

Phase-ordering kinetics in nonconserved scalar systems with long-range interactions

Hisao Hayakawa,* Takamitsu Ishihara, Kenichi Kawanishi,[†] and Takeshi S. Kobayakawa[‡]

Department of Physics, Tohoku University, Sendai 980, Japan

(Received 15 March 1993; revised manuscript received 20 August 1993)

The domain growth of a system with the nonconserved scalar order parameter quenched into the ordered phase from a disorder phase is considered for a system with power-law interactions of the form $1/r^{d+\sigma}$, with $0 < \sigma < 2$. Our numerical simulation is consistent with a prediction by Bray [Phys. Rev. E **47**, 3191 (1993)] in which the characteristic length $l(t)$ obeys a power law $l(t) \sim t^{1/2}$ for $1 < \sigma < 2$ and $l(t) \sim t^{1/(1+\sigma)}$ for $\sigma < 1$ in the late stage.

PACS number(s): 64.60.Cn, 64.60.My

I. INTRODUCTION

When a system with a nonconserved scalar order parameter is quenched from the high-temperature disordered phase into the ordered phase, domains of two pure phases are formed and grow with time [1]. The dynamical scaling [2] is a key concept to understand the late stage of domain growth in which the equal-time two-point correlation function has the form

$$C(r/l(t)) = \langle S(\mathbf{x}, t) S(\mathbf{x} + \mathbf{r}, t) \rangle / \langle S(\mathbf{x}, t)^2 \rangle, \quad (1)$$

where S is the order parameter, $l(t)$ is the characteristic length at time t after the quench, and $C(X)$ is the scaling function. The angular brackets in (1) indicate an average over initial conditions.

For systems with short-range interactions, it is well known that $l(t)$ obeys a power law $l(t) \sim t^{1/2}$ [3]. We also know an approximate analytic form of $C(X)$ for the spatial dimension $d \geq 2$ [4–6]. When analyzing an experiment, one has to be aware of the possible presence of long-range interactions. Thus, it is of interest to study how the long-range interactions affect the phase-ordering processes. Recently, Hayakawa, Rácz, and Tsuzuki (HRT) [7] have analyzed the phase-ordering kinetics for vector order parameter systems with long-range interactions, falling off with distance as $r^{-d-\sigma}$ with $0 < \sigma < 2$ and the spatial dimension d . They predicted a growth law $l(t) \sim t^{1/\sigma}$ which is independent of the dimensionality of the vector nonconserved order parameter, based on the singular perturbation method developed by Kawasaki, Yalabik, and Gunton (KYG). This result was shown to be consistent with the exact solution of the spherical model. Quite recently, Bray [8] has denied the result of HRT and the approximation used by KYG, at least for a system with a scalar order parameter, and predicted $l(t) \sim t^{1/(1+\sigma)}$ for $\sigma < 1$ and $l(t) \sim t^{1/2}$ for $1 < \sigma < 2$.

Bray's argument [8] is more plausible than that of HRT [7], because Bray's theory is based on both the renormalization-group method and the equation of interface kinetics.

In this paper we attempt to check whether Bray [8] is correct from our numerical simulation. After the Introduction, in Sec. II we explain our model and summarize Bray's argument and its controversial point. In Sec. III we perform simulations for two-dimensional systems based on the cell-dynamical-systems (CDS) method [9]. The results of our simulation suggest that in the late stage of domain growth our results are consistent with Bray's prediction for $\sigma = 0.5, 1$, and 1.5 . In Sec. IV we discuss and conclude our results.

II. MODEL

In this section, we explain the time-dependent Ginzburg-Landau (TDGL) model with long-range interactions and with a scalar nonconserved order parameter to describe phase-ordering processes. The time evolution of the order parameter is governed by

$$\frac{\partial S}{\partial t} = \nabla^2 S + g(S) + \beta \int d\mathbf{r}' \frac{S(\mathbf{r}', t) - S(\mathbf{r}, t)}{|\mathbf{r} - \mathbf{r}'|^{d+\sigma}}, \quad (2)$$

where $g(S)$ is an odd function of S with zeros at $S = \pm 1$. In this paper we restrict ourselves to the case of $\beta > 0$, which means that the interaction is attractive.

Here we summarize Bray's argument [8] based on his interfacial picture. Equation (2) is rewritten as

$$\partial_t S(\mathbf{r}, t) = - \frac{\delta H}{\delta S}, \quad (3)$$

where H is the Hamiltonian. If the system has sharp interfaces, (3) can be described by the equation for interfaces [8,10]. In fact, (3) can be rewritten as

$$\begin{aligned} \delta H &\simeq \Sigma \int da \delta q(a) v(a) \\ &\simeq \int da \delta q(a) \left[\Sigma \kappa(a) - \beta \int d\mathbf{r}' \frac{\bar{S}(\mathbf{r}')}{|\mathbf{r}(a) - \mathbf{r}'|^{d+\sigma}} \right], \quad (4) \end{aligned}$$

where Σ , $\delta q(a)$, $v(a)$, $\kappa(a)$, and $\bar{S}(\mathbf{r})$ are the surface tension, the virtual displacement of the interface at a , the velocity of moving interface at a , and the mean profile function of $S(\mathbf{r})$ at the interface a determined by the one-

*Electronic address: hisao@cmpt01.phys.tohoku.ac.jp

[†]Present address: Department of Physics, The University of Tokyo.

[‡]Present address: Institute of Solid State Physics, The University of Tokyo.

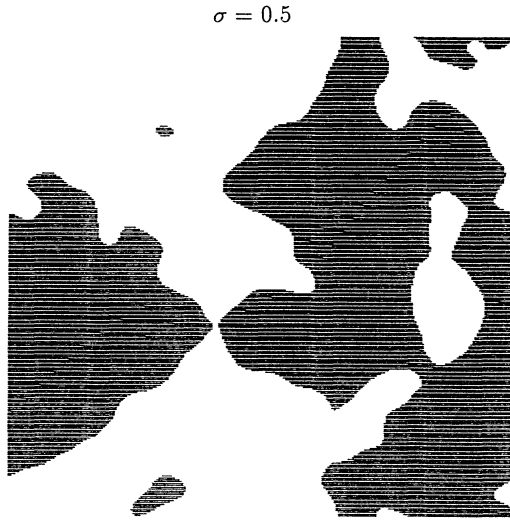


FIG. 1. The configurations of domains for $\sigma=0.5$ at $t=40$ in systems with size 256×256 .

dimensional (1D) equation of $\delta H/\delta S=0$, respectively. To derive (4) we use the well-known facts $\delta H/\delta q(a)=\Sigma\kappa(a)$, $\partial_t S \simeq -\bar{S}'(n)v(a)$, $\delta S \simeq -\bar{S}'(n)\delta q(a)$, and $\Sigma = \int dn \bar{S}'(n)^2$ with the normal coordinate n of the interface a . From (4) we obtain

$$v(a) \simeq \kappa(a) - \frac{\beta}{\Sigma} \int d\mathbf{r}' \frac{\bar{S}(\mathbf{r}')}{|\mathbf{r}(a) - \mathbf{r}'|^{d+\sigma}}. \quad (5)$$

$$\frac{dR}{dt} = -\frac{d-1}{R} - \frac{\beta'}{R} \int_0^\infty dr' r'^{d-2} \left[\frac{1}{|r'-R|^{d-2+\sigma}} - \frac{1}{|r'+R|^{d-2+\sigma}} \right] \text{sgn}(r'-R), \quad (6)$$

where β' is a constant in proportion to β and $\text{sgn}(x)=1$ for $x>0$ and $\text{sgn}(x)=-1$ otherwise. To derive (6) we have used the fact that the profile function is essentially a step function to replace $\bar{S}(n)$ by $\text{sgn}(n)$. The integral in (6) remains finite in the limit of $R \rightarrow \infty$ for $\sigma > 1$. Therefore, in this case, the growth law is given by $l(t) \sim t^{1/2}$. For $\sigma < 1$ the integral diverges as $R \rightarrow \infty$ and is evaluated as $R^{1-\sigma}$. In this case, for large R , the long-range part is dominant and the growth law is given by $l(t) \sim t^{1/(1+\sigma)}$. Note that this growth law without the short-range interactions is the same as that mentioned above. Since Bray's argument [8] is based on a physical picture in which the dynamics is described by the interfacial motions, Bray's argument is plausible, if the picture of sharp kinks is correct.

We feel, however, that the above argument is not complete. In fact, it is not difficult to illustrate the violation of a simple sharp-kink picture which was assumed by Bray. Let us consider the steady-state solution of (2) in a one-dimensional system. For simplicity, we replace $g(S)$ by the piecewise linear function $g(S) = -S + \text{sgn}(S)$.

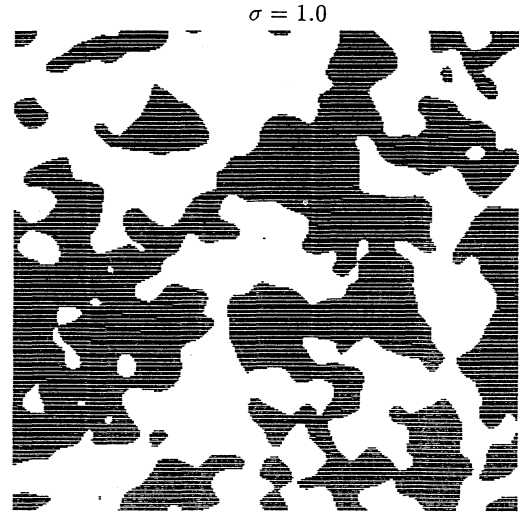


FIG. 2. The configuration of domains for $\sigma=1.0$ at $t=40$ which starts from the initial condition identical to Fig. 1.

This is the equation of interfaces. This equation is a highly nonlinear and integral equation. Therefore, it is difficult to obtain the correlation function based on the linearization of this equation as used in a trick by Ohta, Jasnow, and Kawasaki (OJK) [5] for the short-range case. Bray [8], however, obtained the growth law from the consideration of the time evolution of a spherical droplet. When we consider such a case, (5) is reduced to

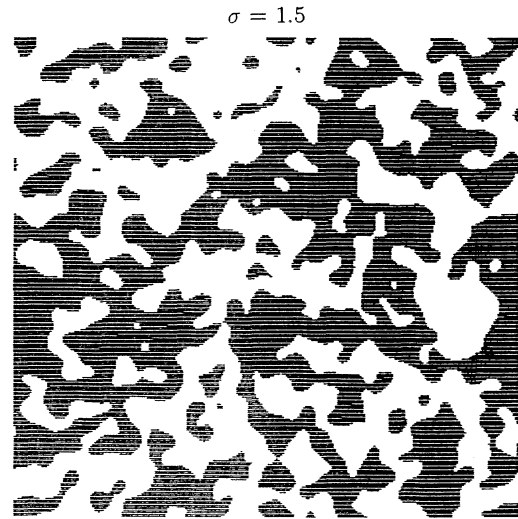


FIG. 3. The configuration of domains for $\sigma=1.5$ at $t=40$ which starts from the initial condition identical to Figs. 1 and 2.

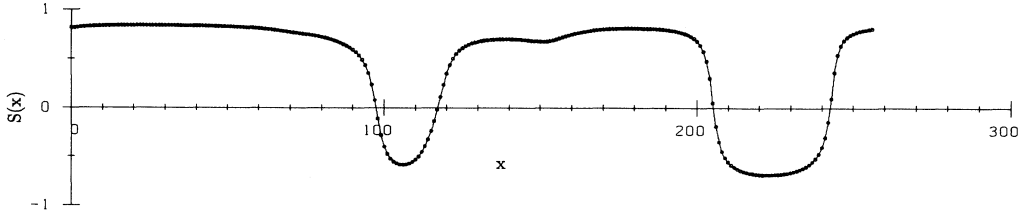


FIG. 4. The values of order parameter along the horizontal lines going through the center of systems for $\sigma=0.5$ corresponding to Fig. 1.

Thus, (2) is reduced to

$$\partial_x^2 S - S + \text{sgn}(S) + \beta \int_{-\infty}^{\infty} dx' \frac{S(x')}{|x-x'|^{1+\sigma}} = 0. \quad (7)$$

When we consider the case that a domain exists near $x=0$, that is, $S > 0$ for $|x| < x_0$, with the boundary condition of $S = -1$ in the limit of $|x| \rightarrow \infty$, (7) can be solved by the Fourier transform as

$$S_q = \frac{2\Psi(q, x_0) - 2\pi\delta(q)}{1 + q^2 + |q|^\sigma}, \quad (8)$$

where $\Psi(q, x_0) = 2 \sin(qx_0)/q$ and we use a suitable β to eliminate the coefficient of $|q|^\sigma$. Using the inverse of the Fourier transform, we obtain an asymptotic form of the profile of S for $|x| \gg x_0$ as

$$S(x) \simeq -1 + \frac{\Gamma(\sigma)}{2\pi} \sin\left[\frac{\sigma\pi}{2}\right] \left[\frac{1}{|x-x_0|^\sigma} - \frac{1}{|x+x_0|^\sigma} \right] + \dots \quad (9)$$

for $\sigma < 1$. Since the order parameter has a long tail as in (9), Bray's argument based on a simple sharp-kink picture may not be appropriate in systems with long-range interactions. Therefore, we need to check the validity of his prediction from numerical simulations.

III. NUMERICAL SIMULATION

In order to examine the validity of Bray's predictions in the preceding section for nonconserved models with long-range interactions, we perform numerical simulations for two-dimensional systems. Our method is based on the cell-dynamical-systems method proposed by Oono and Puri [9]. To extract the essential feature of long-

range interactions we neglect the effects of the short-range interactions.

The method of our simulation is parallel to the paper by Hayakawa and Koga [11] which discussed phase-ordering kinetics in a long-range exchange model. From the CDS spirit we can write the equation for time evolution of $S(\mathbf{n}, t)$ at the cell point \mathbf{n} as

$$S(\mathbf{n}, t+1) = -D(-\nabla^2)^{\sigma/2} S(\mathbf{n}, t) + A \tanh[S(\mathbf{n}, t)], \quad (10)$$

where D and A are constants and $(-\nabla^2)^{\sigma/2}$ is a symbolical representation of the long-range interaction $V(r) \sim r^{-d-\sigma}$. This operator can be interpreted as an operator in the Fourier space

$$\hat{L}(\mathbf{k}) = [1 - \frac{1}{3}\cos(k_x) - \frac{1}{3}\cos(k_y) - \frac{1}{3}\cos(k_x)\cos(k_y)]^{\sigma/2}, \quad (11)$$

where $\mathbf{k} = (k_x, k_y) = (2\pi m_x/N, 2\pi m_y/N)$ with the integers m_x and m_y which are less than the linear size of the system N .

Thus, we can solve (10) as follows. Let FT be the Fourier transform. First, we transform $S(\mathbf{n}, t) \xrightarrow{\text{FT}} \tilde{S}(\mathbf{k}, t)$ into the Fourier space. Second, defining $\tilde{S}'(\mathbf{k}, t) \equiv \hat{L}(\mathbf{k})\tilde{S}(\mathbf{k}, t)$ we come back to the real space $\tilde{S}'(\mathbf{k}, t) \xrightarrow{\text{FT}^{-1}} S'(\mathbf{n}, t)$ with the introduction of the inverse of the Fourier transform. Thus, the symbolic equation (10) is replaced by

$$S(\mathbf{n}, t+1) = -DS'(\mathbf{n}, t) + A \tanh[S(\mathbf{n}, t)] \quad (12)$$

and we come back to the first stage in this paragraph to continue this process.

In our simulation, quenches are carried out at the center of the miscibility gap. The initial values of the or-

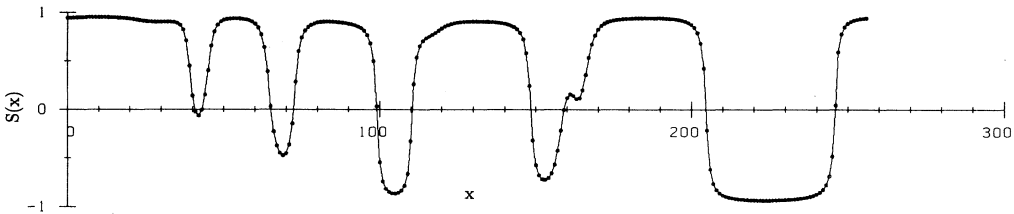


FIG. 5. The values of order parameter along the horizontal lines going through the center of systems for $\sigma=1.0$ corresponding to Fig. 2.

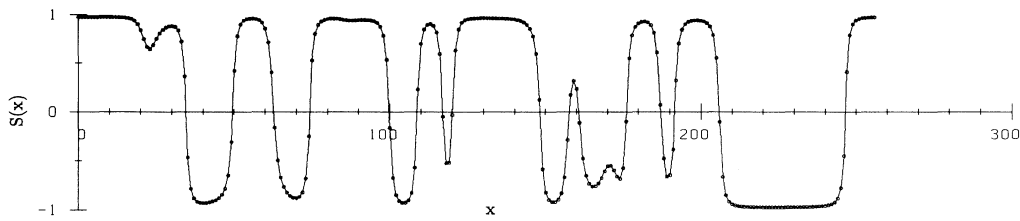


FIG. 6. The values of order parameter along the horizontal lines going through the center of systems for $\sigma = 1.5$ corresponding to Fig. 3.

der parameter on the cell are distributed at random between -0.125 and 0.125 . In order to avoid the dependence of a special initial configuration of the order-parameter field, we have performed ten runs for $\sigma = 0.5, 1.0,$ and 1.5 . Our main results are obtained from simulations up to $t = 100$ with system size 256×256 in the cell unit with the periodic boundary condition and the parameters used in (12) are $D = 0.5$ and $A = 1.3$. Note that a typical domain size in the late stage for small systems is as large as the linear size of systems for small σ . Thus, for $\sigma = 0.5$, we also simulate systems with sizes 512×512 and 1024×1024 up to $t = 800$ to check the finite-size effects.

Figures 1–3 display domain configurations of 256×256 systems for $\sigma = 0.5, 1.0,$ and 1.5 at $t = 40$ from identical initial configurations. In these figures positive regions of the order parameter are shaded. We can recognize that the pattern evolution is faster with decreasing σ . Figures 4–6 display the order-parameter values along horizontal lines going through the center of systems, corresponding to Figs. 1–3, respectively. In contrast to the speed of pattern evolutions, the evolution of the values of order-parameter field is slow with decreasing σ . In particular, we note that the order-

parameter value does not saturate its equilibrium value even in the central part of domains due to long tails as discussed in the preceding section. Thus, a simple picture of sharp kinks assumed by Bray [8] may not be appropriate for small σ .

The time dependence of the characteristic length $l(t)$ is shown in Fig. 7. The characteristic length is defined by the ratio of “the total area” to “the total length of interfaces” where the interface means the lines of $S = 0$. We estimate the values of the growth exponent z defined through $l(t) \sim t^{1/z}$ for $50 \leq t \leq 75$ as $0.88, 1.94,$ and 2.10 for $\sigma = 0.5, 1.0,$ and 1.5 , respectively, from 256×256 simulations, although we are afraid that the determination of z in such a short interval is meaningless. The growth exponent z is almost 2 for both $\sigma = 1.0$ and 1.5 , which is consistent with Bray’s prediction [8]. Note that our estimated value of z for $\sigma = 0.5$ is much smaller than the theoretical value $z = 3/2$. Since this discrepancy may arise from finite-size effects of systems at $\sigma = 0.5$, we examine the plot $l(t)t^{-2/3}$ versus time for simulations with system sizes $256 \times 256, 512 \times 512,$ and 1024×1024 in Fig. 8. This figure displays $l(t) \sim t^{2/3}$ or $z = 1.5$ for $80 \leq t \leq 300$ in systems with size 1024×1024 , while there are no such regions in systems with sizes 256×256 and

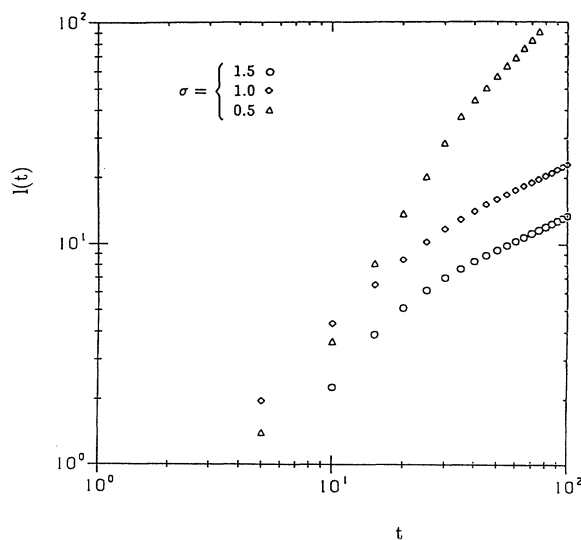


FIG. 7. Log-log plots of the characteristic length $l(t)$ vs time in systems for $\sigma = 0.5, 1.0,$ and 1.5 with size 256×256 after ten times the average of different initial conditions.

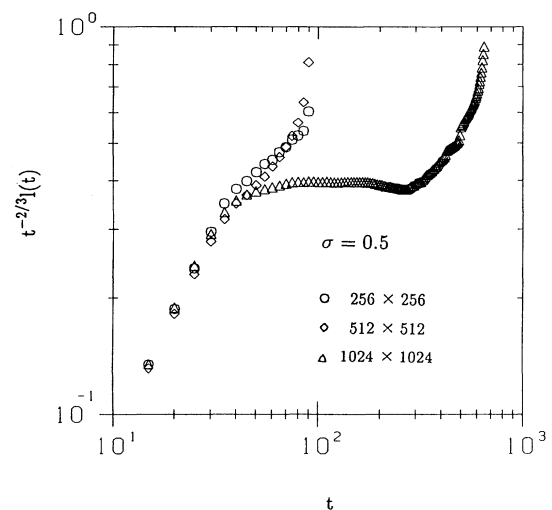


FIG. 8. The plot of $l(t)t^{-2/3}$ vs time for systems at $\sigma = 0.5$ with sizes $256 \times 256, 512 \times 512,$ and 1024×1024 after ten times the average of different initial conditions.

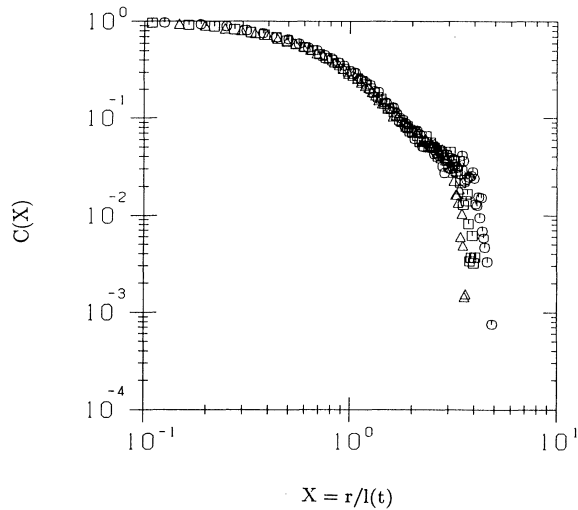


FIG. 9. The scaling plots of the spatial correlation function at $t = 50$ (Δ), 65 (\square), and 80 (\odot) for $\sigma = 1.0$ with system size 256×256 .

512×512 due to finite-size effects. Our result may suggest that Bray's prediction [8], $z = 1 + \sigma$ for $\sigma < 1$ and $z = 2$ for $\sigma > 1$, is correct for large systems in spite of the existence of long tails in order-parameter profile.

We also calculate the equal-time pair-correlation function. The dynamical scaling in systems with size 256×256 seems to be satisfied for $\sigma = 1.0$ and 1.5 after $t = 50$ (Figs. 9 and 10). For $\sigma = 0.5$ we use the data of the spatial correlation function in systems with 1024×1024 . Even in large size systems the dynamical scaling is not good during the time region in which $l(t) \sim t^{2/3}$ is satisfied (Fig. 11). We may need the simulation of larger systems than ours to obtain scaling. Our simulation for $\sigma = 1.0$ and 1.5 also suggests that the tails obey the power

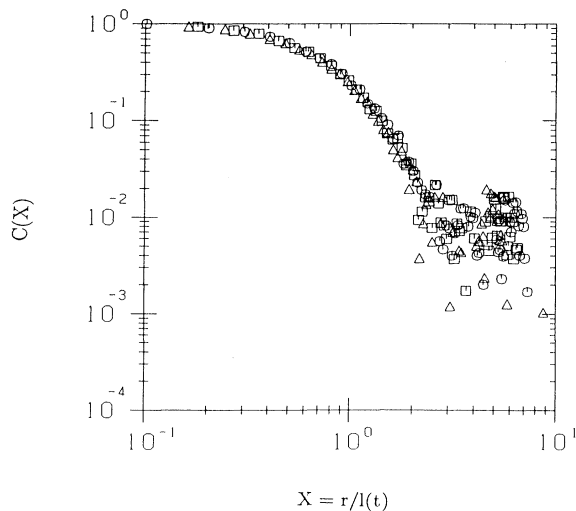


FIG. 10. The scaling plots of the spatial correlation function for $\sigma = 1.5$. The details of this figure are the same as those in Fig. 9.

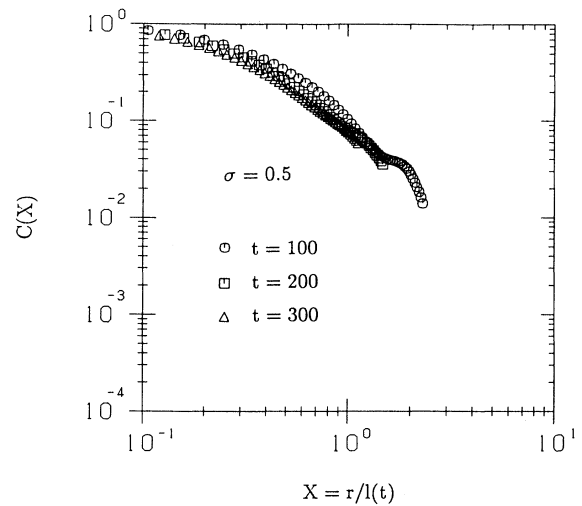


FIG. 11. The scaling plots of the spatial correlation function for $\sigma = 0.5$ in systems with size 1024×1024 .

law as observed by HRT [7]. Note that our data are disordered for large $X = r/l(t)$, because the effects of the periodic boundary condition and long-range interactions lead to confusion as to what cells are close to the observed cell. Thus, the data for $r \sim N/2$ with the linear system size N are almost meaningless for the calculation.

IV. DISCUSSION

Our numerical result for $d = 2$ can be summarized as follows. (i) Our result for $\sigma = 1.0$ and 1.5 with system sizes 256×256 is consistent with Bray's prediction [8] based on interfacial kinetics is correct in the late stage. (ii) For $\sigma = 0.5$ we need to consider the finite-size effects. Our result with 1024×1024 is consistent with Bray's prediction [8], although small systems do not achieve Bray's region. (iii) The dynamical scaling of the spatial correlation function seems to be satisfied for $\sigma = 1.0$ and 1.5 even in small size systems, while scaling cannot be observed at $\sigma = 0.5$ even in large system sizes. (iv) We observe the tail obeying power laws for large $X = r/l(t)$ of the spatial correlation function.

Quite recently, Ohta and Hayakawa [12] have constructed an analytic theory of our systems. Their conclusion supports Bray's simple picture [8] even in the presence of long tails of the order parameter (9), because the order-parameter profile is steep near its zeros. They also predict the analytic form of the spatial correlation function in which (i) the scaling is violated for $\sigma \geq 1$ and it is satisfied for $\sigma < 1$ at finite t and (ii) the scaling form in the long-time limit for $\sigma \geq 1$ is the same as that for short-range interactions [5]. It is interesting that their prediction may not be consistent with our result. We can guess that (a) observed tails of the spatial correlation function in our simulation disappear in the long-time limit and (b) the scaling may be satisfied for large systems even at $\sigma = 0.5$. In fact, if we only focus on the short-time interval between $t = 100$ and 130 , an approximate

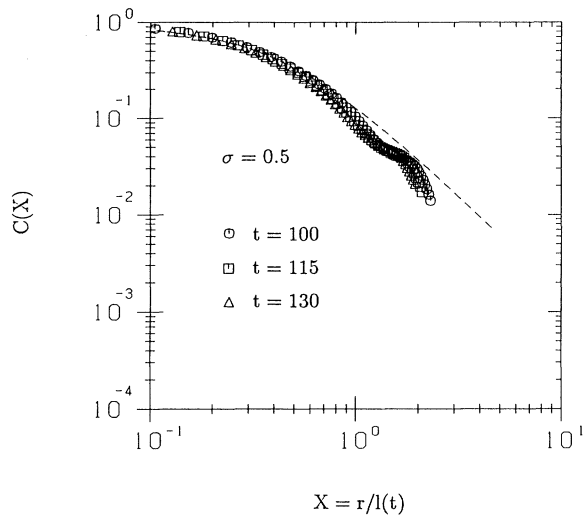


FIG. 12. Comparison of the scaling form of the spatial correlation function between our simulation for $100 \leq t \leq 130$ with the system size 1024×1024 and the theory by Ohta and Hayakawa [12] (dashed line) at $\sigma = 0.5$.

scaling form of $C(X)$ agrees with that of Ohta and Hayakawa [12] (Fig. 12). The details of the discussions have been found in the paper by Ohta and Hayakawa [12].

After submission of this paper, we received some relevant papers related to our work. Lee and Cardy [13] simulated 1D Ising spin by using the Monte Carlo simulation (MCS). Their results are consistent with Bray's prediction for $\sigma = 1.0$ and 1.5 , while they are not consistent for $\sigma = 0.5$. Rutenberg [14] suggested that a consistent result with Bray's prediction [8] can be obtained even in the case of $\sigma = 0.5$ from MCS for 1D Ising spins for large systems. These papers are consistent with our results. There are several papers to generalize our situations. Bray and Rutenberg [15] have generalized Bray's argument [8] to systems with $O(n)$ symmetric order parameters and a global conserved but local nonconserved model. Hayakawa [16] also obtained the spatial correlation function for large n with global conserved but local nonconserved order parameter. In these cases, a simple dimensional counting like that of HRT [7] and KYG [4] is not correct for small n . Using the critical condition by Bray and Rutenberg [15], the HRT result may be correct for $n > 2$.

ACKNOWLEDGMENTS

One of the authors (H.H.) thanks A. J. Bray, S. Puri, A. D. Rutenberg, Z. Rácz, T. Ohta, and T. Tsuzuki for stimulating discussions and helpful comments. This work was partially supported by the Hosokawa-Powder Technology Foundation.

-
- [1] For reviews see, e.g., J. D. Gunton, M. San Miguel, and P. S. Sahni, in *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, New York, 1983), Vol. 8, p. 267; H. Furukawa, *Adv. Phys.* **34**, 703 (1985); K. Binder, *Rep. Prog. Phys.* **50**, 783 (1987).
- [2] K. Binder and D. Stauffer, *Phys. Rev. Lett.* **33**, 1006 (1978); H. Furukawa, *Prog. Theor. Phys.* **59**, 1072 (1978).
- [3] S. M. Allen and J. W. Cahn, *Acta Metall.* **27**, 1085 (1979).
- [4] K. Kawasaki, M. C. Yalabik, and J. D. Gunton, *Phys. Rev. A* **17**, 455 (1978).
- [5] T. Ohta, D. Jasnow, and K. Kawasaki, *Phys. Rev. Lett.* **49**, 1223 (1982).
- [6] G. F. Mazenko, *Phys. Rev. B* **42**, 4487 (1990).
- [7] H. Hayakawa, Z. Rácz, and T. Tsuzuki, *Phys. Rev. E* **47**, 1499 (1993).
- [8] A. J. Bray, *Phys. Rev. E* **47**, 3191 (1993).
- [9] Y. Oono and S. Puri, *Phys. Rev. A* **38**, 434 (1988).
- [10] K. Kawasaki and K. Sekimoto, *Macromolecules* **22**, 3063 (1989).
- [11] H. Hayakawa and T. Koga, *J. Phys. Soc. Jpn.* **59**, 3542 (1990).
- [12] T. Ohta and Hayakawa, *Physica A* (to be published).
- [13] Benjamin P. Lee and J. L. Cardy, *Phys. Rev. E* **48**, 2452 (1993).
- [14] A. D. Rutenberg (private communication).
- [15] A. J. Bray and A. D. Rutenberg (unpublished).
- [16] H. Hayakawa, *Fractals* (to be published).