac{\operatorname{sgn}(T - T_c)}{2} \phi(\mathbf{r}, t)^2 + \frac{1}{4} \phi(\mathbf{r}, t)^4 + \frac{1}{2} (\nabla \phi(\mathbf{r}, t))^2 \right) - G \int d\mathbf{r}\, z \phi(\mathbf{r}, t) \tag{2}$$

In (2), the first three terms terms are the customary ϕ^4 free-energy terms. The last term incorporates the gravitational field (presumed to act in the z direction), whose strength is proportional to G. In the Cahn–Hilliard equation, one usually sets $M(\phi) = M$, i.e., the mobility is order-parameter independent. However, if one does this in (1), it has the unfortunate consequence of omitting the gravitational field from the equation. Previous studies[2] have argued that if the mobility is taken to depend on the order parameter, this will have the effect of retaining the gravitational field. We find this argument somewhat unsatisfactory because it suggests that the order-parameter dependence of trhe mobility is the cause for the action of the gravitational field—though there is no physical relation between the two effects. We do not dispute the order-parameter dependence of the mobility[7] or, for the matter, the appearance of gravitational effects through similar terms. However, we believe that the two should be treated as being unrelated—something which has not emerged clearly in previous studies.[2] Second, the static equilibrium solution for both the nonconserved and conserved cases should be identical because thermodynamic equilibrium is independent of the dynamics. This requirement appears to be respected by (1), where we see that $\delta F\{\phi\}/\delta\phi(\mathbf{r}, t) \equiv 0$ (i.e., the condition for equilibrium in the nonconserved case) also gives rises to a static solution for the conserved case. However, the form of the phenomenological free energy in (2) results in the following equation for the static solution $\phi^s(\mathbf{r})$:

$$-\operatorname{sgn}(T-T_c)\,\phi^s(\mathbf{r}) - \phi^s(\mathbf{r})^3 + \nabla^2\phi^s(\mathbf{r}) + Gz = 0 \tag{3}$$

Equation (3) is clearly unreasonable for $z \to \pm\infty$ and we would have to add an extra saturation term to make the solution well-controlled as $z \to \pm\infty$.

In this paper, we apply the master equation approach to obtain reasonable phenomenological models for both the nonconserved and conserved cases. In previous work[3] we have motivated (from the master equation approach) a phenomenological model for the conserved case. However, that model is appropriate only for early to intermediate stages of phase separation under gravity (or driven diffusive systems[6]), because it gives reasonable results only with periodic boundary conditions in the z direction. These are obviously unsatisfactory for studying the late stages of phase separation under gravity. We should also add that, in our present study, the nonconserved case is not particularly interesting physically as it corresponds to the un usual situation of a magnetic field that varies linearly in the z direction. However, our study of the nonconserved case is useful as it yields the static solution with appropriate boundary conditions, which one must obtain in the conserved case also.

This paper is organized as follows. Section 2 is devoted to the derivation of phenomenological models for both the nonconserved and conserved cases. In Section 3 we present numerical results from a simulation of our model for the conserved case. Section 4 concludes with a summary and discussion.

2. PENOMENOLOGICAL MODELS FOR NONCONSERVED AND CONSERVED CASES

The starting point of our modeling is the Hamiltonian for a nearest-neighbor Ising model in a site-dependent field,

$$\mathscr{H} = -J \sum_{\langle i,j\rangle} s_i s_j - \sum_i h_i s_j \tag{4}$$

where J is the strength of the exchange interaction between spins s_i (which take values ± 1 corresponding to wether the spin at site i is "up" or "down" or whether site i is occupied by an atom of species A or B); and h_i is the field at the site i. For simplicity of presentation and for the purpose of obtaining the structure of the order parameter equation, we confine ourselves to the one-dimensional (1D) case, initially. The generalization to arbitrary dimensions is straightforward. First, we consider the nonconserved case, namely we associate Glauber (or spin-flip) dynamics with the Ising model. The standard procedure for finding the time evolution of the order parameter (in this case, an average "magnetization") $\langle s_k \rangle$ (where the average is over spin configurations) from a master equation is well-documented in the literature[4] and we do not go into it again here. The resultant equation in the mean-field approximation is

$$\tau_s \frac{\partial}{\partial t} \langle s_k \rangle = -\langle s_k \rangle + \tanh \left(\frac{J(\langle s_{k+1} \rangle + \langle s_{k-1} \rangle) + gka}{T} \right) \tag{5}$$

where τ_s is the time scale which characterizes a spin flip. In (5), we have put $h_k = gka$, where g is the strength of the gravitational field; k is the layer index; and a is the lattice spacing. We can now identify $\langle s_k \rangle$ as the order parameter $\phi(z, t)$ (where $z = ka$) and Taylor expand $\langle s_{k \pm 1} \rangle$ to obtain

$$\tau_s \frac{\partial}{\partial t} \phi(z, t) = -\phi(z, t) + \tanh \left[\frac{T_c}{T} \phi(z, t) + \frac{Ja^2}{T} \frac{\partial^2 \phi(z, t)}{\partial z^2} + \frac{gz}{T} \right] \tag{6}$$

where we have introduced the mean-field critical temperature $T_c = qJ$, where q is the coordination number of a site. In (6), we introduce rescaled variables as

$$z' = \left(\frac{T}{Ja^2} \right)^{1/2} z, \qquad t' = \frac{t}{\tau_s} \tag{7}$$

to obtain the dimensionless equation (dropping the primes)

$$\frac{\partial \phi(z, t)}{\partial t} = -\phi(z, t) + \tanh \left(\frac{T_c}{T} \phi(z, t) + \frac{\partial^2 \phi(z, t)}{\partial z^2} + Gz \right) \tag{8}$$

where we put $G = (g/T)(Ja^2/T)^{1/2}$. At this stage, it is customary[4] (when $G = 0$) to Taylor expand the "tanh" function assuming that its argument is small and thus recover the time-dependent Ginzburg–Landau (TDGL) equation. However, we cannot do this in our case because of the explicit z dependence of the argument of the "tanh" function. Thus, we will consider (8) itself to be reasonable phenomenological model for nonconserved phase ordering dynamics in a "gravitational" (linear in space) field.

The static solution $\phi^s(z)$ of (8) is found by putting $\partial/\partial t \equiv 0$ to obtain the implicit equation

$$\phi^s(z) = \tanh\left[\frac{T_c}{T}\phi^s(z) + \frac{d^2\phi^s(z)}{dz^2} + Gz\right] \tag{9}$$

with the boundary conditions $\phi^s(\pm\infty) = \pm 1$. An immediate consequence of (9) is that the static solution has the form $\phi^s(z) \simeq \tanh(Gz)$ as $z \to \pm\infty$. Thus, the system orders for large $|z|$, regardless of the value of T. Higher values of T only increase the width of the interface between the spin-up and spin-down regions, as is natural. Equation (8) easily generalizes to arbitrary dimensions, where it has the form

$$\frac{\partial\phi(\mathbf{r}, t)}{\partial t} = -\phi(\mathbf{r}, t) + \tanh\left[\frac{T_c}{T}\phi(\mathbf{r}, t) + \nabla^2\phi(\mathbf{r}, t) + Gz\right] \tag{10}$$

Next, we consider the more interesting case of conserved order parameter, namely we associate Kawasaki (or spin exchange) dynamics with the Ising Hamiltonian in (4). Again, the standard master equation prescription[3,4] yields the following equation (in one dimension) for $\langle s_k\rangle$ in the mean-field approximation:

$$\begin{aligned} 2\tau_s \frac{\partial}{\partial t}\langle s_k\rangle &= -2\langle s_k\rangle + \langle s_{k+1}\rangle + \langle s_{k-1}\rangle + \sum_{n=\pm 1}[1 - \langle s_k\rangle\langle s_{k+n}\rangle] \\ &\quad\times \tanh\left[\frac{J}{T}\left(\langle s_{k+1}\rangle + \langle s_{k-1}\rangle + \frac{gka}{J} - \langle s_k\rangle - \langle s_{k+2n}\rangle - \frac{g(k+n)a}{J}\right)\right] \end{aligned} \tag{11}$$

where τ_s is the characteristic time scale of a spin exchange; and we have again set $h_k = gka$. Equation (11) is easily confirmed to have the same static solution as the nonconserved case. Introducing the short-hand notation $AQ_p = (J/T)[\langle s_{p+1}\rangle + \langle s_{p-1}\rangle + gpa/J]$, we can rewrite Eq. (11) as

$$\begin{aligned} 2\tau_s \frac{\partial}{\partial t}\langle s_k\rangle &= -\langle s_k\rangle + \langle s_{k+1}\rangle + \langle s_{k-1}\rangle \\ &\quad + \sum_{n=\pm 1}[1 - \langle s_k\rangle\langle s_{k+n}\rangle]\tanh(A_k - A_{k+n}) \end{aligned} \tag{12}$$

Clearly, we can add or subtract zero from the right-hand side of (12) without changing the equation. Thus, we rewrite (12) as

$$2\tau_s \frac{\partial}{\partial t} \langle s_k \rangle$$
$$= -2\langle s_k \rangle + (s_{k+1} \rangle + \langle s_{k-1} \rangle + [1 - \langle s_k \rangle \langle s_{k+1} \rangle] \tanh(A_k - A_{k+1})$$
$$+ [1 - \langle s_k \rangle \langle s_{k-1} \rangle] \tanh(A_k - A_{k-1}) - 2[1 - \langle s_k \rangle^2] \tanh(A_k - A_k) \quad (13)$$

where the last term on the right-hand side (which is identically zero) is introduced so as to enable us to identify the last three terms on the right-hand side as a discrete Laplacian.

As before, the continuum limit is obtained by identifying $\langle s_k \rangle \equiv \phi(z, t)$. Then, we can coarse-grain the first three terms on the right-hand side of (13) as

$$-2\langle s_k \rangle + \langle s_{k+1} \rangle + \langle s_{k-1} \rangle = a^2 \frac{\partial^2 \phi(z, t)}{\partial t^2} + O(a^4) \quad (14)$$

The other three terms in (13) are coarse-grained by introducing the discrete function

$$f_{k,n} \equiv [1 - \langle s_k \rangle \langle s_n \rangle] \tanh(A_k - A_n) \quad (15)$$

and identifying

$$f_{k,k+1} + f_{k,k-1} - 2f_{k,k} = a^2 \left. \frac{\partial^2 f(z, x)}{\partial x^2} \right|_{x=z} + O(a^4) \quad (16)$$

where

$$f(z, x) \equiv [1 - \phi(z, t)\, \phi(x, t)] \tanh[A(z, t) - A(x, t)]$$
$$A(z, t) \equiv \frac{1}{T} \left(\phi(z + a, t) + \phi(z - a, t) + \frac{gz}{J} \right) \quad (17)$$

Using (17), we obtain from (16)

$$f_{k,k+1} + f_{k,k-1} - 2f_{k,k}$$
$$= -a^1 \frac{\partial}{z} \left\{ [1 - \phi(z, t)^2] \frac{\partial}{\partial z} \left[\frac{T_c}{T} \phi(z, t) + \frac{1}{2} \frac{T_c}{T} a^2 \frac{\partial^2 \phi(z, t)}{\partial z^2} + \frac{gz}{T} + O(a^4) \right] \right\} \quad (18)$$

We should emphasize that (18) has been obtained without invoking a small-argument expansion as is the case in "derivations" of the phenomenological Cahn–Hilliard equation using the master equation approach.[4] Combining the results from (14) and (18), we have a phenomenological equation for the case with conserved order parameter as follows:

$$2\tau_s \frac{\partial\phi(z,t)}{\partial t} = a^2 \frac{\partial^2\phi(z,t)}{\partial z^2} - a^2 \frac{\partial}{\partial z}\left\{[1-\phi(z,t)^2]\frac{\partial}{\partial z}\left[\frac{T_c}{T}\phi(z,t) + \frac{1}{2}\frac{T_c}{T}a^2\frac{\partial^2\phi(z,t)}{\partial z^2} + \frac{gz}{T}\right]\right\} \tag{19}$$

To obtain (19), we should emphasize that we have retained all terms of $O(a^2)$; selectively retained only some terms of $O(a^4)$; and neglected all higher-order terms. The inconsistency in our choice of $O(a^4)$ terms and neglect of all higher-order terms is the reason we refer to the arguments above as a "guide to good phenomenology" rather than as a "derivation." Finally, we rescale variables as

$$z' = \left(\frac{T}{Ja^2}\right)^{1/2} a, \qquad t' = \frac{T}{2\tau_s J} t \tag{20}$$

and obtain the following dimensionless equation for the case of conserved order parameter in a gravitational field (dropping the primes):

$$\frac{\partial\phi(z,t)}{\partial t} = -\frac{\partial^2}{\partial z^2}\left[\left(\frac{T_c}{T}-1\right)\phi(z,t) - \frac{1}{3}\frac{T_c}{T}\phi(z,t)^3 + \frac{\partial^2\phi(z,t)}{\partial z^2}\right] + \frac{\partial}{\partial z}\left[\phi(z,t)^2\frac{\partial^3\phi(z,t)}{\partial z^3} + G\phi(z,t)^2\right] \tag{21}$$

where $G = (g/T)(Ja^2/T)^{1/2}$. Equation (21) is the central result of this paper. Notice that it is similar to the Cahn–Hilliard equation but with two additional terms, the second of which is due to the gravitational field and is similar in form to previously proposed modifications of the Cahn–Hilliard equation to account for the gravitational field.[2,3] These extra terms may be interpreted as arising from an order-parameter-dependent mobility $M(\phi) = 1 - \alpha\phi^2$ in (1), where α is some constant.[2] However, (21) contains only a few of the many terms generated by such an assumption. Furthermore, as is easily confirmed, the choice of terms in (21) ensures that (8) and (21) have the same static solutions. This is an essential check on the reasonableness of any phenomenological model for the conserved case.

Equation (21) easily generalizes to that case of arbitrary dimensions and has the form

$$\frac{\partial\phi(\mathbf{r},t)}{\partial t} = -\nabla^2\left[\left(\frac{T_c}{T}-1\right)\phi(\mathbf{r},t)-\frac{T_c}{3T}\phi(\mathbf{r},t)^3+\nabla^2\phi(\mathbf{r},t)\right] + \nabla\cdot[\phi(\mathbf{r},t)^2\,\nabla(\nabla^2\phi(\mathbf{r},t))+G\phi(\mathbf{r},t)^2\hat{k}] \tag{22}$$

where $\hat{k}$ is a unit vector along the z direction.

It is interesting to note that Eq. (22) can be recast in the form of Eq. (1) by identifying $M(\phi)\equiv 1-\phi^2$ and the free energy

$$F\{\phi\} = H_F\{\phi\} + H_I\{\phi\} \tag{23}$$

In (23), the free part $H_F\{\phi\}$ is the entropy of a noninteracting binary mixture[8]

$$H_F\{\phi\} = \int d\mathbf{r}\,\tfrac{1}{2}\{[1+\phi(\mathbf{r},t)]\ln[1+\phi(\mathbf{r},t)]+[1-\phi(\mathbf{r},t)]\ln[1-\phi(\mathbf{r},t)]\} \tag{24}$$

and the interacting part $H_I\{\phi\}$ is

$$H_I\{\phi\} = \int d\mathbf{r}\left\{-\frac{1}{2}\frac{T_c}{T}\phi(\mathbf{r},t)^2+\frac{1}{2}[\nabla\phi(\mathbf{r},t)]^2-Gz\phi(\mathbf{r},t)\right\} \tag{25}$$

Unfortunately, the corresponding nonconserved equation (10) cannot be formulated as a TDGL equation with the above form for $F\{\phi\}$. However, it is easy to see the TDGL equation obtained as $\partial\phi(\mathbf{r},t)/\partial t = -\delta F\{\phi\}/\delta\phi(\mathbf{r},t)$ has the same static solution as (10) and constitutes a reasonable model for the nonconserved case as such.

Before we proceed to describe our numerical results, we should summarize our modeling. In this section, we have motivated phenomenological models for phase ordering dynamics in a gravitational field. Our modeling provides us with certain advantages. First, our modeling clearly delineates the roles of order-parameter-dependent mobility and the gravitational field. Second, our models for the nonconserved and conserved cases provide a consistent description in that they have the same static solution and this is obtained without introducing any artificial saturation terms into a phenomenological TDGL equation. Third our modeling improves on previous master-equation-based approaches to phase ordering dynamics[4] in that we do not invoke proximity to the critical temperature to make small-argument expansions. (Of course, there are still enough approximations that we cannot claim to have "derived" our models from microscopic considerations.) We do not claim that our model for the conserved case is in a different dynamical universality class form extant works.[2,3] However, for the reasons mentioned above, we believe that our modeling clearly elucidates the role of gravity in phase ordering dynamics.

3. NUMERICAL RESULTS

We have numerically simulated (22) in two dimensions using simple Euler discretization on a lattice of size $L_x \times L_z$ with mesh sizes $\Delta t = 0.05$ and $\Delta x = 1.0$. We present here results for $L_x = 128$ and $L_z = 512$. Periodic boundary conditions are applied in the x direction, which is the smaller dimension and is perpendicular to the direction of the gravitational field, i.e., the z direction. The appropriate boundary conditions in the z direction are determined from the static solution, which we know from (9). Recall that $\phi^s(e) \simeq \tanh(Gz)$ as $z \to \pm\infty$. This would mean that $d\phi^s(z)/dz \simeq G(1 - \phi^s(z)^2)$ as $z \to \pm\infty$ and we fix the first pair of boundary conditions for our simulation as

$$\left.\frac{\partial\phi(z, t)}{\partial z}\right|_{z=0, L_z} = G(1 - \phi^2(z, t))|_{z=0, L_z} \tag{26}$$

The second pair of boundary conditions is determined by taking the derivative with respect to z of (9) to obtain (for $z \to \pm\infty$)

$$\frac{d^3\phi^s(z)}{dze^3} + \frac{T_c}{T}\frac{d\phi^s(z)}{dz} = \frac{1}{1 - \phi^s(z)^2}\frac{d\phi^s(z)}{dz} - G \tag{27}$$

The second pair of boundary conditions, consistent with (26) and (27), is then

$$\left.\frac{\partial^3\phi(z, t)}{\partial z^3}\right|_{z=0, L_z} = -\frac{T_c}{T}G(1 - \phi(z, t)^2)\Big|_{z=0, L_z} \tag{28}$$

Thus, the boundary conditions we specify for our simulation correspond to the known equilibrium solution. Notice that, for large $|z|$, the values of $\phi(z, t)$ rapidly saturates out to ± 1 and the boundary conditions (26) and (28) reduce to

$$\begin{aligned} \left.\frac{\partial\phi(z, t)}{\partial z}\right|_{z=0, L_z} &\simeq 0 \\ \left.\frac{\partial^3\phi(z, t)}{\partial z^3}\right|_{z=0, L_z} &\simeq 0 \end{aligned} \tag{29}$$

The initial conditions for our simulation consist of uniformly distributed random fluctuations of amplitude 0.05 around a zero background, i.e., the so-called critical quench. All results for real-space correlation functions presented below are averages over 200 different initial conditions.

First, we describe our results for temperatures $T > T_c$, assuming that the gravitational field is switched on at time $t = 0$. Our numerical results (not shown here) indicate that a layer rich in the lighter component (say A, with $\phi \simeq 1$) forms at the top of the system, whereas a layer rich in the heavier component (say B, with $\phi \simeq -1$) forms at the bottom of the system. Fronts between the ordered ($\phi \simeq \pm 1$) and disordered ($\phi \simeq 0$) regions move toward the center of the system and finally coalesce so that there is only one interface between the lighter and heavier components. The speed of these fronts can be determined by looking for a traveling wave solution of (21) as $\phi(z, t) = \phi(z - vt) \equiv \phi(\eta)$. This yields (after integrating once with respect to η)

$$-v\phi(\eta) = -\left(\frac{T_c}{T} - 1\right)\frac{d\phi(\eta)}{d\eta} + \frac{T_c}{T}\phi(\eta)^2\frac{d\phi(\eta)}{d\eta} - \frac{d^3\phi(\eta)}{d\eta^3} + \phi(\eta)^2\frac{d^3\phi(\eta)}{d\eta^3} + G\phi(\eta)^2 + K \tag{30}$$

where K is a constant of integration. To obtain a front solution between -1 at $\eta = -\infty$ and 0 at $\eta = \infty$ with all derivatives of $\phi(\eta)$ vanishing, we must have $v = G$, which is the velocity of the front between the heavier component and the disordered region. Similarly, the velocity of the front between the lighter component and the disordered region is $-G$. Our numerical simulations are consistent with this.

Next, we describe our results for $T < T_c$, where the system undergoes spinodal decomposition in the bulk and it is of some interest to see how the gravitational field interferes with spinodal decomposition. Results described here are for the parameter values $T_c/T = 2.0$ and $H = 0.1$. Results similar to those described here are obtained for a wide range of parameter values, with the only difference being in the coefficients of growth laws.

Figure 1 shows the evolution pictures from our simulations of (22) with the boundary conditions (26) and (28). Regions rich in the lighter component ($\phi > 0$) are marked in black and regions rich in the heavier component ($\phi < 0$) are not marked. Evolution pictures are shown for dimensionless times ranging from $t = 800$ to $t = 4000$. As in the case $T > T_c$, layers rich in the lighter and heavier components are formed at the top and bottom, respectively, and these grow rapidly. The central region, which shrinks as the enriched layers grow, is comprised of domains of A and B which become highly anisotropic in time, considerably elongated in the direction of gravity.[2,3] Figure 2 shows cross sections (at $x = 64$) of the order-parameter profile along the z direction corresponding to the evolution pictures shown in Fig. 1.

We next focus on the real-space correlation functions. Because of the intrinsic anitropy of the system, we consider correlation function in both the x and z directions. The correlation function in the zs direction is defined as

$$S_{\text{int}}(z, t) = \frac{1}{N} \int_0^{L_x} dx \int_{A(t)}^{B(t)} dz' \, \langle \phi(x, z', t) \, \phi(x, z' + z, t) \rangle \qquad (31)$$

where the subscript "int" refers to integration along the x direction. In (31), the limits of the z' integration are chosen so as to exclude z' and $(z' + z)$ values which lie in the enriched layers. The normalization factor is

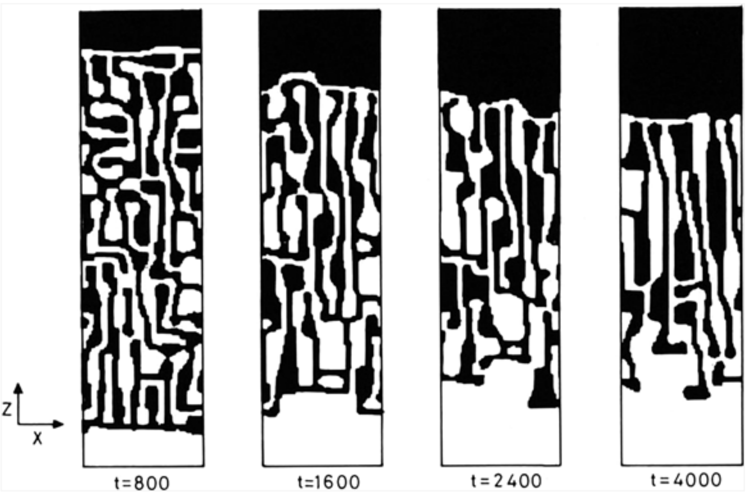

Fig. 1. Evolution pictures obtained from an Euler-discretrized version of our model for the conserved case with a gravitational field [Eq. (22)] in two dimensions. The gravitational field is taken to act along the z direction. Parameter values are $T_c/T = 2.0$ and $G = 0.1$. The discretization mesh sizes are $\Delta t = 0.05$ and $\Delta x = 1.0$ and the system size is $L_x \times L_z$, where $L_x = 128$ and $L_z = 512$. Periodic boundary conditions are applied in the x direction and the boundary conditions derived from the known static solution [Eqs. (26) and (28)] are applied in the z direction. The initial conditions for our simulation consist of uniformly distibuted random fluctuations of amplitude 0.05 around a zero background, corresponding to a critical quench. Sites with positive order parameter (corresponding to the lighter component) are marked in black and sites with negative order parameter (corresponding to the heavier component) are not marked. Pictures shown are for dimensionless times $t = 800$, 1600, 2400, and 4000.

$N = L_x(B(t) - A(t))$ and the angular brackets denote an averaging over 200 independent initial conditions. An analogous definition holds for $S_{\text{int}}(x, t)$, with the subscript "int" referring to an integration along the z direction, excluding the enriched layers. If we assume that there are unique length scales of domain growth in the x and z directions, then the real-space correlation function should exhibit generalized dynamical scaling[3,9] as

$$S(x, z, t) = S(x/L_x(t), z/L_z(t)) \tag{32}$$

where $L_x(t)$ and $L_z(r)$ are characteristic domain sizes in the x and z directions, respectively. Equation (32) implies that the quantities defined above should independently exhibit dynamical scaling as follows:

$$\begin{aligned} S_{\text{int}}(z, t) &= S_1(z/L_z(t)) \\ S_{\text{int}}(x, t) &= S_2(x/L_x(t)) \end{aligned} \tag{33}$$

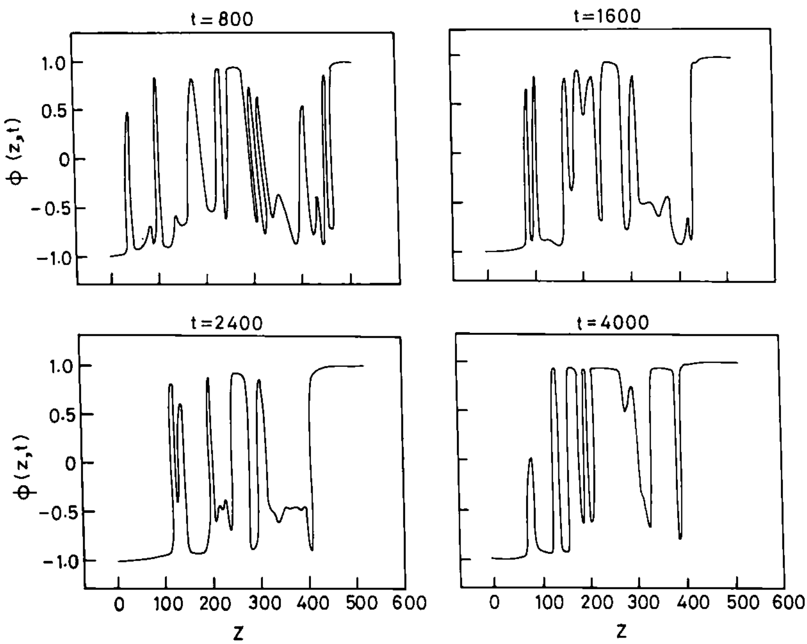

Fig. 2. Cross-section profiles of the order parameter for the temporal evolution shown in Fig. 1. The cross sections are taken at $x = 64$ and we plot $\phi(x = 64, z, t)$ vs. z for dimensionless times $t = 800$, 1600, 2400, and 4000.

We define characteristic length scales as the distances over which the appropriate correlation functions decay to half their maximum values, i.e.,

$$\begin{aligned} S_{\rm int}(L_z(t), t) &= \frac{S_{\rm int}(0, t)}{2} \\ S_{\rm int}(L_x(t), t) &= \frac{S_{\rm int}(0, t)}{2} \end{aligned} \tag{34}$$

Figure 3a shows the real-space correlation function in the z direction $S_{\rm int}(z, t)$ vs. z for dimensionless times $t = 800$, 1600, 3200, and 4000 (denoted by the symbols indicated). The slow decay of the correlation function is indicative of the large characteristic domain size in the z direction. Furthermore, the shape of the correlation function is very different from that in the usual Cahn–Hilliard domain growth, where the correlation function has a markedly oscillatory behaviour.[10] Figure 3b tests for dynamical scaling of $S_{\rm int}(z, t)$ by superposing data for $S_{\rm int}(z, t)/S_{\rm int}(0, t)$ vs. $z/L_z(t)$ from the different times shown in Fig. 3a. Apart from the earliest time in the figure (i.e., $t = 800$), the data collapse rather well onto a single master curve, suggesting that dynamical scaling holds, at least in the z direction.

Figure 4a shows the correlation function in the x direction $S_{\rm int}(x, t)$ vs. x for dimensionless times $t = 800$, 1600, 3200, and 4000 (denoted by the symbols indicated). These correlation functions are reminiscent of the oscillatory form for the case without gravity.[10] Figure 4b tests for dynamical scaling by plotting $S_{\rm int}(x, t)/S_{\rm int}(0, t)$ vs. $x/L_x(t)$ for the various times from Fig. 4a. In this case, the data collapse is not good and dynamical scaling appears to break down in the x direction.

Finally, we show the characteristic length scales as a function of time. Figure 5a shows the characteristic domain size in the z direction $L_z(t)$ plotted as a function of time t. The data exhibit an approximately linear growth up to about $r \approx 2500$ and then there is a saturation which probably signals the onset of unphysical freezing effects. Figure 5b shows the "characteristic domain size" in the x direction $L_x(t)$ plotted as a function of time t. (We use the quotes because, in the absence of clear dynamical scaling, our definition for the length scale will also include the slow modulation in time of the correlation function.) In this case, we do not see any extended growth regime at all—possibly a result of coupling to the extremely rapid growth in the z direction. As a matter of fact, the growth is so limited and so badly affected by freezing that it is not possible to extract even an approximate growth law in the x direction for any reasonable period of time.

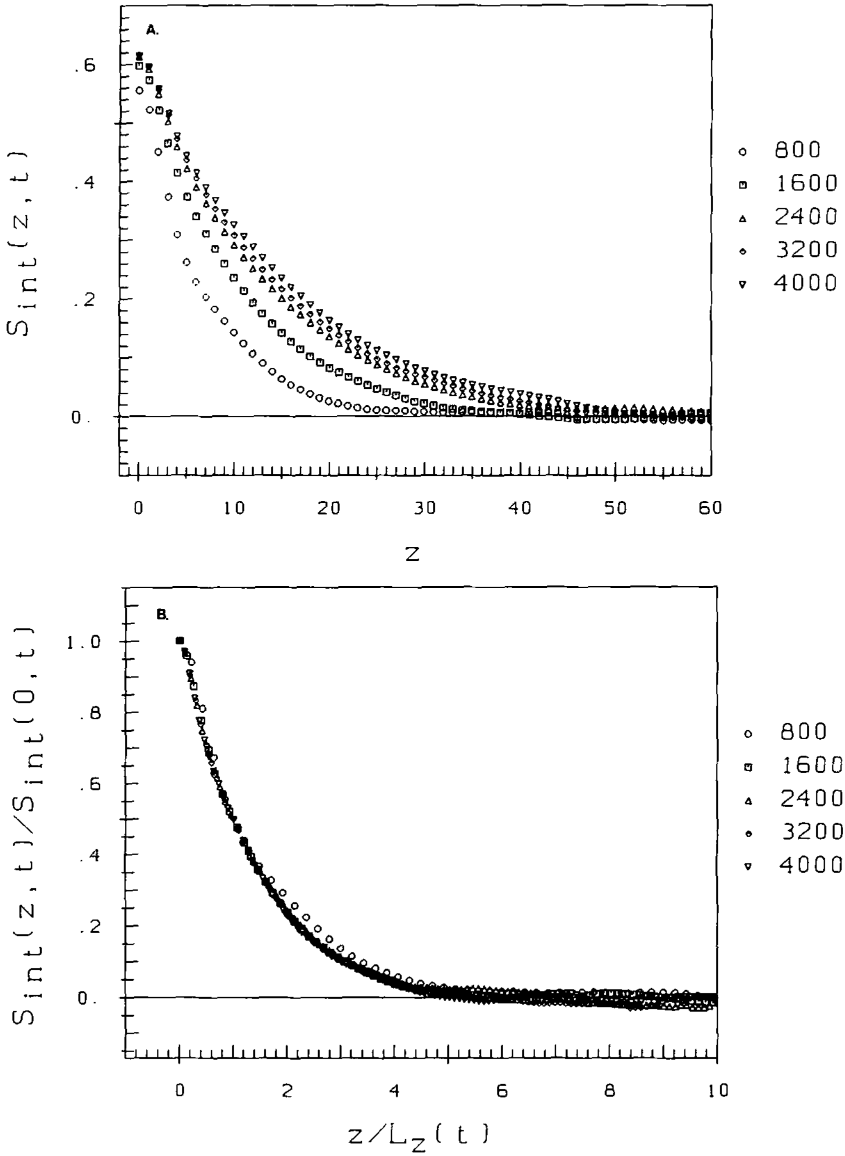

Fig. 3. (a) Real-space correlation function in the z direction (integrated along the x direction) $S_{int}(z, t)$ as a function of z for dimensionless times $t = 800$, 1600, 2400, 3200, and 4000, denoted by the symbols indicated. Correlation functions are obtained as averages over 200 independent runs. (b) Scaled plot for $S_{int}(z, t)$ from part (a). We superpose data for $S_{int}(z, t)/S_{int}(0, t)$ vs. $z/L_z(t)$ from the times in part (a), denoted by the symbols indicated. The characteristic length scale in the z direction $L_z(t)$ is defined in Eq. (30).

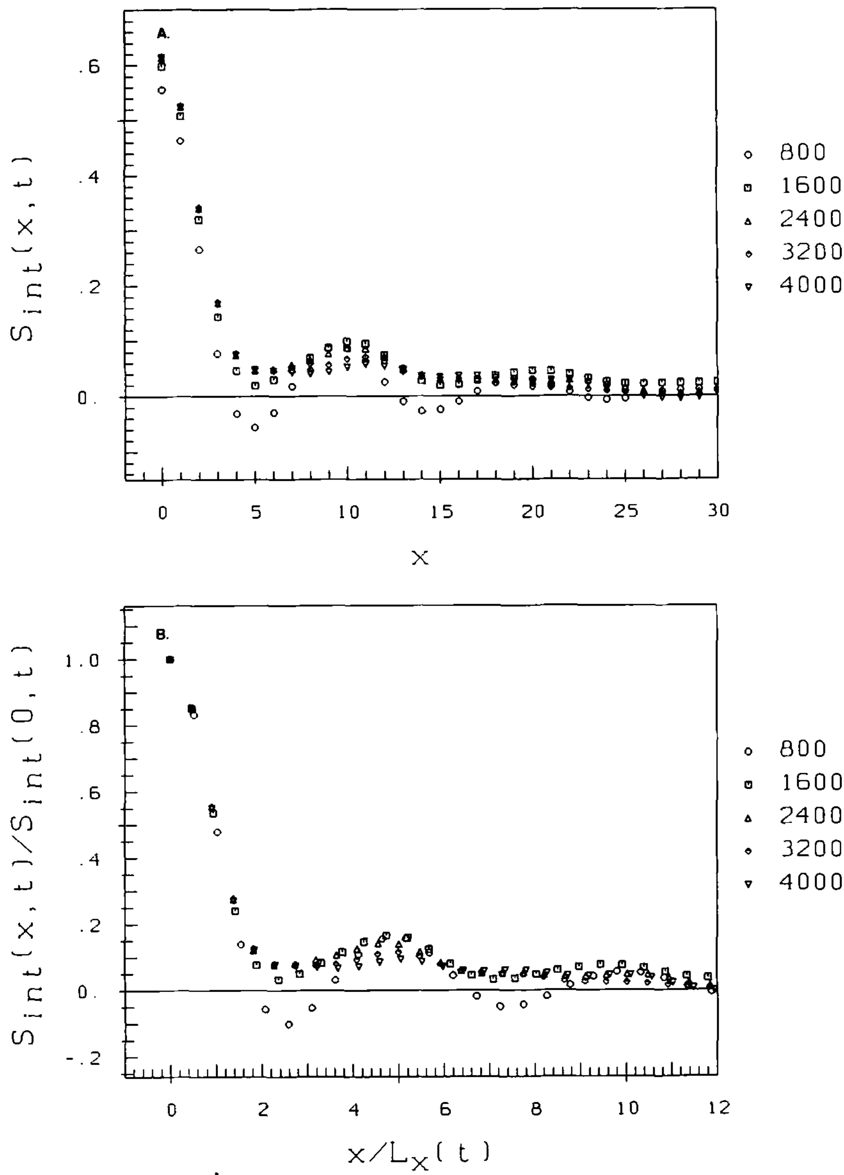

Fig. 4. (a) Real-space correlation function in the x direction (integrated along the z direction) $S_{\mathrm{int}}(x, t)$ as a function of x for dimensionless times $t = 800$, 1600, 2400, 3200, and 4000, denoted by the symbols indicated. (b) Scaled plot for $S_{\mathrm{int}}(x, t)$ from part (a). We superpose data for $S_{\mathrm{int}}(x, t)/S_{\mathrm{int}}(0, t)$ vs. $x/L_x(t)$ from the times in part (a), denoted by the symbols indicated.

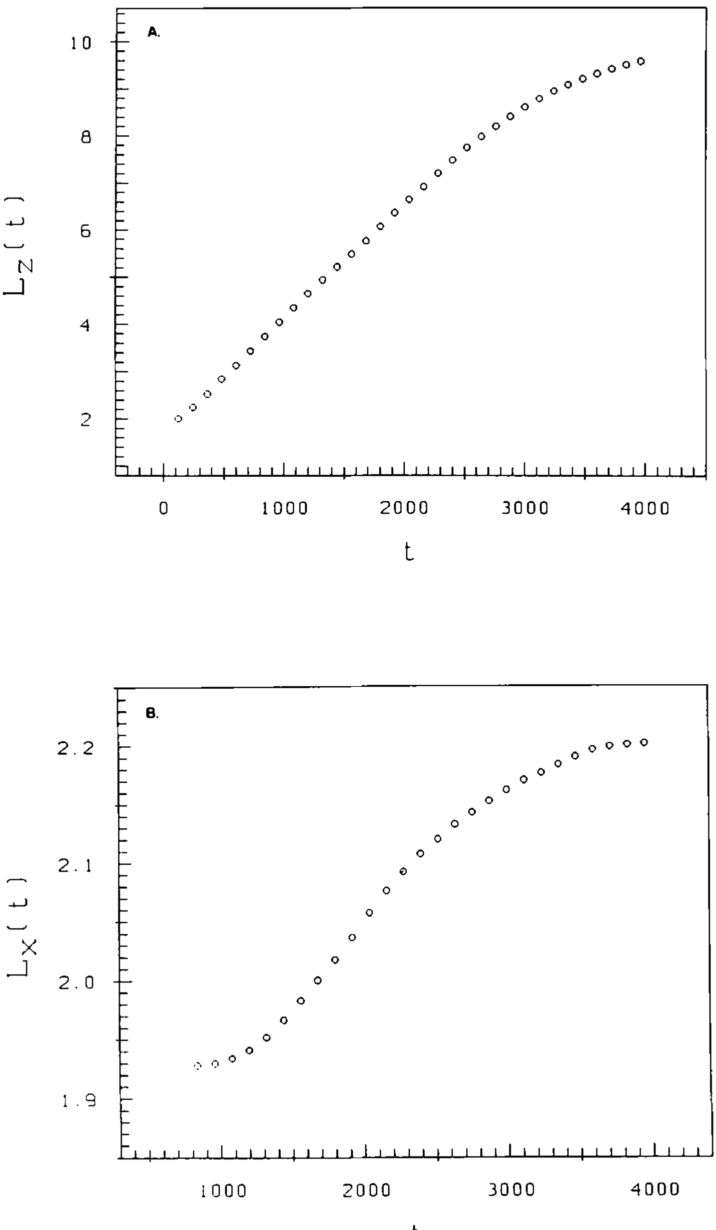

Fig. 5. Temporal dependence of the characteristic length scales in (a) the z direction and (b) the x direction.

Before we end this section, it is useful to compare our results with previous studies (in two dimensions) which have also considered the conserved case under gravity in same detail. The first study we focus on is an earlier one by us[3] where we considered the equation (in dimensionless units)

$$\frac{\partial\phi(\mathbf{r},t)}{\partial t} = -\nabla^2[\phi(\mathbf{r},t)-\phi(\mathbf{r},t)^3+\nabla^2\phi(\mathbf{r},t)] + \frac{\partial}{\partial z}[G\phi(\mathbf{r},t)^2] + G\phi(\mathbf{r},t)\frac{\partial^3\phi(\mathbf{r},t)}{\partial z^3} \tag{35}$$

Equation (35) was also motivated using the master equation approach, but was the result of a small-argument expansion at an intermediate stage of the calculation. It does not have the correct static solution as obtained from our nonconserved equation (10). In ref. 3 we considered the momentum-space structure factor, which was possible because we imposed periodic boundary conditions in both directions. Our numerical results in ref. 3 suggested that the momentum-space structure factor exhibits generalized dynamical scaling for late times, though our results were not conclusive—partly because of the quality of the 1D data in the absence of spherical averaging. We also found that the shape of the structure factor showed strong anisotropy between the x and z directions and the growth in the z direction was much faster (approximately linear) than the growth in the x direction. The second study we discuss here is that of Yeung *et al.*,[2] who considered the equation (in dimensionless units)

$$\frac{\partial\phi(\mathbf{r},t)}{\partial t} = -\nabla^3[\phi(r,t)-\phi(r,t)^3+\nabla^2\phi(r,t)] + \frac{\partial}{\partial z}[G\phi(\mathbf{r},t)^2] \tag{36}$$

Equation (36) was motivated from a phenomenological argument based on an order-parameter-dependent mobility $[M(\phi)=1-\alpha\phi^2]$ in (1). This equation also does not possess a static solution of the form suggested by our nonconserved equation (10). The simulation of Yeung *et al.*[2] was also with periodic boundary conditions and they considered both momentum-space structure factors and real-space correlation functions. Their real-space structure factors appear to exhibit reasonable dynamical scaling in the z direction but not in the x direction (analogous to our results here). Again, they find a much faster domain growth in the z direction (growth exponent $\phi \approx 0.8$–0.9) than in the x direction.

The above comparisons lead us to believe that our conserved equation (22) is not in a different dynamical universality class from previously suggested models. (Of course, thorough investigation is needed before a conclusive statement can be made to this effect.) However, as we have already stressed, our present "derivation" and model have important advantages over previous works.

4. SUMMARY AND DISCUSSION

Let us briefly summarize the major results in this paper. We have applied the master equation approach to obtain coarse-grained models for systems with nonconserved and conserved order parameters in a field which varies linearly in one direction, i.e., a gravitational field in the z direction. We do not use a small-argument expansion in our "derivation," as this is not at all justifiable in the context of a field that goes to $\pm\infty$ as $z \to \pm\infty$. The models we obtain are consistent in that both the nonconserved and conserved cases have the same static solution. Furthermore, our treatment carefully delineates the separate roles of order-parameter-dependent mobilities and the gravitational field.

We use simple Euler discretization to simulate our models and obtain real-space correlation functions as averages over a large number (200) of initial conditions so as to improve the quality of our 1D data. Our results demonstrate that there is reasonable dynamical scaling in the direction of gravity, but there appear to the violations of dynamical scaling in the perpendicular direction. Furthermore, the growth in the direction of gravity is much faster than that in the perpendicular direction. Our results are in broad agreement with numerical results from previous studies of different models, leading us to believe that all these models are in the same dynamical universality class.

Finally, we should remark that gravitational effects are not expected to be so pronounced in binary alloys, where strain effects due to lattice misfits are more dominant. They are far more important in the context of the segregation of binary fluids.[11] In the absence of gravity, the qo-called model H has been successfully used to describe the critical dynamics of binary fluids.[12] This model consists of two coupled partial differential equations, one for the order-parameter field and the other for the hydrodynamic velocity field. The equation for the order parameter is the Cahn–Hilliard equation along with a coupling to the fluid velocity field. The equation for the velocity field is essentially the Navier–Stokes equation with a coupling to the order-parameter field. Both these equations are easily adapted to the case with gravity in a fashion analogous to what we have done above. Of course, the simulation of hydrodynamic effects is numerically very demanding because of the large system sizes needed[13] to account reasonably for long-ranged hydrodynamic effects. We will present details of our numerical numerical studies of model H with a gravitational field elsewhere.

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