Modeling thermal fluctuations: phase mixing and percolation

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Abstract

We consider the nonequilibrium dynamics of a real scalar field in a double-well potential. The system is initially prepared in one well and coupled to a thermal bath. Using a simple analytical model, we compute the equilibrium fraction of the total volume in each phase as a function of the parameters of the potential. We also show how complete phase mixing, i.e. symmetry restoration, is related to percolation, which is dynamically driven by domain instability. Our method describes quantitatively recent numerical results, and is applicable to systems in the Ising universality class. © 1997 Published by Elsevier Science B.V.

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It is well known that an Ising ferromagnet loses its net magnetization above a certain temperature. The simplest mean-field description of this phenomenon is based on the Ginzburg–Landau model, in which the average magnetization $M = (V^{-1}) \int dV\, M(x)$ is the order parameter, and the thermodynamic potential is expanded to the fourth power in M, $V(M) = a(T - T_c)M^2 + bM^4$ [1], where we have omitted the term linear in M because we are only interested in the case of zero external magnetic field. Above the critical temperature T_c, the lowest free energy state of the system has zero net magnetization, while below T_c the material acquires a magnetization $M = \pm[a|T-T_c|/2b]^{1/2}$.

It is also well known that mean-field theory breaks down close to T_c; for example, although mean-field theory correctly predicts that the correlation length diverges as $\xi \sim |(T-T_c)/T_c|^{-\nu}$, it gives the value of the critical exponent $\nu = 0.5$, while numerical simulations find $\nu = 0.630(2)$ [2]. In order to handle the infrared divergences that appear near T_c, the renormalization group is used to relate a given theory to an equivalent theory with smaller correlation lengths and thus better behaved in the infrared. With the ε-expansion, one works in $4 - \varepsilon$ dimensions and finds a fixed point of order ε of the renormalization group equations, taking the limit $\varepsilon \to 1$ in the end. To second order in ε, $\nu = \frac{1}{2} + \frac{1}{12}\varepsilon + \frac{7}{162}\varepsilon^2 \simeq 0.63$, a remarkable result [3]. The continuous field model exhibits the same critical exponents of the discrete Ising model, and one can be mapped into the other for temperatures near T_c.

In the present work, we would like to follow a somewhat orthogonal approach to study a closely related question. Consider again an Ising ferromagnet in the absence of an external magnetic field, which is well be-

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low its critical temperature and has been prepared with all spins initially pointing in one direction. In the thermodynamic limit, this is the broken-symmetric state. As the temperature is increased, thermal fluctuations will flip groups of spins, so that the absolute value of the magnetization will start decreasing. At some temperature $T_c^* < T_c$, $|M| \to 0$. (This is another way of expressing the breakdown of mean-field theory.) The question we would like to address is the following: At a given temperature below T_c, what is the fraction of the volume occupied by each of the two possible phases of the system as a function of the parameters of the potential? Can we provide a method for computing this fraction which somehow encompasses the breakdown of mean-field theory, without resorting to the renormalization group?

We start by writing the homogeneous part of the free-energy density as

$$V(\phi, T) = \frac{a}{2} \left(T^2 - T_2^2 \right) \phi^2 - \frac{\alpha}{3} T \phi^3 + \frac{\lambda}{4} \phi^4 . \qquad (1)$$

It is easy to see that with a simple field redefinition ($\phi \to \phi - T\alpha/3\lambda$), we can rewrite $V(\phi, T)$ as a Ginzburg–Landau potential with a temperature-dependent "magnetic field" coupled linearly to the order parameter ϕ. We define the critical temperature T_c' as the temperature when the two minima of $V(\phi, T)$ are degenerate. At T_c', the "magnetic field" is zero and we recover the degenerate double-well potential with quadratic term given by

$$-\frac{\alpha^2 T_c'^2}{18\lambda} \phi^2 .$$

We will only be interested in investigating this system at T_c'. The critical point will be approached by varying λ. In the language of the analogous Ising model, we will investigate the approach to criticality from below in the absence of an external magnetic field.

Introducing dimensionless variables $\tilde{x} = a^{1/2} T_2 x$, $\tilde{t} = a^{1/2} T_2 t$, $X = a^{-1/4} T_2^{-1} \phi$, and $\theta = T/T_2$, the Hamiltonian is

$$\frac{H[X]}{\theta} = \frac{1}{\theta} \int d^3 \tilde{x} \left[\frac{1}{2} \left| \tilde{\nabla} X \right|^2 + \frac{1}{2} \left(\theta^2 - 1 \right) X^2 \right.$$
$$\left. - \frac{\tilde{\alpha}}{3} \theta X^3 + \frac{\tilde{\lambda}}{4} X^4 \right] , \qquad (2)$$

where $\tilde{\alpha} = a^{-3/4} \alpha$, and $\tilde{\lambda} = a^{-1/2} \lambda$ (henceforth we drop the tildes). At the critical temperature $\theta_c =$

$(1 - 2\alpha^2/9\lambda)^{-1/2}$ the two minima, at $X_0 = 0$ and $X_+ = \frac{\alpha\theta}{2\lambda} [1 + \sqrt{1 - 4\lambda \left(1 - 1/\theta^2 \right) /\alpha^2}]$, are degenerate. In what follows, we are only interested in the system at θ_c.

In a recent work, Borrill and Gleiser (BG) simulated the dynamics of the above system coupled to a Markovian thermal bath [4]. (This is why we wrote the potential as in Eq. (1).) In analogy with Ising ferromagnetism, it is useful to think of the system described by the Hamiltonian above as having two phases, the "0 phase", for $X < X_{max}$, and the "+ phase", for $X \geq X_{max}$, where X_{max} is at the maximum of the double-well potential. The initial conditions were chosen so that the system started in the 0 phase. Thus, $V_0^t/V_T(t = 0) = 1$, where V_0^t is the total volume in the 0 phase, V_T is the constant total volume, and $V_0^t/V_T(t) + V_+^t/V_T(t) = 1$. The coupling of this system to a thermal bath will induce the nucleation of domains of the + phase. For a small free-energy barrier between the two phases, domains of the 0 phase will also nucleate within domains of the + phase, and so on, resulting in a very complicated domain structure. It is necessary to distinguish between two possible kind of domains, connected and disconnected. *Connected domains* percolate throughout the volume, and thus cannot be surrounded by a domain of the opposite phase. *Disconnected domains* have finite volume and are always surrounded by the other phase. In general, $V_{0(+)}^t = V_{0(+)}^c + V_{0(+)}^d$.

Keeping the system at θ_c and fixing $\alpha = 0.065$ (this seemingly ad hoc choice was inspired by the electroweak effective potential, although any other value would do), BG measured the equilibrium fractions, $f_0 \equiv V_0^t/V_T$ and $f_+ \equiv V_+^t/V_T$, as a function of the coupling λ. They found that for $\lambda \geq \lambda_c \simeq 0.025$, $f_0 = f_+ = 0.5$, that is, the two phases completely mix (see Fig. 1). In other words, for $\lambda \geq \lambda_c$, the symmetry is restored, even though the mean-field potential still has a double-well shape. Clearly, for $\lambda \geq \lambda_c$, mean-field theory breaks down, and the system is better described by an effective free-energy density with a single minimum at $X_{max} = 0$. This situation is exactly analogous to an Ising ferromagnet for $T \geq T_c^*$.

In what follows, we will reproduce these results with a simple statistical model for the thermal fluctuations. Our approach is completely general, in that it can be easily adapted to other systems described by a similar double-well potential, i.e. for systems in the
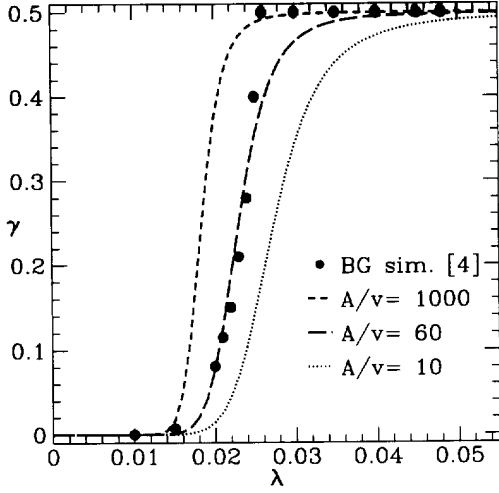
Fig. 1. The fraction of the volume in the + phase. The dots are from the numerical simulations of BG, while the lines are the solutions of the Boltzmann equation for different values of the parameter $A/|v|$.

universality class of the Ising ferromagnet. We will assume that the large-amplitude fluctuations from the 0 (+) phase into the + (0) phase can be modelled by spherically symmetric subcritical bubbles of Gaussian shape of a given radius and amplitude (for previous treatments of subcritical bubbles see Ref. [5]),

$$\phi_c(r) = \phi_c e^{-r^2/R^2},$$
$$\phi_0(r) = \phi_c \left(1 - e^{-r^2/R^2}\right),$$
(3)

where R is the radial size of the configuration, and ϕ_c is the value of the field amplitude at the bubble's core, away from (and into) the 0 phase. For these configurations to interpolate between the two phases in the system, $\phi_c \geq \phi_{\max}$. With this ansatz, the free energy of the fluctuations assumes the general form, $F_{\mathrm{sc}}(R, \phi_c, T) = b\phi_c^2 R + c\beta(\phi_c, T)R^3$, where b and c are numerical constants and $\beta(\phi_c, T)$ is a polynomial which depends on the particular potential used. We will further assume that the nucleation rate for these configurations is obtained from a Gibbs distribution, $G(\phi, R) = A \exp\left[-F_{\mathrm{sc}}/T\right]$, where A is a constant. The nucleation rate per unit volume is then $\Gamma = \int G\, d\phi\, dR$.

The number density of bubbles of, say, the + phase with radii between R and $R + \delta R$ and amplitudes between ϕ and $\phi + \delta\phi$ at time $t + \delta t$ is

$$n_+(R + \delta R, \phi + \delta\phi, t + \delta t) - n_+(R, \phi + \delta\phi, t + \delta t)$$
$$- \left[n_+(R + \delta R, \phi, t + \delta t) - n_+(R, \phi, t + \delta t)\right].$$

Changes in the number density are generated by three different processes: (i) bubbles can shrink into and out of this interval. (We assume the time dependence of the amplitude to be closely related to the radial time dependence, as recent numerical studies have demonstrated [6]); (ii) bubbles can be thermally nucleated into this interval; (iii) bubbles can be thermally destroyed out of this interval by inverse nucleation. Expanding to first order in δR, $\delta\phi$, and δt, we obtain a Boltzmann equation for the bubble distribution function $f_+^d(R, \phi, t)$,

$$\frac{\partial f_+^d(R, \phi, t)}{\partial t} = -|v|\frac{\partial f_+^d}{\partial R} + \frac{V_0^c}{V_T}G_{0\to+} - \frac{V_+^d}{V_T}G_{+\to 0},$$
(4)

where the bubble density distribution function for domains of the + phase (hence the superscript d, for disconnected), is defined as

$$f_+^d(R, \phi, t) \equiv \frac{\partial^2 n_+}{\partial\phi\partial R},$$
(5)

and $G_{0(+)\to+(0)}$ is the Gibbs distribution for the nucleation rate per unit volume of bubbles of the + (0) phase within the 0 (+) phase. Note that we have written the Boltzmann equation to be consistent with the initial conditions used in the simulations, so that only disconnected domains contribute to the fraction of the volume in the + phase. It is straightforward to adapt the equation to different initial conditions.

In order to proceed, we note that the total fraction of volume in the + phase can be written as

$$\gamma \simeq \int_{\phi_{\max}}^{\infty}\int_{R_{\min}}^{\infty}\left(\frac{4\pi R^3}{3}\right)\frac{\partial^2 n_+}{\partial\phi\partial R}\,d\phi\,dR.$$
(6)

For a degenerate double well, $G_{+\to 0} = G_{0\to+} \equiv G$, and the Boltzmann equation can be written as

$$\frac{\partial f_+^d(R, \phi, t)}{\partial t} = -|v|\frac{\partial f_+^d}{\partial R} + (1 - 2\gamma)G.$$
(7)

Imposing the physical condition $f_+^d(R \to \infty, \phi, t) \to 0$, we can solve for the equilibrium distribution function ($\dot{f}_+^d = 0$), and use it to compute the equilibrium fraction of the volume in the + phase, γ_{eq}, which

is the quantity measured in the BG simulation. The general solution is

$$\gamma_{eq} = \frac{I(\phi_{max}, R_{min})}{1 + 2I(\phi_{max}, R_{min})}, \tag{8}$$

where

$$I(\phi_{max}, R_{min}) = \frac{A}{|v|} \int_R \int_{R_{min}} \int_{\phi_{max}}^{\infty} dR' \, dR \, d\phi$$

$$\times \frac{4\pi}{3} R^3 \exp\left[-F_{sc}(R', \phi)\right], \tag{9}$$

and ϕ_{max} is at the maximum of the double-well potential, and the minimum radius is taken to be the lattice spacing in the BG simulation, i.e. $R_{min} = 1$, which sets the coarse-graining scale. An analytical expression for $I(\phi_{max}, R_{min})$ can be obtained if we write $F_{sc}(R', \phi) \approx b\phi^2 R'$. This is a good approximation in the case that fluctuations are small enough that the volume term is sub-dominant.

In Fig. 1, we show γ_{eq} as a function of λ. The dots are the results of BG, while the curves are the results of the integration of the Boltzmann equation, for different values of the single parameter $A/|v|$. It is clear that for $\lambda \lesssim \lambda_c$, we obtain an excellent fit to the data with $A/|v| = 60$.

For larger values of λ, our method underestimates the fraction of volume in the + phase. This can be understood by noting that our kinetic description does not include possible terms which account for the coalescence of nearby domains. As fluctuations become more probable, these terms will play an increasingly important rôle. In fact, it is easy to understand how the onset of domain instability is intimately related to percolation of the + phase. (An excellent introduction to percolation theory can be found in Ref. [7].)

Consider a large spherical domain of the + phase of radius R. There are three ways by which the volume V of this domain can change: (i) it may shrink by surface tension with a velocity v; (ii) a small bubble of the + phase may nucleate just outside it; (iii) a small bubble of the 0 phase may nucleate inside it. Assuming that the bubble of the 0 phase nucleates just inside the large domain (see Fig. 2), we can write an approximate equation for the change in the volume V,
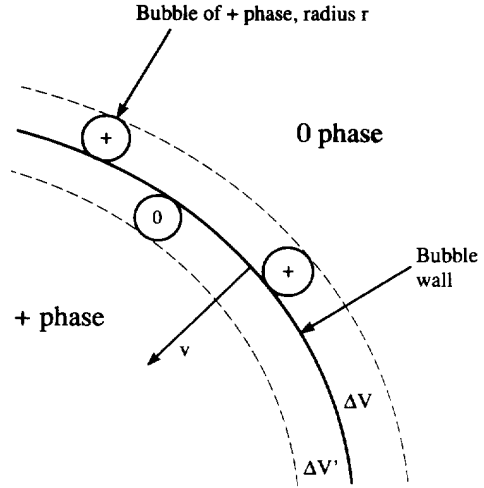

Fig. 2. Schematic of domain instability. The surface tension on the bubble wall will tend to shrink the large bubble with wall velocity v. However, more bubbles of the + phase will nucleate just outside the large bubble wall than bubbles of the 0 phase just inside the wall because $\Delta V > \Delta V'$ (nucleation rates of 0 and + bubbles are equal). This will tend to make the large bubble grow. When the barrier between the phases is small enough, nucleation dominates over bubble shrinking, causing the wall to become unstable to rapid growth.

$$\frac{dV}{dt} = -v 4\pi R^2 + (\Gamma_{0 \to +} \Delta V) \frac{4\pi}{3} r^3$$

$$- (\Gamma_{+ \to 0} \Delta V') \frac{4\pi}{3} r'^3, \tag{10}$$

where $\Gamma_{0(+) \to +(0)} \Delta V^{(')}$ is the nucleation rate for a bubble of the + (0) phase of radius $r^{(')}$ in the neighborhood of the domain wall. Assuming for simplicity that $r = r'$, and recognizing that $\Gamma_{+ \to 0}(r) = \Gamma_{0 \to +}(r)$ for a degenerate double-well potential, the condition for domain instability, $\frac{dV}{dt} > 0$, becomes

$$\Gamma r^4 > \frac{3}{8\pi} \left(\frac{R}{r}\right) v. \tag{11}$$

On the other hand, in order for the + phase to percolate, $\gamma_{eq} > p_c$, where p_c is the critical percolation probability. Using Boltzmann's equation, we can approximately write

$$\gamma_{eq} = \frac{g}{1 + 2g}, \qquad g \simeq \frac{4\pi}{3v} \Gamma r^4. \tag{12}$$

Thus, for percolation, we obtain the inequality

$$\Gamma r^4 > \frac{3}{4\pi} \frac{p_c}{1 - 2p_c} v . \tag{13}$$

For a simple cubic lattice, $p_c = 0.311$. Note that this is remarkably close to the value of γ_{eq} for λ_c, the point where the kinetic description breaks down (see Fig. 1).

Moreover, comparing the two inequalities of Eqs. (11) and (13), it is clear that they are satisfied at similar values of Γr^4. In particular, writing for simplicity $p_c = 1/3$, they are equal for $R = 2r$. This simple argument strongly suggests that the onset of percolation is dynamically driven by the nucleation of small bubbles in the neighborhood of large domains.

As stated before, once the barrier between the phases is small enough, the domain wall becomes unstable and nucleation of small bubbles is the dominant process for changing a volume of space from one phase to another. The equations determining the fraction of volume in each phase can then be approximated as

$$\frac{dV_+}{dt} = \left(\frac{4\pi}{3} r^3 \Gamma_{0 \to +} \right) V_0(t) - \left(\frac{4\pi}{3} r^3 \Gamma_{+ \to 0} \right) V_+(t) ,$$

$$V_0(t) = V_{tot} - V_+(t) , \tag{14}$$

where r is the average radius of a nucleated bubble. The solution to these equations is

$$\frac{V_+(t)}{V_{tot}} = \frac{1}{2} + \left(\frac{V_+(0)}{V_{tot}} - \frac{1}{2} \right) e^{-(8\pi\Gamma r^3/3)t} . \tag{15}$$

Notice that the equilibrium value $V_+(\infty)/V_{tot} = \gamma_{eq} = 1/2$, independently of $V_+(0)$. Therefore, once the domain wall becomes unstable, the system will equilibrate to $\gamma = 1/2$ in a time scale $\sim (\Gamma r^3)^{-1}$, which, at percolation, is of order the light crossing time r (see Eq. (13)). That is, once the system percolates, the stable, equilibrium, mean value of the field is at ϕ_{max}, which is the value exactly between the two minima.

As shown by Eq. (15), even if the system is perturbed away from $\gamma = 1/2$, it will quickly relax back to this value. This is consistent with previous results (see, for example, Ref. [8]), which also found that in 3d the percolation point is closely related to the point of symmetry restoration: the symmetry of the true (coarse-grained) effective potential has been restored, even though the mean-field potential still describes a double-well potential. It is important to note, however, that even if the average value of the field is ϕ_{max}, there

are widespread large-amplitude fluctuations with average volume set by the correlation length; the system is far from being locally homogeneous.

We conclude that our method based on subcritical bubbles gives a quantitatively accurate description of the behavior of thermal fluctuations for models in the Ising universality class. It also provides a dynamical picture of symmetry restoration, and the breakdown of mean-field theory. Furthermore, the method relates the breakdown of mean-field theory to a critical value of a given parameter, which is easily calculable. For values of the parameter larger than the critical value, large domains become unstable to growth due to the nucleation of nearby bubbles, percolation ensues, and symmetry or, more accurately, complete phase mixing, is restored.

Acknowledgements

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