Coarsening dynamics of binary Bose condensates

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We study the dynamics of domain formation and coarsening in a binary Bose-Einstein condensate that is quenched across a miscible-immiscible phase transition. The late-time evolution of the system is universal and governed by scaling laws for the correlation functions. We numerically determine the scaling forms and extract the critical exponents that describe the growth rate of domain size and autocorrelations. Our data is consistent with inviscid hydrodynamic domain growth, which is governed by a universal dynamical critical exponent of $1/z = 0.68(2)$. In addition, we analyze the effect of domain wall configurations which introduce a nonanalytic term in the short-distance behavior of the pair correlation function, leading to a high-momentum “Porod”-tail in the static structure factor, which can be measured experimentally.

Introduction. — The thermodynamic ground state of a system that consists of multiple species is not always spatially homogeneous. Indeed, as the thermodynamic state variables or the interspecies couplings are tuned, often a transition between a miscible and an immiscible ground state takes place [1]. A system that is quenched across such a transition does not phase-separate instantly but exhibits highly nontrivial dynamics which generally proceed in two stages [2–5]: first, domains of one species nucleate over a short time-scale. In a second stage, these domains merge and coarsen until in the infinite-time limit, only one large domain of each species remains. The dynamics in the latter stage are universal in that they do not depend on the microscopic details of the system and are only constrained by symmetries and conservation laws [3, 6]. The time evolution is self-similar, i.e., the time dependence of any ensemble averaged-quantity is captured by a simple rescaling of units by a characteristic length scale $L(t)$ (for example, the average domain size). In classical theories of phase ordering kinetics, this scale diverges with time according to a characteristic power law $L(t) \sim t^{1/z}$. The phase ordering dynamics of different systems can thus be separated into distinct dynamical universality classes that are characterized by the dynamical critical exponent $z$. Here we calculate the dynamical critical exponent for coarsening in a binary superfluid in two dimensions.

While it has been a longstanding problem to study the quantum properties of multicomponent superfluids [7], it has become possible only fairly recently to realize them in experiments with spinor Bose-Einstein condensates (BECs) [1, 8, 12] (see [13] for a review). These ultracold gases are unique quantum fluids as they are largely isolated from the environment and their quantum dynamics can be probed accurately over long times both in-situ [9, 14] and in time-of-flight [1, 8, 11, 12]. Furthermore, the unprecedented control offered by quantum gas experiments makes them an ideal testbed to study the nonequilibrium physics of superfluids following a quench of parameters. Indeed, the short-time dynamics of domain formation following a quench are well understood both theoretically and experimentally [1, 8, 9, 13, 15–18]. However, questions remain about the long-time coarsening dynamics and the nature of phase-ordering kinetics [16–19, 21]. Here, we theoretically establish the power-laws governing the long-time domain growth in a homogeneous, two-dimensional binary Bose gas at zero temperature.

Our study sheds light on ongoing investigations of how isolated quantum systems approach equilibrium, and how (and if) long-range order is established following a quench. Much of our knowledge of these fundamental questions is derived from studies of one-dimensional systems, where powerful analytical and numerical methods can be brought to bear [22, 23]. Here, the absence of true long-range order, combined with kinematic constraints can lead to extremely long relaxation times or relaxation to athermal steady states [24]. In higher dimensions, however, the question of whether or not quasi/true long-range order is established becomes relevant [18, 25]. Here we find that the long-time kinetics of phase separation in a binary Bose superfluid quenched across the miscible-immiscible transition is hydrodynamic, which leads to the formation of macroscopic ferromagnetic domains in the long-time limit.

Theory. — We describe the binary BEC at zero temperature by two classical fields $\psi_1$ and $\psi_2$ and take into account the interaction between the particles on a mean field level. In typical ultra-cold gas experiments, these fields correspond to two hyperfine states of an atom such as $^{23}$Na or $^{87}$Rb ([1, 8, 11]), or two different atomic species ($^{85}$Rb and $^{87}$Rb) as in the experiment of Papp et al. [12]. This yields the Gross-Pitaevskii energy functional:

$$H = \int d^2r \left( \sum_{i=1,2} \left\{ -\psi_i^+ \frac{\nabla^2}{2m} \psi_i - \mu_i |\psi_i|^2 + \frac{g_{1i}}{2} |\psi_i|^4 \right\} \right) + g_{12} |\psi_1|^2 |\psi_2|^2,$$

(1)
where $m$ is the particle mass, $\mu$, the chemical potential, $g_{ii}$ is the interaction between like particles of type $i$, and $g_{12}$ describes the scattering of atoms of spin 1 and 2. In the absence of long-range dipolar interactions [9], the interaction Hamiltonian does not contain spin-flip terms and conserves the total density of each species. Note that the Gross-Pitaevskii equation is strictly applicable only at zero temperature and does not account for quantum fluctuations. More complex models describing the time-evolution of the superfluid mixture, such as the “Model F” in the Hohenberg-Halperin classification [6], reduce to the Gross-Pitaevskii equation in the low-temperature limit [19]. Here we model the Gross-Pitaevskii equation directly and briefly discuss the limitations of our approach later.

In typical spinor BECs such as the hyperfine states of $^{87}$Rb or $^{23}$Na, the scattering length is nearly identical in all channels [29], and we choose $g_{11} = g_{22} = g > 0$ in the following. If the intra-species interaction dominates, $g_{12} < g$, the two condensates can coexist. However if $g_{12} > g$, the ground state is no longer homogeneous and the system phase-separates [8, 27–29]. We investigate how the system evolves when suddenly quenched from the miscible phase with $g_{12} < g$ to the immiscible phase with $g_{12} > g$.

We consider the time-evolution of the polarization $n(r) = (n_1(r) - n_2(r))/(n_1(r) + n_2(r))$ as an order parameter. The spin texture of a spinor gas, and thus the magnetization, can be measured directly using spin-sensitive phase contrast imaging [10, 11]. At early times, domains of opposite spin form due to a spin-wave instability [15].

Taking into account only the most unstable mode, the initial domain size is of order $L_0 \approx \xi_s$, where we define the spin healing length $\xi_s = \sqrt{1/2m(g_{12} - g)}$, and $n = |\psi_1|^2 + |\psi_2|^2$ is the total density. When the domain size becomes much larger than the spin healing length, the dynamics are universal. Expressed in units of the characteristic length scale $L(t)$, all correlation functions of the order parameter $m$ have no explicit time dependence, and collapse to a single, universal scaling function. For example, the pair correlation function, which describes the correlation of the magnetization at two points separated by a distance $r$, can be written as follows:

$$g(r, t) = \frac{1}{V} \int d^2R \langle m(R)m(R + r) \rangle = f(rL^{-1}(t)).$$  

(2)

The bracket $\langle \ldots \rangle$ denotes an ensemble-average. The correlation function is normalized such that $g(0, t) = 1$. Similarly, the static structure factor assumes the scaling form

$$S(q) = \int d^2re^{iqr}g(r, t) = L^2 \hat{f}(qL(t)).$$  

(3)

It should be emphasized that the scaling is a conjecture which must be proven on a case-to-case basis [5].

The equations of motion corresponding to the Hamiltonian (1) are the well-known Gross-Pitaevskii equations:

$$i\partial_t \psi_1 = \left\{ -\frac{\nabla^2}{2m} - \mu_1 + g|\psi_1|^2 + g_{12}|\psi_2|^2 \right\} \psi_1$$

$$i\partial_t \psi_2 = \left\{ -\frac{\nabla^2}{2m} - \mu_2 + g|\psi_2|^2 + g_{12}|\psi_1|^2 \right\} \psi_2.$$  

(4)

We simulate the time evolution (4) on a square lattice of dimension $l = 1024$, and spacing $d$ using a split-step spectral method as introduced in Ref. [30]. Although we only present results for size $l = 1024$, we have performed numerical simulations over a wide range of system sizes $l = 64, 128, 512$, finding the same dynamical critical exponent in each case. We initialize the system in the ground state $\psi_i = \sqrt{\mu/(g + g_{12})}$ and add a small Gaussian noise to seed the instability after a sudden quench. The results are averages over several different ensembles. The chemical potential is chosen such that the initial domain size ($L_0 \sim \xi_s$) is much larger than the lattice spacing but is still much smaller compared to the system size.

Figure 1 shows the domain structure at various times $\hat{t} = md^2t = 300, 1000, 2000$, and 5000 for a quench with...
final couplings \( g = 1 \) and \( g_{12} = 1.1 \). In typical experiments with \(^{87}\text{Rb}\) or \(^{23}\text{Na}\), the coupling strengths are almost identical with \( (g_{12} - g)/g \approx 10^{-3} \), however these can be tuned using a Feshbach resonance \(^{12}\)\(^{20}\)\(^{33}\). The choice of couplings determines the initial domain size after the quench and the onset of the universal late-time scaling regime, but does not affect the scaling behavior itself. Regions with positive (negative) polarization are shown in black (white). Shortly after the quench, distinct domains form (Fig. 1(a)) the size of which grows with time (Figs. 1(b)-(c)). In the following, we compute the universal scaling exponent that governs this time evolution. Note that even at late times, the domains are not fully polarized but contain small patches of opposite polarization. These correspond to vortex or skyrmion defects, which are created during the coarsening \(^{25}\). For the nondissipative time-evolution studied here, these defects are long-lived \(^{25}\), but they are not present if dissipative effects are included into the Gross-Pitaevskii equations \(^{15}\)\(^{18}\)\(^{20}\).

**Results.** — Let us start by considering the radial pair correlation function \( g(r, t) \). Figure 2(a) shows the scaling function \( f \) of the pair correlation function at various times. The inset shows the unrescaled pair correlation function. All results are averaged over 25 initial conditions. For small separation \( r \), the correlation is positive, indicating that two nearby points have predominantly the same polarization. This changes at larger distances, where two points become anticorrelated. We take the position of the first zero in the pair correlation function as a measure for the average domain size \( L(t) \). For sufficiently large domains, the results obtained from this method are consistent with those obtained by extracting the domain size directly from the simulations. Higher oscillations are visible but very weak, and the correlation between two points is lost at large distances. As can be seen from Fig. 2(a) when expressed in terms of the rescaled coordinate \( r/L(t) \), the correlation functions at different times collapse onto a single scaling function. Indeed, the time evolution is consistent with the scaling hypothesis.

The scaling behavior is also visible in the structure factor \( S(q) \) shown in Fig. 2(b). In addition to the scaling, we see that the structure factor decays as a power law \( \sim 1/q^3 \) at large momentum. This feature is a consequence of the presence of domain walls, which determine the short-distance structure of the pair correlations. It can be understood as follows: two points with separation \( r \) are positively correlated if they are in domains of the same type and negatively otherwise. At short distances, this correlation is determined by the probability to cross a single domain wall, which is proportional to \( r/L(t) \) \(^{25}\). This gives rise to a nonanalytic linear term in the pair correlation function \( g(r) = 1 + f'(0) r/L(t) + O(r^2) \). The linear slope is clearly present in our numerical data, Fig. 2(a)\(^{12}\). This implies a universal high-momentum “Porod” tail \(^{11}\), in the structure factor

\[
S(q) = \frac{C}{L^d q^d} + O(1/q^4). \tag{5}
\]

Importantly, this high-momentum tail is not present in the initial stage of the coarsening, where the structure factor is Gaussian. The structure factor changes from its initial Gaussian shape to the form in Fig. 2(b) only after the domains have formed and the system has entered the second coarsening stage. At late times when the density of domain walls in the system decreases, the magnitude of the tail decreases as well and vanishes as \( 1/L(t) \). The emergence of a Porod tail at late stages of coarsening dynamics is an important new prediction of our work.

We proceed to extract the scaling exponent from the measured domain sizes. The scaling argument is strictly valid only in the limit of infinitely large domain sizes, and the exponent has a finite size scaling correction. Huse argued that for a conserved order parameter, this correction is of order \( 1/L(t) \) \(^{34}\). We determine the time-dependent scaling exponent \( \zeta(t) \) by taking the logarithmic differential quotient of the domain size at different times \( t' > t \) : \( 1/\zeta(t) = \log(L'/L_t) / \log(t'/t) \). The result is shown in Fig. 3 The scaling exponent displays a weak drift towards smaller values at later times. Extrapolating to the limit of infinite domain size (red line in Fig. 3) we
obtain $1/z(\infty) = 0.68(2)$. The same dynamical exponent is found in classical binary fluids, where $1/z = 2/3$ [35].

This result indicates that the dominant mechanism driving domain growth is inertial hydrodynamic transport of the superfluid from low-density to high-density regions [3]. The numerical value of this exponent can be understood from dimensional analysis: in a binary fluid, the change in a domain wall’s velocity $dv/dt$ is equal to the gradient of the pressure $-\nabla P$, where the pressure $P$ is proportional to the energy density of the domain wall. The inertial term scales as $dv/dt \sim L/t^2$, and the pressure gradient scales as $-\nabla P \sim \sigma/L^2$, where $\sigma$ is the surface tension. Equating inertial and gradient terms gives the dynamical exponent $1/z = 2/3$ [3]. We remark that in classical binary mixtures, coarsening dynamics is more complicated due to advective and viscous terms which give rise to other scaling exponents and can even lead to a breakdown of scale invariance [36, 37].

Our previous analysis was restricted to the equal-time correlation function. It turns out that a single dynamical exponent is not sufficient to describe the scaling behavior of correlators at different times [3]. Consider the dynamical pair correlation function, which in the scaling limit depends on two length scales:

$$g(r, t; r', t') = \frac{\langle m(r, t)m(r', t') \rangle}{\langle m^2(r, t) \rangle^{1/2} \langle m^2(r', t') \rangle^{1/2}} = f \left( \frac{r}{L(t)}, \frac{r'}{L(t')} \right).$$

(6)

In the limit of $t \gg t'$, the dependence on one length scale separates, and the correlation function becomes a homogeneous function of the ratio $L(t)/L'(t)$:

$$g(r, t; r', t') = \left( \frac{L(t)}{L(t')} \right)^{-\lambda} \hat{f}(r/L(t)).$$

(7)

In general, the exponent $\lambda$ differs from $z$. We show the behavior of the zero-range value of the pair correlation function $g(0, t; 0, t')$ as a function of time in Fig. 4. We assume that the correction arising from the finite domain size are small and perform a direct fit to the data over the whole measurement interval. This procedure gives a dynamical exponent of $\lambda = 3.90(2)$.

Experimental Significance and Limitations.— We now discuss the significance of our results to experiments in binary Bose condensates. In typical non-equilibrium experiments, the spin healing length is of order $\zeta \sim 10 \mu m$ [11, 8, 9], which corresponds to a time of $t \sim 1 s$ beyond which scaling should be observed. On these rather long timescales, the dynamics of the physical system is complicated by particle losses and heating in the trap [11]. Smaller spin healing lengths (hence smaller $t$) can be obtained in strongly interacting binary mixtures such as the one recently realized in Chicago [14]. Here, an effective spin-1/2 system was realized by using lattice modulation to create a double-well potential in the ground band of an optical lattice with $(g_{12} - g)/g \sim 1$. It may be possible to explore the predicted universal dynamical scaling regime in this strongly interacting binary system.

Finally, we note that even at low temperatures $T \ll \mu$, where the Gross-Pitaevskii approach used here is valid, on long timescales of order $t_{\text{col}} \sim (\hbar a/\zeta (na^3/\hbar \omega))^{-1}$, (where $\zeta$ is the axial confinement length), quantum fluctuations which start to become important. A proper modeling of these effects is a challenging and computationally intensive problem, and requires more sophisticated methods such as the c-field techniques currently being developed by several groups [35]. Whether these effects qualitatively modify our conclusions remains to be understood and is an exciting problem for further research.

Conclusions.— In conclusion, we provide numerical evidence that the coarsening dynamics of a binary Bose-Einstein condensate that is quenched across a miscible-immiscible phase boundary obeys universal scaling laws.
Equal-time correlation functions depend implicitly on time through a single characteristic length scale which grows according to a power law with time. The exponent governing the power-law growth is found to be $1/z = 0.68(2)$, which is consistent with inertial hydrodynamic growth. The presence of domain walls induces a high-momentum tail in the structure function which decays as a power-law of the momentum. This power-law decay is a key signature of coarsening dynamics, and is not present in the initial stages of domain growth. Our findings can be verified experimentally either via direct imaging of magnetic domains in situ or in time-of-flight, or by measuring the structure factor, which can be probed by imaging density fluctuations in situ, or using Bragg spectroscopy.

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