Crossover from Fluctuation-Driven Continuous Transitions to First-Order Transitions

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Near a tricritical point of an n-component spin system, fluctuations turn the first-order transition (predicted by the Landau theory) into second order. We show that when this happens, quadratic anisotropies turn the transition first order again. In systems which exhibit fluctuation-driven first-order transitions, increasing anisotropies yield two consecutive tricritical points. These effects are predicted to result from the application of magnetic fields or uniaxial stresses to MnO, $BaTiO_3$, $KTa_xNb_{1-x}O_3$ (KTN), TbP, etc.

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In most cases, Landau's theory[1] provides a correct qualitative description of phase transitions, including their order. It was only recently realized that a variety of transitions, predicted by Landau's theory to be continuous, are *driven by fluctuations to be first order.*[2,3] Technically this happens when there exists no fixed point which is accessible under the renormalization-group (RG) iterations. As the RG is iterated, and the fluctuations are gradually eliminated, the effective Hamiltonian flows into a range of instability where even the Landau theory predicts a first-order transition.

Much less attention has been given to *fluctuation-driven continuous transitions*. In the present Letter we emphasize that *such transitions always occur in the vicinity of tricritical points*. Starting with the usual Landau-Ginzburg-Wilson Hamiltonian for n-component spins $\{\vec{S}(\vec{x})\}$ in d dimensions,

$$\mathcal{H} = \int d^dx \, \{\tfrac{1}{2}|\nabla\vec{S}|^2 + \tfrac{1}{2}r|\vec{S}|^2 + u_4|\vec{S}|^4 + u_6|\vec{S}|^6 + O(|\vec{S}|^8)\}, \qquad (1)$$

the Landau theory predicts that the transition becomes first order for $u_4 < 0$ ($u_6 > 0$). In fact, fluctuations shift the tricritical point down to $\tilde{u}_4 = 0$, with[4-6]

$$\tilde{u}_4 = u_4 + C(n)u_6, \quad C(n) = \tfrac{3}{2}K_4(n+4), \quad K_4 = 1/8\pi^2. \qquad (2)$$

In the range $-C(n)u_6 < u_4 < 0$ we can thus consider the continuous phase transition as being driven by fluctuations.[7] The crucial role played by u_6, which is essential for stability when $u_4 < 0$, has been ignored in many earlier discussions.

A very useful tool in the study of critical behavior has been the application of symmetry-breaking fields.[8] In particular, the quadratic anisotropy

$$\mathcal{H}_g = \tfrac{1}{2}g\int d^dx \, [m|\vec{S}_{n-m}|^2 - (n-m)|\vec{S}_m|^2]/n, \qquad (3)$$

where $\vec{S}_{n-m}$ and $\vec{S}_m$ are the $(n-m)$- and m-component parts of the vector $\vec{S}$, will generate a crossover from the n-component critical behavior to that of the m- [or $(n-m)$-] component one for $g > 0$ [< 0]. For convenience, we consider only g

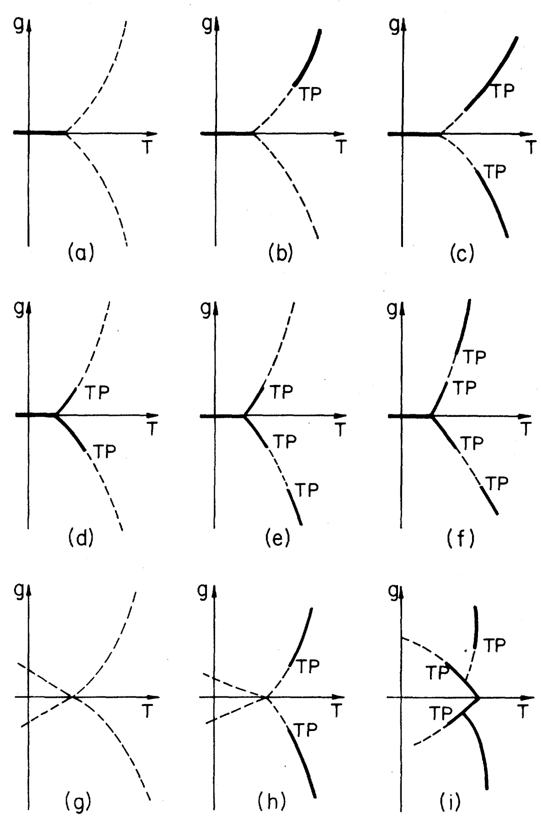

FIG. 1. Schematic g-T phase diagrams. Dashed (full) lines represent second- (first-) order transitions. TP is a tricritical point. The (high-T) transitions for $g > 0$ (< 0) are into an m- [$(n-m)$-] component phase [we chose $m < (n-m)$]. (a)–(c) are for the isotropic case; (d)–(f) are for the cubic case, with $u_6 < \bar{u}_6$ and $v < 0$; and (g)–(i) are for the cubic case and $v > 0$. Each "triplet" of figures corresponds to decreasing values of u_4.

>0, the results for $g<0$ being obtainable by replacing $g \to -g$ and $m \to (n-m)$. If $u_4>0$, Eq. (3) generates the well-studied *bicritical* phase diagram,[8] shown in Fig. 1(a), observable in many anisotropic antiferromagnets under a magnetic field,[9] in structural transitions under uniaxial stress,[10] etc. In the present Letter we show that when $-C(n)u_6<u_4<-C(m)u_6$, then the application of the anisotropy field g may *turn the fluctuation-driven continuous transition,* expected for the n-component system, *back into first order* [Figs. 1(b) and 1(c)]. As function of g, the tricritical point ($\tilde{u}_4=0$ at $g=0$) splits into two tricritical lines (Fig. 2), given for small $g>0$ by

$$\tilde{u}_{4,t}=[u_4+C(n)u_6]_t=B_m g_t^{\psi}, \quad \psi=\tfrac{1}{2}d-1. \tag{4}$$

A similar expression, with B_{n-m} and $-g_t$ replacing B_m and g_t, describes the tricritical line for $g<0$. The ratio $B_m/B_{n-m}=(n-m)/m$ is universal. Since $\psi<1$, the two tricritical lines approach the u_4 axis tangentially. Similarly, the tricritical points in Figs. 1(b) and 1(c) are given by $g_t=A_m t_t$ and $g_t=-A_{n-m}t_t$, with $t_t=[T_t(g)-T_t(g=0)]/T_t(g=0)$ and $A_m/A_{n-m}=m/(n-m)$. These results are valid for $d>3$. At $d=3$ they may be modified by logarithmic corrections,[4] and the exponents describing the curves in the u_4-g and g-t planes will have a different dependence on d for $d<3$.[5]

It has recently been shown[11-14] that symmetry-breaking fields like Eq. (3) may turn fluctuation-driven *first-order* transitions *back to second order* [(Fig. 1(d)]. This effect has indeed been observed in MnO (Ref. 15) and in $RbCaF_3$ (Ref. 16) under appropriate uniaxial stresses. Note that *the new effect predicted in this Letter is the "inverse" of the one observed there.* Moreover, we find that *if the fluctuation-driven first-order transition occurs in the vicinity of a tricritical point* (which bounds the range of attraction of an accessible fixed point) *then there is a range in which the symmetry breaking first turns the fluctuation-driven first-order transition into second order, and then turns it back into first order, via two consecutive tricritical points* [Figs. 1(e) and 1(f)].

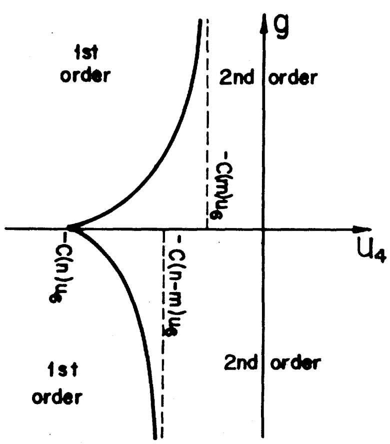

FIG. 2. Schematic g-u_4 phase diagram, $m<(n-m)$. The (tricritical) lines separate regions of second- and first-order transitions.

The new effects predicted in Figs. 1(b), 1(c), and 2 will occur near *isotropic* n-component tricritical points, with $n \geq 2$. In the simple examples of this kind, e.g., that of ^{3}He-^{4}He mixtures,[17] it is impossible to break the symmetry experimentally. However, we predict the effects to be observable near tricritical points such as that of MnO.[2,11,15] A uniaxial stress $p>p_t \simeq 5$ kbar[15] along [111] turns the fluctuation-driven first-order transition of the eight-component antiferromagnetic order parameter into a continuous one, described by an isotropic two-component order parameter vector [in the (111) plane]. For $p \gtrsim p_t$, we predict that a magnetic field in the (111) plane will yield Figs. 1(b), 1(c), and 2 (u_4 is represented here by p, and $m=1$).

Figures 1(e) and 1(f) will be realized, e.g, for the cubic to tetragonal ferroelectric transitions in $BaTiO_3$,[18] or $KTa_xNb_{1-x}O_3$ (KTN).[19] In such systems, there is an additional cubic interaction[8]

$$\mathcal{H}_v=v\sum_{\alpha=1}^{n}(S^\alpha)^4, \quad v<0. \tag{5}$$

Landau's theory[1] predicts a first-order transition for $u_4+v<0$, while we find that fluctuations shift the tricritical point to $w=\tilde{u}_4+3v/(4-n)\simeq 0$. Increasing the hydrostatic pressure on $BaTiO_3$,[18] or the concentration x in KTN,[19] moves the parameters u_4, v, and u_6 through this tricritical surface. As this pressure (concentration) is increased we predict that additional uniaxial stress along, e.g., [100] will yield the sequence of diagrams shown in Figs. 1(f), 1(e), 1(d), and 1(a) ($n=3$, $m=1,2$).

Another possible realization is TbP.[2,14,20] A uniaxial stress or a magnetic field along [111] may turn this $n=4$ fluctuation-driven first-order transition into an $n=3$ (cubic) continuous one. Additional uniaxial stress along $[\bar{1}11]$, $[\bar{1}\bar{1}1]$, or $[1\bar{1}1]$ will then yield our Figs. 1(e) and 1(f).

Our analysis starts with the Hamiltonians (1) and (3). Equation (2) simply follows from the fact that under the RG iterations u_6 generates new contributions to u_4. The correct scaling field near the Gaussian fixed point ($u_4 = u_6 = 0$) describing the tricritical point is thus $\tilde{u}_4$, and not u_4. Higher-order terms are not expected to modify this qualitative picture. For $g \gg 1$, the fluctuations in the $(n-m)$-components of $\vec{S}_{n-m}$ become small, and we can integrate $\vec{S}_{n-m}$ out of the partition function, leaving an effective m-component spin Hamiltonian.[12] In this Hamiltonian, which has the same form as Eq. (1), the new coefficients will be $u_6^{\rm eff} \simeq u_6$ and $u_4^{\rm eff} \simeq u_4 + 3(n-m)\, I_1(r_{n-m})\, u_6$, where $r_{n-m} = r + mg/n$, $I_k(x) = \int_{\vec{q}} (x+q^2)^{-k}$, and where we ignore corrections of higher order in u_4 and u_6.[21] This m-component Hamiltonian will now have a tricritical point at $\tilde{u}_4^{\rm eff} = 0$, i.e.,

$$\tilde{u}_{4,t}^{\rm eff} = [u_4^{\rm eff} + C(m) u_6^{\rm eff}]_t = \tilde{u}_{4,t} + 3(n-m)[I_1(r_{n-m}) - \tfrac{1}{2}K_4]u_6 = 0. \quad (6)$$

Since $I_1(r)$ is monotonically decreasing with r, it follows that if $-C(n)u_6 < u_4 < -C(m)u_6$ then $\tilde{u}_4^{\rm eff}$ will change sign as function of g, becoming negative for sufficiently large g (Fig. 2). For very large g, the tricritical point occurs at $g_t \simeq -3(n-m)K_4 u_6/\{4[u_4 + C(m)u_6]\}$. Similar results are found for $g < 0$.

For small g we must first eliminate some of the fluctuations.[6, 12] We iterate the RG transformation until $r_{n-m}(l^*) \simeq 1$ (for $g > 0$), and then integrate $\vec{S}_{n-m}$ out of the partition function. In the vicinity of the Gaussian fixed point, in $d = 4 - \epsilon$ dimensions, one recovers Eq. (6), in which $\tilde{u}_4$, u_6, and r_{n-m} are replaced by $\tilde{u}_4 \exp(\epsilon l^*)$, $u_6 \exp[-2(1-\epsilon)l^*]$, and 1. Demanding also that the effective temperature scaling field, $t^{\rm eff}(l^*) \simeq [t - (n-m)g/n] \exp(2l^*) + O(u_4, u_6)$ $\{$where $t = [T - T_t(g=0)]/T_t(g=0)$ is a combination of r, u_4, and $u_6\}$, should vanish, we end up with Eq. (4) and $B_m = [\frac{3}{2}K_4 - 3I_1(1)](n-m)u_6 = \frac{3}{2}K_4 \ln 2 (n-m)u_6$. The ratio B_m/B_{n-m} thus follows immediately. Similarly, we find that $A_m = n/(n-m)$.

In terms of Hamiltonian flows in the u_4-u_6 plane, we start above the line $\tilde{u}_4 = u_4 + C(n)u_6 = 0$ and iterate l^* times. For small g, the flow crosses the m-component tricritical line, $u_4(l^*) + C(m)\, u_6(l^*) = 0$, and the m-component transition remains second order. For large g the flow ends below this line, and the transition becomes first order.

To obtain Figs. 1(d)-1(f), we now add the cubic Hamiltonian, Eq. (5).[22] In the presence of v, the condition for tricriticality becomes $w = \tilde{u}_4 + 3v/(4-n) = 0$, representing a plane in the u_4-u_6-v space. Points below this plane will have a first-order transition (no accessible fixed point), points on this plane will have a tricritical behavior (flow to the "cubic" fixed point),[8] and points above this plane will have a continuous transition (flow to the "Heisenberg" fixed point, with $v = 0$). We next eliminate $\vec{S}_{n-m}$ (either directly, for $g \gg 1$, or after l^* RG iterations), and obtain an effective m-component Hamiltonian. To leading orders, $u_4^{\rm eff}$ and $u_6^{\rm eff}$ are the same as before, and $v^{\rm eff} \simeq v$. We then find $w^{\rm eff}$ as a function of g, and solve $w^{\rm eff}(g) = 0$ for tricriticality. Including terms of order u_4^2, this equation has *two acceptable solutions* if $u_6 < \bar{u}_6 = -2v/[K_4(4-n)(4-m)]$ and $u_4 + C(m)\, u_6 + 3v/(4-m) < 0$.[23] This generates Fig. 1(f). In terms of flows, one should note that although u_6 is "irrelevant" (decaying to zero for large l), it drives u_4 towards higher values in the first few iterations.[24] Later, v takes over in driving $w^{\rm eff}$ towards negative values. If one starts sufficiently close to the m-component tricritical plane $u_4 + C(m)\, u_6 + 3v/(4-m) = 0$ (and below it), with $u_6 < \bar{u}_6$, then the flow crosses the plane twice. For $u_6 > \bar{u}_6$ and $w > 0$ we again predict the diagrams of Fig. 1(b) and 1(c). Both the m-component tricritical points found for $g > 0$ in Fig. 1(f) will now be given by $g_t = A_m t_t^{\varphi}$, with $\varphi = 1 + \epsilon/6 + O(\epsilon^2)$ being the anisotropy crossover exponent at the cubic fixed point[8] and with[12] $A_1/A_2 \simeq (\frac{9}{134})^{1/3}$.

The above results are all for $v < 0$, i.e., for *bicritical* phase diagrams. When $v > 0$ and $u_4 > 0$, *tetracritical* points are expected [Fig. 1(g)].[25] We expect that for an appropriate range of $u_4 < 0$ and $u_6 > 0$ this phase diagram will turn into one of those shown in Figs. 1(h) and 1(i).[23]

In conclusion, we have shown that the interplay between fluctuations and symmetry breaking yields many new kinds of tricritical points. We hope that the many physical realizations listed above will stimulate experimental checks of our predictions.

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[21]The perturbation (3) also generates quartic (and higher-order) anisotropies. However, these are of order $u_4^2 g$, and we consistently keep only terms of first order in u_4 and u_6.

[22]Additional cubic terms, e.g., $\Sigma(S^\alpha)^4(S^\beta)^2$ and $\Sigma(S^\alpha)^6$, are assumed to be absent. Their presence will modify the expressions for w and w^{eff} and the relevant range of parameters, but will otherwise not affect our conclusions.

[23]More details will be presented elsewhere.

[24]u_6 is thus a "dangerous irrelevant variable"; see M. E. Fisher, in *Renormalization Group in Critical Phenomena and Quantum Field Theory: Proceedings of a Conference*, edited by J. D. Gunton and M. S. Green (Temple Univ. Press, Philadelphia, 1974).

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