Avoided Critical Behavior in $O(n)$ Systems

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Long-range frustrating interactions, even if their strength is infinitesimal, can give rise to a dramatic proliferation of ground or near-ground states. As a consequence, the ordering temperature can exhibit a discontinuous drop as a function of the frustration. We have found this phenomenon in an entire class of models: amphiphilic systems, Mott insulators, and gauge theories of metallic glasses, to name a few.

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A wide variety of systems display equilibrium domain patterns characterized by periodic (or nearly periodic) variations of an order parameter. These patterns are stabilized by competing interactions. Linear arrays of stripes and hexagonal arrays of bubbles are ubiquitous in thin films of magnetic garnets and ferrofluids. Similar morphologies are also seen in Langmuir films, membranes, semiconductor surfaces, and many other systems in which an otherwise uniform ground state is thwarted by a competing "frustrating" interaction of one sort or another [1]. Lately, stripe structures have been detected [2] in doped Mott insulators, including the high T_c superconductors: the ordered states in these compounds consist of arrays of charged stripes which form antiphase domain walls between antiferromagnetically ordered spin domains. In the absence of a frustrating Coulomb interaction (i.e., for neutral holes), a lightly doped Mott insulator is unstable to phase separation into a hole-rich "metallic" phase and a hole-deficient antiferromagnetic phase. Electrostatic repulsions forbid macroscopic charge separation; the compromise leads to the formation of stripe morphologies on an intermediate scale [3,4].

In this Letter, we explore the effect of fluctuations on the periodic structures in a simple model of uniformly frustrated $O(n)$ spins. We study the problem using two complementary approaches: a low temperature, spin-wave expansion, and a perturbative expansion for large n, which we carry through to order $1/n^2$. It is found that the ordering temperature, $T_c(Q)$, as a function of the strength of the frustrating interaction "Q" may, in certain instances, satisfy the inequality

$$T_c(Q = 0) > \lim_{Q\to 0} T_c(Q) . \tag{1}$$

In other words, an infinitesimal amount of frustration depresses the ordering temperature discontinuously. Specifically, we shall argue on the basis of a low temperature expansion about stripelike ground states, that, in the absence of lattice effects, $T_c(Q) = 0$ for $n > 2$ and $Q > 0$. Lattice anisotropies elevate $T_c(Q)$ from zero, but the discontinuity in $T_c(Q)$ persists for $2 < d \leq 3$ and $n > 2$. For $n = 2$, the lower critical dimension is three, and here the finite temperature "ordered" phase exhibits power law decay of correlations; the model with $n = 2$ has the same hydrodynamic description as a smectic liquid crystal.

For low frustration Q, the behavior of the system is controlled by the proximity to the "avoided critical temperature" $T_c(Q = 0)$. The following picture emerges of the thermal evolution of the model, as summarized in Fig. 1: At temperatures somewhat above $T_c(Q = 0)$, *two large lengths* govern the exponential decay of correlations. As the temperature is lowered below a crossover temperature $T_1(Q) \sim T_c(Q = 0)$, the system enters a low temperature regime characterized by an oscillatory spin structure function with a *single length* controlling the exponential decay of correlations at long distances. $T_1(Q)$ is a

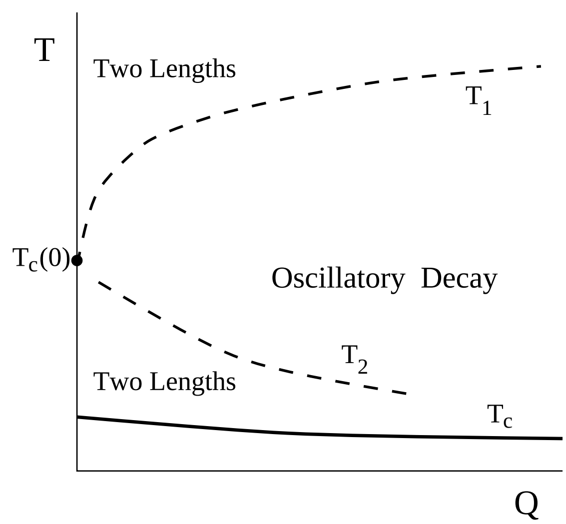

FIG. 1. Schematic phase diagram: Q is the strength of the frustration. For $T > T_1(Q)$ and $T_2(Q) > T > T_c(Q)$, there are two long lengths governing the fall of correlations. For $T < T_1(Q)$, the spin-spin correlation function exhibits long distance oscillatory structure. The thick black dot marks $T_c(Q = 0)$, the ordering temperature in the absence of frustration; this is what we term "the avoided critical point." In the continuum limit, $T_c(Q > 0) = 0$; lattice effects result in a nonzero, yet small $T_c(Q)$.

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"disorder line" in the sense that as T approaches T_1 from below, the wavelength of the oscillations diverges, but no phase transition occurs. As T is lowered further, the wavelength decreases until, as $T \to T_c(Q)$, it smoothly approaches the period of the ordered phase that appears below $T_c(Q)$. However, an additional crossover occurs at a temperature $T_2(Q)$ which lies between $T_c(Q)$ and $T_1(Q)$, such that for $T_2(Q) \gg T \gg T_c(Q)$, there are again two long lengths characterizing the falloff of correlations, where the new length is akin to the Josephson length in the ordered phase of the unfrustrated system. This second length can be seen only in the context of a $1/n$ expansion. The existence of multiple correlation and modulation lengths is a common feature of the physics of all the various frustrated systems alluded to above [1]. A finite size scaling analysis, which is a simple extension of an argument presented previously [5] allows us to identify the longest length in the temperature regime above T_1 and below T_2 as a "domain" size, R, within which the physics is essentially that of the unfrustrated system, and to extract the scaling relation (which is reproduced by the large n results)

$$R \sim \sqrt{Q/\xi_0}\,, \tag{2}$$

where $\xi_0 \sim [T_c(Q=0) - T]^{-\nu}$ is the correlation length in the unfrustrated system at temperature T.

The Coulomb frustrated ferromagnet.—As a concrete example, we consider a system with a short-range tendency to phase separation which is frustrated by a long-range Coulomb interaction. A simple spin Hamiltonian which represents these competing interactions is

$$H_0 = -\sum_{\langle \vec{x},\vec{y}\rangle} S(\vec{x})S(\vec{y}) + \frac{Q}{2}\sum_{\vec{x}\neq\vec{y}} \frac{S(\vec{x})S(\vec{y})}{|\vec{x}-\vec{y}|}\,. \tag{3}$$

Here, $S(\vec{x})$ is a coarse grained scalar variable which represents the local charge density. Each site $\vec{x}$ lies on a cubic lattice (of size N) and represents a small region of space in which $S(\vec{x}) > 0$, and $S(\vec{x}) < 0$ correspond to the positively and negatively charged phases, respectively. The first "ferromagnetic" term represents the short-range (nearest-neighbor) tendency to phase separation, while the second term is the Coulomb interaction. Nonlinear terms in the full Hamiltonian typically fix the locally preferred values of $S(\vec{x})$. One may consider $d \neq 3$ dimensional variants wherein the spins lie on a hypercubic lattice, and the Coulomb kernel in H_0 is replaced by $Q|\vec{x}-\vec{y}|^{2-d}$. H_0 can be Fourier transformed as

$$H_0 = \sum_{\vec{k}} J(\vec{k})\,|S(\vec{k})|^2, \tag{4}$$

where the kernel

$$J(\vec{k}) = \frac{1}{2}\,[Qk^{-2} + r_0 + k^2 + \ldots], \tag{5}$$

where $r_0 = -2d$, and the ellipsis represents higher order terms in powers of k. We will neglect these terms for now, as they are unimportant in the continuum; however, we will need to include some of these terms when we treat lattice effects since they are the ones that reduce the full rotational symmetry of free space to the point group symmetry of the lattice [6].

We now generalize this model, allowing the spins to have n components, and replacing all two spin products in H_0 with a scalar product. We treat both the "soft-spin" version of this model, in which we include the nonlinear interaction

$$H_{\mathrm{soft}} = H_0 + u\sum_{\vec{x}}[\mathbf{S}^2(\vec{x}) - 1]^2 \tag{6}$$

with $u > 0$, or the "hard-spin" version, which can be viewed as the $u \to \infty$ limit of the soft-spin model, in which we instead enforce the local constraint, $|\mathbf{S}(\vec{x})| = 1$.

When $n \geq 2$, we can construct a set of ground-state configurations which are simple spirals of the form

$$\mathbf{S}^g(\vec{x}) = \mathbf{a}\cos(\vec{k}_{\min}\cdot\vec{x}) + \mathbf{b}\sin(\vec{k}_{\min}\cdot\vec{x})\,, \tag{7}$$

where $\vec{k}_{\min}$ denotes any wave vector which minimizes the interaction kernel, $J(\vec{k})$, in H_0, and the prefactors satisfy

$$\mathbf{a}\cdot\mathbf{b} = 0; \qquad \mathbf{a}\cdot\mathbf{a} = \mathbf{b}\cdot\mathbf{b} = 1\,. \tag{8}$$

It is readily seen that such states are unstable to transverse fluctuations. One may expand H_{soft} to quadratic order in fluctuations about the ground state $\Delta\mathbf{S}(\vec{x}) = [\mathbf{S}(\vec{x}) - \mathbf{S}^g(\vec{x})]$ and estimate the thermal average of $\Delta\mathbf{S}^2(\vec{x})$. For $d = 3$ and a vanishing lower cutoff ϵ on $||\vec{k}| - |\vec{k}_{\min}||$,

$$\frac{\langle(\Delta\mathbf{S})^2\rangle}{T} = \frac{(n-2)\sqrt{Q}}{4\pi^2\epsilon} - \frac{1}{16\pi}\,Q^{1/4}\ln|\epsilon|\,. \tag{9}$$

For $n > 2$, the leading order divergence is $O(\epsilon^{-1})$, independent of d; for XY spins ($n = 2$) the leading order divergence, in $2 \leq d < 3$, is $O(\epsilon^{d-3})$. In $d = 3$, XY spins exhibit power law correlations at low temperatures. As we show, for small Q and $n = 2, 3$, these simple spirals are the only possible ground states; for $n \geq 4$ other types of "multispiral" ground states are possible.

The three-dimensional spherical model.—To make the phase diagram nontrivial, yet tractable, we may solve the scalar spin model subject to the single mean spherical constraint [1,7]

$$\sum_{\vec{x}}\langle S^2(\vec{x})\rangle = N\,. \tag{10}$$

It is known [8] that, in many respects, the spherical model [9] is equivalent to the $n \to \infty$ limit of the $O(n)$ model. Here, the effective Hamiltonian is the same H_0 defined above, with $r_0 \to r$, where r is a Lagrange multiplier determined implicitly from the constraint equation (10). In order that all modes have a bounded Boltzmann weight it is necessary that $r \geq -2\sqrt{Q}$. By equipartition, $\langle|S(\vec{k})|^2\rangle = T[k^2 + Q/k^2 + r]^{-1}$, so the mean spherical constraint reads

$$\frac{1}{T} = \int_{|\vec{k}|<\Lambda}\frac{d^3k}{(2\pi)^3}\,\frac{1}{k^2 + Qk^{-2} + r}\,, \tag{11}$$

where Λ is an ultraviolet cutoff. If this equation cannot be satisfied for any value of $r \geq -2\sqrt{Q}$, then the system is at or below criticality.

Observe, from Eq. (11), that for $Q > 0$, the integral diverges when $r \to -2\sqrt{Q}$. Thus, the constraint can be satisfied for any nonzero T: $T_c(Q > 0) = 0$. By contrast, when $Q = 0$ (which is the standard three-dimensional short-range ferromagnet) T_c is nonzero. Thus a discontinuity in $T_c(Q)$ is seen to exist. However, even though $T_c = 0$ for $Q > 0$, there is a genuine zero temperature phase transition with the usual $n \to \infty$ critical exponents, e.g., $\nu = 1$ and $\gamma = 2$ in $d = 3$. As we shall see, lattice effects elevate $T_c(Q)$ but do not change the critical properties, nor, in $d = 3$, eliminate the discontinuity.

The pair correlator is given by

$$G(\vec{x}) = \frac{1}{(2\pi)^3} \int d^3k \, \langle |S(\vec{k})|^2 \rangle \exp[i\vec{k} \cdot \vec{x}]$$
$$= \frac{T}{2\pi^2|\vec{x}|} \int_0^\infty dk \, \frac{k^3[\mathrm{Im}\{e^{ik|\vec{x}|}\}]}{(k^2 + \alpha^2)(k^2 + \beta^2)}, \quad (12)$$

where

$$\alpha^2, \beta^2 = \frac{r \mp \sqrt{r^2 - 4Q}}{2}. \quad (13)$$

When $r > 2\sqrt{Q}$, the integral can be readily evaluated by applying the residue theorem to the poles lying on the imaginary axis at $k = \pm\imath\alpha, \pm\imath\beta$,

$$G(\vec{x}) = \frac{T(\beta^2 e^{-\beta|\vec{x}|} - \alpha^2 e^{-\alpha|\vec{x}|})}{4\pi|\vec{x}|(\beta^2 - \alpha^2)}. \quad (14)$$

Note the existence of two macroscopic correlation lengths—a consequence of charge neutrality: In H_0, the spins portray charges and therefore must sum to zero,

$$\int G(\vec{x})\, d^3x = \left\langle \left| \int S(\vec{x})\, d^3x \right|^2 \right\rangle = 0. \quad (15)$$

Whenever G is dominated by its long-distance behavior, the integral can vanish only if $G(x)$ contains positive and negative contributions, as in Eq. (14). The latter integral can be made to vanish only if $G(\vec{x})$ contains at least two length scales. At high temperatures, the length

$$\xi_1 \equiv |\mathrm{Re}\{\beta\}|^{-1} \approx r^{-1/2} \quad (\text{for } r \gg 2\sqrt{Q}). \quad (16)$$

plays the role of the correlation length of the canonical short-range ferromagnet (i.e., with $Q = 0$). Note that now, however, an additional correlation length appears:

$$\xi_2 \equiv |\mathrm{Re}\{\alpha\}|^{-1} \approx Q^{-1/2}/\xi_1. \quad (17)$$

Thus, $\xi_2 \gg \xi_1$ in the limit of weak frustration, $Q \ll 1$. The analytic continuation of Eq. (14) to low temperatures, $r < 2\sqrt{Q}$, is

$$G(\vec{x}) = \frac{T}{4\pi} \exp(-\alpha_1|\vec{x}|) \times \left[\frac{(\alpha_2^2 - \alpha_1^2)\sin\alpha_2|\vec{x}| + 2\alpha_1\alpha_2\cos\alpha_2|\vec{x}|}{4\alpha_1\alpha_2|\vec{x}|} \right], \quad (18)$$

where $\alpha \equiv \alpha_1 + \imath\alpha_2$. The temperature T_1, defined by $r(T = T_1) = 2\sqrt{Q}$, marks a dramatic crossover. At low temperatures ($T < T_1$), the system possesses a single correlation length $\xi = |\alpha_1|^{-1} = 2[r + 2\sqrt{Q}]^{-1/2}$ and a single modulation length $L_D = 2\pi/|\alpha_2| = 4\pi[-r + 2\sqrt{Q}]^{-1/2}$; at high temperatures ($T > T_1$), the system possesses two distinct correlation lengths. When $T = T_1^-$, the modulation length diverges as $L_D \sim (T_1 - T)^{-1/2}$. Many quantities of interest (e.g., the specific heat C_V) albeit analytic, display a crossover at $T_1(Q)$. As Q tends to zero, the crossover temperature $T_1(Q)$ tends to $T_c(Q = 0)$. Thus despite the nonexistence, for $Q = 0^+$, of a phase transition at or near $T_c(Q = 0)$, the system is governed, in part, by the proximity to the *avoided* critical temperature $T_c(Q = 0)$.

Avoided critical behavior to $O(n^{-2})$.—We will now examine corrections to the spherical limit. In a $(1/n)$ expansion [10], the soft term of constraint, $[H_{\mathrm{soft}} - H_0]$, is taken to be small with $u = O(1/n) > 0$. The perturbation theory in u is then selectively resummed treating $1/n$ as the small parameter. As our unperturbed Hamiltonian, we take H_0 in Eq. (3) with a temperature dependent chemical potential, $r_0 + 2\sqrt{Q}$, which changes sign at $T = T_{MF}$, and is increasingly negative at low T. The Dyson equation implies

$$G^{-1}(\vec{k}) = G_0^{-1}(\vec{k}) + \Sigma(\vec{k}), \quad (19)$$

where, in the continuum limit, $G_0^{-1} = r_0 + k^2 + Qk^{-2}$, and $[-\Sigma(\vec{k})]$ is the self-energy. T_c, if it exists, is determined implicitly from the solution of the equation

$$\min_{\vec{k}}\{G^{-1}(\vec{k})\} = 0. \quad (20)$$

To zeroth order in $1/n$,

$$G^{-1}(\vec{k}) = r + k^2 + Qk^{-2}. \quad (21)$$

Here $r = r_0 + \Sigma^0$, where $[-\Sigma^0]$ denotes the self-consistently computed $O(n^0)$ correction to the self-energy. At low temperatures,

$$\Sigma^0(Q, r) \approx \Sigma^0(Q = 0, r = 0) + \frac{nu}{\pi}\sqrt{\frac{Q}{r + 2\sqrt{Q}}}, \quad (22)$$

where $\Sigma^0(Q = 0, r = 0)$ is the value of the $O(n^0)$ self-energy at criticality for the standard three-dimensional ferromagnet and the second term is the $O(n^0)$ self-energy of a one-dimensional spin chain with a nearest-neighbor exchange interaction proportional to $1/Q$. Since Σ^0 is manifestly positive and diverges as $r \to r_{\min} = -2\sqrt{Q}$, Eq. (20) is satisfied only in the limit $r_0 = -\infty$; to this order $T_c(Q > 0) = 0$. We have extended this analysis [7] to $O(n^{-2})$. By evaluating diagrams self-consistently, one observes that all $O(n^{-1})$ and $O(n^{-2})$ self-energy contributions are explicitly positive or cancel against more divergent positive contributions. We outline here how this is done to $O(n^{-1})$. In Fig. 2, the $\vec{k}$-independent $\Sigma^0 > 0$ is the single zeroth order $[O(n^0)]$ contribution. To $O(n^{-1})$ there are two additional diagrams: $\Sigma^A(\vec{k})$ and the

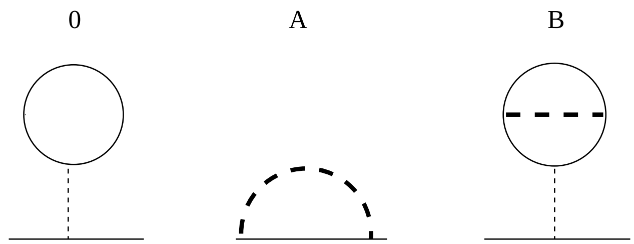

FIG. 2. The self-energy corrections: The thin dashed lines denote bare interaction, the thick dashed lines represent dressed interactions (i.e., bare interactions screened by a geometric series of bubble diagrams), and the solid lines denote propagators.

$\vec{k}$-independent Σ^B. Inserting, self-consistently, $G(\vec{k}) = [G_0^{-1}(\vec{k}) + \Sigma^0 + \Sigma^A(\vec{k})]^{-1}$ into the integral expression $\Sigma^0 = \int \frac{d^3k}{(2\pi)^3} G(\vec{k})$ automatically generates Σ^B, as well as higher order diagrams. This integral diverges as $r \to r_{\min}$. The self-energy Σ^A is positive and thus can only further thwart any tendency to order. A similar analysis [7] may be repeated to $O(n^{-2})$.

All this indicates that to $O(n^{-2})$, $r = r_{\min}$ is attainable only at $T_c = 0$. Unfortunately, the results of the $1/n$ expansion are not independent of Q for small Q; we cannot safely draw conclusions concerning the $Q \to 0$ limit as there could, in principle, be a change in the behavior of the system when $Q \sim 1/n$. Nevertheless, the results strongly support the contention that the $n \to \infty$ limit is not singular, and that the spherical model captures the important physics of the system for any large n.

Algebraic crossover.—We have also computed the pair correlator to $O(n^{-1})$. At very low temperatures, where $0 < r + 2\sqrt{Q} \ll \sqrt{Q}$, the propagator at intermediate momenta ($1 \gg |\vec{k}| \gg Q^{1/4}$) is

$$G^{-1}(\vec{k}) \approx k^2 + [2\Sigma^0/(n^2u)]|\vec{k}| + r + Qk^{-2}. \quad (23)$$

We note that

$$\begin{aligned} G(|\vec{x}|) &\sim |\vec{x}|^{-2} \quad \text{for } \ell_J \ll |\vec{x}| \ll L_D \ll \xi \\ G(|\vec{x}|) &\sim |\vec{x}|^{-1} \quad \text{for } |\vec{x}| \ll \ell_J\,, \end{aligned} \quad (24)$$

where the correlation length $\ell_J \equiv n^2u/(2\Sigma^0)$ is defined in a way analogous to the Josephson length [11] in the ordered phase of a system with Goldstone modes. Thus at sufficiently low temperatures, $T < T_2$, the (nonoscillatory) spatial behavior of the correlators is again governed by two length scales.

Lattice effects.—The fact that the lattice system has discrete rather than continuous rotational symmetry is reflected in higher order terms in powers of k, in the kernel $J(\vec{k})$ in Eq. (5); the lowest order term of this sort is $\lambda \sum_{a=1}^d k_a^4$. The effects of these terms was determined previously [6] for $n \to \infty$; they produce a $T_c(Q > 0) > 0$, but the avoided critical phenomena, i.e., the fact that $\lim_{Q\to 0} T_c(Q) < T_c(0)$, survives for $2 < d \leq 3$. More generally, if we apply the above spin-wave analysis and a Lindemann criterion for T_c, then the same calculation leads to the conclusion that, once again, the large n results are qualitatively correct for finite n.

Multispiral states.—Whenever $n \geq 2$, any ground-state configuration can be decomposed into Fourier components, $\mathbf{S}^g(\vec{x}) = \sum_{i=1}^M \{\mathbf{a}_i \cos[\vec{k}_{\min}^{(i)} \cdot \vec{x}] + \mathbf{b}_i \sin[\vec{k}_{\min}^{(i)} \cdot \vec{x}]\}$, where $\vec{k}_{\min}^{i}$ are chosen from the set of wave vectors which minimize $J(\vec{k})$. So long as these wave vectors are "nondegenerate," in the sense that the sum of any pair of wave vectors, $\vec{k}_{\min}^{i} \pm \vec{k}_{\min}^{j}$ is not equal to the sum of any other pair of wave vectors, and "incommensurate" in the sense that for all i and j, $2(\vec{k}_{\min}^{i} + \vec{k}_{\min}^{j})$ is not equal to a reciprocal lattice vector, it is straightforward to prove [7] that the condition $[\mathbf{S}^g(\vec{x})]^2 = 1$ can be satisfied only if $M \leq n/2$. (These conditions are always satisfied for $Q < 4$.) Thus, for $n \leq 3$ only simple spiral ($M = 1$) ground states are permitted, while for $n = 4$, a double spiral saturates the bound.

Metallic glasses.—Metallic glasses have been modeled by an SO(4) Landau-Ginzburg theory with a uniform frustrating background [12]—the fields represent projections of the mass density onto a 4-sphere. The curvature κ of the 4-sphere is an inherent geometric frustration. It is straightforward to demonstrate that in the minimal model there is an avoided critical point: $T_c(\kappa > 0)$ vanishes, while $T_c(\kappa = 0)$ is finite, lending support to [5].

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