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Information-entropic signature of the critical point

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ABSTRACT

We investigate the critical behavior of continuous (second-order) phase transitions in the context of $(2+1)$-dimensional Ginzburg–Landau models with a double-well effective potential. In particular, we show that the recently-proposed configurational entropy (CE)—a measure of the spatial complexity of the order parameter in momentum space based on its Fourier-mode decomposition—can be used to identify the critical point. We compute the CE for different temperatures and show that large spatial fluctuations near the critical point (T_c)—characterized by a divergent correlation length—lead to a sharp decrease in the associated configurational entropy. We further show that the CE density goes from a scale-free to an approximate scaling behavior $|k|^{-5/3}$ as the critical point is approached. We reproduce the behavior of the CE at criticality with a percolating many-bubble model.

1. Introduction

From materials science [1] to the early universe [2], phase transitions offer a striking illustration of how changing conditions can affect the physical properties of matter [3]. In very broad terms, and for the simplest systems described by a single order parameter, it is customary to classify phase transitions as being either discontinuous or continuous, or as first or second order, respectively. First-order phase transitions can be described by an effective free-energy functional (or an effective potential in the language of field theory) where an energy barrier separates two or more phases available to the system. The system may transition from a higher to a lower free-energy state (or from a higher to a lower vacuum state) either by a thermal fluctuation of sufficient size (a critical bubble) or, for low temperatures, by a quantum fluctuation. Generally speaking, this description of thermal bubble nucleation is valid as long as $\mathcal{F}[\phi_b]/k_B T \gg 1$, where $\mathcal{F}[\phi_b]$ is the 3d Euclidean action of the spherically-symmetric critical bubble or bounce $\phi_b(r)$, k_B is Boltzmann's constant, and T is the environmental temperature. For quantum tunneling, one uses instead $\mathcal{S}_4[\phi_b]/\hbar$, where $\mathcal{S}_4[\phi_b]$ is the $O(4)$-symmetric Euclidean action of the 4d bounce.

For second-order transitions the order parameter varies continuously as an external parameter such as the temperature is changed [3]. A well-known example is that of an Ising ferromagnet, where the net magnetization of a sample is zero above a critical temperature T_c, the Curie point, and non-zero below it. Below T_c the transition unfolds via spinodal decomposition, whereby long-wavelength fluctuations become exponentially-unstable to growth. This growth is characterized by the appearance of domains with the same net magnetization which compete for dominance with their neighbors. In the continuum limit, systems in the Ising universality class can be modeled by a Ginzburg–Landau (GL) free-energy functional with an order parameter $\phi(\mathbf{x})$ [4]. In the absence of an external source (or a magnetic field), the GL free-energy functional is simply

$$E[\phi] = \int d^d x \left[\frac{\gamma}{2}(\nabla\phi)^2 + \frac{a}{2}t\phi^2 + \frac{b}{4}\phi^4\right], \quad (1)$$

where $t \equiv (T - T_c)/T_c$, and γ, a, b are positive constants. For $T > T_c$ the system has a single free-energy minimum at $\phi = 0$, while for $T < T_c$ there are two degenerate minima at $\phi_0 = \pm(-at/b)^{1/2}$. This mean-field theory description works well away from the critical point. In the neighborhood of T_c one uses perturbation theory and the renormalization group to account for the divergent behavior of the system. This behavior can be seen through the two-point correlation function $G(\mathbf{r})$: away from T_c $G(\mathbf{r})$ behaves as $\sim\exp[-\mathbf{r}/\xi(T)]$, where $\xi(T)$ is the correlation length, a measure of the spatial extent of correlated fluctuations of the order parameter. In mean-field theory, $\xi(T) \sim |T - T_c|^{-\nu}$, where $\nu = 1/2$, independently of spatial dimensionality. In the neighborhood of T_c, where the mean-field description breaks down, the behavior of spatial fluctuations is corrected using the renormal-

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ization group. Within the ε-expansion, one obtains, in 3d, $\nu = 1/2 + \varepsilon/12 + 7\varepsilon^2/162 \simeq 0.63$ [4].

For continuous transitions in GL-systems, the focus of the present letter, the critical point is characterized by having fluctuations on all spatial scales. This means that while away from T_c large spatial fluctuations are suppressed, near T_c they dominate over smaller ones. In this letter, we will explore this fact to obtain a new measure of the critical point based on the information content carried by fluctuations at different momentum scales. For this purpose we will use a measure of spatial complexity known as configurational entropy (CE), recently proposed by Gleiser and Stamatopoulos [5]. The CE has been used to characterize the information content [5] and stability of solitonic solutions of field theories [5,6], to obtain the Chandrasekhar limit of compact Newtonian stars [6], the emergence of nonperturbative configurations in the context of spontaneous symmetry breaking [7] and in post-inflationary reheating [8] in the context of a top-hill model of inflation [9]. (Note that our usage of the name "configurational entropy" differs from other instances in the literature, as for example in protein folding [10].) Here we show that in the context of continuous phase transitions the CE provides a very precise signature and a marked scaling behavior at criticality.

2. Model and numerical implementation

We consider a $(2+1)$-dimensional GL model where the system is in contact with an ideal thermal bath at temperature T. The role of the bath is to drive the system into thermal equilibrium. This can be simulated as a temperature-independent GL functional (so, setting $t = -1$ in Eq. (1)) with a stochastic Langevin equation

$$\ddot{X} + \eta\dot{X} - \nabla^2 X - X + X^3 + \xi = 0, \tag{2}$$

where we have introduced dimensionless variables $x^\mu = \frac{1}{\sqrt{a}} y^\mu$ and $\phi = \sqrt{\frac{a}{b}}X$, and we took $\gamma = 1$. In Eq. (2), η is the viscosity and $\xi(\mathbf{x}, t)$ is the stochastic driving noise of zero mean, $\langle\xi\rangle = 0$. The two are related by the fluctuation–dissipation relation, $\langle\xi(\mathbf{x}, t)\xi(\mathbf{x}', t')\rangle = 2\eta\theta\delta(\mathbf{x} - \mathbf{x}')\delta(t - t')$. $\theta \equiv T/a$ is the dimensionless temperature and we take $k_B = \hbar = 1$.

We use a staggered leapfrog method and periodic boundary conditions to implement the simulation in a square lattice of size L and spacing h. We used $L = 200$ and $h = 0.25$. Simulations with larger values of L produce essentially similar results, apart from typical finite-size scaling effects [4]. Different values of h can be renormalized with the addition of proper counter terms, as has been discussed in Refs. [11] and [12]. Since all we need here is to simulate a phase transition with enough accuracy, we leave such technical issues of lattice implementation of effective field theories aside. We follow Ref. [12] for the implementation of the stochastic dynamics, so that the noise is drawn from a unit Gaussian scaled by a temperature-dependent standard deviation, $\xi = \sqrt{2\eta\theta/\Delta t h^2}$. To satisfy the Courant condition for stable evolution we used a time-spacing of $\Delta t = h/4$. The discrete Laplacian is implemented via a maximally rotationally invariant convolution kernel [15] with error of $O(h^2)$.

We start the field X at the minimum at $X = -1$ and the bath at low temperature, $\theta = 0.01$. We wait until the field equilibrates, checked using the equipartition theorem: in equilibrium, the average kinetic energy per degree of freedom of the lattice field, $\langle\dot{X}_{ij}^2/2\rangle$, is $\langle\dot{X}_{ij}^2\rangle = \theta$. Once the field is thermalized, which typically takes about 1,000 time steps, we use ergodicity to take 200 readings separated by 50 time steps each to construct an ensemble average. We then increase the temperature in increments of 0.01 and repeat the entire procedure until we cover the interval $\theta \in [0.01, 0.83]$.

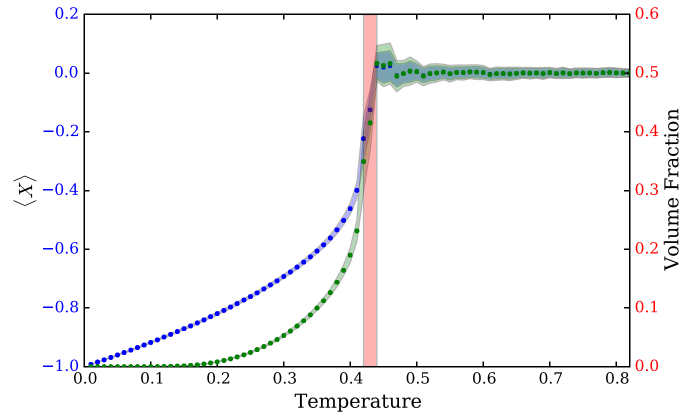

Fig. 1. (Color online.) The order parameter $\langle X\rangle$ [top (blue) line] and the volume fraction (p_V) occupied by the $X > 0$ phase [bottom (green) line] vs. temperature. The shaded regions correspond to 1σ deviations from the mean. Within the accuracy of our simulation, the critical temperature is $\theta_c \simeq 0.43 \pm .01$, marked by the vertical band.

We then obtain the ensemble-averaged $\langle X\rangle$ vs. θ. The coupling to the bath induces temperature-dependent fluctuations which, away from the critical point, can be described by an effective temperature-dependent potential, as in the Hartree approximation [13]. The critical point occurs as $\langle X\rangle \to 0$, when the $\mathbb{Z}_2$ symmetry is restored.

In Fig. 1 we plot the results. The top (blue) line is $\langle X\rangle$, while the bottom (green) line is the ensemble-averaged fraction of the volume occupied by $X > 0$ (p_V). Symmetry restoration corresponds to this fraction approaching 0.5. Shadowed regions correspond to 1σ deviation from the mean. Within the accuracy of our simulation, the critical temperature is $\theta_c \simeq 0.43 \pm .01$. In the top row of Fig. 2 we show the field at different temperatures, including at $\sim T_c$, where large-size fluctuating domains are apparent, indicative of the divergent correlation length.

3. Configurational entropy of the critical point

Consider the set of square-integrable bounded periodic functions with period L in d spatial dimensions, $f(\mathbf{x}) \in L^2(\mathbb{R}^d)$, and their Fourier series decomposition, $f(\mathbf{x}) = \sum_{\mathbf{k_n}} F(\mathbf{k_n})e^{i\mathbf{k_n}\cdot\mathbf{x}}$, with $\mathbf{k_n} = 2\pi(n_1/L, \ldots, n_d/L)$, and n_i integers. Now define the modal fraction $f_{\mathbf{k_n}} = |F(\mathbf{k_n})|^2/\sum|F(\mathbf{k_n})|^2$. (For details and the extension to nonperiodic functions, see [5].) The configurational entropy for the function $f(\mathbf{x})$, $S_C[f]$, is defined as

$$S_C[f] = -\sum f_{\mathbf{k_n}} \ln[f_{\mathbf{k_n}}]. \tag{3}$$

The quantity $\sigma(\mathbf{k_n}) \equiv -f_{\mathbf{k_n}} \ln[f_{\mathbf{k_n}}]$ gives the relative entropic contribution of mode $\mathbf{k_n}$. In the spirit of Shannon's information entropy [14], $S_C[f]$ gives an informational measure of the relative weights of different k-modes composing the configuration: it is maximized when all N modes carry the same weight, the mode equipartition limit, $f_{\mathbf{k_n}} = 1/N$ for any $\mathbf{k_n}$, with $S_C[f] = \ln N$. If only a single mode is present, $S_C[f] = 0$. For the lattice used here, with $N = 800^2$ points, the maximum entropy is $S_C^{\max} = 13.37$.

Plane waves in momentum space have equally distributed modal fractions, and their position space representations are highly localized. Conversely, singular modes in momentum space have plane wave representations in position space which are maximally delocalized. Localized distributions in position space maximize CE (many momentum modes contribute), while delocalized distributions minimize it. $S_C[f]$ is, in a sense, an entropy of shape, an informational measure of the complexity of a given spatial profile