Transitions in a gauge model for nematic ordering

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(Received 4 August 1994)

We study the phase diagram of the $Z(2)$ gauge model coupled to classical three-component spins in a cubic lattice. This model has been introduced to describe the nematic transition with the gauge term representing a disclination energy. We give the phase diagram in a mean-field approximation, also at negative gauge couplings where two ordered frustrated phases are found. Moreover, by perturbative methods and by expansion on the dual lattice, we study at positive gauge couplings the transitions in the extreme regions of the phase diagram and consider the possibility that the nematic-isotropic transition becomes critical at a tricritical point.

PACS number(s): 64.70.Md, 11.15.Ha, 75.10.−b, 61.30.Jf

Gauge models are introduced in condensed matter physics to represent annealed disorder or defects [1]. Recently, a classical Heisenberg model coupled to Ising gauge variables has been considered [2] to describe the nematic-isotropic transition in liquid crystals. Here the gauge term is interpreted as an energy for disclination defects, and the transition is related to a condensation of defects. Usually, the nematic transition is described in terms of a Landau free energy with a cubic term explaining the first-order behavior [3]. In [2] it is observed that a sufficiently high defect energy cost would make the nematic transition critical. As a different physical interpretation of the same Heisenberg-gauge model we observe that this model could also describe a magnetic system coupled to annealed disorder.

The phase diagram given in [2] is based on numerical simulations and on some expansions at extreme values of the parameters. In this Brief Report we first give the result of a mean-field calculation reproducing the correct topology of the phase diagram. We consider also the case of negative gauge couplings, when the fluid system crystallizes from the nematic phase into a fully frustrated phase [4] through two first-order transitions separating a phase with an intermediate frustration content. Second, we accurately study the transition lines in the extreme regions of the phase diagram by a type of high-temperature or low-temperature expansion. We show how interacting terms arising in these expansions could change the initial critical character of the transitions into a first-order behavior moving inside the phase diagram. In particular, at next to first order in the expansion at large gauge couplings, the model becomes equivalent to a model introduced by Krieger and James [5], which exhibits a tricritical point [5,6]. Therefore the possible appearance of tricritical points in the gauge model of [2] is discussed.

The partition function of the model introduced in [2] is

$$\mathcal{Z}(\beta_M,\beta_G) = \sum_{\{U_{ij}\},\{\mathbf{S}_i\}} \exp\left[\beta_M \sum_{\langle ij\rangle} U_{ij}\mathbf{S}_i\cdot\mathbf{S}_j + \beta_G \sum_{\text{pla}} U_{ij}U_{jk}U_{kl}U_{li}\right], \quad (1)$$

where the $\mathbf{S}_i$'s are three-component unit vectors on the sites of a cubic lattice and the U_{ij}'s are Ising variables defined on the bonds. The sums in the exponent are over nearest neighbors and plaquettes. The model is locally invariant with respect to the gauge transformations $U_{ij}\to\gamma_i U_{ij}\gamma_j$, $\mathbf{S}_i\to\gamma_i\mathbf{S}_i$, with $\gamma_i=\pm1$. It can describe liquid crystals if the vector $\mathbf{S}_i$ represents the molecular-axis direction field. The sum over U_{ij} takes into account the irrelevance of the reciprocal orientation of the spins $\mathbf{S}_i$ and $\mathbf{S}_j$. In particular, at $\beta_G=0$ the sum over U_{ij} gives $\cosh\beta_M\mathbf{S}_i\cdot\mathbf{S}_j$, which has the same physical content of the Maier-Saupe model [7] and coincides with it at small β_M. The plaquette term can be intended as an energy for disclinations [2]. To illustrate this point in a simpler case, consider for example two-component spins on a square lattice. There are two ways depicted in Fig. 1 to realize a frustrated plaquette with $U_{ij}U_{jk}U_{kl}U_{li}=-1$. The corresponding ground-state configurations are characterized by a rotation of 2π [Fig. 1(a)] and 4π [Fig. 1 (b)] of the spin axis around the plaquette [4]. Therefore, if the spin represents the director field, the frustrated plaquette can describe a disclination.

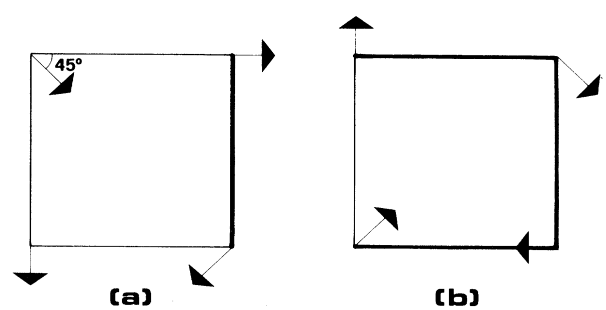

FIG. 1. Two-component spin ground states corresponding to the two bond configurations giving a frustrated plaquette [4]. Bold bonds are antiferromagnetic. Angles between spins are always multiples of $\pi/4$. In (a) the spin rotates by 2π around the plaquette. The rotation angle is calculated by always rotating the spin in the same direction and considering the minimum global rotation. In (b) the spin rotates by 4π. Two other ground states with spins rotating in opposite directions are also possible.

1063-651X/95/51(2)/1590(4)/$06.00

The phase diagram of the model (1) can be studied in the mean-field approximation based on the following expression of the free energy:

$$\mathcal{F}(\beta_M,\beta_G)=-\beta_M\sum_{\langle ij\rangle} l_{ij}\mathbf{m}_i\cdot\mathbf{m}_j-\beta_G\sum_{\rm pla} l_{ij}l_{jk}l_{kl}l_{li}+\sum_i\left[|\mathbf{m}_i|h_i-\frac{\sqrt{2\pi}}{2}\frac{I_{1/2}(h_i)}{\sqrt{h_i}}\right]+\sum_{\langle ij\rangle}\left[\frac{1+l_{ij}}{2}\ln\frac{1+l_{ij}}{2}+\frac{1-l_{ij}}{2}\ln\frac{1-l_{ij}}{2}\right], \quad (2)$$

where l_{ij} and $\mathbf{m}_i$ are the approximated mean values of U_{ij} and $\mathbf{S}_i$, h_i is implicitly defined by $|\mathbf{m}_i|=I_{3/2}(h_i)/I_{1/2}(h_i)$, and $I_{1/2}$ and $I_{3/2}$ are Bessel functions of order $\frac{1}{2}$ and $\frac{3}{2}$, respectively. It can be shown that it is sufficient to study the minima of the free energy (2) over a single cube [8]. The resulting phase diagram is shown in Fig. 2. At positive β_G we find the nematic phase N and the two isotropic phases T and I described in [2]. The vertical line starting from $\beta_G=\infty$, $\beta_M=\frac{1}{2}$ is a critical line separating the region T with $\mathbf{m}_i=\mathbf{0}$ and $l_{ij}l_{jk}l_{kl}l_{li}\approx 1$ from the nematic region at large β_M, where $|\mathbf{m}_i|>0$ and $l_{ij}l_{jk}l_{kl}l_{li}\approx 1$. Here there are 2^N equivalent ground states, corresponding to the gauge degeneracy (N is the number of the sites of the lattice), with all the spins in the same direction coupled ferromagnetically or antiferromagnetically depending on the sign of the bond linking them. The vertical line intersects the first-order line, limiting the high-temperature phase I with $\mathbf{m}_i=\mathbf{0}$, $l_{ij}l_{jk}l_{kl}l_{li}=0$ at the triple point $\beta_M=0.505$, $\beta_G=0.69$. The first-order line starts from the β_G axis at $\beta_G=0.69$ and crosses the horizontal axis at $\beta_M=1.55$, which has to be compared with the value $\beta_M\approx 1.95$ found in Monte Carlo simulations [2]. The N-I transition is also present at small negative values of β_G. By diminishing further the value of β_G, defects proliferate and at sufficiently negative values of β_G and large values of β_M, there is a first-order transition from the nematic phase to a partially frustrated phase PF with four frustrated plaquettes for each cube and a magnetization different from zero. At still more negative values of β_G, after another first-order transition, a fully frustrated phase FF with all plaquettes frustrated is stable. In the gauge with the lowest number of antiferromagnetic links, the bond configuration corresponds to the *odd model* introduced by Villain [4], which has at low temperatures a net magnetization different from zero. Finally, at large negative β_G there is another vertical critical line separating an isotropic frustrated phase FT with $\mathbf{m}_i\approx 0$ and $l_{ij}l_{jk}l_{kl}l_{li}\approx -1$ from the fully frustrated phase. This line intersects the first-order line at the triple point $\beta_M=0.99$, $\beta_G=-0.69$. We observe that, differently from the gauge-invariant Ising model, where the Ising spin variables can be washed away by a gauge transformation, the spins here are not fictitious degrees of freedom and the transition at $\beta_G=0$ is well described in the mean-field approximation.

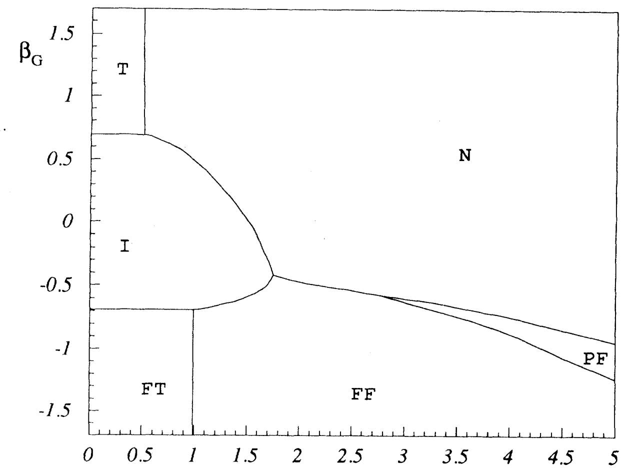

FIG. 2. Phase diagram of the model (1) in the mean-field approximation. The phases T, N, I, FT, PF, and FF are described in the text. The T-N and the FT-FF transitions are continuous, all the other transitions are first order.

The mean-field approximation, on the other hand, does not correctly describe everywhere the nature of the transitions. For example, at $\beta_M=0$ and $\beta_G>0$ the model is dual to the Ising model with a continuous transition at $\beta_G=0.7613=-\frac{1}{2}\ln\tanh\beta_{\rm cr}$, where $\beta_{\rm cr}=0.2217$ is the critical Ising inverse temperature in $d=3$ [9]. A more accurate description of the phase diagram at $\beta_G>0$ can be given by expanding the partition function in the two regions at small β_M and large β_G. The first expansion is a high-temperature expansion of a Heisenberg model with variable exchange interactions. Since only gauge-invariant quantities have to be considered, the expansion reads as

$$Z(\beta_M,\beta_G)=\sum_{\{U_{ij}\}}\exp\left[\beta_G\sum_{\rm pla}U_{ij}U_{jk}U_{kl}U_{li}\right]\sum_{\{\mathbf{S}_i\}}\prod_{\langle ij\rangle}\cosh\beta_M\mathbf{S}_i\cdot\mathbf{S}_j\sum_{\Gamma}\prod_{\langle ij\rangle\in\Gamma}U_{ij}(\tanh\beta_M\mathbf{S}_i\cdot\mathbf{S}_j)\ , \quad (3)$$

where the last sum is over the closed loops Γ of the lattice. If we expand to order β_M^6 and trace over the spins $\mathbf{S}_i$, we get the expression

$$Z(\beta_M,\beta_G)\sim\sum_{\{U_{ij}\}}\exp\left[\beta_G\sum_{\rm pla}U_{ij}U_{jk}U_{kl}U_{li}\right]\left[1+\left[\frac{\beta_M^4}{27}-\frac{4}{405}\beta_M^6\right]\sum_{\rm pla}U_{ij}U_{jk}U_{kl}U_{li}+\frac{\beta_M^6}{243}\sum_{\Gamma^{(6)}}\prod_{\langle ij\rangle\in\Gamma^{(6)}}U_{ij}\right], \quad (4)$$

where $\Gamma^{(6)}$ are the loops of length 6. We see that at the order β_M^4 only the effects of the smaller loops have to be considered, which produce a shift of the gauge coupling β_G as $\beta_G \to \beta_G^{\text{eff}} = \beta_G + \beta_M^4/27$. Therefore, at this order of the expansion, one can predict a critical line given by $\beta_G = 0.7613 - \beta_M^4/27$ and conclude that the Ising transition is stable moving inside the phase diagram, as observed in [2]. However, loops larger than a plaquette could be relevant for the nature of the transition. This can be understood by writing the expression (4) as an Ising spin system on the dual lattice. Following the same procedure discussed in [10], we get the Ising reduced Hamiltonian

$$\mathcal{H}\{s_i\} = \mathcal{J}_{\langle\rangle} \sum_{\langle ij\rangle} s_i s_j + \mathcal{J}_{nnn} \sum_{nnn} s_i s_j + \mathcal{J}_{\text{pla}} \sum_{\text{pla}} s_i s_j s_k s_l + \mathcal{J}_{\text{corn}} \sum_{\text{corn}} s_i s_j s_k s_l \ , \tag{5}$$

where the sums are over nearest neighbors, next nearest neighbors, plaquettes, and corners, that is, clusters of four spins with three of them nearest neighbors to another one on a single cube. In terms of the original parameters the new couplings are given by

$$\mathcal{J}_{\langle\rangle} = \tilde{\beta}_G^{\text{eff}} - \tfrac{4}{243}\beta_M^6 (3\mathcal{C}\mathcal{S} + \mathcal{C}^2\mathcal{S}) \ , \tag{6a}$$

$$\mathcal{J}_{nnn} = \tfrac{2}{243}\beta_M^6 (\mathcal{S}^2 + \mathcal{C}\mathcal{S}^2) \ , \tag{6b}$$

$$\mathcal{J}_{\text{pla}} = \tfrac{2}{243}\beta_M^6 \mathcal{S}^2 \ , \tag{6c}$$

$$\mathcal{J}_{\text{corn}} = -\tfrac{1}{486}\beta_M^6 \mathcal{S}^3 \ , \tag{6d}$$

where

$$\mathcal{C} = \cosh 2\tilde{\beta}_G^{\text{eff}}, \quad \mathcal{S} = \sinh 2\tilde{\beta}_G^{\text{eff}} \ , \tag{7}$$

$$\tilde{\beta}_G^{\text{eff}} = -\tfrac{1}{2} \ln \tanh \beta_G^{\text{eff}} \ , \tag{8}$$

$$\beta_G^{\text{eff}} = \beta_G + \frac{\beta_M^4}{27} - \frac{4}{405}\beta_M^6 \ . \tag{9}$$

The critical line resulting from the study of the model (5)–(9) is shown in Fig. 3, as obtained by Monte Carlo renormalization group calculations (see [10] and Ref. [21] therein). As regards the nature of the transition, we see that the loops of length 6 generate on the dual lattice interactions between four spins, which are expected to change the critical behavior into a first-order behavior. For example, in a mean-field approximation, the model (5)–(9) has a critical line with a tricritical point at $\beta_M = 1.83$. We will discuss later the relevance of this tricritical point for the phase diagram of the model (1).

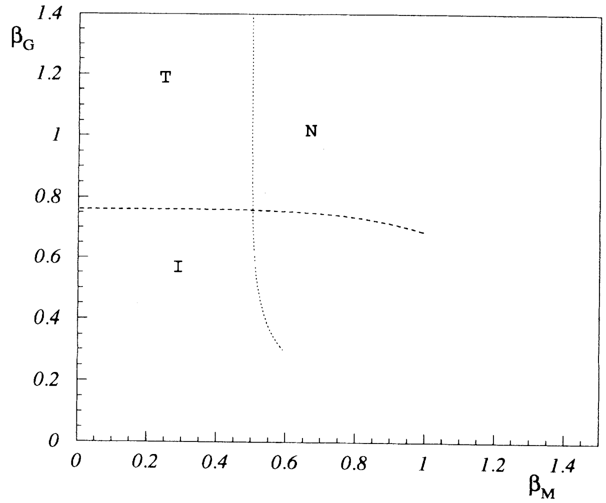

FIG. 3. Critical lines of the model (1) resulting from the expansions (3) and (10).

In principle, a tricritical point could also occur on the vertical transition at positive β_G. The model (1) can be expanded at large β_G. At $\beta_G = +\infty$ each plaquette is not frustrated and the variables U_{ij} can be represented as the product of Ising variables on the sites of the lattice. Then these Ising variables can be adsorbed into a redefinition of the Heisenberg spins and the model is equivalent to the Heisenberg model with a critical transition at $\beta_M \approx 0.69$ [11]. At finite large β_G a few of the plaquettes are frustrated. Considering only excitations with four frustrated plaquettes, we get

$$Z(\beta_M, \beta_G) \approx \frac{2^N}{2} e^{3N\beta_G} \sum_{\{\mathbf{S}_i\}} \left[\exp\left[\beta_M \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j\right] + e^{-8\beta_G} \sum_{\langle kl\rangle} \exp\left[-\beta_M \mathbf{S}_k \cdot \mathbf{S}_l + \beta_M \sum_{\langle ij\rangle \neq \langle kl\rangle} \mathbf{S}_i \cdot \mathbf{S}_j\right]\right]$$
$$\approx \frac{2^N}{2} e^{3N\beta_G} \sum_{\{\mathbf{S}_i\}} \exp\left[\beta_M \sum_{\langle ij\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j + e^{-8\beta_G} e^{-2\beta_M \mathbf{S}_i \cdot \mathbf{S}_j})\right] \ , \tag{10}$$

which gives at small β_M a model described by the reduced Hamiltonian

$$\mathcal{H}\{\mathbf{S}_i\} = \beta_M^{\text{eff}} \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \beta^{(4)} \sum_{\langle ij\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j)^2 \ , \tag{11}$$

with

$$\beta_M^{\text{eff}} = \beta_M (1 - 2e^{-8\beta_G}) \ , \tag{12a}$$

$$\beta^{(4)} = 2e^{-8\beta_G} (\beta_M)^2 \ . \tag{12b}$$

The phase diagram of the model (11) is known in the mean-field approximation [5], in the multicomponent limit [6], and by numerical simulations [12]. The mean-field approximation gives a critical transition at $\beta_M^{\text{eff}} = 0.5$ with a tricritical point at $\beta^{(4)}/\beta_M^{\text{eff}} = \frac{5}{9}$. This corresponds to the critical line $\beta_M = 0.5(1 + 2e^{-8\beta_G})$ with a tricritical point at $\beta_G \approx 0.072$. The approximation of [6] gives the critical line $\beta_M^{\text{eff}} = w/2 - 2\beta^{(4)}(1 - 1/3w)$, where $w \approx 0.505$, with a tricritical point at $\beta^{(4)} = 0.191$. This corresponds in the model (1) to the critical line $\beta_M = w\{1+2[1-w(1-1/3w)]e^{-8\beta_G}\}/2$ with a tricritical point at $\beta_G \approx -0.05$. The position of the tricritical point coming out from simulations [12] is at $\beta^{(4)}/\beta_M^{\text{eff}} = 0.6$. In the following we will use mean-field results since other approximations do not give any significant improvement as regards the phase diagram of the model (1).

The transition line $\beta_M = 0.5(1+2e^{-8\beta_G})$ intersects the other critical line (see Fig. 3) at the point $\beta_M = 0.502$, $\beta_G = 0.758$, which we know from the mean-field approximation and simulations to be a triple point [13]. We have found on these lines tricritical points which occur beyond the triple point so that they are irrelevant at this order of approximation. In this respect the situation is the same as in the gauge-invariant Ising model where tricritical points are analytically predicted beyond the triple point [10]. However, simulations [14] of the gauge-invariant Ising model give tricritical points before the triple point, while here, simulations [2] exclude this possibility. Therefore the tricritical points we have found seem to be really irrelevant. In any case, it is interesting to observe that, differently from what was generally expected, terms of higher order in the expansions (3) and (10) can change the order of the transition.

In conclusion we summarize our results, consisting of a careful description of the phase diagram of the Heisenberg-gauge model (1) and also at negative gauge couplings where new frustrated phases have been found. At positive gauge couplings we have discussed the possibility—not confirmed from simulations [2]—that the nematic-isotropic transition becomes critical at a tricritical point, not at a triple point. Of course, the experimental relevance of this observation is related to the possibility of independently varying the energy of disclinations and the nematic interaction strength [2]. From the theoretical point of view, we say that a better approximation is needed to study the phase diagram of gauge models coupled to matter variables close to the triple point.

The author would like to thank Amos Maritan and Hans van Leeuwen for discussions about the subject of this paper.

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