

Quantum spinodal decomposition

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We study the process of spinodal decomposition in a scalar quantum field theory that is quenched from an equilibrium disordered initial state at $T_i > T_f$ to a final state at $T_f \approx 0$. The process of the formation and growth of correlated domains is studied in a Hartree approximation. We find an approximate scaling law for the size of the domains $\xi_D(t) \approx \sqrt{t} \xi_0$ at long times for weakly coupled theories, where ξ_0 is the zero-temperature correlation length.

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The process of phase separation through spinodal decomposition is well understood within the context of classical nonequilibrium statistical mechanics [1–3]. When the quench is at criticality, it is primarily associated with the onset and growth of unstable longwavelength modes (we will not discuss nucleation here).

Spinodal decomposition is conjectured to have taken place during phase transitions in the early Universe typically described by scalar quantum field theories [4–6]. Thus it becomes an important issue to understand and describe the mechanism of phase separation in quantum field theory with the definite motivation provided by cosmological phase transitions. An attempt to study some of these issues was reported by Mazenko and collaborators [7]. Understanding the process of phase separation in quantum many-body systems may also prove relevant within the context of mesoscopic systems and quantum phase transitions in condensed matter. In this paper, we introduce the techniques of nonequilibrium quantum statistical mechanics to study the process of phase separation in a typical scalar field theory.

From the outset we recognize fundamental differences between classical theories of spinodal decomposition, and the description of phase separation in a quantum system. In the former, the equations of motion are purely dissipative, whereas in the latter, the Heisenberg operator equations of motion are second order and thus time-reversal invariant. Furthermore, thermal fluctuations are incorporated in the classical description via a Langevin noise term, typically uncorrelated and satisfying the fluctuation-dissipation relation, whereas in the quantum description, both thermal and quantum fluctuations are present in the initial *density matrix* that describes the initial ensemble.

We model the physical situation of a “critical quench”

via a time-dependent Hamiltonian

$$H(t) = \int_{\Omega} d^3x \left\{ \frac{1}{2} \Pi^2(x) + \frac{1}{2} [\nabla \Phi(x)]^2 + \frac{1}{2} m^2(t) \Phi^2(x) + \frac{\lambda}{4!} \Phi^4(x) \right\}, \quad (1)$$

$$m^2(t) = m_i^2 \Theta(-t) - m_f^2 \Theta(t), \quad (2)$$

$$m_i^2 = \mu^2 \left[\frac{T_i^2}{T_c^2} - 1 \right], \quad m_f^2 = \mu^2 \left[1 - \frac{T_f^2}{T_c^2} \right], \quad (3)$$

with $\mu^2 > 0$, $T_i > T_c$, $T_f \approx 0$, and $\Theta(t)$ the step function. The initial state of the system (at $t < 0$) is assumed to be described by an equilibrium density matrix at the initial temperature T_i .

$$\hat{\rho}_i = e^{-\beta_i H_i}, \quad (4)$$

$$H_i = H \quad (t < 0). \quad (5)$$

In the Schrödinger picture, the density matrix evolves in time as

$$\hat{\rho}(t) = U(t) \hat{\rho}_i U^{-1}(t), \quad (6)$$

with $U(t)$ the time evolution operator. In the present case, the order parameter $[\text{Tr} \rho(t) \int_{\Omega} d^3x \Phi(\mathbf{x})] / \text{Tr} \rho_i$ obeys a Heisenberg equation of motion and is *not conserved*. The expectation value of operators may be computed by introducing the generating functional

$$Z[J^+, J^-] = \text{Tr} U(T - i\beta_i, T) \times U(T, T'; J^-) U(T', T; J^+), \quad (7)$$

with $T \rightarrow -\infty$, $T' \rightarrow \infty$. It is found that

$$Z[J^+, J^-] = \exp \left\{ i \int_T^{T'} dt [\mathcal{L}_{\text{int}}(-i\delta/\delta J^+) - \mathcal{L}_{\text{int}}(i\delta/\delta J^-)] \right\} \exp \left\{ \frac{i}{2} \int_T^{T'} dt_1 \int_T^{T'} dt_2 J_a(t_1) J_b(t_2) G_{ab}(t_1, t_2) \right\}, \quad (8)$$

with G_{ab} the Green's function on a contour [8]. The quantities of interest are

$$S(\mathbf{r};t) = \langle \Phi(\mathbf{r},t) \Phi(\mathbf{0},t) \rangle, \quad (9)$$

$$S(\mathbf{r};t) = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} \langle \Phi_{\mathbf{k}}(t) \Phi_{-\mathbf{k}}(t) \rangle. \quad (10)$$

The equal-time correlation function at zeroth order (“tree level”) is thus found to be

$$\langle \Phi_{\mathbf{k}}(t) \Phi_{-\mathbf{k}}(t) \rangle = \frac{1}{2\omega_{<}(k)} \mathcal{U}_{\mathbf{k}}^+(t) \mathcal{U}_{\mathbf{k}}^-(t) \coth[\beta_i \omega_{<}(k)/2] \quad (11)$$

with the mode functions obeying

$$\left[\frac{d^2}{dt^2} + \mathbf{k}^2 + m^2(t) \right] \mathcal{U}_{\mathbf{k}}^\pm = 0 \quad (12)$$

with $m^2(t)$ given by (2).

The boundary conditions on the homogeneous solutions are

$$\mathcal{U}_{\mathbf{k}}^\pm(t < 0) = e^{\mp i\omega_{<}(k)t}, \quad \omega_{<}(k) = [\mathbf{k}^2 + m_i^2]^{1/2} \quad (13)$$

corresponding to positive frequency (particles) and negative frequency (antiparticles) [$\mathcal{U}_{\mathbf{k}}^+(t)$, $\mathcal{U}_{\mathbf{k}}^-(t)$, respectively].

The “free field” mode functions are easily found. For $t > 0$, they consist of stable modes ($\mathbf{k}^2 > m_f^2$) and unstable modes ($\mathbf{k}^2 < m_f^2$). These unstable modes are responsible for the growth of correlations. The zeroth-order equal-time correlation function becomes

$$\langle \Phi_{\mathbf{k}}(t) \Phi_{-\mathbf{k}}(t) \rangle = \frac{1}{2\omega_{<}(k)} \coth[\beta_i \omega_{<}(k)/2] \quad (14)$$

for $t < 0$, and

$$\begin{aligned} \langle \Phi_{\mathbf{k}}(t) \Phi_{-\mathbf{k}}(t) \rangle = & \frac{1}{2\omega_{<}(k)} [(1 + 2A_k B_k \{ \cosh[2W(k)t] - 1 \}) \Theta(m_f^2 - \mathbf{k}^2) \\ & + (1 + 2a_k b_k \{ \cos[2\omega_{>}(k)t] - 1 \}) \Theta(\mathbf{k}^2 - m_f^2)] \coth[\beta_i \omega_{<}(k)/2] \end{aligned} \quad (15)$$

with $\omega_{>}(k) = (\mathbf{k}^2 - m_f^2)^{1/2}$ and $W(k) = (m_f^2 - \mathbf{k}^2)^{1/2}$, for $t > 0$.

The first term, the contribution of the unstable modes, reflects the growth of correlations because of the instabilities and will be the dominant term at long times in this approximation.

It is convenient to introduce the dimensionless quantities

$$\begin{aligned} \kappa &= \frac{k}{m_f}, \quad L^2 = \frac{m_i^2}{m_f^2} = \frac{[T_i^2 - T_c^2]}{[T_c^2 - T_f^2]}, \\ \tau &= m_f t, \quad \mathbf{x} = m_f \mathbf{r}, \end{aligned} \quad (16)$$

and the critical temperature $T_c^2 = 24\mu^2/\lambda$ [4–6], in terms of which the “tree-level” subtracted structure factor $S^{(0)}(k,t) - S^{(0)}(k,0) = (1/m_f) \mathcal{S}^{(0)}(\kappa,\tau)$ becomes

$$\begin{aligned} \mathcal{S}^{(0)}(\kappa,\tau) = & \left[\frac{24}{\lambda \left[1 - \frac{T_f^2}{T_c^2} \right]} \right]^{1/2} \left[\frac{T_i}{T_c} \right] \frac{1}{2\omega_\kappa^2} \left[1 + \frac{\omega_\kappa^2}{W_\kappa^2} \right] \\ & \times [\cosh(2W_\kappa\tau) - 1], \end{aligned} \quad (17)$$

$$\omega_\kappa^2 = \kappa^2 + L^2, \quad W_\kappa = 1 - \kappa^2. \quad (18)$$

To obtain a better idea of the growth of correlations, it is convenient to introduce the scaled correlation function

$$\mathcal{D}(x,\tau) = \frac{\lambda}{6m_f^2} \int_0^{m_f} \frac{k^2 dk}{2\pi^2} \frac{\sin(kr)}{(kr)} [S(k,t) - S(k,0)]. \quad (19)$$

The reason for this is that the minimum of the tree-level potential occurs at $\lambda\Phi^2/6m_f^2 = 1$, and the inflexion (spinodal) point, at $\lambda\Phi^2/2m_f^2 = 1$, so that $\mathcal{D}(0,\tau)$ measures the excursion of the fluctuations to the classical spinodal

and beyond as the correlations grow in time.

At large τ (time), $\kappa^2 \mathcal{S}(\kappa,\tau)$ has a sharp peak at $\kappa_s = 1/\sqrt{\tau}$ with amplitude $\exp[2\tau]/\tau$ (see Fig. 1). We find for $x < \tau$ and $T_f \approx 0$

$$\mathcal{D}(x,\tau) \approx \mathcal{D}(0,\tau) \exp \left[-\frac{x^2}{8\tau} \right] \frac{\sin(x/\sqrt{\tau})}{(x/\sqrt{\tau})}, \quad (20)$$

$$\mathcal{D}(0,\tau) \approx \left[\frac{\lambda}{12\pi^3} \right]^{1/2} \left[\frac{\left[\frac{T_i}{2T_c} \right]^3}{\left[\frac{T_i^2}{T_c^2} - 1 \right]} \right] \frac{\exp[2\tau]}{\tau^{3/2}}. \quad (21)$$

Restoring dimensions, and recalling that the zero-temperature correlation length is $\xi(0) = 1/\sqrt{2\mu}$, we find that for $T_f \approx 0$ the amplitude of the fluctuation inside a “domain” $\langle \Phi^2(t) \rangle$, and the “size” of a domain $\xi_D(t)$ grow as

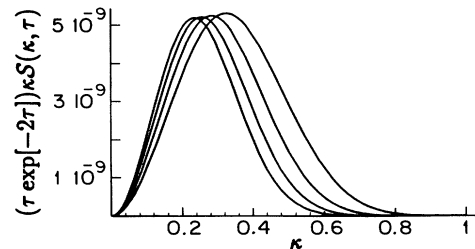


FIG. 1. $(\tau \exp[-2\tau]) \kappa \mathcal{S}(\kappa,\tau)$ for $\lambda = 10^{-12}$; $T_i/T_c = 2$ and $\tau = 10, 13, 16, 19$.

$$\langle \Phi^2(t) \rangle \approx \frac{\exp[\sqrt{2}t/\xi(0)]}{[\sqrt{2}t/\xi(0)]^{3/2}}, \quad \xi_D(t) \approx (8\sqrt{2})^{1/2} \sqrt{t\xi(0)}. \quad (22)$$

The presence of the instabilities precludes a well-defined perturbative expansion. Consider a one-loop contribution to the equal-time correlation function. The “external legs” obtain a contribution from the unstable modes, but in the loop integral, the integration over the momenta also includes a contribution from the unstable modes. It is clear that eventually the one-loop correction dominates and perturbation theory breaks down, even for the case of very weak couplings. This feature will persist to all orders in a perturbative expansion. The *dynamics of the phase transition cannot be studied in perturbation theory.*

Our nonperturbative approach is based on a Hartree approximation, which is similar to the early approach of Langer [9] for classical spinodal decomposition. It is implemented by the replacement

$$m^2(t) \rightarrow m^2(t) + \frac{\lambda}{2} \langle \Phi^2(t) \rangle$$

(where we used spatial translational invariance).

This leads to the self-consistent set of equations

$$\left[\frac{d^2}{dt^2} + \mathbf{k}^2 + m^2(t) + \frac{\lambda}{2} \langle \Phi^2(t) \rangle \right] \mathcal{U}_k^\pm = 0, \quad (23)$$

with $T_i > T_c$ and $T_f \ll T_c$. With the self-consistent solution and boundary condition for $t < 0$

$$[\langle \Phi^2(t < 0) \rangle - \langle \Phi^2(0) \rangle] = 0, \quad (30)$$

$$\mathcal{U}_k^\pm(t < 0) = \exp[\mp i\omega_<(k)t],$$

$$\omega_<(k) = (\mathbf{k}^2 + m_{iR}^2)^{1/2}. \quad (31)$$

This set of Hartree equations is extremely complicated to be solved exactly. However, it accounts for the process of coarsening [1]. Consider the equations for $t > 0$, at very early times, when (the renormalized) $\langle \Phi^2(t) \rangle - \langle \Phi^2(0) \rangle \approx 0$ the mode functions are the same as in the zeroth-order approximation, and the unstable modes grow exponentially. By computing the expression (27) self-consistently with these zero-order unstable modes, we see that the fluctuation operator begins to grow exponentially.

$$\langle \Phi^2(t) \rangle = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_<(k)} \mathcal{U}_k^+(t) \mathcal{U}_k^-(t) \times \coth[\beta_i \omega_<(k)/2]. \quad (24)$$

The composite operator $\langle \Phi^2(\mathbf{r}, t) \rangle$ needs one subtraction and multiplicative renormalization. The subtraction is absorbed in a renormalization of the bare mass, and the multiplicative renormalization into a renormalization of the coupling constant. The Hartree approximation provides a self-consistent nonperturbative scheme that sums an infinite series of Feynman diagrams [10]. For $t < 0$ there is a self-consistent solution given by

$$\langle \Phi^2(t) \rangle = \langle \Phi^2(0) \rangle, \quad \mathcal{U}_k^\pm(t) = \exp[\mp i\omega_<(k)t], \quad (25)$$

$$\omega_<(k) = \mathbf{k}^2 + m_i^2 + \frac{\lambda}{2} + \langle \Phi^2(0) \rangle = \mathbf{k}^2 + m_{i,R}^2, \quad (26)$$

and $m_{i,R}^2 = \mu_R^2 [(T_i^2/T_c^2) - 1]$. For $t > 0$ we subtract the composite operator at $t=0$ absorbing the subtraction into a renormalization of m_f^2 which we now parametrize as $m_{f,R}^2 = \mu_R^2 [1 - (T_f^2/T_c^2)]$. This choice of parametrization only represents a choice of the bare parameters. The logarithmic multiplicative divergence of the composite operator will be absorbed in a coupling-constant renormalization consistent with the Hartree approximation [10]. However, for the purpose of understanding the dynamics of growth of instabilities associated with the long-wavelength fluctuations, we will not need to specify this procedure. After this renormalization, the Hartree equations read as

$$[\langle \Phi^2(t) \rangle - \langle \Phi^2(0) \rangle] = \int \frac{d^3k}{(2\pi)^3} \frac{1}{2\omega_<(k)} [\mathcal{U}_k^+(t) \mathcal{U}_k^-(t) - 1] \coth[\beta_i \omega_<(k)/2], \quad (27)$$

$$\left[\frac{d^2}{dt^2} + \mathbf{k}^2 + m_R^2(t) + \frac{\lambda_R}{2} [\langle \Phi^2(t) \rangle - \langle \Phi^2(0) \rangle] \right] \mathcal{U}_k^\pm(t) = 0, \quad (28)$$

$$m_R^2(t) = \mu_R^2 \left[\frac{T_i^2}{T_c^2} - 1 \right] \Theta(-t) - \mu_R^2 \left[1 - \frac{T_f^2}{T_c^2} \right] \Theta(t), \quad (29)$$

As $\langle \Phi^2(t) \rangle - \langle \Phi^2(0) \rangle$ grows larger, its contribution to the Hartree equation tends to balance the negative mass term, thus weakening the instabilities, so that only longer wavelengths can become unstable. Even for very weak-coupling constants, the exponentially growing modes make the Hartree term in the equation of motion for the mode functions become large and compensate for the negative mass term. Thus when

$$\frac{\lambda_R}{2m_{f,R}^2} [\langle \Phi^2(t) \rangle - \langle \Phi^2(0) \rangle] \approx 1$$

the instabilities shut off; this equality determines the “spinodal time” t_s . The modes will still continue to grow further after this point because the time derivatives are fairly (exponentially) large, but eventually the growth will slow down when fluctuations sample deep inside the stable region.

After the subtraction, and multiplicative renormalization (absorbed in a coupling-constant renormalization), the composite operator is finite. The stable mode functions will make a *perturbative* contribution to the fluctuation which will be always bounded in time. The most important contribution will be that of the *unstable modes*. These will grow exponentially at early times and their effect will dominate the dynamics of growth and formation of correlated domains. The full set of Hartree equations is extremely difficult to solve, even numerically, so we will restrict ourselves to account *only* for the unstable modes. From the above discussion it should be clear that

$$\left[\frac{d^2}{d\tau^2} + q^2 - 1 + \int_0^1 dp \left\{ \frac{p^2}{p^2 + L^2} [\mathcal{U}_p^+(\tau) \mathcal{U}_p^-(\tau) - 1] \right\} \right] \mathcal{U}_q^\pm(\tau) = 0 \quad (32)$$

with the boundary conditions (30) for $t < 0$ and

$$g = \frac{\sqrt{24\lambda_R}}{4\pi^2} \frac{T_i}{[T_c^2 - T_f^2]^{1/2}}. \quad (33)$$

The effective coupling (33) reflects the enhancement of quantum fluctuations by high-temperature effects; for $T_f/T_c \approx 0$, and for couplings as weak as $\lambda_R \approx 10^{-12}$, $g \approx 10^{-7}(T_i/T_c)$. This value of the coupling has particular significance in inflationary models and arises from bounds on density fluctuations [4–6]. Equations (32) may now be integrated numerically for the mode functions; once we find these, we can then compute the contribution of the unstable modes to the subtracted correlation function equivalent to (19) (HF stands for Hartree-Fock):

$$\begin{aligned} \mathcal{D}^{(\text{HF})}(x, \tau) \\ = \frac{\lambda_R}{6m_{f,R}^2} [\langle \Phi(\mathbf{r}, t) \Phi(\mathbf{0}, t) \rangle - \langle \Phi(\mathbf{r}, 0) \Phi(\mathbf{0}, 0) \rangle], \end{aligned} \quad (34)$$

$$\begin{aligned} 3\mathcal{D}^{(\text{HF})}(x, \tau) \\ = g \int_0^1 dp \left[\frac{p^2}{p^2 + L^2} \right] \frac{\sin(px)}{(px)} [\mathcal{U}_p^+(t) \mathcal{U}_p^-(t) - 1]. \end{aligned} \quad (35)$$

In Fig. 2 we show $3[\mathcal{D}^{(\text{HF})}(0, \tau) - \mathcal{D}^{(\text{HF})}(0, 0)]$ (solid line) and also for comparison, its zeroth-order counterpart $3[\mathcal{D}^{(0)}(0, \tau) - \mathcal{D}^{(0)}(0, 0)]$ (dashed line) for $\lambda_R = 10^{-12}$, $T_i/T_c = 2$. (This value of the initial temperature does not have any particular physical significance and was chosen as a representative.) We clearly see what we expected; whereas the zeroth-order correlation grows indefinitely, the Hartree correlation function is bounded in time and oscillatory. At $\tau \approx 10.52$, $3[\mathcal{D}^{(\text{HF})}(0, \tau) - \mathcal{D}^{(\text{HF})}(0, 0)] = 1$, fluctuations are sampling field configurations near the classical spinodal; fluctuations continue to grow, however, because the derivatives are still fairly large. After this time, the modes begin to probe the stable region in which there is no exponential growth. At this point $(\lambda_R/2m_{f,R}^2)[\langle \Phi^2(\tau) \rangle - \langle \Phi^2(0) \rangle]$, becomes small again because of the small coupling $g \approx 10^{-7}$, and the correction

these are the only relevant modes for the dynamics of formation and growth of domains, whereas the stable modes, will always contribute perturbatively for weak coupling after renormalization.

Introducing the dimensionless ratios (16) in terms of $m_{f,R}$, $m_{i,R}$ (all momenta are now expressed in units of $m_{f,R}$), dividing (28) by $m_{f,R}^2$, using the high-temperature approximation $\coth[\beta_i \omega_<(k)/2] \approx 2T_i/\omega_<(k)$ for the unstable modes, and expressing the critical temperature as $T_c^2 = 24\mu_R^2/\lambda_R$, the set of Hartree equations (27) and (28) becomes the following integrodifferential equation for the mode functions for $t > 0$:

term becomes small. When it becomes smaller than 1, the instabilities set in again, the unstable modes begin to grow, and the process repeats. This gives rise to an oscillatory behavior around $(\lambda_R/2m_{f,R}^2)[\langle \Phi^2(\tau) \rangle - \langle \Phi^2(0) \rangle] = 1$ as shown in Fig. 2. We clearly see that for very weakly coupled theories, the zeroth-order correlation function provides a fairly good approximation to the Hartree correlations up to the “spinodal time.” Thus for very weakly coupled theories correlation functions will be approximately given by (20) and (21) and this permits us to find an approximate result for the spinodal time (at which fluctuations begin probing the stable region),

$$\tau_s = \frac{t_s}{\sqrt{2\xi(0)}} \approx -\ln \left[\left(\frac{3\lambda}{4\pi^3} \right)^{1/2} \frac{\left[\frac{T_i}{2T_c} \right]^3}{\left[\frac{T_i^2}{T_c^2} - 1 \right]} \right]. \quad (36)$$

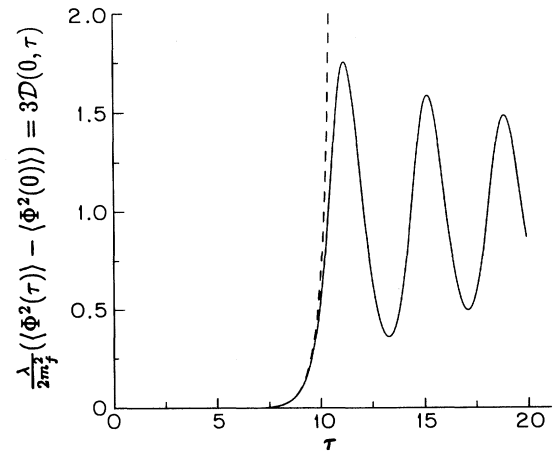


FIG. 2. Hartree (solid line) and zeroth-order (dashed line) results for $(\lambda/2m_{f,R}^2)[\langle \Phi^2(\tau) \rangle - \langle \Phi^2(0) \rangle] = 3\mathcal{D}(0, \tau)$, for $\lambda = 10^{-12}$, $T_i/T_c = 2$.

It is remarkable that the domain size scales as $\xi_D(t) \approx t^{1/2}$ just like in classical theories of spinodal decomposition, in which the order parameter is *not conserved*, as is the case in this relativistic scalar field theory, but certainly for completely different reasons. At the tree level, we can identify this scaling behavior as arising from the relativistic dispersion relation, a situation very different from the classical description of the Allen-Cahn-Lifshitz [11] theory of spinodal decomposition based on a time-dependent Landau-Ginzburg model. For strong coupling, the Hartree result and the zeroth-order result depart at very early times [12]. It is well known within the context of classical spinodal decomposition

that the Hartree approximation is not correct at intermediate and long times. We are currently studying a consistent treatment beyond the Hartree approximation. Details of the calculation and possible extensions will be presented elsewhere [12]. Of particular importance will be the study of the interface dynamics, known to be the relevant description in classical theories [13].

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