INTERMEDIATE SCALING REGIME IN THE PHASE ORDERING KINETICS*

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We have investigated the intermediate scaling regime in the phase ordering/separating kinetics of the three-dimensional system of the non-conserved scalar order parameter. It is demonstrated that the observed scaling behavior can be described in terms of two length scales $L_H(t) \sim t^{2/5}$ and $L_K(t) \sim t^{3/10}$. The quantity $L_H(t)$ is related to the geometrical properties of the phase interface and describes time evolution of the characteristic domain size, surface area, and the mean curvature. The second length scale, $L_K(t)$, determining the Gaussian curvature and the Euler characteristic, can be regarded as the topological measure of the phase interface. Also, we have shown that the existence of the two length scales has a simple physical interpretation and is related to the domains-necks decoupling process observed in the intermediate regime.

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1. Introduction

Perhaps the simplest example of a system exhibiting the phase separating/ordering kinetics [1–4] is a ferromagnet quenched from a temperature above its critical temperature T_c to a temperature below T_c. After lowering the temperature, such a system is brought into thermodynamically unstable, two-phase region. The two phases are characterized by positive or negative magnetization. The system starts to evolve towards one of the two equilibrium states. Since both the coexisting $\pm$ phases are equally likely to appear, the system consists of domains of these two phases. During the phase separating/ordering process the domains coarsen and the system orders over larger and larger length scales.

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At early stages of the phase ordering process the order parameter is small and the $\pm$ domains are separated by broad interfaces. In this regime the dynamics of the system is linear [5, 6] and its evolution advances diffusively. In the late stage the order parameter is saturated and the walls separating the domains are sharp. The dynamics of the system is then determined by the local curvature of the phase interface. Lifshiz [7], Allen and Cahn [8] showed that in the late stage of the evolution the domain coarsening is driven by local displacement of the domain walls, which move with the velocity v proportional to the local mean curvature H of the interface. According to the Lifshiz–Cahn–Allen (LCA) theory, typical time t needed to close the domain of size $L(t)$ is $t \sim L(t)/v = L(t)/H(t)$, where $H(t)$ is the characteristic mean curvature of the system. Thus, under the assumption that

$$H(t) \sim 1/L(t)\,, \tag{1.1}$$

the LCA theory predicts the growth law $L(t) \sim t^{1/2}$. The late scaling with the growth exponent $n = 0.5$ has been confirmed for the non-conserved systems in many 2D simulations [9–11].

Although both the early and the late stage of the phase ordering kinetics seem to be rather well described theoretically, the pathway of the transition from the early to the late stage is far from being understood. A new insight into the phase separating/ordering kinetics provided however the method developed recently in Ref. [12], based on the geometry and topology of the phase interface. In the paper cited the nature of the crossover from the early to the intermediate stage scaling was precisely stated and related to the saturation of the order parameter inside the domains. Here, we continue the study of the phase ordering kinetics, based on the analysis of the morphology of the phase interface, which was started in [12]. It is the purpose of this paper to investigate the intermediate stage of the evolution. In particular, we seek to explain the scaling behavior observed in the system in this regime.

The rest of the paper proceeds as follows. The dynamical scaling hypothesis is briefly summarized in the next section. Scaling properties of the system, obtained in computer simulations of the phase ordering process, are presented in Sec. 3. In Sec. 4 the concept of the two length scales is introduced and used to describe the scaling properties exhibited by the system in the intermediate regime. The paper ends with the concluding Sec. 5.

2. Dynamical scaling

The systems undergoing phase transitions, such as the phase separating/ordering process considered here, exhibit usually scaling phenomena [1–4]. Qualitatively, this means that a morphological pattern of the domains at earlier times looks statistically similar to a pattern at later times, apart from the global change of scale implied by the growth of the average domain size. Quantitatively, the scaling hypothesis says that, for example, the correlation function $g(\boldsymbol{r},t)$ of the order parameter (here: the magnetization density) satisfies the following relation: $g(\boldsymbol{r},t) = g(\boldsymbol{r}/L(t))$, where $L(t)$ is the characteristic length scale in the system, which scales algebraically with time t,

$$L(t) \sim t^n . \tag{2.1}$$

The growth exponent n depends on the universality class [1] of the system. Note that the system of the non-conserved order parameter following a quench which is considered in the present paper belongs to the universality class characterized by the exponent $n = 0.5$. In the theory of critical phenomena [13] it is also referred to as the model A.

Assuming the scaling hypothesis, we can derive all the scaling laws for different morphological measures such as: the Euler characteristic, $\chi(t)$, surface area, $S(t)$, the distribution of the mean, $P_H(H,t)$, and Gaussian, $P_K(K,t)$, curvatures. The scaling hypothesis implies the following scaling laws for any phase separating/ordering symmetric system irrespective of the universality class:

$$S(t) \sim L(t)^{-1}, \tag{2.2}$$

$$\chi(t) \sim L(t)^{-d}, \tag{2.3}$$

$$P_H(H,t) = \frac{P_H^*\,(HL(t))}{L(t)}\,, \tag{2.4}$$

$$P_K(K,t) = \frac{P_K^*\left(KL(t)^{(d-1)}\right)}{L(t)^{(d-1)}}\,. \tag{2.5}$$

where d is the dimensionality of the system. The first law follows from the congruency of the domains [14]. The scaling law (2.3) results from the Gauss–Bonnet theorem [15], which relates the Euler characteristic to the Gaussian curvature and the surface area

$$\chi = \gamma \int K(S)dS\,, \tag{2.6}$$

where $\int dS$ denotes the integral over the surface, and γ is twice the inverse of the volume of a $(d-1)$-dimensional sphere of the unit radius ($\gamma = 1/2\pi$ for $d = 3$).

$$K(t) \sim L(t)^{-d+1}\,, \tag{2.7}$$

and $S(t) \sim L(t)^{-1}$ we find scaling (2.3). The probability densities $P_H(H,t)$ and $P_K(K,t)$ are normalized to unity. The relation (2.4) is a simple consequence of the scaling of the mean curvature

$$H(t) \sim L(t)^{-1}\,. \tag{2.8}$$

The last relation results from the scaling (2.7) of the Gaussian curvature. Note that for $d = 2$ the scalings (2.4) and (2.5) are equivalent.

3. Results of numerical simulations

3.1. The model

The dynamics of the system of the non-conserved scalar order parameter $\psi(\boldsymbol{r},t)$ following a quench from the temperature $T=\infty$ to $T=0$ is governed by the Time Dependent Ginzburg–Landau (TDGL) equation [1,7,8,13]:

$$\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} = -\frac{\delta F[\psi]}{\delta\psi}\,, \tag{3.1}$$

with the free-energy functional taken to have the form of the coarse-grained Ginzburg–Landau free energy:

$$F[\psi] = \int d\boldsymbol{r}\left[\frac{1}{2}\left|\nabla\psi(\boldsymbol{r})\right|^2 + f(\psi(\boldsymbol{r}))\right]. \tag{3.2}$$

The bulk potential $f(\psi)$ has the Landau–Ginzburg double-well structure

$$f(\psi) = \frac{1}{4}\psi^4 - \frac{1}{2}\psi^2 \tag{3.3}$$

with two degenerate minima at $\psi=\pm1$. The TDGL equation with the potential given by (3.3) leads to the following kinetic equation governing the time evolution of the field $\psi(\boldsymbol{r},t)$:

$$\frac{\partial}{\partial t}\psi(\boldsymbol{r},t) = \Delta\psi(\boldsymbol{r},t) + \psi(\boldsymbol{r},t) - \psi^3(\boldsymbol{r},t)\,, \tag{3.4}$$

where Δ stands for the Laplacian.

The results discussed in this paper were obtained by numerical solving of the TDGL equation (3.4) on the cubic lattice, using simple Euler integration scheme with the time step $\Delta t = 0.05$ and the mesh size $\Delta x = 1$. The initial condition were chosen from the uniform distribution of the field ψ with zero mean.

3.2. Scaling regimes

It was found in Ref. [12] that the system described by the TDGL equation exhibits two scaling regimes: (*i*) the early regime where the characteristic domain size $L(t)$ scales with $t^{1/2}$, and (*ii*) the intermediate regime where $L(t)\sim t^{2/5}$. The transition between the early and the intermediate regimes was found to be marked by the saturation of the order parameter inside the domains. The late stage dynamics predicted by the LCA theory with the growth exponent $n = 0.5$ was not observed due to finite-size effects. During the whole evolution the system has a *bicontinuos* morphology with a single interface and two percolating $\pm$ domains.

The early stage of the phase ordering kinetics is governed by the saturation of the order parameter inside the domains. The phase interface follows then the bulk evolution and the exponent $n = 0.5$ results simply from the linearized TDGL equation. If we drop the ψ^3 term in Eq. (3.4), the solution $\psi_{\boldsymbol{k}}(t)$ in the Fourier space reads

$$\psi_{\boldsymbol{k}}(t) = \psi_{\boldsymbol{k}}(0) \exp\left[-\left(k^2 - 1\right) t\right], \tag{3.5}$$

where $k = |\boldsymbol{k}|$; the function $\psi_{\boldsymbol{k}}(0)$ is assumed to be a constant, what corresponds to the initial conditions with the uncorrelated field $\psi(\boldsymbol{r}, 0)$. Since in the early stage the average domain size is very small, we have $k \gg 1$ and the argument of the exponent in (3.5) can be approximated by $-k^2 t$. The linearized equation (3.4) describes then a purely diffusive process and its real space solution is written as

$$\psi(\boldsymbol{r}, t) \sim \exp\left(-\boldsymbol{r}^2/4t\right) \equiv \exp\left[-\left(\boldsymbol{r}/L(t)\right)^2\right]. \tag{3.6}$$

In view of the above solution, it is clear why in the early stage of the evolution the characteristic length scale $L(t)$ growths as $t^{1/2}$. Note that the four scaling relations (2.2)–(2.5) are satisfied in the early stage.

The behavior of the system in the intermediate regime is much more interesting; In this regime the order parameter is saturated and the $\pm$ domains are separated by sharp walls. The time evolution of the system is driven by the local curvature of the interface. However, the LCA assumption (1.1) does not hold; instead, it was found that in this regime the morphological measures of the phase interface behave as:

$$L(t) \sim t^{2/5}, \tag{3.7}$$

$$\chi(t) \sim t^{-1}, \tag{3.8}$$

$$S(t) \sim t^{-2/5}. \tag{3.9}$$

It was also found that the distribution of the curvatures satisfies the relations $P_H(H,t) = P_H^*\left(HL(t)\right)/L(t)$, with $L(t)$ given by (3.7), and $P_K(K,t) = P_K^*(Kt^{3/5})/t^{3/5}$ Thus, the scaling relations (2.2)–(2.5), based on a single length scale $L(t)$, do not hold in the intermediate regime. In the next section we demonstrate that the scaling behavior observed in the intermediate regime is successfully described in terms of two length scales, which can be inferred from the scaling properties of the distributions of the mean and the Gaussian curvatures.

4. The concept of two length scales in the intermediate regime

Scaling of the distributions of the mean H and the Gaussian K curvatures in the intermediate regime are shown in Fig. 1(a) and Fig. 1(b), respectively. As seen, for different times the data collapse onto single master curves.

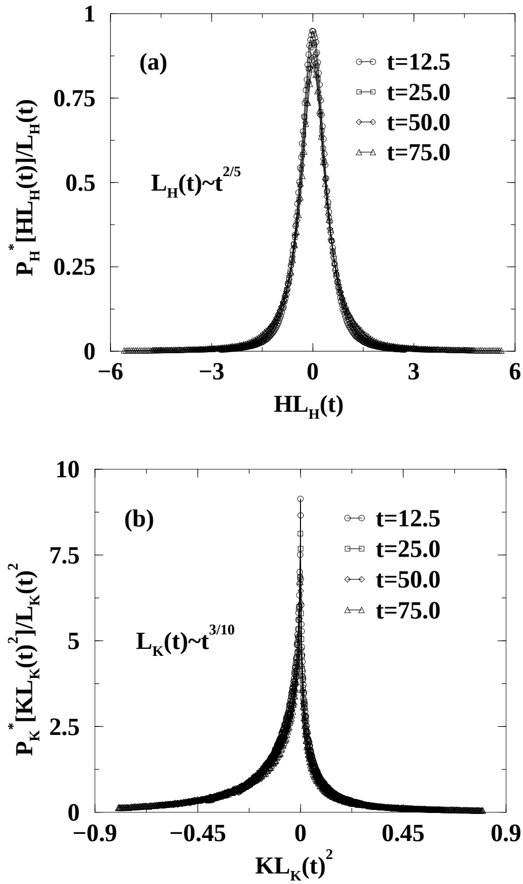

Fig. 1. The rescaled distributions of the mean (a) and the Gaussian (b) curvature in the intermediate regime. The distributions obey the scaling relations $P_H(H,t) = P_H^*\left(HL_H(t)\right)/L_H(t)$, with $L_H(t) \sim t^{2/5}$, and $P_K(K,t) = P_K^*\left(KL_K(t)^2\right)/L_K(t)^2$, with $L_K(t) \sim t^{3/10}$. The curvatures are given in dimensionless units. The system size is $50 \times 50 \times 50$.

This means that the scaling relations (2.4) and (2.5) are satisfied. However, there is not one common length scale for the mean and Gaussian curvatures. Instead, the curvatures H and K scale independently with two different length scales, $L_H(t)$ and $L_K(t)$, respectively. They vary with time t as:

$$L_H(t) \sim t^{2/5}, \tag{4.1}$$

$$L_K(t) \sim t^{3/10}. \tag{4.2}$$

In terms of the two quantities $L_H(t)$ and $L_K(t)$ the scaling relations (2.2)–(2.5) can be rewritten in the following form:

$$S(t) \sim L_H(t)^{-1}, \tag{4.3}$$

$$\chi(t) \sim L_K(t)^{-2} L_H(t)^{-1}, \tag{4.4}$$

$$P_H(H,t) = \frac{P_H^\star(H L_H(t))}{L_H(t)}, \tag{4.5}$$

$$P_K(K,t) = \frac{P_K^\star\Big(K L_K(t)^2\Big)}{L_K(t)^2}. \tag{4.6}$$

Note that the second relation, Eq. (4.4), expresses the Gauss–Bonnet theorem (2.6), with the average Gaussian curvature $K(t) \sim L_K(t)^{-2}$.

In view of the four relations (4.3)–(4.6), we see that that the length scale $L_H(t)$ can be interpreted as the *geometrical* measure of the phase interface. It determines such quantities as the characteristic domain size, the area of the interface, and the mean curvature. The second length scale, $L_K(t)$, is related to the *topology* of the system and characterizes its Euler characteristic and the Gaussian curvature.

The existence of the two length scales in the intermediate regime has a simple physical interpretation and can be explained in terms of the LCA theory, which links the velocity of the interface with its local curvature. Below, we demonstrate that it is related to the domains-necks decoupling processes [12] taking place in the intermediate stage of the evolution. Let us denote by $n(t)$ the average number of domains in the system, which are assumed to be spheres of the radius $L_H(t)$. The Euler characteristic is then proportional to the product

$$\chi(t) \sim n(t) p(t), \tag{4.7}$$

where $p(t)$ is the number of necks or passages piercing the surface of the sphere. On the other hand, according to the Gauss–Bonnet theorem, the Euler characteristic can be written as $\chi(t) \sim K(t)S(t)$. Since the total area $S(t)$ of the interface is proportional to the product of the surface of the sphere of radius $L_H(t)$ and the number $n(t)$ of the domains, we get

$$\chi(t) \sim L_K(t)^{-2} n(t) L_H(t)^2. \tag{4.8}$$

By comparing Eqs. (4.7) and (4.8) we obtain

$$p(t) \ \sim \ \left(\frac{L_H(t)}{L_K(t)}\right)^2 . \tag{4.9}$$

In the early regime we have $L_H(t) = L_K(t) = L(t) \sim t^{1/2}$ and, therefore, $p(t) \sim 1$ is independent of time. This means that for each sphere of size $L(t)$ we have the same number of passages. In the intermediate regime we have $L_H(t) \sim t^{2/5}$ and $L_K(t) \sim t^{3/10}$, what gives $p(t) \sim t^{1/5}$ indicating the decoupling between the domains and the connections joining them.

Since in the intermediate regime the average mean curvature is equal to zero and its distribution is peaked at $H = 0$ (Fig. 1(a)), we deduce that the phase interface possesses large patches of the minimal-like (saddle-like) shape [16] with zero mean curvature. Furthermore, the apparence of the domains-necks decoupling process indicates that these areas are localized mainly at the necks connecting the domains. This means that in the intermediate regime the necks are in “partially frozen” state and slow down the kinetics of the system. They evolve slower (with the exponent $n = 0.3$) compared to the domains following the evolution with the growth exponent $n = 0.4$. Of course, the LCA argument, based on the assumption (1.1), does not work in the intermediate regime. However, during the evolution the morphology of the system changes and transforms successively from the “minimal-like” structure (with the mean curvature $H(t)$ equal to zero) to the “constant mean curvature like” structure [17], where the average mean curvature is proportional to the inverse of the characteristic size of the domains, *i.e.* $H(t) \sim 1/L(t)$. Once the morphological transformation is completed the LCA argument works and the late scaling with the growth exponent $n = 0.5$ is reached.

To sum up, in the intermediate regime the evolution of the morphology of the phase interface splits off and the “geometry” and the “topology” start to evolve independently with two different growth exponents, $n = 0.4$ and $n = 0.3$, respectively. This process manifests as the breaking down of the scaling laws, Eqs. (2.2)–(2.5). The existence of the two length scales in the intermediate regime is a consequence of the fact that the late-stage morphology and the early-stage morphology differ significantly and by no means cannot be transformed each to other by scaling operations based on a single length scale.

5. Summary

In this paper we have investigated the intermediate regime of the phase separating/ordering process of the system with non-conserved order parameter, using tools based on the morphology of the phase interface. As the main result, we have demonstrated that the observed scaling properties of the morphological measures of the interface can be successfully described in terms of two lengths scales $L_H(t)$ and $L_K(t)$. They characterize, respectively, scaling of the distributions of the mean H and Gaussian K curvatures. $L_H(t)$ varies with the time as $t^{2/5}$ and is related to the *geometrical* properties of the system such as the average size of the domains, the surface area, and characteristic radius of the curvature. The second length scale, $L_K(t) \sim t^{3/10}$, is associated with the *topological* features of the system's interface and determines its Euler characteristic and the Gaussian curvature. We have also demonstrated that the appearance of the two length scales in the intermediate regime is related to the domains-necks decoupling process and accompanies the morphological transformation from the "minimal-like" structure formed at the early stage of the evolution to the "constant mean curvature like" structure, which is characteristic for the late-stage dynamics. Although both the early- and the late-stage morphologies are bicontinuos, they differ significantly and the system cannot be brought from the early stage to the late stage by simple scaling. For this reason the scaling is broken in the intermediate regime and the two length scales appear.

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