Tricritical Points in Three-Dimensional *XY* Model with Mixed Action

W. Janke[(a)] and H. Kleinert[(a)]
University of California, San Diego, La Jolla, California 92093
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We present theoretical arguments (using mean fields and strong-coupling graphs) for a line of first-order phase transitions in the three-dimensional XY model with the mixed action $\beta\cos(\nabla_i\theta)+\gamma\cos(2\nabla_i\theta)$, where $\gamma\in(0.35,0.40)$, and verify its existence by a Monte Carlo simulation.

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According to a well-known and often cited argument by Coleman and Weinberg,[1] the Abelian Higgs model in four dimensions should always undergo a first-order phase transition if the mass parameter turns negative. Some time ago it was pointed out by one of us[2] that the Monte Carlo finding[3] of a continuous transition in the pure U(1) lattice gauge model suggested, via duality arguments,[4] the existence of a tricritical point in the Abelian Higgs model. Thus there are unforeseen subtleties in the Coleman-Weinberg argument which are worth investigating. This suggestion was taken up in a number of recent papers[5,6] which by now seem to agree that such a tricritical point does indeed exist.

In the three-dimensional Abelian Higgs model, the same argument was put forward once more by Halperin, Lubensky, and Ma.[7] Here, the experimental smoothness of the smectic-A–nematic transition in liquid crystals gave rise to first doubts about its validity.[8] The doubts were confirmed by Monte Carlo studies of the so-called lattice superconductor which showed clearly a continuous transition of the (inverted) λ type.[9]

Making use of the duality of the Abelian Higgs model and the XY model, one of the authors[10] found a theoretical explanation for these simulation data and predicted, in addition, the presence of a tricritical point whenever the two length scales of the model, penetration depth and coherence length, have a ratio smaller than 0.7.

The predicted tricritical point was subsequently observed in two different Monte Carlo simulations of the Abelian Higgs model.[11] Unfortunately, as a result of the large number of fluctuating variables (one complex Higgs field and three real gauge fields) both simulations were unable to determine the important tricritical ratio of the two length scales.

It is obvious that, just as in four dimensions, it will be easier to investigate the tricritical behavior in the dual form of the theory which has only one fluctuating angular variable $\theta\in(0,2\pi)$. This is the planar spin, or XY model. In its standard form, this model is known to have a continuous phase transition. Thus, if we want to study first-order transitions, the standard form needs some modification. From an analysis of the strong-coupling expansion which describes an ensemble of nonbacktracking random loops we know[12] that we have to enhance the loops of strength 2, making it easier for them to condense. The intertwining of the strength-1 and strength-2 loops is what drives the transition first order.

The desired enhancement is made possible by use of a mixed energy

$$-\beta E=\sum_{\mathbf{x},i}[\beta\cos(\nabla_i\theta)+\gamma\cos(2\nabla_i\theta)] \qquad (1)$$

[in this notation, $\nabla_i\theta=\theta(\mathbf{x}+\mathbf{i})-\theta(\mathbf{x})$ are the lattice gradients across the links i] with positive γ. Our analysis is confirmed by the observation[6] that positive γ increases the discontinuity of the transition in the U(1) lattice gauge theory (which is similarly driven by the intertwining of random surfaces of strengths 1 and 2).

In order to see what is happening in the present case and to estimate which value of γ is relevant, it is useful to rewrite the partition function associated with the energy (1) as a field theory of two complex fields u_1 and u_2 and their conjugates α_1 and α_2.[13,14] The fluctuating energy is simply

$$-\beta E=\sum_{\mathbf{x}}\left[\sum_i \tfrac{1}{2}[\beta u_1(\mathbf{x})u_1^\dagger(\mathbf{x}+\mathbf{i})+\gamma u_2(\mathbf{x})u_2^\dagger(\mathbf{x}+\mathbf{i})+\text{c.c.}]-(\alpha_1^\dagger u_1+\alpha_2^\dagger u_2+\text{c.c.})+\ln\tilde I_0(2\alpha_1,2\alpha_2)\right], \qquad (2)$$

where $\tilde I_0(2\alpha_1,2\alpha_2)$ is a generalization of the modified Bessel function,

$$\tilde I_0(2\alpha_1,2\alpha_2)=\int_{-\pi}^{\pi}(d\theta/2\pi)\exp(\alpha_1^\dagger U+\alpha_2^\dagger U^2+\text{c.c.}), \qquad (3)$$

with $U=e^{i\theta}$.

The fields u_1 and u_2 have a simple physical meaning. They are the *disorder fields*[15] of the nonbacktracking random loops of strengths 1 and 2, respectively. If they have a nonzero expectation value, this signals the presence of a condensate of such loops. In the case of $\langle u_1\rangle\neq 0$ this also implies that there are infinitely long loops of strength 1. If $\langle u_2\rangle$ is nonzero, this has a somewhat more indirect meaning. Remembering that $|\langle u_2\rangle|^2$ is also the $|\mathbf{x}|\to\infty$ limit of the correlation function $\langle u_2(\mathbf{x})u_2^\dagger(\mathbf{0})\rangle$ we see that $\langle u_2\rangle\neq 0$ is related to the finiteness of the $|\mathbf{x}|\to\infty$ limit which is caused by the repeated splitup and recombination of finite pieces of lines of strength 2 into long pairs of lines of strength 1. It is the propagation of the latter which causes $|\langle u_2\rangle|^2$ to be nonzero.

We shall now demonstrate how the coupling between these two sets of lines causes the model to have two tricritical points. The position of one, which lies at low γ, is found quite easily by expansion of

$$\ln \tilde{I}_0(2\alpha_1, 2\alpha_2) = \{ |\alpha_1|^2 - \tfrac{1}{4}|\alpha_1|^4 + \tfrac{1}{2}[\alpha_1^2\alpha_2^\dagger + \text{c.c.}] + |\alpha_2|^2 + \tfrac{1}{9}|\alpha_1|^6 - \tfrac{1}{3}|\alpha_1|^2[\alpha_1^2\alpha_2^\dagger + \text{c.c.}] + \dots \} + O(\alpha_1^8, \alpha_1^6\alpha_2, \alpha_1^4\alpha_2^2, \alpha_1^2\alpha_2^3, \alpha_2^4), \tag{4}$$

which, after elimination of the fields u_1, u_2 via the field equations $u_1 = \alpha_1/D\beta$, $u_2 = \alpha_2/D\gamma$, leads to a Landau type of free energy, at constant fields,[16]

$$\beta f = (1/D\beta - 1)|\alpha_1|^2 + (1/D\gamma - 1)|\alpha_2|^2 + \tfrac{1}{4}|\alpha_1|^4 - \tfrac{1}{2}[\alpha_1^2\alpha_2^\dagger + \text{c.c.}] - \tfrac{1}{9}|\alpha_1|^6 + \tfrac{1}{3}|\alpha_1|^2[\alpha_1^2\alpha_2^\dagger + \text{c.c.}] + \dots . \tag{5}$$

Minimizing in α_2 gives

$$\alpha_2 = \tfrac{1}{2}(1/D\gamma - 1)^{-1}[\alpha_1^2 - \tfrac{2}{3}|\alpha_1|^2\alpha_1^2 + \dots], \tag{6}$$

and the free energy takes the form

$$\beta f = (1/D\beta - 1)|\alpha_1|^2 + c_4(\gamma)|\alpha_1|^4 + c_6(\gamma)|\alpha_1|^6 + \dots , \tag{7}$$

with

$$c_4(\gamma) = \frac{1}{4}\left(\frac{1-2D\gamma}{1-D\gamma}\right), \quad c_6(\gamma) = \frac{1}{9}\left(\frac{4D\gamma - 1}{1-D\gamma}\right),$$

revealing the point $(\beta,\gamma)_{\text{tr}} = (1/D, 1/2D)$ as the desired tricritical point [where $(1/D\beta_{\text{tr}} - 1) = 0$, $c_4(\gamma_{\text{tr}}) = 0$, $c_6(\gamma_{\text{tr}}) > 0$]. It obviously belongs to the universality class of a *complex* $|\psi|^6$ theory with vanishing $|\psi|^4$ coupling.

In the random-loop interpretation, the generation of the tricritical point is easy to understand. For small γ and small β, the loops of strength 2 are frozen out. If β exceeds the critical value $1/D$, the loops of strength 1 grow in a continuous λ transition and α_1 becomes nonzero. We now observe that because of the coupling $(\alpha_1\alpha_1\alpha_2^\dagger + \text{c.c.})$, the condensate of strength 1 loops acts as a source (approximately equal to the magnetic field) for the strength-2 line pieces (which might be split along their way into pairs of strength-1 lines). In Feynman-diagram language, the term $\alpha_1\alpha_1\alpha_2^\dagger$ corresponds to the merging of two lines of strength 1 into a bound state of strength 2.

As γ approaches the tricritical value $1/2D$, the number of links occupied by such bound states increases dramatically. This has the consequence that, for $\gamma > 1/2D$, the energy can be lowered even *before* β hits the second-order transition point $1/D$. [There is a certain similarity with the joint condensation of dislocation and disclination lines in the melting process, which is strongly of first order (the former being bound states between two of the latter lines).[17]] At this precocious point, both types of lines condense in an avalanchelike discontinuous phase transition.

The analysis of the upper tricritical point is somewhat more involved. Here $\gamma > 1/D$, and the high-temperature phase is one in which loops of strength 2 are condensed from the beginning with $\alpha_0^0 = D\gamma I_1(2\alpha_2^{(0)})/I_0(2\alpha_2^{(0)})$. In this background the disorder field of loops of strength 1 changes its symmetry properties. If $\alpha_2^{(0)}$ is chosen to be real, α_1 is coupled via $\alpha_2^{(0)}(\alpha_1^2 + \alpha_1^{\dagger 2})$, and hence pairs of *equally* oriented

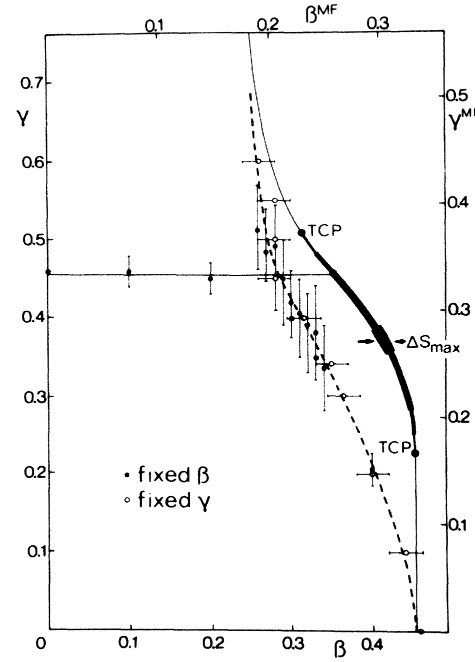

FIG. 1. The phase diagram of the mixed-action XY model as obtained from the Monte Carlo simulations on 16^3 lattices as well as from our mean-field analysis (the latter curves are rescaled in the β and γ directions by a factor 0.45/0.333 in order to account heuristically for the fluctuation corrections). The thickness of the mean-field curve is graded according to steps of $\Delta s = 0.1$. The region where Δs is maximal at the mean-field level is studied further in Figs. 2 and 3 and is found to have a first-order transition, also after including fluctuations.

lines can emerge at and disappear into one site, thus changing the orientational properties of these lines. For large γ, the transition is of second order and therefore in the same universality class as the loops of the high-temperature expansion of the Ising model. The usual symmetry argument relies on the reduction of the U(1) symmetry $\alpha_1 \to e^{i\theta}\alpha_1$ to the Ising symmetry $\alpha_1 \to -\alpha_1$ via $\alpha_2^{(0)}(\alpha_1^2+\alpha_1^{\dagger 2})$. [Notice that previously near the lower tricritical point, the same coupling $(\alpha_2^\dagger\alpha_1^2+\alpha_2\alpha_1^{\dagger 2})$ did not destroy this symmetry since the α_2 field was fluctuating *symmetrically* around the origin.] When γ is no longer large, the expectation of the α_2 field decreases. It is easy to verify that this leads to a *decrease* in the quartic term in α_1. In fact, this term can be expressed via the ratio of modified Bessel functions $q_n = I_n(2\alpha_2^{(0)})/I_0(2\alpha_2^{(0)})$ as follows:

$$c_4(\gamma) = -\frac{1}{32}\,\frac{1-q_1/2\alpha_2^{(0)}-q_1^2}{q_1/\alpha_2^{(0)}+q_1^2-1}+\frac{1}{64}+\frac{1}{24}q_1-\frac{1}{32}\left[\frac{1}{6}q_2-q_1^2\right]. \tag{8}$$

It turns negative at $\gamma=0.3749$. Using $c_2(\beta,\gamma) = \frac{1}{4}(1/D\beta-1-q_1)$ we locate the upper tricritical point at

$$(\beta,\gamma)_{\rm tr} = (3/D)(0.2293, 0.3749). \tag{9}$$

Clearly, this tricritical point is in the same universality class as the *real* ϕ^6 field theory with vanishing ϕ^4 term.

The full mean-field diagram is shown in Fig. 1. We have dilated it by a factor $\beta_c/\beta_c^{\rm MF} \approx 1.35$ so that the pure XY phase-transition points on the β and γ axes agree with the known values $\beta_c = 0.45$ and $\gamma_c = 0.45$, respectively.

In the neighborhood of $\gamma^{\rm MF} \approx 0.275$ ($\gamma \approx 0.37$) the mean-field entropy jump is maximal ($\Delta s^{\rm MF} \approx 0.3$).

In order to confirm the calculated phase structure, we have studied the model by Monte Carlo techniques in the crucial regime $\gamma \in (0.3, 0.4)$, $\beta \in (0.30, 0.35)$ (using the heat-bath algorithm). In Fig. 2, we have shown various cycles over the internal energy which exhibit a hysteresis in the same region in which Δs was

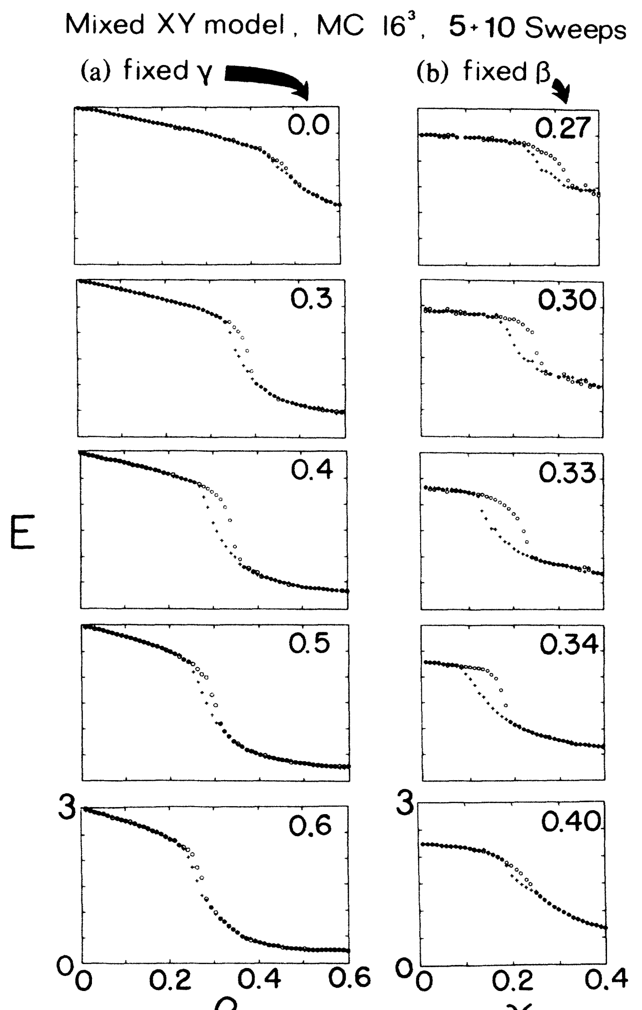

FIG. 2. (a) Thermal cycles in β for various fixed γ showing a hysteresis at $\gamma \approx 0.30$–0.40 as a rough indication for a first-order transition. (b) Thermal cycles in γ for various fixed β showing a hysteresis at $\beta \approx 0.30$–0.35.

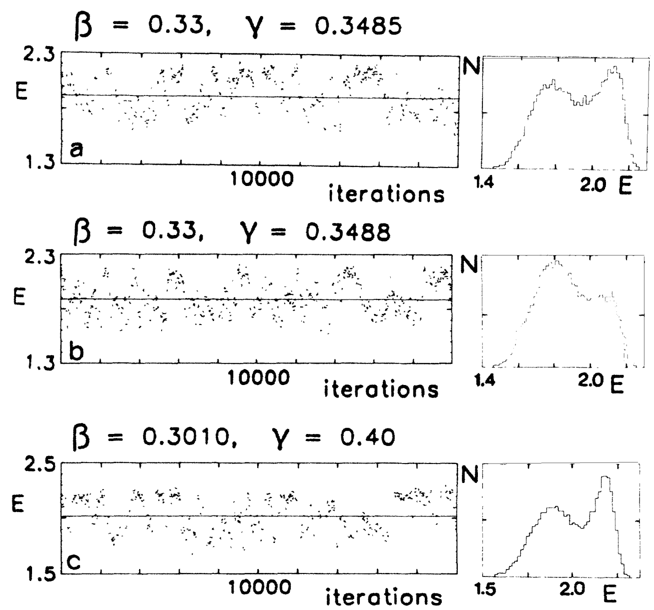

FIG. 3. The time evolution of the internal energy on a 16^3 lattice at three different points (β,γ) near the transition line. They show the jumping back and forth between two minima separated by a barrier typical for a first-order transition. At the right end of each evolution diagram we show the corresponding histograms displaying clearly the double peak of a first-order transition.

found to be large at the mean-field level. In order to verify that Δs is nonzero we have iterated ordered and random initial configurations 20000 times and observed the metastability of these states (see Fig. 3). On the basis of these data we claim evidence for a first-order transition in the range $(\beta,\gamma)=(0.30, 0.40)-(0.33, 0.35)$ with a small entropy jump of $\Delta s \approx 0.1$. Thus we conclude that in three dimensions, fluctuations are still moderate enough to allow for the survival of part of the mean-field jump (remember that for $D \rightarrow \infty$, mean-field results are exact[14]).

Similar runs in two dimensions did not show any sign of a discontinuity.

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[a]On leave from Institut für Theorie der Elementarteilchen, Freie Universität Berlin, Arnimallee 14, 1000 Berlin 33, Germany.

[1]S. Coleman and E. W. Weinberg, Phys. Rev. D **7**, 1888 (1973).

[2]H. Kleinert, Phys. Lett. **93A**, 86 (1982).

[3]B. Lautrup and M. Nauenberg, Phys. Lett. **95B**, 63 (1980).

[4]H. Kleinert, in *Gauge Interactions*, edited by A. Zichichi (Plenum, New York, 1982).

[5]Y. Munehisa, Phys. Rev. D **30**, 1310 (1984), and **31**, 1522 (1985) [also Phys. Lett. **155B**, 159 (1985), for the three-dimensional case]; D. Toussaint and R. Sugar, Phys. Rev. D **32**, 2061 (1985); G. Koutsoumbas, Phys. Lett. B **140**, 379 (1984).

[6]J. Jersák, T. Neuhaus, and P. Zerwas, Phys. Lett. **133B**, 103 (1983); H. G. Everts, J. Jersák, and T. Neuhaus, Nucl. Phys. **B251 [FS13]**, 279 (1985).

[7]B. I. Halperin, T. C. Lubensky, and S. K. Ma, Phys. Rev. Lett. **32**, 292 (1974).

[8]B. I. Halperin and T. C. Lubensky, Solid State Commun. **14**, 997 (1974).

[9]C. Dasgupta and B. I. Halperin, Phys. Rev. Lett. **47**, 1556 (1981).

[10]H. Kleinert, Lett. Nuovo Cimento **35**, 405 (1982).

[11]J. Bartholomew, Phys. Rev. B **28**, 5378 (1983); Y. Munehisa, Phys. Lett. **155B**, 159 (1985).

[12]W. Janke and H. Kleinert, Nucl. Phys. **B270 [FS16]**, 135 (1986).

[13]J. M. Drouffe and J.-B. Zuber, Phys. Rep. **102**, 1 (1983).

[14]E. Dagotto, Phys. Rev. D **30**, 1276 (1984); V. Alessandrini and Ph. Boucaud, Nucl. Phys. **B225 [FS9]**, 303 (1983).

[15]For an introduction into this concept and an analysis of the *XY* model according to it, see H. Kleinert, *Gauge Theory of Stresses and Defects* (Gordon and Breach, New York, 1986).

[16]There is, accidentally, no $\alpha_1^\dagger\alpha_1\alpha_2^\dagger\alpha_2$ coupling.

[17]See H. Kleinert, Phys. Lett. **95A**, 381 (1983).