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Fluid *n*-vector model and its hydrodynamic ordering processes

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We introduce a fluid n-component vector model for the study of the phase ordering dynamics. We examine several hydrodynamic growth laws of length scale for both conserved and nonconserved order parameters, with and without the thermal fluctuation. Several growth laws for fluids with the scalar order parameter are generalized, by taking the bulk energy and the defect core energy into consideration. Numerical simulation is also presented for the case of a conserved order parameter for $n=2$ and 3 in two and three dimensions, respectively. Different growth laws are observed between in two and in three dimensions. [S1063-651X(97)01008-8]

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I. INTRODUCTION

Over more than two decades great attention has been paid to the ordering dynamics in thermodynamically unstable systems. It began with studies of ordering dynamics in unstable systems with *scalar* order parameters (see for reviews [1–3]), and then with *vector* order parameters (see for the reviews [4,5]). The n-vector model is equivalent to the scalar model for $n=1$ and is applied to binary mixtures. For $n=2$ and 3 the model is applied to liquid crystals. The case of $n=\infty$ is called the spherical model. The ordering dynamics with vector order parameters for $n>2$ have been extensively discussed rather recently [6–28]. Vector models are subjects of applications of theoretical methods [21,29–32] and/or numerical methods [33]. The vector model also provides models of liquid crystals [34–37], though the liquid crystal may also be a model of a scalar order parameter [38,39].

In this paper we shall introduce a fluid vector model, which we shall abbreviate as the ''vector fluid'' or the ''vector liquid.'' One motivation of this is that usually used vector models are those with the real order parameter. In such models order parameters have no intrinsic velocity field (complex order parameter has it). The other motivation comes from the fact that for fluid systems with the scalar order parameter several kinds of examinations have been done, i.e., theoretical predictions [40–43], experimental studies [44–50], numerical studies, [51–70] and the studies of shear induced phase separations [71–76]. How is the ordering dynamics in the vector fluid? We shall explore hydrodynamic growth laws of the vector fluid.

We consider the isothermal ordering process. The isothermal process is appropriate in a slowly varying phase ordering like in polymers or in a late stage of ordering in any system, where the effect of the heat production can be neglected. The relevant free energy in such isothermal processes is the Helmholtz free energy. The order parameter of the n-vector model is written as

$$\vec{\psi}\equiv(\psi_1,\psi_2,\ldots,\psi_n). \tag{1}$$

The nonhydrodynamic part of the Helmholtz free energy is given by

$$F=\int\left(\frac{g}{2}\sum_{i=1}^{n}|\vec{\nabla}\psi_i|^2+\frac{1}{4}\alpha(1-|\vec{\psi}|^2)^2\right)d\mathbf{r}, \tag{2}$$

where g and α are positive constants and

$$|\vec{\psi}|^2\equiv\sum_{i=1}^{n}|\psi_i|^2. \tag{3}$$

The equation of motion for the order parameter is then given applying the thermodynamics of irreversible process as

$$\frac{\partial\psi_i}{\partial t}=-L(i\vec{\nabla})^{2\theta}\frac{\delta F}{\delta\psi_i}=L(i\vec{\nabla})^{2\theta}[g\nabla^2\psi_i+\alpha(1-|\vec{\psi}|^2)\psi_i], \tag{4}$$

where $i=\sqrt{-1}$ in the brackets, and $\theta=0$ corresponds to the case where $\vec{\psi}$ is not conserved, whereas $\theta=1$ corresponds to the case where $\vec{\psi}$ is conserved. When the system is quenched from a state with a high temperature into an unstable state, the phase ordering takes place. A complete set of growth laws of the length scale R in the ordering process of this system was examined by the energy scaling method and it is classified into three cases [4,77]:

$$R\sim\begin{cases} t^{1/2}, & \text{for } n<2-2\theta \quad (5)\\ t^{1/(n+2\theta)} & \text{for } 2-2\theta<n<2 \quad (6)\\ t^{1/(2+2\theta)} & \text{for } n>2. \quad (7)\end{cases}$$

Logarithmic corrections are obtained at the thresholds in the above classification [77], but we have disregarded those corrections here.

In the next section we obtain a set of kinetic equations for the vector order parameter and the velocity field. In Sec. III we explore several hydrodynamic growth laws. In Sec. IV some discussions will be presented. We also present some numerical results.

II. KINETIC EQUATIONS FOR VECTOR FLUID

We here derive a suitable set of kinetic equations for $\vec{\psi}$ and ϕ. The hydrodynamic term can be added to the above free energy (2) as follows. Let us assume that each part of the system is drifting. By the Galilean transformation we can observe a local part in a comoving frame. In this frame the free energy density of the local part is given by Eq. (2). The kinetic energy of the fluid is therefore added to Eq. (2). Let $\mathbf{v}$ be the local velocity field and $\mathbf{v}+\delta\mathbf{v}_i$ be the velocity of the ith constituent which carries mass. Then the total kinetic energy density is $\rho v^2/2 + \rho\langle\delta\mathbf{v}^2\rangle/2$, where the second term corresponds to the thermal energy. The linear term in $\mathbf{v}$ does not appear. Except for the thermal energy we obtain a relevant Helmholtz free energy

$$F=\int\left(\frac{1}{2}\rho v^2+\frac{1}{2}\chi^{-1}(\phi-\phi_0)^2+\frac{g}{2}\sum_{i=1}^{n}|\vec{\nabla}\psi_i|^2+\frac{1}{4}\alpha(1-|\psi|^2)^2\right)d\mathbf{r}. \tag{8}$$

Here we have added the energy due to the compression (the second term). χ is the compressibility of fluid, ϕ is a quantity corresponding to the total number density, and ϕ_0 is the average of ϕ.

We here explore hydrodynamic kinetic equations for the vector fluid. This may be the generalization of the so-called H model [78]. Under constant temperature, constant volume, and constant total particle number the Helmholtz free energy does not increase. Therefore

$$\begin{aligned}\frac{dF}{dt}&=\int\left(\dot{\mathbf{v}}\frac{\delta F}{\delta\mathbf{v}}+\dot{\phi}\frac{\delta F}{\delta\phi}+\sum_i\dot{\psi}_i\frac{\delta F}{\delta\psi_i}\right)d\mathbf{r}\\&=\int\left[\dot{\mathbf{v}}\vec{\mu}_v+\dot{\phi}\left(m\frac{v^2}{2}+\mu_\phi\right)+\sum_i\dot{\psi}_i\mu_i\right]d\mathbf{r}\leqslant 0,\end{aligned} \tag{9}$$

where the dot denotes the time derivative, $m=\rho/\phi$ corresponds to mass, μ_ϕ and μ_i are static chemical potentials for ϕ and ψ_i $(i=1,2,\dots,n)$, and $\vec{\mu}_v$ is a kind of chemical potential for the velocity field:

$$\begin{aligned}\vec{\mu}_v&\equiv\frac{\delta F}{\delta\mathbf{v}}=\rho\mathbf{v},\qquad \mu_\phi\equiv\frac{\delta F^{(0)}}{\delta\phi}=\chi_0^{-1}(\phi-\phi_0),\\ \mu_i&\equiv\frac{\delta F}{\delta\psi_i}=-g\nabla^2\psi_i-\alpha(1-|\psi|^2)\psi_i,\end{aligned} \tag{10}$$

and $F^{(0)}$ is the static part of the free energy, i.e., $F^{(0)}\equiv F(\mathbf{v}=0)$.

In order to derive kinetic equations for ϕ and ψ's we notice the following. If there is no dissipation of particles and the order parameter by the diffusions and/or the chemical reactions, only the source for changes in these quantities is the drift velocity $\mathbf{v}$. Then the local currents of these quantities are products of the local drift velocity $\mathbf{v}$ and local densities of corresponding quantities. In this case ϕ's and ψ's should satisfy continuity equations. Thus we obtain

$$\frac{\partial\phi}{\partial t}=-\vec{\nabla}\cdot\mathbf{v}\phi,\qquad \frac{\partial\psi_i}{\partial t}=-\vec{\nabla}\cdot\mathbf{v}\psi_i\qquad (i=1,2,\dots,n). \tag{11}$$

If there are dissipations, then changes by the dissipations are added to the above equations. These changes occur through the second derivative of the free energy:

$$\frac{\partial\phi}{\partial t}=-\vec{\nabla}\cdot\mathbf{v}\phi+L_\phi\nabla^2\left(m\frac{v^2}{2}+\mu_\phi\right), \tag{12}$$

$$\frac{\partial\psi_i}{\partial t}=-\vec{\nabla}\cdot\mathbf{v}\psi_i-L(i\nabla)^{2\theta}\mu_i\qquad (i=1,2,\dots,n). \tag{13}$$

Here $\theta=1$ and $\theta=0$ correspond to conserved and nonconserved order parameters, respectively. Coefficients L, which are assumed to be constant, should be positive.

For the velocity field $\mathbf{v}$ we may write the equation of motion as

$$\rho\frac{\partial\mathbf{v}}{\partial t}=\mathbf{F}^*+\eta\nabla^2\mathbf{v}. \tag{14}$$

Here the first term on the right hand side represents the time-reversible part, and the second term represents the dissipative part which may be of more complicated form. The ambiguity in the relation between the chemical potential and the pressure or the hydrodynamic force in the case where abstract order parameters are associated as in the present case will be removed with the help of an identy:

$$\int\left\{\mathbf{v}\cdot\left[\mathbf{F}^*+\phi\vec{\nabla}\left(m\frac{v^2}{2}+\mu_\phi\right)+\sum_i\psi_i\vec{\nabla}\mu_i\right]\right\}d\mathbf{r}=0. \tag{15}$$

To prove this identity let us remember that the time derivative of the free energy (9) is identically zero for $L_\phi=L=\eta=0$, because all equations are now time reversible. By substituting Eqs. (11) and (14) for $L_\phi=L=\eta=0$ into Eq. (9), and performing a partial integration once for each term, we arrive at Eq. (15). Using $\frac{1}{2}\mathbf{v}\cdot\vec{\nabla}v^2=\mathbf{v}\cdot[(\mathbf{v}\cdot\vec{\nabla})\mathbf{v}]$ Eq. (15) is transformed into

$$\int\left[\mathbf{v}\cdot\left(\mathbf{F}^*+\rho(\mathbf{v}\cdot\vec{\nabla})\mathbf{v}+\phi\vec{\nabla}\mu_\phi+\sum_i\psi_i\vec{\nabla}\mu_i\right)\right]d\mathbf{r}=0. \tag{16}$$

In order for Eq. (16) to hold identically we choose

$$\mathbf{F}^*=-\rho(\mathbf{v}\cdot\vec{\nabla})\mathbf{v}-\phi\vec{\nabla}\mu_\phi-\sum_i\psi_i\vec{\nabla}\mu_i. \tag{17}$$

Thus a desired equation of motion for $\mathbf{v}$ is given by

$$\rho\frac{\partial\mathbf{v}}{\partial t}=-\rho(\mathbf{v}\cdot\vec{\nabla})\mathbf{v}+\eta\nabla^2\mathbf{v}-\phi\vec{\nabla}\mu_\phi-\sum_i\psi_i\vec{\nabla}\mu_i. \tag{18}$$

Similar or equivalent equations for $n=1$ were used previously, [51–53,59,68,69]. It is easy to show that Eq. (18) for $n=1$ is equivalent to the Navier-Stokes equation of binary mixture, which has a single component order parameter [59]. By substituting Eqs. (12), (13), and (18) into the right hand side of Eq. (9) we find that the right hand side of Eq. (9) is really of a nonpositive form:

$$\frac{dF}{dt} = -\int \left[-\eta \mathbf{v}\cdot\nabla^2\mathbf{v} + L_\phi \left| \vec{\nabla}\left(m\frac{v^2}{2} + \mu_\phi \right) \right|^2 + \sum_i L|\vec{\nabla}\mu_i|^{2\theta} \right] d\mathbf{r} \leqslant 0. \tag{19}$$

Therefore the present dynamical equations are consistent with the second law of thermodynamics. The extension of the present equations to the case where extra variables exist is straightforward.

If the chemical potential is a local quantity, then the pressure is a well-defined thermodynamic quantity, i.e., dP $\phi d\mu_\phi + \Sigma \psi_i d\mu_i$ is a total derivative. However, if the chemical potential is nonlocal, then the derivative of the local quantity $\delta P(\mathbf{r}) = -\phi(\mathbf{r})\delta\mu_\phi(\mathbf{r}) - \Sigma_i \psi_i(\mathbf{r})\delta\mu_i(\mathbf{r})$ is not a total derivative, in general. Let us explain this for a simplified case where $\mu_\psi(\mathbf{r}) = \int g(|\mathbf{r}-\mathbf{r}'|)\psi(\mathbf{r}')d\mathbf{r}'$. Then $\delta P(\mathbf{r}) = -\psi(\mathbf{r})\delta\mu_\psi(\mathbf{r})$. Thus $[\delta/\delta\psi(\mathbf{r}'')][\delta/\delta\psi(\mathbf{r}')]P(\mathbf{r}) = -\delta(\mathbf{r}-\mathbf{r}'')g(|\mathbf{r}''-\mathbf{r}'|)$. This is not equivalent to $[\delta/\delta\psi(\mathbf{r}')][\delta/\delta\psi(\mathbf{r}'')]P(\mathbf{r})$, if the function $g(r)$ is not of a local form $[\propto \delta(\mathbf{r})]$. Therefore the local pressure $P(\mathbf{r})$ is not a conserved quantity if the interaction is nonlocal. For this reason sometimes only the third term on the right hand side of Eq. (18) is identified with the pressure.

III. HYDRODYNAMIC GROWTH LAWS

According to the dynamical scaling assumption $S_k(t) = R(t)^d \tilde{S}(kR(t))$ the ordering process is characterized by the time dependence of the length scale $R(t)$, where S is the structure function $S_k(t) \equiv \Sigma_i^n \langle |\psi_{i,\mathbf{k}}|^2 \rangle$. Here $\psi_{i,\mathbf{k}} = \int e^{i\mathbf{k}\cdot\mathbf{r}}\psi_i(\mathbf{r})d\mathbf{r}$ is the Fourier coefficient of the order parameter ψ_i. In the cases of $n=1$ with and without the hydrodynamic term and in the cases of $n>1$ without the hydrodynamic term growth laws are well established. Here we examine the growth laws $R \sim t^a$ in the case of $n>1$ with the hydrodynamic term. Let us notice that the hydrodynamic growth is governed by the hydrodynamic equation (18), and therefore there is no distinction between conserved and nonconserved order parameters. A dimensional analysis is a useful tool to obtain the growth laws. For this purpose we need the potential energy density of the system. In the binary system ($n=1$) this is the energy of the domain wall. The domain wall is regarded as a kind of defect, where the order parameter becomes singular. The defect for $n=1$ is a line in two dimensions, and a wall in three dimensions. The defect for $n=2$ is a point in two dimensions and a line in three dimensions. Generally the spatial dimensionality D of the defect is given by

$$D = d - n. \tag{20}$$

For $D<0$ there is no defect. Generally for $n=1$ and 2 the relevant energy is the defect core energy. However, for $n>2$ that is the bulk energy. This was shown using a generalized Porod law for the tail of the structure function [79, 80]:

$$\tilde{S}(x) \sim x^{-d-n}. \tag{21}$$

To evaluate the energy we notice that the temporal change in the order parameter $\vec{\psi}$ is very slow, enough for the system to be in a local equilibrium state. The local equlibrium assumption was successfully applied to the scalar order parameter to evaluate the interfacial energy [81]. The local equilibrium assumption for the vector order parameters may also be valid. However, it is certainly different from that for the scalar order parameter. Let the typical length scale at time t be R. For instance, R is the average curvature of defect core or average distance for which the direction of the order parameter changes its angle by the amount 2π. The spatial structure cannot relax to the equilibrium one independently of surrounding structures. The surrounding structures play a role of external constraints. Assuming that the local structure is in a local equilibrium state under the surrounding constraints, the determination of the local structure of the order parameter is treated as the problem of solving the equation giving the minimum of the free energy under a given constraint:

$$\frac{\delta F}{\delta\psi_i} = -g\nabla^2\psi_i - \alpha(1-|\psi|^2)\psi_i \approx 0 \quad \text{with constraints.} \tag{22}$$

If we honestly apply Eq. (22) to the dynamics, then the time derivative of the order parameter seems to vanish. However, this is not true since the constraints of this equation depend on time. Equation (22) should be regarded as the balance between two forces under a given constraint. Such a constraint may be replaced by the condition of a fixed length scale R. As an example we consider the simplest one dimensional case without loss of generality. Let $\vec{\psi}(x)$ be a one dimensional vector order parameter and let the constraints be $\psi_i(0) = a_i$ and $\psi_i(R) = -a_i$. Under such constraints the vector order parameter gradually changes as a function of coordinate x, because such a gradual change does not cost much energy. For instance, we have $\psi \sim a\cos(\pi x/R)$. Therefore

$$\vec{\nabla}\psi_i \sim R^{-1}\psi_i, \quad \nabla^2\psi_i \sim R^{-2}\psi_i. \tag{23}$$

Such estimations generally hold for vector order parameters without singularity. The use of the evaluation (23) gives the following energy scaling:

$$|\vec{\nabla}\vec{\psi}|^2 \sim R^{-2}, \tag{24}$$

$$(1-\psi^2)^2 \sim R^{-4}. \tag{25}$$

The second scaling is obtained with the use of Eq. (22) and the second relation in Eq. (23), since we have $(1-\psi^2)\psi \sim \nabla^2\psi \sim R^{-2}$. The same result is also given for energy density around spherically symmetric defect cores [4]. In this case the static equation is solved. Then the result is applied to the dynamics. These procedures correspond to the local equilibrium assumption. The energy density of the vector order parameter is thus captured only by the gradient term in the late stage of the ordering process for the vector order parameter:

$$F \approx \frac{g}{2}\int d\mathbf{r}\sum_{i=1}^{n} |\vec{\nabla}\psi_i|^2 = \frac{gV}{2}\int k^2 S(k,t)d\mathbf{k}, \tag{26}$$

where V is the total volume of the system. Notice that the energy density for the scalar order parameter is also given by an equation similar to Eq. (26), where, however, the contribution from the local energy $\alpha(1-\psi^2)^2/4$ is equal to $g|\vec{\nabla}\psi|^2/2$ and hence a factor of 2 should be added to Eq. (26) for the scalar order parameter [81].

Two comments are needed for Eq. (26). First, the defect core energy can be captured also by Eq. (26), in general. This is because the defect core energy is given by the defect core size (length, area, or volume) times some proportionality constant. The defect core size is captured by means of singularity of Eq. (24) or Eq. (25), since Eqs. (24) and (25) become equally singular at the defect core. Second, the conserved scalar order parameter has a nonvanishing bulk chemical potential $\mu \sim O(1/R)$ in nonequilibrium state (Gibbs-Thomson), which is the deviation from Eq. (22). This bulk chemical potential gives deviations of the order parameter from those in equilibrium single phase states, $\psi_{\mathrm{eq}} = \pm 1$. The deviation is given as $\Delta\psi \equiv \psi - \psi_{\mathrm{eq}} \sim 1/R$ except near the defect core region. This gives the following scalings of bulk energies for the scalar order parameter:

$$|\vec{\nabla}\psi|^2 \sim R^{-4}, \tag{27}$$

$$(1-\psi^2)^2 \sim \Delta\psi^2 \sim R^{-2}. \tag{28}$$

The corresponding defect core energy density is of the order $1/R$. Therefore bulk energies (27) and (28) for the scalar order parameter can be neglected compared with the corresponding defect core energy, justifying that the dominant contribution to the energy comes from the defect core which can be captured by Eq. (26).

Substituting Eq. (21) into the last side of Eq. (26) the contribution from large wave numbers is given as $F \sim gVR^{-2}(Rk_c)^{2-n}$, where k_c is the upper cutoff of the integration. Therefore if $n<2$ then the energy becomes larger as k_c becomes larger. In this case the dominant contribution comes from large wave numbers. Since the energy should be finite we must fix the microscopic upper cutoff of the wave number, i.e., $k_c \sim \xi$, where ξ is the microscopic thermal correlation length. We then obtain $F \sim gVR^{-n}\xi^{n-2}$. On the other hand, for $n>2$ the contribution from large wave number is not important and we set $k_c \sim 1/R$. We then obtain $F \sim gV/R^{-2}$. The usefulness of these evaluations of the energy was examined by applying it to the growth laws for arbitrary values of n, d, and θ, Eqs. (5)–(7) [4,77].

Since the hydrodynamic driving force $\mathbf{F}$ given by Eq. (18) is the superposition of contributions from all components of $\vec{\psi}$, the contributions from the bulk energy is expected to be small. Therefore we cannot simply apply the above method to the hydrodynamic case. To investigate the hydrodynamic growth laws we separate the energy into two parts, i.e., the defect core energy ($\sim R^{-n}$) and the bulk energy ($\sim R^{-2}$), and we investigate the hydrodynamic growth laws using these energies separately. The bulk energy density for the vector order parameter is captured simply by the gradient term of the free energy $|\vec{\nabla}\psi|^2/2$ assuming there is no singularity:

$$\epsilon_B \sim gR^{-2} \sim \sigma\xi R^{-2}, \tag{29}$$

where σ is a quantity corresponding to the surface tension. A similar energy is given for the conserved scalar order parameter by the local term (28), but this bulk energy is not effective since the defect core energy is dominant in this case. The defect core energy is proportional to the defect core size:

$$\epsilon_D \sim \sigma\xi^{n-1}R^D/R^d = \sigma\xi^{n-1}R^{-n}. \tag{30}$$

These evaluations give the same results as the above evaluations by the integration of the gradient energy term with a generalized Porod law. It is considered that the defect core energy ϵ_D is not relevant for $n>2$ in the purely relaxational case (with no hydrodynamic term). However, if the bulk energy ϵ_B becomes ineffective to the hydrodynamic driving force, then ϵ_D should be important even for $n>2$, if defects exist.

Let us now examine hydrodynamic growth laws using these energies. Orderings independent of the velocity field $\mathbf{v}$ are not the hydrodynamic ones but the purely relaxational ones. Therefore we may examine only the case where the defect is comoving with the order parameter by the velocity $\mathbf{v}$. This allows us to have the following picture of the ordering. The potential energy is released according to the coarsening. The balance between the released defect energy and the fluid kinetic energy or the dissipated energy determines the growth law of the length scale R. This allows us to use the dimensional analysis for the energy balance or the force balance.

The driving force is of the order ϵ/R, where ϵ is ϵ_D or ϵ_B. The acceleration of the fluid of unit volume is of the order R/t^2 and the friction by the dissipation is of the order $\eta/(Rt)$. Then the velocity field equation (18) is transformed into a dimensional equation:

$$\rho R/t^2 + \eta/(Rt) \approx \epsilon/R. \tag{31}$$

Let us introduce the Reynolds number Re:

$$\mathrm{Re} = \frac{\rho R/t^2}{\eta/(Rt)} = \frac{\rho R^2}{\eta t}. \tag{32}$$

For Re>1 the inertial term, the first term on the left hand side of Eq. (31), is effective, while for Re<1 the dissipative term, the second term, is effective. The condition Re$=1$ gives $R \propto t^{1/2}$.

A. Growth by defect core energy

Let us consider the case where the defect core energy ϵ_D is the relevant driving force. Then we obtain

$$R \sim \left(\frac{\sigma\xi^{n-1}}{\rho}\right)^{1/(n+2)} t^{2/(n+2)} \quad \text{for} \quad \mathrm{Re}>1. \tag{33}$$

We have

$$R \sim \left(\frac{\sigma\xi^{n-1}}{\eta}\right)^{1/n} t^{1/n} \quad \text{for} \quad \mathrm{Re}<1. \tag{34}$$

Let $R \sim t^a$. Then Re increases indefinitely for $a>1/2$. Therefore the leading growth law in the long time limit is Eq. (33) for $n<2$, whereas it is Eq. (34) for $n>2$. In the intermediate time the leading growth law depends on the value of Re. For

$n=1$ Eq. (33) gives a $t^{2/3}$ growth law [43] and Eq. (34) gives t-linear growth laws [42]. A comment on the above growth laws may be needed. The global connectivity of defects is important for the defect core energy to be effective to the hydrodynamic growth laws. If the defect core is not connective, then the coarsening by the shrinking of defect cores does not continue. Let us consider only the case where the averages of compositions are the same for all components, i.e., $\langle|\psi_i|^2\rangle=1/n$ for $i=1,2,\ldots,n$. Then for defects, which are globally connective, the spatial dimensionality of the defect should be larger than or equal to 1:

$$D\equiv d-n\geqslant 1. \tag{35}$$

For the bulk energy ϵ_B no such a restriction as Eq. (35) exists. The other comment is given on Eq. (33). For this growth law the dissipation term is neglected, but this does not mean that the hydrodynamic dissipation, represented by the second term on the right hand side of Eq. (18), plays no role, but plays a role of energy dissipation at shorter length scales. If the kinetic energy released at the coarsening redestroys the order, then the growth law (33) will be modified. This was discussed for $n=1$ [59].

B. Growth by bulk energy

The effect of the bulk energy for the vector case $(n\geqslant 2)$ to the hydrodynamic growth laws is very ambiguous. The following is one of the possible estimations, but is not conclusive. A straightforward application of the bulk energy (29) gives another growth law:

$$R\sim Ct^{1/2}. \tag{36}$$

The coefficient C is given by a simple dimensional analysis as $C\sim(\sigma\xi/\rho)^{1/3}$. However, this value of C or Eq. (36) may be questioned. If Eq. (36) is observed, then this must occur for very large length scales. This is because the hydrodynamic force due to the bulk energy from each component of the order parameter would be canceled out. We here present a very crude estimation of the hydrodynamic growth law by the bulk energy. The hydrodynamic force associated with the order parameter ψ is estimated (except near the defect core region) as

$$\mathbf{F}_{\psi,B}\sim\sum_i \psi_i\vec{\nabla}\nabla^2\psi_i\sim R^{-2}\sum_i \psi_i\vec{\nabla}\psi_i\sim R^{-2}\vec{\nabla}|\vec{\psi}|^2\sim R^{-5}, \tag{37}$$

where we have used Eq. (25) to obtain the last side. This corresponds to replacing ϵ_B/R by ϵ_B/R^3. Therefore Eq. (36) may be replaced by

$$R\sim C' t^{1/3} \quad \text{for} \quad \text{Re}>1 \tag{38}$$

and

$$R\sim C'' t^{1/4} \quad \text{for} \quad \text{Re}<1, \tag{39}$$

where C' and C'' are constants. In the long time limit the leading growth law is Eq. (39). Due to the approximation used here estimated growth laws in this subsection are not conclusive, yet. Therefore further investigation should be done. In the present paper we also report some results of the numerical simulation to investigate the effect of the bulk energy on the hydrodynamic growth. This is presented in Sec. IV.

C. Growth by thermal fluctuation (hydrodynamic case)

The reason the thermal fluctuation can be the driving force of the ordering process is that the state we are considering is unstable and therefore any motion of the order parameter contributes to the reduction of the free energy of the system. The effect of the thermal fluctuation on the hydrodynamic growth law is examined by adding the fluctuating force $\mathbf{Q}_f$ to Eq. (18),

$$\rho\frac{\partial\mathbf{v}}{\partial t}=-\rho(\mathbf{v}\cdot\vec{\nabla})\mathbf{v}+\eta\nabla^2\mathbf{v}-\phi\vec{\nabla}\mu_\phi-\sum_i \psi_i\vec{\nabla}\mu_i+\rho\mathbf{Q}_f. \tag{40}$$

The fluctuating force $\mathbf{Q}_f$ is that of the fluid

$$\langle\mathbf{Q}_f(t,\mathbf{r})\cdot\mathbf{Q}_f(t',\mathbf{r}')\rangle=-\frac{2dk_BT\eta}{\rho^2}\nabla^2\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'), \tag{41}$$

in d dimensions. Then one can show that the thermal equilibrium fluctuation of the velocity field satisfies the equipartition law:

$$\rho\langle|\mathbf{v}_\mathbf{k}|^2\rangle=dk_BT. \tag{42}$$

This relation represents the thermal fluctuation of the velocity field with the length scale k^{-1}. Applying this relation to the velocity field with the length scale R, and setting $\langle|\mathbf{v}_\mathbf{k}|^2\rangle\sim R^d(R/t)^2$, we obtain a growth law in the case where the viscosity is not important and hence the inertia is dominant:

$$R\sim\left(\frac{k_BT}{\rho}\right)^{1/(d+2)} t^{2/(d+2)} \quad \text{for} \quad \text{Re}>1. \tag{43}$$

We can also find a different kind of a growth law associated with the inertia. By retaining only the fluctuating force in the right hand side of Eq. (40) we obtain

$$\frac{\partial\mathbf{v}}{\partial t}=\mathbf{Q}_f. \tag{44}$$

This gives

$$\frac{\partial\langle|\mathbf{v}_\mathbf{k}|^2\rangle}{\partial t}\sim\int^t dt'\langle\mathbf{Q}_{f,\mathbf{k}}(t)\cdot\mathbf{Q}_{f,\mathbf{k}}(t')\rangle\sim\frac{k_BT\eta k^2}{\rho^2}. \tag{45}$$

Corresponding to this relation we obtain

$$R\sim\left(\frac{k_BT\eta}{\rho^2}\right)^{1/(d+4)} t^{3/(d+4)}, \tag{46}$$

where we have used the relations $\mathbf{v}_k^2\sim R^d(R/t)^2$ and $kR\sim 1$. This growth law is obtained for $n=1$ in [59] by the dimensional analysis and is explained as the growth law associated both with the dissipation and the inertia. We consider that Eq. (46) is valid when the inertial term and the dissipative term are of the same order, i.e., Re ~ 1. Therefore Eq. (46) is not valid over long temporal range, in general.

When the inertial term can be neglected we retain only the second and the last terms of Eq. (40):

$$\mathbf{v}_{\mathbf{k}} \sim k^{-2}\nu^{-1}\mathbf{Q}_{f,\mathbf{k}}. \tag{47}$$

Notice that the velocity $\mathbf{v}_{\mathbf{k}}$ in this case does not obey the equipartition law (42), since it is dissipative. Most convincing ways of extracting the dissipative behavior of the ordering process are to combine Eq. (47) with the equation for $\vec{\psi}$ and then to use a scaling analysis. The same result can be obtained by using a convenient relation $\mathbf{Q}^2_{f,\mathbf{k}}t \sim k_B T \eta k^2/\rho^2$:

$$R \sim \left(\frac{k_B T}{\eta}\right)^{1/d} t^{1/d} \quad \text{for} \quad \mathrm{Re}<1. \tag{48}$$

Prefactors of these growth laws are only qualitative. These growth laws are the same as originally given for the scalar order parameter, i.e., Eq. (48) by [40] and Eq. (43) by [43].

D. Growth by thermal fluctuation (purely relaxational case)

The growth law by the thermal fluctuation in the purely dissipative case is given by adding the random force Q to the kinetic equation (13):

$$\frac{\partial \psi_i}{\partial t} = -L(i\vec{\nabla})^{2\theta}\mu_i + \nabla^\theta Q_i \qquad (i=1,2,\ldots,n). \tag{49}$$

The random forces Q are given to produce the thermal equilibrium fluctuation of ψ:

$$\langle Q_i(t,\mathbf{r})Q_j(t',\mathbf{r}')\rangle = 2k_B T L \delta_{i,j}\delta(t-t')\delta(\mathbf{r}-\mathbf{r}'). \tag{50}$$

Disregarding the first term on the right hand side of Eq. (49) and applying the dimensional analysis we obtain

$$R^{d+2\theta} \sim k_B T L t. \tag{51}$$

The precoefficient is only qualitative, too. The above growth law for $\theta=1$ was originally given for the scalar order parameter [2,40].

Finally we note the relation between the above several hydrodynamic growth laws and the continuity equation (11). In the case of $n=1$, which corresponds to the binary mixture, the value of each component is 1 or -1. Without changing this local value the coarsening proceeds with the hydrodynamic motion. However, for $n \geqslant 2$ the local value of each component ψ_i of the vector $\vec{\psi}$ continuously changes. In the hydrodynamic growth such changes are done not by the dissipational motion but by the drift motion obeying the continuity equations (11). Because the continuity equations (11) have no dimensional restriction, the above hydrodynamic growth laws are not affected by the continuity equations.

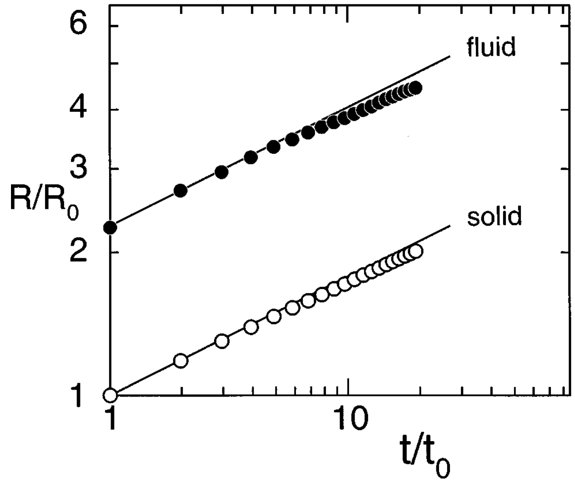

FIG. 1. $R(t)$ for $n=2$ in two dimensions. Open circles indicate the case of purely dissipative, and closed circles indicate the hydrodynamic case. $t_0=512$ and R_0 is the value of R at $t=t_0$ in the nonhydrodynamic case. Two straight lines have a slope 0.25.

IV. DISCUSSIONS AND REMARKS

As noted, the hydrodynamic growth laws in Sec. III evaluated using the bulk energy (29) are very ambiguous. In order to examine the effect of the bulk energy on the hydrodynamic motion we have performed the numerical simulation for the conserved order parameter with $n=2$ in two dimensions and with $n=3$ in three dimensions. In this simulation we disregarded the compressibility term in the hydrodynamic equation. Namely, we used Eq. (13) with $\theta=1$ and Eq. (18) without the third term associated with ϕ. For two dimensional simulation we have chosen $\alpha=1$, $L=1/4$, $m=1$ ($\phi=\rho$), $g=1/4$, and $\eta=0.1$. The numerical method is the Euler method or the method of the cell dynamical system [33]. In this simulation we did only a single run for the system with 512^2 cells. A discrete time $\delta t=0.1$ was used and the final computation time is 20×512. The length scale R is calculated by

$$R(t)=\left(\frac{\int k^{\Delta}S_k(t)dk}{\int S_k(t)dk}\right)^{-1/\Delta}, \qquad \Delta\sim 0. \tag{52}$$

Here the result is almost independent of the value of Δ. Time-dependent length scales $R(t)$ with and without the hydrodynamic term are shown for $n=2$ (Fig. 1). In this figure $t_0=512$, and R_0 is the length scale at $t=t_0$ in the nonhydrodynamic case. Two straight lines indicate $R \propto t^{0.25}$. The hydrodynamic length scale is about two times larger than the nonhydrodynamic one at the same time. The growth law in the nonhydrodynamic case supports Eq. (6) or Eq. (7) for the conserved order parameter [82]. The growth law in the hydrodynamic case seems to support Eq. (39). Since the defect core is a point in this case, no defect core energy is relevant to the hydrodynamic force.

We have also performed a simulation for $n=3$ in three dimensions. The system size is 128^3. In this case we used $g=1/6$. Other parameters are the same as in two dimensions. The final simulation time is 40×64. The defect is a point in this case, too. In this case we calculated the length scale by a different method from Eq. (52). Namely, we calculated it by the relation

$$R(t)\propto N_D(t)^{-1/d}, \tag{53}$$

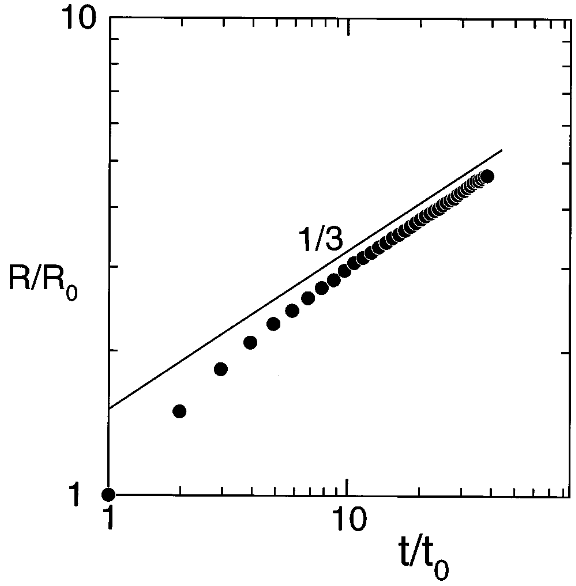

FIG. 2. $R(t)$ in hydrodynamic case for $n=2$ in three dimensions. The straight line has the slope 1/3. $t_0=64$ and R_0 is the value of R at $t=t_0$.

where N_D is the number of defect cores. We defined the defect core by $|\vec{\psi}|^2<0.8$, and actually N_D is identified with the number of cells satisfying this inequality. Figure 2 shows the length scale in this case. Although the final time is 1/4 times shorter than that in two dimensions and the simulation was done only for the single run, the length scale exhibits the $t^{1/3}$ dependence. Although Eq. (34) gives the same exponent 1/3 for $n=3$, this growth law cannot be applied to the present case because the defect morphology is a point in this case. The present simulation may support Eq. (38). But it is not clear why different growth exponents are observed in two and in three dimensions.

We have proposed a fluid vector model and we have studied its ordering processes from theoretical and numerical viewpoints. The hydrodynamic growth laws in the vector fluid are rather complicated. Further theoretical and numerical analyses are desired to clarify the nature of the hydrodynamic growth for the vector model. If the bulk energy (29) is not effective to the hydrodynamic growth, then the hydrodynamic growth laws by the defect core energy (33) and (34) together with Eq. (35) become important even for $n>2$ in the case of the conserved order parameter. In this case the condition $D\equiv d-n>1$ must be satisfied. For the present simulation $D=1$ and therefore these growth laws are not applied. Since Eqs. (33) and (34) become smaller as n increases, the growth laws by the nonhydrodynamic growth laws and those by the thermal fluctuation becomes important, and the classification of growth laws becomes complicated.

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[1] J. D. Gunton, M. San Miguel, and P. S. Sani, *Phase Transition and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, London, 1983), Vol. 8.
[2] H. Furukawa, Adv. Phys. **34**, 703 (1984).
[3] K. Binder, in *Material Sciences and Technology*, edited by R. W. Cohen, P. Haasen, and E. J. Kramer (VCH, Weinheim, 1991) Vol. 5, p. 405.
[4] A. J. Bray, Adv. Phys. **43**, 357 (1994).
[5] H. Toyoki, in *Formation, Dynamics and Statistics of Patterns*, edited by K. Kawasaki and M. Suzuki (World Scientific, Singapore, 1993), p. 309.
[6] G. F. Mazenko and M. Zanetti, Phys. Rev. Lett. **53**, 2106 (1984); Phys. Rev. B **32**, 4565 (1985); Phys. Rev. B **35**, 4565 (1987).
[7] F. de Pasquale and P. Tartaglia, Phys. Rev. B **33**, 2081 (1986); F. de Pasquale, G. F. Mazenko, P. Tartaglia, and M. Zanetti, *ibid.* **37**, 296 (1988).
[8] H. Toyoki and K. Honda, Prog. Theor. Phys. **78**, 237 (1987).
[9] R. Loft and T. A. DeGrand, Phys. Rev. B **35**, 8528 (1987).
[10] H. Nishimori and T. Nukkii, J. Phys. Soc. Jpn. **58**, 563 (1989).
[11] A. J. Bray and K. Humayun, J. Phys. A **23**, 5897 (1990); A. J. Bray, Phys. Rev. B **41**, 6724 (1990); A. J. Bray and S. Puri, Phys. Rev. Lett. **67**, 2670 (1991).
[12] H. Toyoki, Phys. Rev. A **42**, 911 (1990).
[13] S. Puri and C. Roland, Phys. Lett. A **151**, 500 (1990); H. Toyoki J. Phys. Soc. Jpn. **60**, 1433 (1991); Phys. Rev. B **45**, 1965 (1992).
[14] M. Mondello and N. Goldenfeld, Phys. Rev. A **42**, 5865 (1990); F. Liu and G. F. Mazenko, Phys. Rev. B **45**, 6989 (1992); M. Mondello and N. Goldenfeld, Phys. Rev. A **42**, 5865 (1990); **45**, 657 (1992).
[15] B. Yurke, A. N. Pargellis, T. Kovacs, and D. A. Huse, Phys. Rev. E **47**, 1525 (1993).
[16] R. E. Blundell and A. J. Bray, Phys. Rev. E **49**, 4925 (1994).
[17] Jong-Rim Lee, Sung Jong Lee, and Bongsoo Kim, Phys. Rev. E **52**, 1550 (1995); Jong-Rim Lee, Sung Jong Lee, and Bongsoo Kim, and Iksoo Chang, Phys. Rev. E **54**, 3257 (1996).
[18] F. Liu, M. Mondello and N. Goldenfeld, Phys. Rev. Lett. **66**, 3071 (1991). This paper treats a complex order parameter for superconducting transition.
[19] A. D. Rutenberg and A. J. Bray, Phys. Rev. Lett. **74**, 3836 (1995); A. D. Rutenberg, Phys. Rev. E **51**, R2715 (1995).
[20] M. Zapotocky and W. Zakrzewski, Phys. Rev. E **51**, R5189 (1995).
[21] A. Coniglio and M. Zanetti, Europhys. Lett. **10**, 575 (1989); A. Coniglio, Y. Oono, A. Shinozaki, and M. Zanetti, *ibid.* **18**, 59 (1992).
[22] A. J. Bray and K. Humayun, Phys. Rev. Lett. **68**, 1559 (1992).
[23] M. Mondello and N. Goldenfeld, Phys. Rev. E **47**, 2384 (1993).
[24] M. Siegert and M. Rao, Phys. Rev. Lett. **70**, 1956 (1993).
[25] M. Rao and A. Chakrabarti, Phys. Rev. E **49**, 3727 (1994).
[26] S. Puri, A. J. Bray, and F. Rojas, Phys. Rev. E **52**, 4699 (1995).

[27] Z. Zhang, Phys. Rev. E **51**, 4155 (1995).

[28] C. Castellano and M. Zannetti, Phys. Rev. E **53**, 1430 (1996).

[29] T. Ohta, D. Jasnow, and K. Kawasaki, Phys. Rev. Lett. **49**, 1223 (1982).

[30] K. Kawasaki, M. C. Yalabik, and J. D. Gunton, Phys. Rev. A **17**, 455 (1978).

[31] G. F. Mazenko, Phys. Rev. Lett. **63**, 1605 (1989); Phys. Rev. B **42**, 4487 (1990); **43**, 5747 (1990).

[32] A. J. Bray and K. Humayun, Phys. Rev. E **48**, 1609 (1993).

[33] Y. Oono and S. Puri, Phys. Rev. Lett. **58**, 863 (1987); Phys. Rev. A **38**, 434 (1988); S. Puri and Y. Oono, *ibid.* **38**, 1542 (1988).

[34] T. Shiwaku, A. Nakai, H. Hasegawa, and T. Hashimoto, Polym. Commun. **28**, 174 (1987).

[35] I. Chuang, N. Turok, and B. Yurke, Science **251**, 1336 (1991); Phys. Rev. Lett. **66**, 2472 (1991).

[36] A. N. Pargellis, P. Finn, J. W. Goodby, P. Panizza, B. Yurke, and P. E. Cladis, Phys. Rev. A **46**, 7765 (1992).

[37] R. Snyder, A. N. Pargellis, P. A. Graham, and B. Yurke, Phys. Rev. A **45**, R2169 (1992).

[38] H. Orihara and Y. Ishibashi, J. Phys. Soc. Jpn. **55**, 2151 (1986); T. Nagaya, H. Orihara, and Y. Ishibashi, *ibid.* **56**, 3086 (1987).

[39] H. Tutu and H. Fujisaka, Phys. Rev. B **50**, 9274 (1994).

[40] K. Binder and D. Stauffer, Phys. Rev. Lett. **33**, 1006 (1974).

[41] K. Kawasaki and T. Ohta, Prog. Theor. Phys. **59**, 362 (1978).

[42] E. D. Siggia, Phys. Rev. A **20**, 595 (1979).

[43] H. Furukawa, Phys. Rev. A **31**, 1103 (1985); Physica A **204**, 237 (1994).

[44] N. C. Wang and C. M. Knobler, J. Chem. Phys. **69**, 725 (1978); Phys. Rev. A **24**, 3205 (1981).

[45] Y. C. Chou and W. I. Goldburg, Phys. Rev. A **20**, 2105 (1979); **23**, 858 (1981).

[46] N. Kuwahara, M. Tachikawa, K. Hamano, and Y. Kenmochi, Phys. Rev. A **25**, 3449 (1982).

[47] J. K. Hoffer and D. N. Sinha, Phys. Rev. A **33**, 1918 (1986).

[48] D. Beysens, P. Guenoun, and F. Perrot, in *Dynamics of Ordering Processes in Condensed Matter*, edited by S. Komura and H. Furukawa (Plenum Press, New York, 1988), p. 373.

[49] P. Guenoun, R. Gastaud, F. Perrot, and D. Beysen, Phys. Rev. A **36**, 4876 (1987).

[50] T. Hasimoto, in *Materials Science and Technology*, edited by R. W. Cohen, P. Haasen, and E.J. Kramer (VCH, Weinheim, 1993), Vol. 12, p. 252.

[51] O. T. Valls and G. F. Mazenko, Phys. Rev. B **38**, 11 643 (1988).

[52] J. E. Farrel and O. T. Valls, Phys. Rev. B **40**, 7027 (1989); **42**, 2353 (1990).

[53] Y. Wu, F. J. Alexander, T, Lookman, and S. Chen, Phys. Rev. Lett. **74**, 3852 (1995).

[54] W. J. Ma, A. Maritan, J. Banavar, and J. Koplik, Phys. Rev. A **45**, 5347 (1992).

[55] E. Valasco and S. Toxvaerd, Phys. Rev. Lett. **71**, 388 (1993).

[56] P. Ossadnik, M. F. Gryre, H. E. Stanley, and S. Glotzer, Phys. Rev. Lett. **72**, 2498 (1994).

[57] G. Leptoukh, B. Strickland, and C. Roland, Phys. Rev. Lett. **74**, 3636 (1995).

[58] E. Velasco and S. Toxvaerd Phys. Rev. E **54**, 605 (1996).

[59] H. Furukawa, Phys. Rev. E **55**, 1150 (1997).

[60] F. F. Abraham, S. W. Koch, and R. C. Desai, Phys. Rev. Lett. **49**, 923 (1982).

[61] F. I. Alexander, S. Chen, and D. W. Grunau, Phys. Rev. B **48**, 634 (1993).

[62] S. Bastea and J. L. Lebowitz, Phys. Rev. E **52**, 3821 (1995).

[63] W. R. Osborn, E. Orlandini, M. F. Swift, J. M. Yeomans, and J. R. Banavar, Phys. Rev. Lett. **75**, 4031 (1995).

[64] P. B. S. Kumar and M. Rao, Phys. Rev. Lett. **77**, 1067 (1996).

[65] M. Laradji, S. Toxvaerd, and O. G. Mouritsen, Phys. Rev. Lett. **77**, 2253 (1996).

[66] M. Laradji, O. G. Mouritsen, and S. Toxvaerd, Phys. Rev. E **53**, 3673 (1996).

[67] T. Koga and K. Kawasaki, Phys. Rev. A **44**, R817 (1991); T. Koga and K. Kawasaki, Physica A **196**, 389 (1993).

[68] S. Puri and B. Dünweg, Phys. Rev. A **45**, R6977 (1992).

[69] O. T. Valls and J. E. Farrell, Phys. Rev. E **47**, R36 (1993).

[70] A. Shinozaki and Y. Oono, Phys. Rev. E **48**, 2622 (1993).

[71] A. Onuki, Phys. Rev. A **34**, 3528 (1986).

[72] *Dynamics and Patterns in Complex Fluids*, edited by A. Onuki and K. Kawasaki (Springer, Berlin, 1990).

[73] T. Hashimoto, T. Takebe, and K. Asakawa, Physica A **194**, 338 (1993).

[74] J. Casas-Vazquez, M. Criado-Sancho, and D. Jou, Europhys. Lett. **23**, 469 (1993).

[75] T. Hashimoto, K. Matsuzaka, E. Moses, and A. Onuki, Phys. Rev. Lett. **74**, 126 (1995).

[76] J. Läuger, C. Laubner, and W. Gronski, Phys. Rev. Lett. **75**, 3576 (1995).

[77] A. J. Bray and A. D. Rutenberg, Phys. Rev. E **49**, 27 (1994); **51**, 5499 (1995).

[78] K. Kawasaki, Ann. Phys. (N.Y.) **61**, 1 (1970); B. I. Halperin, P. C. Hohenberg, and E. D. Siggia, Phys. Rev. Lett. **32**, 1289 (1974). See also [51].

[79] A. J. Bray and S. Puri, Phys. Rev. Lett. **67**, 2670 (1991); F. Rojas and A. J. Bray, Phys. Rev. E **53**, 4686 (1996).

[80] H. Toyoki, Phys. Rev. B **45**, 1965 (1992); Phys. Mod. Phys. Lett. B **7**, 397 (1993).

[81] J. W. Cahn and J. E. Hilliard, J. Chem. Phys. **28**, 258 (1958).

[82] The growth law $R\sim t^{0.25}$ was predicted by the renormalization group method [A. J. Bray, Phys. Rev. Lett. **62**, 2841 (1989); Phys. Rev. B **41**, 6724 (1990)], and observed by numerical simulations [23–26] for the purely dissipative case of conserved vector order parameter.