Criterion for Dominance of Directional over Size Fluctuations in Destroying Order

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(Received 17 August 1999)

For systems that exhibit a second-order phase transition with a spontaneously broken continuous O(N) symmetry at low temperatures, we give a criterion for judging at which temperature T_K long-range directional fluctuations of the order field destroy the order when approaching the critical temperature from below. The temperature T_K lies always significantly below the famous Ginzburg temperature T_G at which size fluctuations of finite range become important.

PACS numbers: 05.40.–a, 64.60.–i

Although the fluctuation behavior of systems in a second-order phase transition is universal in the immediate vicinity of the transition, and the theory is well established [1], there are still disputes concerning the dominant fluctuation mechanism which drives a number of important phase transitions. A typical example is the question whether the superfluid transition in liquid helium is initiated by the proliferation of vortex lines, which are the defects in all systems with pure angular fluctuations of a complex order parameter, or by the size fluctuations of the associated complex *order field* $\phi(x)$. At first sight, this question may seem meaningless since all critical exponents of the transition can be calculated with great accuracy either from an order field theory with ϕ^4 interaction [2], where size and directional fluctuations seem to be equally important, or from a Heisenberg model on a lattice, which contains only directional fluctuations. In fact, the two descriptions are completely equivalent. The equivalence can easily be proved for superfluids, where the Heisenberg model reduces to an XY model. After a duality transformation, the XY model can be reexpressed as a sum over a grand-canonical ensemble of non-self-backtracking vortex lines [3,4] whose proliferation completely describes all properties of the superfluid transitions. They produce the same critical exponents as a complex ϕ^4 theory, and the reason for this is simple: the XY model may be converted into a complex ϕ^4 theory by a transformation of integration variables in the functional integral of the partition function [4].

The question whether directional or size fluctuations drive a phase transition does therefore not concern the immediate vicinity of the transition where the properties are universally governed by a critical exponent ω. It is only a meaningful question in the *precritical* regime of the transition, where a mean-field description of a system breaks down. There it possesses an answer similar to the Ginzburg criterion which estimates the temperature range where this happens due to *size fluctuations* of the order field. The new criterion to be presented in this note will tell us where the breakdown is caused by *directional fluctuations*. In the case of a complex order field, these lead to an early proliferation of vortex lines before size fluctuations become large.

The new criterion serves to understand the dominance of directional fluctuations in the recently discovered restoration of continuous symmetry in Gross-Neveu [5] and Nambu–Jona-Lasinio models [6], and, more importantly, the generation of a pseudogap phase above the superfluid phase in strong-coupling superconductors [7].

In order to lead up to the new criterion, we briefly recall the relevant features of the field-theoretic approach to the critical exponents in the immediate vicinity of second-order phase transitions [1]. Since critical properties are caused by the long-wavelength fluctuations of a system, it is sufficient to identify these, assign to each of them a real order field $\phi_A(x)$, $A = 1, \ldots, N$, the local generalization of Landau's order parameter [8], and set up a Ginzburg-Landau energy density. Its fluctuations are studied with the help of a functional integral over all field configurations, weighted by a Boltzmann factor of the total field energy.

At a moderate temperature distance $|T - T_c|$ from the critical temperature T_c, the functional integral may be evaluated by the saddle point approximation. This is the mean-field regime of the field theory. When approaching the critical point, the fluctuations of the order parameter increase. They become important in a temperature regime ΔT_G around T_c, whose width was first estimated by the famous Ginzburg criterion [9]: It is the regime where the fluctuations of the order parameter in pockets of coherence size reach into the normal phase.

The Ginzburg-Landau field energy density is found from phenomenological studies of a system in some neighborhood of the critical temperature [8]. One expands the energy density in powers of the order field and its derivatives. Then one identifies the temperature interval where all expansion terms are irrelevant except for those appearing in a simple ϕ^4 theory. At some *mean-field critical temperature* $T_c^{\rm MF} \neq T_c$, correlation lengths become infinite in the mean-field approximation. The mass term goes through zero linearly in $T/T_c^{\rm MF}$, i.e., the bare square mass m^2 is proportional to $\tau \equiv T/T_c^{\rm MF} - 1$.

As the system enters the critical regime, fluctuations of the order parameter become important and must be accounted for. This is done by perturbative methods. Each physical quantity of interest is expanded into a Taylor

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series of the reduced interaction strength g/m^{4-D}, and a resummation of these in the limit $m \to 0$ allows us to extract power laws m^{power}, which determine the critical exponents [10].

We shall now demonstrate that in systems with a continuous symmetry, the Ginzburg criterion is not sufficient to characterize the temperature range where fluctuations are important. A system will exhibit strong directional fluctuations before the size fluctuations of the order parameter become noticeable, leading to a phase transition at a temperature T_K far below the Ginzburg temperature T_G.

For simplicity, we restrict the argument to N order fields ϕ_A with O(N) symmetry in D dimensions. With a convenient choice of field and mass normalization, the Ginzburg-Landau energy density in D dimensions may be written as

$$\varepsilon(\phi_A, \partial\phi_A) = \frac{1}{2a^D}\left\{\alpha^2 a^2[\partial\phi_A(x)]^2 + \tau\phi_A^2(x) + \frac{g}{2}[\phi_A^2(x)]^2\right\}.$$

From here on we use natural units with $k_B T_c^{\text{MF}} = 1$. The fields have zero engineering dimension; a denotes some microscopic length scale of the system, usually the size of atoms or molecules, and g is some interaction strength. The parameter α specifies the zero-temperature coherence length of the system in units of a as being $\xi_0 = \alpha a/\sqrt{2}$. This can vary greatly from system to system. In superconductors, for example, α can lie anywhere between a few thousand, and less than ten in high-temperature superconductors.

In this note, we shall be concerned only with the destruction of the ordered state which lies *below* the critical temperature where $\tau < 0$: There the fields in the energy density fluctuate around an ordered ground state with a constant vector $\langle\phi_A\rangle \equiv \Phi_A \equiv \langle\phi\rangle N_A \equiv \Phi N_A$ in field space, whose direction vector N_A breaks spontaneously the O(N) symmetry, and whose magnitude is $\Phi = \sqrt{\Phi_A^2} = \sqrt{-\tau/g}$, where the energy density is minimal, fluctuating around the condensation energy density $\varepsilon_0 = \varepsilon(\Phi_A, 0) = -\tau^2/4ga^D$. The temperature-dependent coherence length $\xi = \alpha a/\sqrt{2|\tau|}$ describes the range of the size fluctuations of the order field.

The magnitude is estimated by assuming the field to live in patches on a simple cubic lattice of spacing $\xi_l = l\xi$, choosing eventually a spacing parameter between $l = 1$ and $l = 2$ to ensure the independence of the patches. Then

$$\langle[\phi(x) - \Phi]^2\rangle/\Phi^2 = l^{2-D}(2|\tau|)^{D/2-2} g\alpha^{-D} v_{l^2}(0), \quad (1)$$

where $v_{m^2}^D(0) = \int_{-\pi}^{\pi} d^D k/(2\pi)^D[\sum_{i=1}^D (2 - 2\cos k_i) + m^2]$ is the lattice Coulomb potential of reduced mass m. It is equal to $\int_0^\infty ds\, e^{-s(m^2+2D)}[I_0(2s)]^D$. For $D = 3, 4, \ldots$, $v_1^D(0)$ has the values [11]

$$v_1^D(0) \approx 0.1710, 0.1270, \ldots, 1/2D. \quad (2)$$

Mean-field behavior breaks down if (1) is of the order unity, which happens at the reduced Ginzburg temperature

$$|\tau_G| \approx [K v_{l^2}^D(0)/l^{D-2}]^{2/(4-D)}, \qquad D < 4, \quad (3)$$

where

$$K \equiv 2^{D/2-1} g/\alpha^D, \quad (4)$$

i.e., at a Ginzburg temperature $T_G \equiv T_c^{\text{MF}}(1 - |\tau_G|)$. Ginzburg, in his original paper [9], estimated $v_1^D(0)$ in three dimensions by an integral $\int d^3p/(2\pi)^3(p^2 + 1) \approx (2\pi^2)^{-1}\int_0^\pi dp\, p^2/(p^2 + 1) \approx 1/4\pi$, and assumed $l = 1$, which lead to $|\tau_G| \approx (g/\alpha^3)^2/8\pi^2$. In "old-fashioned" type-II superconductors, $|\tau_G|$ can be as small as 10^{-8} [12], which explains why conventional superconductors are well described by mean-field theory. In modern high-T_c superconductors, on the other hand, Ginzburg's estimate leads to $|\tau_G| \approx 0.01$ [13], such that critical exponents become observable.

For $D > 4$, the right-hand side in (1) decreases when approaching the critical point, so only mean-field behavior is observed. If $D = 4 - \varepsilon$ lies only slightly below 4, the right-hand side of (3) behaves like $|\tau|^{-\varepsilon/2}$, implying a good mean-field description until $|\tau|$ is extremely small.

The derivation of the new criterion is based on the observation that the kinetic term defines a second, completely independent, energy scale of the system. For its identification, we split the fields according to size and direction in O(N) field space as $\phi_A = \phi n_A$, $n_A^2 = 1$. The directions n_A describe the long-range fluctuations of the Goldstone modes. Sufficiently far from the critical regime, we may neglect the gradient term of the size $\phi(x)$, and approximate the energy density by

$$\varepsilon(\phi, \partial n_A) = \frac{1}{2a^D}\left\{\alpha^2 a^2 \phi^2(x)[\partial n_A(x)]^2 + \tau\phi^2(x) + \frac{g}{2}\phi^4(x)\right\}.$$

The fluctuations of the Goldstone modes are controlled by the gradient term whose magnitude depends on the size Φ of ϕ at the minimum of the potential. The gradient energy density is

$$\varepsilon_{n_A}(\partial n_A) = \frac{\beta}{2\xi_l^{D-2}}[\partial n_A(x)]^2, \quad (5)$$

with

$$\beta = \beta(\Phi) = \alpha^2(\xi_l/a)^{D-2}\Phi^2 = \alpha^D l^{D-2}/(2|\tau|)^{D/2-2} g.$$

This is the second energy scale. It measures how much energy is spent when reversing the direction vector n_A over the distance ξ_l, and is called the *stiffness* of the directional field.

From studies of O(N)-symmetric classical Heisenberg models it is known that directional fluctuations disorder a system if the bending stiffness drops below a certain critical value $\beta_{\rm cr}$. For large N, this value can easily be estimated by a simple manipulation of the functional integral for the partition function associated with the energy (5). It may be written as [14]

$$Z_{n_A} = \int \mathcal{D} n_A\, \mathcal{D}\lambda\, e^{-(\beta/2\xi^{D-2})\int d^D x \{[\partial n_A(x)]^2 + \lambda(x)\,[n_A^2(x)-1]\}},$$

where the unit length of $n_A(x)$ is enforced by a Lagrange multiplier field $\lambda(x)$. Integrating out the $n_A(x)$ fields leaves us with a pure $\lambda(x)$-field theory, with an energy functional

$$E[\lambda] = \frac{N}{2}\,\mathrm{Tr}\log[-\partial^2 + \lambda(x)] - \frac{\beta}{2\xi^{D-2}} \int d^D x\, \lambda(x)\,. \tag{6}$$

For large N, the fluctuations of the λ field are frozen, and the disordered state has an energy density given by the extremum of (6), where $\lambda(x)$ is a constant satisfying the gap equation $\beta = \beta_\lambda \equiv N v_\lambda^D(0)$. The order is destroyed at a critical stiffness at $\beta_{\rm cr} = \beta_0$. On a simple cubic lattice, we find in three, four, and large-D dimensions [11]:

$$\beta_{\rm cr} = N v_0^D(0) \approx N0.2527, N0.1549, N/2D\,, \tag{7}$$

respectively. Formula (7) is reliable only for large N. However, Monte Carlo simulations show that the critical value (7) can be trusted already for $D = 3$ and $N = 2$ to within about 10%, where simulations yield $\beta_{\rm cr}^{\rm MC} \approx 0.45$ (see [15]), in good agreement with the value 0.5054 from (7). The simulations are done by putting the Heisenberg model on a lattice of unit spacing, so that the energy density for $N = 2$ takes the *XY* model form $\varepsilon_{n_A}(\partial n_A) \approx \beta \sum_{\mu=1,\ldots,D}[1 - \cos\nabla_\mu \gamma(x)]$, where ∇_i denotes the lattice gradient in the ith coordinate direction, and $\gamma \equiv \arctan n_2/n_1$. Since the quality of the approximation increases with N and D, we can trust Eq. (7) to within 10% for all N and $D \geq 3$. This accuracy will be sufficient for the criterion to be derived here.

The critical stiffness can, incidentally, be also estimated by calculating its renormalized version from a sum of an infinite number of terms in a perturbation expansion. Expanding the cosine into a Taylor series, and calculating the harmonic expectation values of quartic, sextic, etc., terms, we find in a self-consistent approximation of the Hartree-Fock-Bogoliubov type that the stiffness has a renormalized value [16] $\beta_R = \beta e^{-1/2D\beta_R}$. This softens with increasing temperature $1/\beta$, until β reaches a critical value $\beta_{\rm cr} = e/2D$, where β_R drops to zero (see Fig. 1). In $D = 3$ dimensions, this happens at $\beta_{\rm cr} = 0.4530, \ldots$, a value which is in excellent agreement with the Monte Carlo number $\beta_{\rm cr}^{\rm MC} \approx 0.45$. The prediction of such sharp drop is true only in two dimensions, as shown by Kosterlitz and Thouless [17]. For $D > 2$ it is an artifact of the approximations, and the true ρ_s goes to zero like $|T_c - T|^{(D-2)\nu}$, with a critical exponent $\nu \approx 1/2 + (4 - D)/10 + \ldots$.

The estimate for the critical stiffness (7) leads now directly to the announced criterion: The phase fluctuations will disorder the system if the stiffness β in Eq. (5) drops below the critical value (7), which happens at a reduced temperature

$$|\tau_K| \approx [NK v_0^D(0)/l^{D-2}]^{2/(4-D)}, \qquad D < 4, N \geq 2\,. \tag{8}$$

Thus we obtain the important result that

$$|\tau_K| \approx [N v_0(0)/v_{l^2}^D(0)]^{2/(4-D)}|\tau_G|, \qquad D < 4, N \geq 2\,. \tag{9}$$

This implies that for all systems with $N \geq 2$, directional fluctuations destroy the order *before* size fluctuations become large. They cause a phase transition below the Ginzburg temperature, at $T_K \equiv T_c^{\rm MF}(1 - |\tau_K|)$. For $D = 3$, and $l = (1, 3/2, 2)$, the relation becomes $|\tau| \approx (2.20, 3.48, 5.56)N^2|\tau_G|$. Thus, if the critical regime is approached in a ϕ^4 theory with a well-formed mean-field regime, the transition is *always* initiated by directional fluctuations. In particular, the estimates for the critical regime of the high-$|T_c|$ superconductors [13] will receive a factor of ≈ 9.

The dominance of directional fluctuations is, of course, most prominent for the limit of large N, and it is therefore not surprising that the critical exponents of the ϕ^4 theory and the Heisenberg model have the same $1/N$ expansions in any dimension $D > 2$, as a pleasant demonstration of the universality of critical phenomena.

By adding to the field energy density $\varepsilon(\phi, \partial n_A)$ the energy density of directional fluctuations with the field-dependent stiffness $\beta = \beta(\phi) = \alpha^D \phi^2 l^{D-2}/(2|\tau|)^{D/2-1}$ we can study, as in Ref. [6], the combined energy density in the disordered phase where the symmetry is restored but the average Φ of the size of the order field ϕ in nonzero.

How do we determine experimentally the fluctuation parameter K to estimate $|\tau_G|$ and $|\tau_K|$? In magnetic systems, one measures the susceptibility tensor $\chi_{AB}(k) \equiv \int d^D x\, e^{ikx}\langle\phi_A(x)\phi_B(0)\rangle$ at wave vector k, and decomposes it into parallel and perpendicular parts as $\chi_{AB}(k) = (\Phi_A\Phi_B/\Phi^2)\chi_\parallel(k) + (\delta_{AB} - \Phi_A\Phi_B/\Phi^2)\chi_\perp(k)$. The

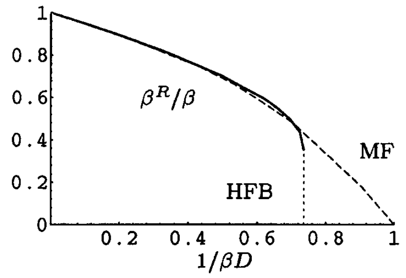

FIG. 1. Softening of the stiffness of the *XY* model derived from a self-consistent approximation *à la* Hartree-Fock-Bogoliubov. The dashed curve shows the mean-field approximation given by $\rho_s = \alpha^2/4D^2\beta^2$, $\beta = \alpha I_0(\alpha)/2DI_1(\alpha)$ [$I_n(\alpha)$ = modified Bessel functions] which goes to zero linearly in $|\tau|$. The exact stiffness goes to zero like $|T_c - T|^{(D-2)\nu}$, with the critical exponent ν ($\approx$0.6705 for $D = 3$ [2]).

mean-field behaviors of these quantities are $\chi_{\|}(k) \approx a^3/(\alpha^2 a^2 k^2 + 2|\tau|)$ and $\chi_{\perp}(k) \approx a^3/\alpha^2 a^2 k^2$. Combining these at $k = 0$ with the mean-field behavior of the spontaneous magnetization $\Phi = \sqrt{|\tau|/g}$, and with the temperature-dependent coherence length ξ, we see that the size of K can immediately be estimated from a plot, versus $t \equiv T/T_c - 1$, of either of the dimensionless experimental quantities

$$K_{\rm exp} \approx |t|^{2-D/2} \frac{k^2}{\xi^{D-2}} \frac{\chi_{\perp}(k)}{k_B T \Phi^2}\bigg|_{k\to 0} \qquad (10)$$

or

$$K_{\rm exp} \approx |t|^{2-D/2} \frac{1}{\xi^{D}} \frac{\chi_{\|}(0)}{k_B T \Phi^2}, \qquad (11)$$

these being written down in physical units. Note that t measures the temperature distance from the experimental T_c, in contrast to $\tau \equiv T/T_c^{\rm MF} - 1$. In the mean-field regime, where $t \approx \tau$, $K_{\rm exp}$ is constant, and can be inserted into Eq. (8) to find the temperature T_K where directional fluctuations destroy the order.

In superfluid helium we may plot, in analogy to the transverse susceptibility expression for $K_{\rm exp}$, the quantity $K_{\rm exp} \approx |t|^{2-D/2} M^2 k_B T/\xi^{D-2}\hbar^2 \rho_s$, where M is the atomic mass and ρ_s the superfluid mass density, which at the mean-field level is defined by writing the gradient energy (5) as $(\rho_s/2k_B T)(\hbar^2/M^2)[\partial n_A(x)]^2$. In the critical regime, the three expressions for $K_{\rm exp}$ go universally to zero like $|t|^{2-D/2}$, since $\xi \propto |t|^{-\nu}$, $\chi_{\|}(0) \approx |t|^{(\eta-2)\nu}$, $k^2\chi_{\perp}(k)|_{k\to 0} \approx |t|^{\eta\nu}$, $\Phi^2 \approx |t|^{\nu(D-2+\eta)}$, $\rho_s \approx |t|^{(D-2)\nu}$, with $\eta \approx [(N + 2)/2(N + 8)^2](4 - D)^2 + \dots$.

Experimentally, the superfluid density of helium for $D = 3$ shows no mean-field behavior *à la* Ginzburg-Landau down to $T \approx T_c/4$, such that the above formulas cannot properly be applied. Let us nevertheless estimate orders of magnitude of a would-be mean-field behavior: $\rho_s/\rho \approx 2|\tau|$ [18], where $\rho = M/a^3$ is the total mass density, with $a \approx 3.59$ Å [19]. Then the factor $k_B T_c$ at $T_c = 2.18$ K can be expressed as $k_B T_c \approx 2.35\hbar^2/Ma^3$ [19]. With $\xi_0 \approx 2$ Å, we obtain an estimate $K \approx 1.2a/\xi_0 \approx 2$. Inserting this into Eq. (8) and relation (9), we obtain for $l = 1$ and $l = 2$

$$(|\tau_K|, |\tau_G|) \approx (1, 0.12) \quad \text{and} \quad (1/4, 0.03). \qquad (12)$$

The large size of $|\tau_K|$ reflects the bad quality of a mean-field description. The larger l gives the more physical estimate.

The author is grateful to B. Van den Bossche for many discussions, and to Dr. E. Babaev, Dr. J. Jersak, Dr. A. Pelster, Dr. A. Schakel, and Dr. K. Wiese for useful comments.

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