Phase ordering kinetics of the Bose gas

Kedar Damle, Satya N. Majumdar, and Subir Sachdev
Department of Physics, P.O. Box 208120, Yale University, New Haven, Connecticut 06520-8120
(Received 22 March 1996)

We study the approach to equilibrium of a Bose gas to a superfluid state. We point out that dynamic scaling, characteristic of far from equilibrium phase-ordering systems, should hold. We stress the importance of a nondissipative Josephson precession term in driving the system to a new universality class. A model of coarsening in dimension $d=2$, involving a quench between two temperatures below the equilibrium superfluid transition temperature (T_c), is exactly solved and demonstrates the relevance of the Josephson term. Numerical results on quenches from above T_c in $d=2,3$ provide evidence for the scaling picture postulated. [S1050-2947(96)07408-2]

PACS number(s): 03.75.−b, 75.10.Hk, 64.60.Cn, 64.60.My

The recent observation of Bose condensation in neutral, trapped atomic gases [1] and excitons in Cu_20 [2] opens up exciting possibilities on experimental studies of time-dependent nonequilibrium phenomena in a heretofore inaccessible regime. In particular, an issue which could be experimentally investigated, and which we shall address theoretically in this paper is the following—upon quenching a Bose gas to a final temperature (T) below T_c, how does the condensate density grow with time before attaining its final equilibrium value? A few recent papers [3,4] have addressed just this question, but they have focused on the early-time (on the order of a few collision times), nonuniversal dynamics. However, as has also been noted recently in Ref. [5], the interesting experimental questions are instead associated with the long-time dynamics involving the coarsening of the Bose condensate order parameter. This dynamics is ''universal'' in a sense that will be clarified below.

A natural and precise language for describing the evolution of the condensate is offered by recent developments in the theory of phase-ordering dynamics in dissipative classical spin systems, as reviewed in the article by Bray [6]. In this theory, one considers the evolution of a classical spin system after a rapid quench from some high T to a low T in the ordered phase. The dynamics is assumed to be purely relaxational, and each spin simply moves along the steepest downhill direction in its instantaneous energy landscape. Locally ordered regions will appear immediately after the quench, but the orientation of the spins in each region will be different. The coarsening process is then one of alignment of neighboring regions, usually controlled by the motion and annihilation of defects (domain walls for Ising spins, vortices for XY spins, etc.). A key step in the theory is the introduction of a single length scale $l(t)$, a monotonically increasing function of the time t, which is about the size of a typical ordered domain at time t. Provided $l(t)$ is greater than microscopic length scales, like the range of interactions or the lattice spacing, it is believed that the late stage morphology of the system is completely characterized by $l(t)$, and is independent of microscopic details, i.e., it is universal. This morphology is characterized by various time-dependent correlation functions which exhibit universal scaling behavior.

We turn then to the Bose gas. The order parameter in this case is the boson annihilation field $\psi(r,t)$ (where r is a spatial coordinate); the phase of the expectation value of ψ is aligned across the system in the equilibrium Bose-condensed state. A key point is that after relatively few atomic collisions, once the domain size $l(t)$ is large enough (e.g., larger than the de Broglie wavelength), it is permissible [4] to treat $\psi(r,t)$ as a *classical* field which obeys Hamilton-Jacobi equations of motion (for a related discussion on the emergence of classical dynamics in the equilibrium properties of an antiferromagnet, see Ref. [7]). It must be kept in mind that it is only the equations of motion for the collective order parameter which are classical—the very existence of the complex order parameter is due entirely to quantum mechanics, and the fact that there is a wave function for the condensate.

An important property of the equations of motion for ψ, discussed below, is that they are not simply relaxational. Instead, they contain nondissipative, kinematical ''streaming'' or ''Poisson bracket'' terms [8]. One such term is responsible for the Josephson precession of the phase of ψ at a rate determined by the local chemical potential. A central objective of this paper is to understand the consequences of such terms on the phase-ordering theories of Ref. [6]. We will argue that the Josephson term constitutes a relevant perturbation on the dynamics and that the resulting coarsening process belongs to a new universality class. Specifically, in the remainder of the paper we will (i) exactly solve a model of a $d=2$ Bose gas always in contact with a reservoir, where the temperature of the reservoir is suddenly switched between two temperatures below T_c [10]; (ii) present numerical results on the time evolution of an isolated Bose gas in $d=2,3$, where the initial state has no superfluid fraction, while the final state is superfluid.

We will begin by considering a solvable coarsening problem which illustrates the possible consequences of the Josephson term in a simple setting. A $d=2$ Bose gas is superfluid for $T<T_{KT}$, the well-known Kosterlitz-Thouless phase-transition temperature; consider the phase-ordering process in which the Bose gas is moved at time $t=0$ from contact with a reservoir at an initial $T=T_i$, to a reservoir with a final $T=T_f$, such that $T_f<T_i<T_{KT}$; a similar quench was considered in Ref. [10] for the purely dissipative XY model. In the long-time limit, all vortices and fluctuations in the amplitude of ψ can be neglected, and we may param-

etrize $\psi = e^{i\phi}$. The free-energy density in the purely dissipative XY model [10] is now determined simply by the gradients of the phase $\sim(\nabla\phi)^2$. In the case of the Bose gas, it is also necessary to take the conserved number density into account. Let m be proportional to the deviation of the particle density from its mean value; then the free-energy density we shall work with is

$$\mathcal{F} = \frac{1}{2}\int d^2r[(\nabla\phi)^2 + m^2]. \tag{1}$$

We have rescaled spatial coordinates and m to obtain convenient coefficients in $\mathcal{F}$. The Josephson precession term, whose effects we wish to study, is contained in the Poisson bracket

$$\{m(r), \phi(r')\} = g_0\delta(r-r'), \tag{2}$$

where g_0 is a constant. The method reviewed in Ref. [8] now leads to the *linear* equations of motion [11]

$$\frac{\partial\phi}{\partial t} = \Gamma_0\nabla^2\phi + g_0 m + \theta, \quad \frac{\partial m}{\partial t} = \lambda_0\nabla^2 m + g_0\nabla^2\phi + \zeta, \tag{3}$$

where the coefficients $\Gamma_0, \lambda_0 > 0$ represent the dissipation arising from the coupling of the system to the reservoir. The effects of the reservoir are also contained in the Gaussian noise sources θ and ζ with zero mean and (for $t>0$) correlations appropriate to $T = T_f$: $\langle\theta(r,t)\theta(r',t')\rangle = 2\Gamma_0 T_f\delta(r-r')\delta(t-t')$, $\langle\zeta(r,t)\zeta(r',t')\rangle = -2\lambda_0 T_f\nabla^2\delta(r-r')\delta(t-t')$, and $\langle\zeta(r,t)\theta(r',t')\rangle = 0$ ($k_B = 1$). Equations (3) are linear, can be easily integrated, and all correlations can be computed exactly.

Let us first recall the structure of the solutions expected from naive scaling [6] for $d \geq 2$. For our models we expect the domain size $l(t) \sim t^{1/z}$ where z is a nonequilibrium dynamic exponent. We consider the behavior of two correlation functions: (i) The equal-time correlator $G(r,t) = \langle\psi^*(r,t)\psi(0,t)\rangle$ (the $k=0$ component of the spatial Fourier transform of G is proportional to the condensate fraction). Under scaling we expect for large r and t, $G(r,t) \sim r^{-\eta_f} g(r/t^{1/z})$ where g is a universal scaling function $\eta_f = 0$ for $d>2$ while in $d=2$, η_f ($= T_f/2\pi$ for $\mathcal{F}_1$) is the equilibrium exponent of the quasi-long-range order at $T = T_f$. (ii) The unequal-time correlation function $C(r,t) = \langle\psi^*(r,t)\psi(0,0)\rangle$ for which we expect for large r and t, $C(r,t) \sim t^{-\lambda/z} f(r/t^{1/z})$ where f is a universal scaling function, and λ is a dynamic exponent.

It turns out that our model $\mathcal{F}$ does not completely obey the simple scaling hypotheses as stated above. This becomes clear upon considering the two-time correlation C which turns out to depend upon *two* large length scales $l_1(t) \sim (at)^{1/2}$ and $l_2(t) \sim g_0 t$ (with $a = (\Gamma_0 + \lambda)/2$): it obeys the scaling form $C(r,t) \sim t^{-(3\eta_i + \eta_f)/4}\tilde{f}(r/(at)^{1/2}, r/(g_0 t))$ (where $\eta_i = T_i/2\pi$). The dependence of these scales on g_0 suggests that g_0 is a relevant perturbation with renormalization group eigenvalue 1, in the language of Ref. [6]. The scaling function $\tilde{f}$ was determined to be

$$\tilde{f}(x_1, x_2) = \exp\left[-\eta_i\int_0^\infty \frac{dy}{y}\{1 - J_0(y)\}\cos(y/x_2)e^{-y^2/x_1^2}\right]. \tag{4}$$

For $r \sim l_1(t)$, we use $\tilde{f}(x_1, x_2 \to 0) = 1$: this shows that the autocorrelation $C(0,t) \sim t^{-(3\eta_i + \eta_f)/4}$ in contrast to the result in the model of Ref. [10] $C(0,t) \sim t^{-(\eta_i + \eta_f)/4}$. On the contrary, one could insist on a scaling picture using only the single larger length scale $r \sim l_2(t)$, and would then need $\tilde{f}(x_1 \to \infty, x_2)$ which equals $[1 + \sqrt{1 - x_2^2}]^{-\eta_i}$ for $x_2 < 1$ and equals $x_2^{-\eta_i}$ for $x_2 \geq 1$. It can also be checked that one recovers the initial equal-time equilibrium result for $C(r,t)$ when $r \to \infty$ with t large but fixed. We also note that the relevance of g_0 is evident in the autocorrelations of m. We find $\langle m(0,t)m(0,0)\rangle \sim (1/t) f_1(g_0\sqrt{t/a})$ where

$$f_1(\tau) = 4\pi^2\eta_i\left[1 - \int_0^\infty \sin y e^{-y^2/2\tau^2} dy\right]; \tag{5}$$

clearly, for $g_0 = 0$, this autocorrelator decays as $1/t$ for large t, while for nonzero g_0 it decays faster as t^{-2}. Finally, results on the equal-time ψ correlator G. It has a crossover at a time $t_1 \sim \tilde{a}/g_0^2$ with $\tilde{a} = |\Gamma_0 - \lambda_0|$; this time is similar to the crossover time in $\langle m(0,t)m(0,0)\rangle$, except that $\tilde{a}$ has replaced a. Both for $t \ll t_1$ and for $t \gg t_1$, G obeys a scaling form similar to that obtained in the relaxational model of Ref. [10] (which has $g_0 = 0$): $G(r,t) \sim r^{-\eta_f} g(r/(\gamma t)^{1/2})$ where g is a scaling function described in Ref. [10]; however, the rate $\gamma = \Gamma_0$ for $t \ll t_1$ and $\gamma = a$ for $t \gg t_1$.

While this phase only model $\mathcal{F}$ is not relevant for studying quenches from above the transition temperature (since it neglects the nonlinear terms), the exact solution of this linear model is quite instructive. It clearly emphasizes the importance of the nondissipative Josephson coupling term. In fact as seen above, the presence of this term ($g_0 \neq 0$) changes the universality class of the system. Thus it is reasonable to expect that even for quenches from above the transition temperature, this term would play an important role. In this case, after the quench the system has defects (e.g., vortices in two-dimensions). As time progresses, these defects move around and annihilate each other and the system becomes more and more ordered. To study this coarsening process that proceeds via the annealing of defects it is necessary to study the evolution of both the phase and amplitude of ψ. This growth of long-range order in the system can be studied in two different ways. In one case one considers the time evolution of an *isolated* Bose gas, not in contact with a reservoir. Though the dynamics in this case is nondissipative, the system still exhibits an irreversible approach to equilibrium. In the other case, the Bose gas is in contact with a heat bath. These are the analogues of microcanonical and canonical ensembles in equilibrium statistical mechanics. It is reasonable to expect that both descriptions would lead to the same results for universal scaling properties. Most previous studies on coarsening have been done in the ''canonical'' ensemble. However in this paper, we use the ''microcanonical'' approach. To the best of our knowledge, this approach has never been used before to study coarsening in any system. As we will see below, the dynamics in the ''microcanonical'' ensemble is completely specified by the Hamiltonian of the system

with no additional phenomenological parameters. The ''canonical'' dynamics, on the other hand, needs several phenomenological constants as input parameters.

For the isolated Bose gas (''microcanonical'' ensemble), an excellent approximation for the total energy of an order-parameter configuration $\psi(r,t)$ is $\mathcal{H}=\int d^d r[|\nabla\psi|^2 + \frac{u}{2}|\psi|^4]$, where we have rescaled lengths to make the coefficient of the gradient term unity, and $u>0$ is the two-particle T matrix at low momentum. The Hamilton-Jacobi equation of motion for ψ follows from the Poisson bracket $\{\psi,\psi^*\}=i$

$$i\frac{\partial\psi}{\partial t}=[-\nabla^2+u|\psi|^2]\psi, \tag{6}$$

and is the well-known [12] Gross-Pitaevski (GP) or nonlinear Schrödinger equation. We can also add a quadratic $|\psi|^2$ term to $\mathcal{H}$, and it leads to a term linear in ψ in the GP equation; however this linear term can be eliminated by an innocuous global phase change in ψ. The GP equation conserves the total number of particles $\int d^d r|\psi|^2$, the total momentum, and $\mathcal{H}$, and hence there is no global dissipation of energy. Nevertheless, in the thermodynamic limit, the GP equation does display irreversible coarsening, as will be abundantly clear from our numerical results to be described later: a random initial state with a negligible number of particles in the zero momentum (k) state (i.e., short-range initial correlations), evolves eventually to a state with a condensate fraction equal to that expected at equilibrium in the microcanonical ensemble at the total energy of the initial state.

In the ''canonical'' approach on the other hand, it is permissible to add dissipative terms to the equation of motion of ψ. A simple additional damping term to the GP equation leads to a model expected to be in the same universality class of the so-called Model A [8,6]; this model is, however, not acceptable: it violates local conservation of the particle density, and, as discussed near (3), it is necessary [8,13] to introduce the density fluctuation field, $m(r,t)$; the value of $|\psi(r,t)|^2$ is then the contribution to the particle density from low-momentum states, while $m(r,t)$ represents the density fluctuation from all states; the Poisson bracket in this case is $\{m(r),\psi(r')\}=ig_0\psi(r)\delta(r-r')$. This is model F in the language of Ref. [8] (see also [9]). Note that the strength of the crucial precession term in the dynamics is controlled by g_0 which is an adjustable phenomenological parameter (however, in the Hamiltonian dynamics considered earlier, there is no such freedom). Numerical study of coarsening using model F could thus be complicated by crossover effects associated with the adjustable value of g_0 ($g_0=0$ corresponds to the purely dissipative model-A dynamics, which is clearly in a different universality class).

We therefore restrict our numerical study here to the GP model. All of the numerical results obtained so far are consistent with the simplest naive scaling hypotheses described earlier, and do not require the introduction of two length scales, as was necessary in the linear model above (though we have not yet obtained numerical results on unequal-time correlations, for which the linear model $\mathcal{F}$ clearly displayed two length scales). We will present results both in $d=2$ and $d=3$. The $d=2$ system allowed us to study larger sizes with better finite-size scaling properties.

We discretized (6) on a lattice, and integrated in time using a fast Fourier transform based algorithm which conserved energy and particle number to a high accuracy. We work in units where the lattice spacing is unity and choose the scale of the lattice field to make the density one. We set u to be approximately 0.25 so that we are considering a dilute gas. We choose an ensemble of initial conditions with a narrow distribution of energy, whose width goes to zero in the thermodynamic limit. We assign initial values to the Fourier components $\psi(k,0)$ as follows: $\psi(k,0)=\sqrt{n_0(k)}\exp[i\phi(k)]$ where the $\phi(k)$'s are independent random variables chosen from a uniform distribution with range $[0,2\pi]$ and the function $n_0(k)$ is chosen to ensure that initial real-space correlations are short-ranged (corresponding to a ''high-temperature'' configuration) while still having low enough energy so that the equilibrium state corresponding to this energy is superfluid. Though the ensemble of initial conditions is not strictly the Gibbs distribution at any temperature, it is however expected that the precise details of the initial conditions do not matter for the late time universal properties as long as the initial correlations are short ranged.

More specifically we chose $n_0(k)=c/([\epsilon(k)+\mu_1](\exp[(\epsilon(k)-\mu_2)/T]+1))$ where $\epsilon(k)$ is the Fourier representation of the lattice version of the Laplacian and c sets the overall scale of $n_0(k)$. Here one chooses the parameters μ_1, μ_2, and T to achieve the appropriate trade-off between energy and correlation length. Note that this careful choice of initial conditions is needed as the GP equation does not have any explicit dissipation and the system evolves in phase space on a constant energy surface.

We used finite-size scaling to model the results in a finite system of linear dimension L: it predicts a scaling form $G(r,t)=L^{-\eta}\Phi_G[r/L,t/L^z]$ for the equal-time correlation function. In $d=3$ the exponent $\eta=0$, while in $d=2$, it is associated with the final equilibrium state and varies continuously with temperature. The structure factor $S(k,t)$ is obtained by a spatial Fourier transform of $G(r,t)$, and the number of particles in the $k=0$ mode is clearly $S(0,t)$; the latter should satisfy $S(0,t)\sim L^{2-\eta}\Phi[t/L^z]$ in $d=2$ and $S(0,t)\sim L^3\Phi[t/L^z]$ in $d=3$. The scaling function Φ goes to a constant for $t\gg L^z$ and the system attains equilibrium after a time $t\sim L^z$.

Results for $d=2$ are shown in Fig 1. We performed finite-size scaling analysis for $L=16$, 32, and 64 and found reasonable data collapse with $\eta\approx 0.27$ and $z\approx 1.1$. The value of η indicates that we are at a nonzero temperature close to T_{KT}; strictly speaking we must have $\eta<1/4$, but the value of η is relatively T independent near T_{KT}, and the discrepancy is within our numerical errors. The value of z is in sharp contrast to the $z=2$ (with logarithmic corrections) result obtained by various groups [14,15] for the purely dissipative Model-A dynamics [8] (obtained from Model F by setting $g_0=0$ and ignoring m) of classical XY spins. Although we have determined the value of z for a quench to a particular temperature T_f, we expect that z is the same for all $0<T_f<T_{KT}$. Results for $d=3$ are shown in Fig. 2 for linear sizes $L=16,32$. The data collapse is not as good as that in $d=2$, but again we obtained a $z\approx 1.1$. Thus our numerical results, both in $d=2$ and 3, are consistent with a value of

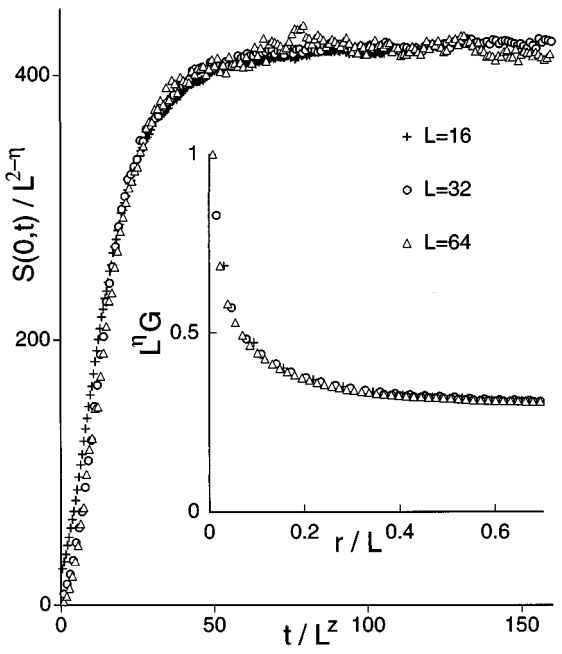

FIG. 1. Numerical results from the simulation of the GP equation in $d=2$. The number of particles in the zero momentum state is $S(0,t)$ and the figure shows its scaling properties as a function of system size L and time t. The inset shows the scaling of the equilibrium equal-time correlation function $G(r,t\to\infty)$. The best scaling collapse was obtained in both plots for $\eta\approx 0.27$ and $z\approx 1.1$. The scale of all axes (except the values of r/L) are arbitrary.

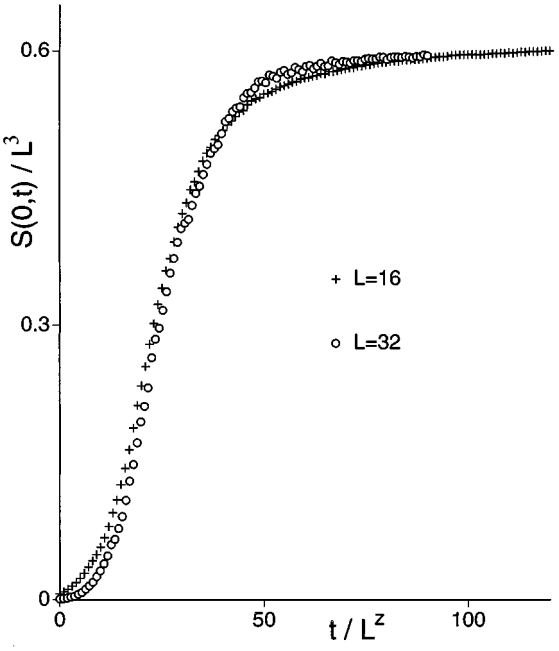

FIG. 2. Numerical results for the GP equation in $d=3$. The notation is as in Fig. 1, with the exponent $z\approx 1.15$.

$z=1$, which is also the result suggested by the exact calculation in the phase only model.

Finally, we close with some physical discussion on reasons for the difference between the GP model, and quenches in the purely dissipative Model A [14,15]. The dynamics in the GP model proceeds via the annihilation of nearby vortex-antivortex pairs (in $d=2$) as in Model A. However there is an important difference between the two in the details of the vortex motion. In Model A, oppositely charged vortices attract each other with a force that falls off as the inverse of their separation (apart from logarithmic corrections). Since the dynamics is overdamped, this implies $l(t)\sim t^{1/2}$. In the GP model, on the other hand, the situation is more complex. In addition to vortices, the system also has a propagating ''spin-wave'' mode arising from the streaming terms. A pair of oppositely charged vortices, apart from attracting each other, also interacts with the spin-wave background. In addition, it experiences a Magnus force which causes the pair to move with uniform velocity in a direction perpendicular to the line joining them. These qualitative differences in the nature of the defect dynamics change the universality class of the coarsening process.

In summary, we have presented evidence, both analytical and numerical, that the phase-ordering dynamics of the Bose gas belongs to a new universality class. A particular conclusion of this work is that the condensate density of the Bose gas, following a sudden quench from the normal to the superfluid phase in dimensions $d\geqslant 2$, will grow at late times as $t^{d/z}$. We have presented evidence, both analytical and numerical, that $z=1$.

We thank D. Kleppner for stimulating our interest in this problem, and M.P.A. Fisher and A. Bhattacharya for useful discussions. This research was supported by NSF Grants DMR-92-24290 and DMR-91-20525.

[1] M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, and E.A. Cornell, Science **269**, 198 (1995); C.C. Bradley, C.A. Sackett, J.J. Tollett, and R.G. Hulet, Phys. Rev. Lett. **75**, 1687 (1995).

[2] D.W. Snoke, J.P. Wolfe, and A. Mysyrowicz, Phys. Rev. Lett. **64**, 2543 (1990); Phys. Rev. B **41**, 11 171 (1990); J.-L. Lin and J.P. Wolfe, Phys. Rev. Lett. **71**, 1223 (1993).

[3] H.T.C. Stoof, Phys. Rev. A **45**, 8398 (1992); B.V. Svistunov, J. Moscow Phys. Soc. **1**, 373 (1991); D.V. Semikoz and I.I. Tkachev, Phys. Rev. Lett. **74**, 3093 (1995).

[4] Yu.M. Kagan, B.V. Svistunov, and G.V. Shlyapnikov, Zh. Eksp. Teor. Fiz. **74**, 279 (1992) [Sov. Phys. JETP **75**, 387 (1992)].

[5] Y. Kagan and B.V. Svistunov, Zh. Eksp. Teor. Fiz. **105**, 353 (1994) [Sov. Phys. JETP **78**, 187 (1994)].

[6] A.J. Bray, Adv. Phys. **43**, 357 (1994).

[7] S. Chakravarty, B.I. Halperin, and D.R. Nelson, Phys. Rev. B **39**, 2344 (1989); A.V. Chubukov, S. Sachdev, and J. Ye, *ibid.* **49**, 11 919 (1994).

[8] P.C. Hohenberg and B.I. Halperin, Rev. Mod. Phys. **49**, 435 (1977).

[9] It may also be necessary to introduce additional fields to account for other conserved quantities: a momentum density as in model H or an energy density as in model C of Ref. [8].

[10] A.D. Rutenberg and A.J. Bray, Phys. Rev. E **51**, R1641 (1995).

[11] D.R. Nelson and D.S. Fisher, Phys. Rev. B **16**, 4945 (1977).

[12] E.P. Gross, Nuovo Cimento **20**, 454 (1961); L.P. Pitaevski, Zh. Eksp. Teor. Fiz. **39**, 216 (1960) [Sov. Phys. JETP **12**, 155 (1961)].

[13] B.I. Halperin, P.C. Hohenberg, and E.D. Siggia, Phys. Rev. B **13**, 1299 (1976).

[14] B. Yurke, A.N. Pargellis, T. Kovacs, and D.A. Huse, Phys. Rev. E **47**, 1525 (1993).

[15] M. Mondello and N. Goldenfeld, Phys. Rev. A **42**, 5865 (1990).