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Phase diagram for the generalized Villain model

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Berge *et al.* have generalized Villain's fully frustrated XY model on a square lattice by multiplying the antiferromagnetic exchange constant by a factor η. Using the Monte Carlo method, they find that the specific heat displays both Ising-type and Kosterlitz-Thouless-type phase transitions with $T_{\rm I} < T_{\rm KT}$, where $T_{\rm I}(\eta) \rightarrow T_{\rm KT}(\eta)$ as $\eta \rightarrow 1$, thus implying a multicritical point. Using mean-field theory we find a phase diagram in good qualitative agreement with that found by Berge *et al.*, explicitly producing the tetracritical point at $\eta=1$, and providing a physical picture for the structure of the phases. The nonferromagnetic, collinear phase for $\eta>1$ is found to possess antiferromagnetic order. When a magnetic field H is included, the paramagnetic and ferromagnetic phases coalesce to a single collinear phase, and the antiferromagnetic and noncollinear phases coalesce to a single noncollinear phase. The critical surface $H_c(T,\eta)$ separating these phases (which should be characterized by a divergence in the staggered susceptibility) has been determined, again within mean-field theory. A phase-only mode-fluctuation analysis is also presented, yielding results consistent with the mean-field analysis, as well as explicitly revealing the fluctuating modes that become unstable at the transitions; with these modes one can explain the presence (and absence) of susceptibility peaks for the four phase transitions found by Berge *et al.* For $T_{\rm I} < T < T_{\rm KT}$, one and only one mode condenses, leading to a standard KT phase transition.

I. INTRODUCTION

A. Summary of related work

Systems with competing interactions are well known in physics and lead to rich thermodynamic phase diagrams; examples are the antiferromagnetic next-nearest-neighbor Ising (ANNNI) model,[1] and various representatives of XY spin symmetry (such as helimagnets,[2] frustrated models,[3] and arrays of Josephson junctions in an applied magnetic field[4]). Competing interactions lead to frustration, with the result that the true symmetry of the model is not simply given by the number of spin components: for instance, the actual symmetry group of a frustrated XY model is $\mathrm{U}(1)\times\mathbb{Z}_2$ where, in addition to the underlying overall orientational, or U(1), symmetry of the spins, frustration adds a discrete up-or-down, or $\mathbb{Z}_2$, symmetry.[3,5]

For frustrated XY models in two spatial dimensions, the possibility exists that the discrete $\mathbb{Z}_2$ symmetry (the ground state is doubly degenerate) may give rise to an Ising-type transition at a temperature $T_{\rm I}$. This would be in addition to the U(1) symmetry giving rise to the usual Kosterlitz-Thouless (KT) vortex transition at a temperature $T_{\rm KT}$. Arguments based on mean-field (MF) theory indicate that, if two transitions do occur, then $T_{\rm I} \le T_{\rm KT}$. This is because noncollinear ordering (needed in order to obtain the $\mathbb{Z}_2$ symmetry) can only be defined if the spin system already possesses some XY rigidity over a reasonably long length scale, and this happens only when $T_{\rm I} < T_{\rm KT}$ (see also Dzyaloshinskii[6]). On the other hand, arguments based upon considerations of topological defects indicate that one should rather expect $T_{\rm I} \ge T_{\rm KT}$.[7,8] In this case it is argued that vortices of fractional "charge" are localized on domain-wall corners, so that when the domain walls associated with an Ising transition become unstable, the corner vortices unbind, thereby disrupting the XY order.

Nevertheless, for the specific case of Villain's "odd" model of fully frustrated XY spins on the square lattice[3] (where each plaquette has three ferromagnetic and one antiferromagnetic nearest-neighbor bonds of equal strength), numerous studies all suggest that $T_{\rm I}=T_{\rm KT}$. Numerical simulations by Teitel and Jayaprakash[9] were consistent with this result, and the mean-field theory of Shih and Stroud,[10] as well as the renormalization-group analyses by Yosefin and Domany,[11] and by Choi and Stroud,[12] gave this result exactly.

For the fully frustrated antiferromagnetic triangular lattice, with nearest-neighbor antiferromagnetic interactions (FFTR), Monte Carlo (MC) calculations by Miyashita and Shiba[13] indicated that perhaps $T_{\rm I}\neq T_{\rm KT}$, with $T_{\rm I}$ the larger of the two. However, Monte Carlo calculations by Lee *et al.*[14] which also considered the effect of a magnetic field H (thereby lowering the symmetry of the Hamiltonian) supported $T_{\rm I}=T_{\rm KT}$ for $H=0$. (These authors also argued that $T_{\rm I} \ge T_{\rm KT}$ because the Ising transition should trigger the KT transition.) A mean-field analysis, including the effect of H, yielded the exact result $T_{\rm I}=T_{\rm KT}$ for $H=0$.[15] (Note that, in finite H, the structure of the phase diagram in mean-field theory differed substantially from that obtained using Monte Carlo. Specifically, a Potts-type phase was found in Monte Carlo, which does not occur in mean-field theory.) In addition, renormalization-group analyses by Yosefin and Domany,[11] and Choi and Stroud[12] gave $T_{\rm I}=T_{\rm KT}$ exactly.

Additional work on the fully frustrated XY model in two dimensions has been devoted to models that, when an extra parameter is chosen properly, reduce to the triangular FFTR or square Villain models with nearest-neighbor exchange. Van Himbergen[16] has used Monte Carlo calculations to study a triangular model with the same symmetry as the FFTR, but a slightly different interaction, finding results consistent with $T_{\rm I}=T_{\rm KT}$. A number of authors have studied models whose extra parameter can give different symmetries: Berge *et al.*[17,18] studied the square lattice using Monte Carlo techniques; van Himbergen[19] studied the triangular lattice using Monte Carlo techniques; Granato studied the square lattice using renormalization-group techniques;[20] Choi, Chung, and Stroud[21] studied the square lattice using both Monte Carlo and renormalization-group techniques; and Thijssen and Knops[22] studied the square lattice using Monte Carlo techniques. In these cases, the symmetry groups of the models break into two subgroups representing the Ising and XY symmetries, allowing for the possibility of two separate transitions. When these models reduce to the FFTR or the Villain model, they yield $T_{\rm I}=T_{\rm KT}$.

We wish to focus on the model considered by Berge *et al.*[17] These authors introduced a symmetry-breaking field by replacing the antiferromagnetic bonds $-J$ by $-\eta J$ (see Fig. 1). (We shall refer to this as the *generalized Villain model.*) Although the symmetry of the Hamiltonian has changed, one expects, by continuity, that results obtained in the limit $\eta\rightarrow 1$ pertain to the original fully frustrated model of Villain.

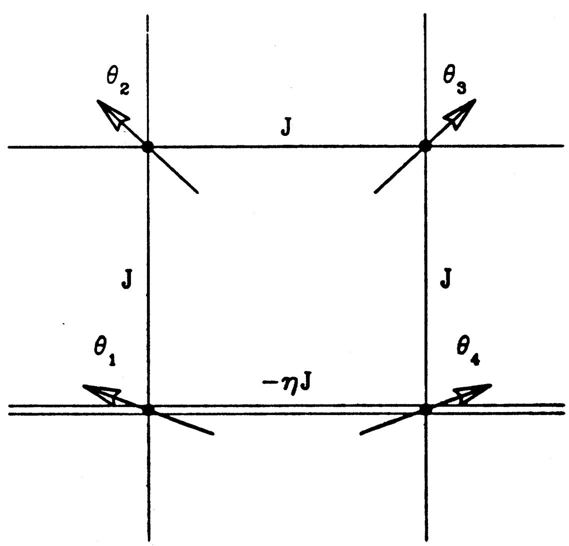

FIG. 1. Generalized Villain model, where the double horizontal lines represent nearest-neighbor bonds of strength $-\eta J$.

Berge *et al.* performed Monte Carlo simulations to obtain the (η,T) phase diagram of this model. For $\frac{1}{3}\leq\eta<1$, on lowering the temperature there was (in the sense of a weak specific-heat peak) a transition of a KT nature, from the paramagnetic phase P to an implicitly ferromagneticlike phase (which we will denote F), accompanied by a divergence in the susceptibility. This was followed by (in the sense of a strong specific-heat peak) a transition of Ising nature, from the F phase to a complex noncollinear phase, with no accompanying divergence in the susceptibility. We denote this phase C (its ground state has two chiralities). For $\eta>1$, on lowering the temperature there was a transition of KT nature from the paramagnetic phase P to a nonferromagnetic, collinear phase, with no accompanying divergence in the susceptibility, followed by a transition of Ising nature, from the nonferromagnetic, collinear phase to the noncollinear phase C, accompanied by a divergence in the susceptibility. Thus, $T_{\rm KT}(\eta)>T_{\rm I}(\eta)$ for $\eta\neq 1$ (in agreement with the mean-field argument). It was also found that $T_{\rm I}(\eta)\rightarrow T_{\rm KT}(\eta)$ for $\eta\rightarrow 1$ (see Fig. 2). Subsequently, Granato and Kosterlitz,[23,24] and later Arosia, Vallat, and Beck,[25] performed a renormalization-group calculation in the Coulomb-gas representation, showing that such a phase diagram is expected for two coupled XY models.

B. Overview of present work

It is the purpose of the present work to study the generalized Villain model both within the context of mean-field theory and a phase-only mode-fluctuation (or

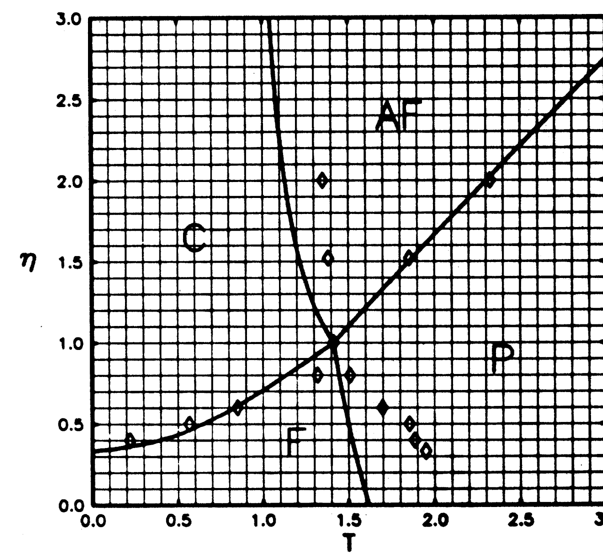

FIG. 2. Mean-field phase diagram for the generalized Villain model in the $H=0$ plane. P stands for the paramagnetic phase, F for the ferromagnetic phase, AF for the antiferromagnetic phase, and C for the noncollinear chiral phase. The diamonds give the Monte Carlo values from Ref. 17, scaled in temperature to make the critical temperatures match. Monte Carlo finds $(T_c/J)_{\rm MC}\approx 0.45$, which is much lower than the mean-field value $(T_c/J)_{\rm MF}=\sqrt{2}$. Thus $(T_c)_{\rm MF}/(T_c)_{\rm MC}\approx 3.14$.

Landau-Ginzburg-Wilson) analysis. These less rigorous approaches have the advantage that they permit an analytic study, from which it is possible to determine the symmetries of each of the states involved. It is not obvious that mean-field theory should yield the same sort of phase diagram as Monte Carlo, but since (as will be seen) there is such a close correspondence [in contrast to the FFTR (Refs. 14 and 15)], it is possible to employ mean-field theory to make more explicit identifications of the various phases. In particular, the mean-field analysis indicates that the nonferromagnetic, collinear phase for $\eta > 1$ is antiferromagneticlike (an identification that has not been made previously), so that in what follows we will refer to that phase as AF. This implies that as one passes from $\eta < 1$ to $\eta > 1$, there is a qualitative change in the local symmetry of the collinear phases that appear, a result that can be tested by further Monte Carlo calculations. Unless in this case mean-field theory is wrong qualitatively (not merely quantitatively), it would appear that for *some* value of η such a symmetry change should occur, at which $T_I = T_{KT}$. From this viewpoint, only the value of η at which this occurs would be in dispute, and mean-field theory concurs with the value $\eta = 1$ obtained by other methods.[17,20,21] Moreover, mean-field theory makes it possible to employ simple arguments to explain: (1) the nature of the phase diagram (and a related phase diagram obtained earlier by DeGennes[26]); (2) the presence (and absence) of peaks in the uniform susceptibility (two of the phase transitions correspond to the onset of ferromagnetic order, and two correspond to the onset of antiferromagnetic, or staggered, order); and (3) the unusual structure of the states for $\eta = 1$.

Using the mode-fluctuation analysis it will be shown that for $\eta \neq 1$ there is a regime ($T_I < T < T_{KT}$) for which the Coulomb-gas analysis, which assumes that two types of XY phases are condensed, is inapplicable because in fact only one type of XY phase is condensed. The coupling of the two types of condensed phases presumably causes the lower transition to be of Ising nature.

In Sec. II we employ the Stratanovich-Hubbard transformation to derive the mean-field equations for the generalized Villain model. From these we obtain the corresponding (η, T) phase diagram. It is strikingly similar to that obtained by Monte Carlo simulations and shows the singular role of the line $\eta = 1$. A discussion is given of the susceptibility maxima found by Berge *et al.* in light of the mean-field theory. We also consider the effect of a magnetic field H on the phase diagram, finding the critical surface $H_c(T, \eta)$ (which should be characterized by a divergence in the staggered susceptibility) that separates the ferromagnetic-collinear (F and P in H) and ferromagnetic-noncollinear (C and AF in H) phases (see Fig. 3). We argue briefly that if a staggered field H_s is included, then in (H_s, T, η) space a surface $H_{sc}(T, \eta)$ exists, characterized by a divergence in the ordinary susceptibility, and separating the antiferromagnetic collinear (AF and P in H_s) and antiferromagnetic noncollinear (C and F in H_s) phases.

In Sec. III we derive the Landau-Ginzburg-Wilson functional appropriate to the present model, in the framework of a phase-only approximation that applies at temperatures for which the amplitudes are frozen but the phases are not. We compute the amplitudes of the fluctuating modes, and briefly reanalyze the critical properties of the model. Its structure is somewhat richer than that of the model studied by Granato and Kosterlitz,[23,24] and its analysis casts light on the role of the fluctuating modes and on the nature of the various transitions. We also remark that $\eta = 1$ and $T > T_I = T_{KT}$ appears to be a disorder line,[27] where correlation functions change over form monotonic to oscillatory behavior. Section IV provides a summary and some concluding remarks.

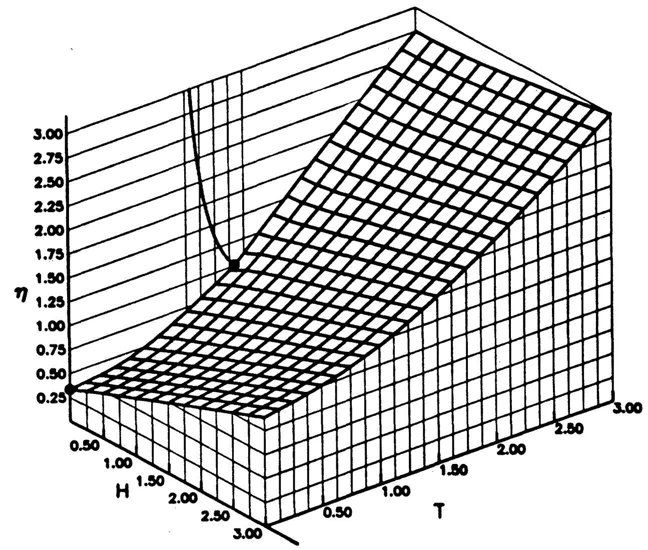

FIG. 3. Critical surface $H_c(T, \eta)$ for the generalized Villain model, from mean-field theory. For H above this surface the system is in the noncollinear phase; for H below this surface the system is in the collinear phase.

II. MEAN-FIELD ANALYSIS

Consider the following Hamiltonian on the square lattice:

$$\mathcal{H} = -\tfrac{1}{2}\sum_{i,j} J_{ij}\mathbf{S}_i \cdot \mathbf{S}_j - \sum_i \mathbf{H}\cdot\mathbf{S}_i \ , \tag{1}$$

where the (double-counting) sum is over nearest-neighbor pairs separated by a unit lattice spacing, the $\mathbf{S}_i$ are classical XY spins of unit length, $\mathbf{H}$ is a magnetic field pointing in the y direction, and the bond couplings J_{ij} are equal to $-\eta J$ on every other row and to $+J$ elsewhere (Fig. 1). The partition function of the model is given by

$$Z = \int \left[\prod_i (D\mathbf{S}_i)\right] \exp(-\beta\mathcal{H}\{\mathbf{S}_i\}) \ , \tag{2}$$

where $\beta = 1/T$.

A Stratonovich-Hubbard transformation of the form

$$\exp\left[\frac{\beta}{2}\sum_{i,j}J_{ij}\mathbf{S}_i\cdot\mathbf{S}_j\right]=\frac{1}{\sqrt{\det\beta \mathrm{J}}}\int\left[\prod_i\left[\frac{D\mathbf{h}_i}{\sqrt{2\pi}}\right]\right]\exp\left[-\tfrac{1}{2}\sum_{i,j}\mathbf{h}_i([\beta \mathrm{J}]^{-1})_{ij}\mathbf{h}_j+\beta\sum_i\mathbf{h}_i\cdot\mathbf{S}_i\right], \quad (3)$$

where $J_{ij}\equiv[\mathrm{J}]_{ij}$, allows one to integrate out each of the angular variables $\mathbf{S}_i$, each integration producing 2π times a Bessel function $I_0(\beta|\mathbf{H}+\mathbf{h}_i|)$. The change of variables

$$\boldsymbol{\Psi}_i=\sum_j([\beta\mathrm{J}]^{-1})_{ij}\mathbf{h}_j \quad (4)$$

then leads to

$$Z=\int\left[\prod_i\left[\frac{D\boldsymbol{\Psi}_i}{\sqrt{2\pi}}\right]\right]\exp(-\beta F\{\boldsymbol{\Psi}_i\}) . \quad (5)$$

Here the $\boldsymbol{\Psi}_i$'s are two-component Gaussian variables with units of magnetization, and

$$-\beta F\{\boldsymbol{\Psi}_i\}=-\tfrac{1}{2}\sum_{i,j}\boldsymbol{\Psi}_i\cdot\beta J_{ij}\boldsymbol{\Psi}_j+\sum_i\ln 2\pi I_0\left[\beta\left|\sum_j J_{ij}\boldsymbol{\Psi}_j+\mathbf{H}\right|\right]+\tfrac{1}{2}\ln\det(\beta\mathrm{J}) . \quad (6)$$

Setting $\delta F/\delta\boldsymbol{\Psi}_i=0$, and employing the local mean-field $\mathbf{H}_i$, one obtains the mean-field equations for the thermal average of the ith spin,

$$\boldsymbol{\Psi}_i^0=\hat{\mathbf{H}}_iR(\beta H_i),\quad \mathbf{H}_i\equiv\sum_j J_{ij}\boldsymbol{\Psi}_j^0+\mathbf{H},\quad R(u)\equiv\frac{I_1(u)}{I_0(u)} , \quad (7)$$

where $I_n(x)$ is the modified Bessel function of order n. Clearly, $R(\beta H_i)$ is the magnitude of the thermal average of the ith spin, and $\hat{\mathbf{H}}_i$ is its direction.

Symmetry considerations and the requirement that the overall magnetization point along $\hat{\mathbf{y}}$ dictate the choice

$$\boldsymbol{\Psi}_i^0=\begin{bmatrix}M_1\sin\theta_1\\ M_1\cos\theta_1\end{bmatrix},\quad \boldsymbol{\Psi}_j^0=\begin{bmatrix}M_2\sin\theta_2\\ M_2\cos\theta_2\end{bmatrix},$$
$$\boldsymbol{\Psi}_k^0=\begin{bmatrix}-M_1\sin\theta_1\\ M_1\cos\theta_1\end{bmatrix},\quad \boldsymbol{\Psi}_l^0=\begin{bmatrix}-M_2\sin\theta_2\\ M_2\cos\theta_2\end{bmatrix} \quad (8)$$

for $\{i,j,k,l\}$ equivalent to $\{1,2,3,4\}$ of Fig. 1. Here

$$M_1=R(\beta H_1),\quad M_2=R(\beta H_2) , \quad (9)$$

$$\tan\theta_1=\frac{2M_1\eta\sin\theta_1+2M_2\sin\theta_2}{-2M_1\eta\cos\theta_1+2M_2\cos\theta_2+H/J} , \quad (10a)$$

$$\tan\theta_2=\frac{-2M_2\sin\theta_2+2M_1\sin\theta_1}{2M_2\cos\theta_2+2M_1\cos\theta_1+H/J} . \quad (10b)$$

The corresponding free energy per plaquette f is given by

$$f=\frac{J}{2}[2M_1M_2\cos(\theta_1-\theta_2)+M_2^2\cos 2\theta_2-\eta M_1^2\cos 2\theta_1]$$
$$-\frac{T}{2}\ln[I_0(\beta H_1)I_0(\beta H_2)] . \quad (11)$$

A. Zero-field case

Simple analytical results may be obtained in the (η,T) plane along three lines: at $T=0$, and along both KT lines, P-F and P-AF. The F-C and AF-C lines must be determined by solving two coupled transcendental equations.

1. *Zero-temperature limit*

At zero temperature one has $M_1=M_2=1$. Then, from Eqs. (10a) and (10b) it follows that $s\equiv\theta_1-\theta_2=2\theta_2$[28] (so $\theta_1=3\theta_2$), and that (with $3s=2\theta_1$)

$$\sin s=\eta\sin 3s ,$$
$$f=(J/2)(3\cos s-\eta\cos 3s) .$$

We thus recover the result of Berge *et al.* that the ground state is ferromagnetic ($s=0$) for $\eta\le\frac{1}{3}$, and canted for $\eta>\frac{1}{3}$. In particular, the canting angle is given by

$$\sin s=\left[\frac{3\eta-1}{4\eta}\right]^{1/2} . \quad (12)$$

2. *The mean-field KT lines*

The P-F and P-AF transitions are of second order, characterized by $M_1,M_2\to 0$. From Eqs. (9) and (10) we obtain

$$\beta_{P\text{-}F}J=\frac{-(1-\eta)+[(1+\eta)^2+4]^{1/2}}{2(1+\eta)}\quad\text{for } \eta<1 ,$$
$$\beta_{P\text{-}AF}J=\frac{(1-\eta)+[(1+\eta)^2+4]^{1/2}}{2(1+\eta)}\quad\text{for } \eta>1 . \quad (13)$$

3. *The noncollinear, or Ising, lines*

The F-C and AF-C transitions are also of second order, characterized by $\theta_1,\theta_2\to 0$ for the F-C boundary and by $\theta_1,\theta_2\to\pi/2$ for the AF-C boundary. From Eqs. (9) we obtain

$$M_1=R(2\beta J|\eta M_1-M_2|) ,$$
$$M_2=R(2\beta J(M_1+M_2)) , \quad (14)$$

and from Eqs. (10a) and (10b) we obtain

$$\left[\frac{M_1}{M_2}\right]_{F\text{-}C}=\frac{-\eta+(\eta^2+\eta)^{1/2}}{\eta}\quad\text{for } \eta<1\ ,$$
$$\left[\frac{M_1}{M_2}\right]_{AF\text{-}C}=\frac{\eta+(\eta^2+\eta)^{1/2}}{\eta}\quad\text{for } \eta>1\ . \tag{15}$$

To find the F-C and AF-C lines, Eqs. (14) are solved numerically.

These results of Eqs. (12)–(14) are summarized in the (η,T) phase diagram of Fig. 2, which clearly has all the features of the MC phase diagram of Berge *et al.* Note, however, that the temperatures at which the phase transitions take place in MC are lower because of the fluctuations included in the MC calculations.

4. *The multicritical point $\eta=1$*

This limit is quite singular in that the minimum of f, Eq. (11), subject to the stationarity conditions [(9) and (10)], is given by $\theta_1+\theta_2=\pi/2$,

$$M_1=M_2\ ,$$
$$\theta_1=3\pi/8,\quad \theta_2=\pi/8 \tag{16}$$

for all T where the system is ordered. In that case, the magnetizations disappear when $\beta J<\beta_c J=\sqrt{2}/2$, where β_c is obtained from (14) with $R(u)\to u/2$, since $u\to 0$ as $\beta\to\beta_c$. (Thus $T_c/J=\sqrt{2}$ in mean-field theory, compared to the Monte Carlo result $T_c/J\approx 0.45$.[17]) Such behavior cannot be obtained by approaching the value $\eta=1$ along the noncollinear or KT lines. Indeed, for $\beta\to\beta_c$, Eqs. (15) yield

$$\frac{M_1}{M_2}\to\sqrt{2}-1\quad\text{when } \eta\to 1^-\ ,$$
$$\frac{M_1}{M_2}\to\sqrt{2}+1\quad\text{when } \eta\to 1^+\ .$$

B. Nonzero field: The collinear-noncollinear surface

As usual, a magnetic field suppresses the P-F line because the moment induced in the P phase gives that phase the same symmetry as the F phase. Thus, in a field, the P and F phases are no longer distinct. Similarly, a magnetic field also suppresses the AF-C line, because the moment induced in the AF phase gives that phase the same symmetry as the C phase. Thus, in a field, the AF and C phases are no longer distinct. The effect is that a critical surface separates the noncollinear phase (AF in a field, and C) from the collinear phase (F in a field, and P).

This result may also be seen from the fluctuation analysis given in Sec. III. There it is shown that the P-F and AF-C transitions are both associated with the uniform fluctuation mode **O**, thus explaining the peaks in the uniform susceptibility found in Ref. 17. Moreover, the P-AF and F-C transitions are both associated with the fluctuation mode $\mathbf{Q}_1=(\pi,0)$; one expects a peak in the staggered susceptibility at wave vector $\mathbf{Q}_1$ to be associated with these transitions.

For $\eta<1$, the equation for the collinear-noncollinear surface is obtained from (10a) and (10b) by taking the limit as $\theta_1,\theta_2\to 0$:

$$\left[2\eta M_1-M_2-\frac{H}{2J}\right]\left[2M_2+M_1+\frac{H}{2J}\right]+M_1M_2=0\ , \tag{17}$$

where

$$M_1=R(2\beta J|-\eta M_1-M_2+H/2J|)\ ,$$
$$M_2=R(2\beta J|M_1-M_2+H/2J|)\ . \tag{18}$$

Since both M_1 and M_2 are less than unity, there exists a critical field above which the left-hand side of (17) must be negative, and thus for which noncollinear ordering cannot occur. This defines the surface $H_c(T,\eta)$ presented in Fig. 3, which was found by solving Eqs. (17) and (18) simultaneously. If Eqs. (18) are satisfied, but the left-hand side of (17) is negative, one is below the critical surface, as can be seen by considering the high-temperature limit, where the system is paramagnetic.

At $T=0$, the critical field is given by

$$H_c/2J=\eta-2+[(\eta+1)^2+1]^{1/2}\ , \tag{19}$$

which follows from Eq. (17) for $M_1=M_2=1$. Note that $H_c=0$ for $\eta=\frac{1}{3}$, as expected from Sec. II A 1.

C. Discussion of phase diagram

Mean-field theory enables one to identify the nature of each phase, and to provide a straightforward explanation for why $\eta=1$ is a multicritical point. By Eq. (7) and Sec. II A 1, in the canted state ($\eta>\frac{1}{3}$) for $T=0$ and $H=0$ the mean fields on sites one and two satisfy

$$(H_1^2-H_2^2)/(2J)^2=[1+\eta^2-2\eta\cos(\theta_1+\theta_2)]$$
$$-[2+2\cos(\theta_1+\theta_2)]$$
$$=(\eta^2-1)(\eta+1)/\eta\ .$$

As a consequence, for $\eta=1$ the mean fields H_i on each site (see Fig. 1) are of the same magnitude (but in different directions). As the temperature increases, each spin is thus subject to the same relative thermalizing influence, so their mean-field lengths $R(\beta H_i)$ change in the same way, and therefore the mean fields they produce also change in the same way. Thus the relative orientations of the spins do not change with temperature, a result found in the MC studies of Berge *et al.*[17]

On the other hand, by the above equation, for $\eta<1$ the spins 1 and 4 have a smaller mean field than do spins 2 and 3. Therefore, thermal energy more easily overwhelms the mean fields on spins 1 and 4, causing these antiferromagnetically coupled spins to "melt" more easily than spins 2 and 3. As spins 1 and 4 melt, their influence in causing spins 2 and 3 to cant decreases. Thus the system becomes more ferromagnetic as the temperature increases, leading eventually to an F-C transition. Eventually, the "ferromagnetic" F phase (which is not truly ferromagnetic, because site inequivalence causes the spins to vary from site to site) undergoes a transition to the paramagnetic phase.[29]

Similarly, for $\eta > 1$ the spins 1 and 4 have a larger mean-field than do spins 2 and 3. Therefore, thermal energy more easily overwhelms the mean-fields on spins 2 and 3, causing these ferromagnetically coupled spins to melt more easily than spins 1 and 4. As spins 2 and 3 melt, their influence in causing spins 1 and 4 to cant decreases. Thus, the system becomes more antiferromagnetic as the temperature increases, leading eventually to an AF-C transition. Eventually, the "antiferromagnetic" AF phase (which is not truly antiferromagnetic, because site inequivalence causes the spins to vary from site to site) undergoes a transition to the paramagnetic phase.

With this identification of the phases, it is possible to interpret the uniform (i.e., zero wave vector) susceptibilities computed by Berge *et al.*, using Monte Carlo methods. For $\eta < 1$ they found a susceptibility peak at the P-F transition, but not at the F-C transition. This is as expected: In the P-F case uniform magnetic order develops, so one expects a peak (indeed, a divergence) in the uniform susceptibility (which is a correlation function of the uniform magnetization), whereas in the F-C case (involving the development of staggered magnetic order) one does not expect such a peak. For $\eta > 1$, Berge *et al.* found a uniform susceptibility peak at the AF-C transition, but not at the P-AF transition. This also is expected: In the P-AF case staggered order develops, so one expects no uniform susceptibility peak, whereas in the AF-C case (involving the development of uniform magnetic order) one does expect a uniform susceptibility peak (again, a divergence). This point will be made again in the following section, which is devoted to the fluctuations that signal the onset of magnetic order. Note that a remarkably similar phase diagram was found much earlier by DeGennes[26] in the context of a magnetic alloy with competing interactions. A similar discussion can be given to explain the mean-field phase diagram found in that case.

III. PHASE-ONLY MODE-FLUCTUATION ANALYSIS

Because of strong fluctuations in two dimensions, one expects the actual phase transitions to occur at temperatures much smaller than predicted by the mean-field theory of Sec. II. It is then justified to consider fluctuations of the phase of the order parameter while keeping the amplitude found by a mean-field treatment. We consider only the case $\mathbf{H}=\mathbf{0}$ and temperatures high enough that, in Eq. (6), one may expand the second term using

$$\ln I_0(x)=x^2/4-x^4/64+O(x^6) \ . \tag{20}$$

The term in x^2 determines the transition temperature for the fluctuations, and the term in x^4 leads to a coupling of the fluctuations. Using the identities

$$\frac{1}{N}\sum_{n\ \text{even}} e^{-iq_y n}=\tfrac{1}{2}(\delta_{q_y,0}+\delta_{q_y,\pi}) \ , \tag{21a}$$

$$\frac{1}{N}\sum_{n\ \text{odd}} e^{-iq_y n}=\tfrac{1}{2}(\delta_{q_y,0}-\delta_{q_y,\pi}) \ , \tag{21b}$$

where $n\in[1,N]$ and N is the total number of sites, one can compute the Fourier transform $J(\mathbf{q},\mathbf{q}')$ of the exchange constant matrix J_{ij}, written more explicitly as $J(m_i, n_i; m_j, n_j)$. One then finds that

$$J(\mathbf{q},\mathbf{q}')=\frac{1}{N}\sum_{\substack{n_1,m_1\\ n_2,m_2}} \exp[-i(q_x m_1+q_y n_1-q_x' m_2-q_y' n_2)]J(m_1,n_1;m_2,n_2)=JR(\mathbf{q},\mathbf{q}')\delta_{q_x,q_x'} \ , \tag{22}$$

where

$$R(\mathbf{q},\mathbf{q}')=[2\cos q_y+(1-\eta)\cos q_x]\delta_{q_y,q_y'}+(1+\eta)\cos q_x\,\delta_{q_y,q_y'+\pi} \ . \tag{23}$$

Doubling the periodicity in the y direction has introduced a coupling between the fluctuations $\mathbf{O}=(0,0)$ and $\mathbf{Q}=(0,\pi)$. Because of the translational invariance along the x direction, $J(\mathbf{q},\mathbf{q}')$ is diagonal in q_x and q_x'.

The eigenvalues of $JR(\mathbf{q},\mathbf{q}')$ are given by

$$J_\pm(\mathbf{q})=J\{(1-\eta)\cos q_x\pm[4\cos^2 q_y+(1+\eta)^2\cos^2 q_x]^{1/2}\} \ . \tag{24}$$

[Note that in going to the basis that diagonalizes J_{ij}, one must restrict $|q_y|<\pi/2$, compensating for this halving of the Brillouin zone by including both $(\pm)$ modes.] One can obtain the transition temperature by reexpressing Eq. (6) in terms of the eigenvectors that diagonalize J_{ij}. One then finds, as in Choi and Doniach,[12] that the terms quadratic in the fluctuation amplitudes are proportional to $1/[\beta J_\pm(\mathbf{q})]-\frac{1}{2}$. The system then becomes unstable when the largest of the eigenvalues satisfies

$$\beta=2/[J_\pm(\mathbf{q})]_{\max} \ . \tag{25}$$

For $\eta<1$ the largest eigenvalue is $J_+(\mathbf{O})$ and the corresponding normalized eigenvector is

$$\langle \mathbf{q}|0+\rangle \equiv \Phi_1(\mathbf{q}) = a\delta_{\mathbf{q},0} + b\delta_{\mathbf{q},\mathbf{Q}} ,$$
$$a = \frac{1+\eta}{C}, \quad b = \frac{[(1+\eta)^2+4]^{1/2}-2}{C}, \quad C^2 = 2(1+\eta)^2+8-4(1+\eta^2+4)^{1/2} . \tag{26}$$

The instability condition, Eq. (25), for $\eta < 1$ then leads to the first of Eqs. (13), for $\beta_{P\text{-}F}$.

For $\eta > 1$ the largest eigenvalue is $J_+(\mathbf{Q}_1)$, where $\mathbf{Q}_1 = (\pi, 0)$, and the normalized eigenvector is

$$\langle \mathbf{q}|\mathbf{Q}_1+\rangle \equiv \Phi_2(\mathbf{q}) = a\delta_{\mathbf{q},\mathbf{Q}_1} - b\delta_{\mathbf{q},\mathbf{Q}_1+\mathbf{Q}} . \tag{27}$$

The instability condition, Eq. (25), for $\eta > 1$ then leads to the second of Eqs. (13), for $\beta_{P\text{-}AF}$.

The Fourier transform of the mean-field magnetization is given by $\mathbf{M}_{\mathbf{q}} = (M_{\mathbf{q}}^x, M_{\mathbf{q}}^y)$, where

$$\langle \mathbf{q}|M^x\rangle \equiv M_{\mathbf{q}}^x = \tfrac{1}{2}(M_1\sin\theta_1 + M_2\sin\theta_2)\delta_{\mathbf{q},\mathbf{Q}_1} + \tfrac{1}{2}(M_2\sin\theta_2 - M_1\sin\theta_1)\delta_{\mathbf{q},\mathbf{Q}_1+\mathbf{Q}} , \tag{28a}$$

$$\langle \mathbf{q}|M^y\rangle \equiv M_{\mathbf{q}}^y = \tfrac{1}{2}(M_1\cos\theta_1 + M_2\cos\theta_2)\delta_{\mathbf{q},0} + \tfrac{1}{2}(M_2\cos\theta_2 - M_1\cos\theta_1)\delta_{\mathbf{q},\mathbf{Q}} . \tag{28b}$$

For $\eta < 1$ the *P-F* transition is associated with fluctuations about **O** and the *F-C* transition is associated with fluctuations about $\mathbf{Q}_1$. For $\eta > 1$ the *P-AF* transition is associated with fluctuations about $\mathbf{Q}_1$ and the *AF-C* transition is associated with fluctuations about **O**.

The amplitudes describing the *P-F* and *AF-C* magnetization fluctuations, in the basis that diagonalizes J_{ij}, are, from Eqs. (25) and (28b),

$$\langle 0+|M^y\rangle \equiv \Psi_0^1 = \frac{a}{2}(M_1\cos\theta_1 + M_2\cos\theta_2) + \frac{b}{2}(M_2\cos\theta_2 - M_1\cos\theta_1) , \tag{29a}$$

and those describing the *P-AF* and *F-C* fluctuations are, from Eqs. (25) and (28b)

$$\langle \mathbf{Q}_1+|M^x\rangle \equiv \Psi_{\mathbf{Q}_1}^2 = \frac{a}{2}(M_1\sin\theta_1 + M_2\sin\theta_2) - \frac{b}{2}(M_2\sin\theta_2 - M_1\sin\theta_1) . \tag{29b}$$

In the free-energy density of Eq. (6), we now include terms fourth order in the fields Ψ_i. This yields the desired phase-only approximation. For $\eta \neq 1$, only one mode contributes to the phase-only Hamiltonian when $T > T_{\rm I}(\eta)$. As a result, both the *P-F* and the *P-AF* transitions are true KT lines (see Berge *et al.*[17]). On the other hand, across $T_{\rm I}(\eta)$ one recovers the Hamiltonian of two coupled *XY* models, the coupling term being proportional to $(\Psi_{\rm O}^1)^2(\Psi_{\mathbf{Q}_1}^2)^2$. For the special case $\eta = 1$, one has $\Psi_{\rm O}^1 = \Psi_{\mathbf{Q}_1}^2$ and $T_{\rm I}(1) = T_{\rm KT}(1)$. At this multicritical point, both fluctuations become critical simultaneously.

Using Eqs. (29) and the *XY* fields defined by $\Psi_1(\mathbf{x}) = \Psi_{\rm O}^1 e^{i\varphi_1(\mathbf{x})}$, $\Psi_2(\mathbf{x}) = \Psi_{\mathbf{Q}_1}^2 e^{i\varphi_2(\mathbf{x})}$, the phase-only part of the free-energy density of Eq. (6) takes the form

$$\beta f \propto \tfrac{1}{2}\Gamma_1[c_1(\partial\varphi_1/\partial x)^2 + (1-c_1)(\partial\varphi_1/\partial y)^2] + \tfrac{1}{2}\Gamma_2[c_2(\partial\varphi_2/\partial x)^2 + (1-c_2)(\partial\varphi_2/\partial y)^2] + u\cos 2(\varphi_1 - \varphi_2) , \tag{30}$$

where

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \frac{\pm(1-\eta) + (1+\eta)^2/[4+(1+\eta)^2]^{1/2}}{\pm(1-\eta) + [4+(1+\eta)^2]^{1/2}} , \tag{31}$$

$$\Gamma_1 = |\Psi_{\rm O}^1|^2(k_BT/J), \quad \Gamma_2 = |\Psi_{\mathbf{Q}_1}^2|^2(k_BT/J) , \tag{32}$$

and $u \propto (\Psi_{\rm O}^1)^2(\Psi_{\mathbf{Q}_1}^2)^2$.

In the collinear regime ($T_{\rm I} < T < T_{\rm KT}$), for $\eta \neq 1$ one has nonisotropic helicity moduli Γ_x and Γ_y, since $c_1 \neq 1 - c_1$ and $c_2 \neq 1 - c_2$ except for $\eta = 1$. Specifically, for $\eta < 1$ one has

$$\frac{\Gamma_x}{\Gamma_y} = \frac{c_1}{(1-c_1)} = \frac{(1-\eta)[4+(1+\eta)^2]^{1/2} + (1+\eta)^2}{4} , \tag{33}$$

and for $\eta > 1$ one has

$$\frac{\Gamma_x}{\Gamma_y} = \frac{c_2}{(1-c_2)} = \frac{-(1-\eta)[4+(1+\eta)^2]^{1/2} + (1+\eta)^2}{4} . \tag{34}$$

In the noncollinear regime, the $u\cos 2(\varphi_1 - \varphi_2)$ term couples φ_1 and φ_2. Assuming that this causes them to lock together, the helicity moduli are given by

$$\Gamma_x = \Gamma_1 c_1 + \Gamma_2 c_2, \quad \Gamma_y = \Gamma_1(1-c_1) + \Gamma_2(1-c_2) . \tag{35}$$

These are typically not equal, so that again the system is not expected to be isotropic. For $T_I > T > T_{\rm KT}$ one has $\Gamma_2 = 0$, and for $\eta = 0.5$ Eqs. (31) and (35) give $\Gamma_x/\Gamma_y = 0.875$. For $T_{\rm I} > T > T_{\rm KT}$, Fig. 2 of Ref. 30 gives $\Gamma_x/\Gamma_y \approx 0.5$. (Note that Ref. 30 employs a rotated set of negative bonds relative to Fig. 2, so their x and y axes must be interchanged to correspond to the present work. See also Ref. 31.) There is only qualitative agreement between these two results (both ratios are less than unity).

In the vicinity of $T_{\rm KT}(\eta)$ (where either Ψ_1 or Ψ_2 is zero, so that either φ_1 or φ_2 is irrelevant), minimization of Eq. (30) leads to

$$\Delta'\varphi = 0 \pmod{2\pi} ,$$

where

$$\Delta' \equiv (\partial^2/\partial x^2)c_1 + (\partial^2/\partial y^2)(1-c_1)$$

for $\eta < 1$, and

$$\Delta' \equiv (\partial^2/\partial x^2)c_2 + (\partial^2/\partial y^2)(1-c_2)$$

for $\eta > 1$. Thus, topological excitations correspond to angles of the form

$$\varphi = \sum q_\alpha \text{Im}[\ln(z - z_\alpha)] ,$$

where the q_α are integers located at arbitrary positions z_a on the lattice

$$z = x/\sqrt{c_1} + iy/\sqrt{1-c_1}$$

for $\eta < 1$, or on the lattice

$$z = x/\sqrt{c_2} + iy/\sqrt{1-c_2}$$

for $\eta > 1$. They lead to a term in the free energy proportional to

$$\sum q_\alpha q_\beta \ln \left[\frac{L}{|z_{\alpha\beta}|} \right] ,$$

where L is the linear size of the system.

In the vicinity of $T_{\text{I}}(\eta)$, on the other hand, both φ_1 and φ_2 are relevant. The problem simplifies for $\eta \approx 1$, where the system is nearly isotropic. In that case, with $\varphi_1 - \varphi_2 = v$, $\varphi_1 + \varphi_2 = w$, minimization of Eq. (30) leads to

$$\Delta w = 0 \ (\text{mod}\, 2\pi), \quad \Delta v + \lambda \sin 2v = 0 ,$$

where $\lambda \propto (\Psi_{\text{O}}^1)^2(\Psi_{\text{Q}_1}^2)^2$. Thus topological excitations correspond to angles φ of the form

$$\varphi = \sum q_\alpha \text{Im}[\ln(z - z_\alpha)] + F(z)$$

where $F(z)$ describes a soliton (Bloch wall). As noted by Garel and Doniach,[2] strings are attached to the vortices and the energy of the soliton yields the line tension of the string, of order $\sqrt{\lambda}$ (see Refs. 2 and 32). For η not close to unity, the nonisotropic nature of the system complicates the situation, and the above analysis does not apply.

IV. SUMMARY AND CONCLUDING REMARKS

We have studied the generalized Villain model (i.e., the Berge *et al.*[17] generalization of the fully frustrated XY model on the square lattice[3]), using both mean-field theory and an analysis of the phase-only fluctuations. The amplitude of the fluctuating fields describing the transitions were obtained from a mean-field analysis. Mean-field theory yields a phase diagram strikingly similar to that obtained by Berge *et al.*, using Monte Carlo methods. Most important, it supports the hypothesis (that $T_{\text{I}} = T_{\text{KT}}$ for $\eta = 1$) which motivated Berge *et al.* to generalize the original model of Villain.

Mean-field theory indicates clearly the special nature of the value $\eta = 1$, since in that case there is only a paramagnetic-to-noncollinear transition; moreover, the structure of the noncollinear phase (i.e., the relative spin orientations) does not change with temperature. Furthermore, for $\eta \neq 1$ the mean-field solutions help clarify the nature of the transitions across the critical lines in the (η, T) plane: (i) When only one XY phase is condensed, pure XY transitions occur along the two higher-temperature lines (see Fig. 2), defined to be $T_{\text{KT}}(\eta)$. The mode analysis further indicates that when only one XY phase is condensed, one expects a standard KT transition at the P-F boundary, although (as pointed out in Sec. III) the vortex-vortex interaction will be strictly logarithmic only in the isotropic ($\eta = 1$) limit. (ii) when both XY phases are condensed—and couple with one another (as indicated by the phase-only fluctuation analysis), so that chirality can be preserved for each plaquette—Ising-type transitions occur along the two lower-temperature lines (see Fig. 2), defined to be $T_{\text{I}}(\eta)$. The mode analysis further indicates that, when the second XY mode condenses, the modes interact. This causes strings to be attached to the vortices (as noted in Sec. III), so that vortex pairs experience an interaction varying linearly with distance. Above $T = T_{\text{I}}$ the strings melt (i.e., the coupling term of the XY variables, which corresponds to the line tension, vanishes).

In addition, the phase-only mode-fluctuation analysis indicates that the mode describing the XY fluctuations for $\eta > 1 (\eta < 1)$ describes the Ising transition for $\eta < 1 (\eta > 1)$. This provides a natural explanation for the peaks in the susceptibility and heat capacity obtained by Berge *et al.*[17]

For the case $\eta = 1$, all four transition lines merge and two modes describe four instabilities. This line may be identified as a disorder line,[27] for the following reasons. First, for $T > T_{\text{KT}} = T_{\text{I}}$ the mode structure shows that correlations display dimensional reduction (the isotropy of the x and y directions is restored, so that they only depend on $(x^2 + y^2)^{1/2}$, whereas, e.g., for $\eta < 1 (\eta > 1)$, these correlations would show a ferromagnetic (antiferromagnetic) oscillation in the x direction. Second, this line intersects the critical manifold (i.e., the critical surface of Fig. 3) at a multicritical point.

It would be of interest to study this model for $H \neq 0$ using the Monte Carlo approach. Specifically, both uniform susceptibility peaks should disappear for sufficiently large H, but a peak in the staggered susceptibility (at wave vector $\mathbf{Q}_1$) should remain on crossing the critical surface $H_c(T, \eta)$. Moreover, if one were to apply a staggered field H_s at wave vector $\mathbf{Q}_1$, one would expect to find a surface $H_{sc}(T, \eta)$ separating the collinear (but now in the sense of antiferromagnetism) and noncollinear phases. In that case, one would expect to find a peak in the uniform susceptibility on crossing the surface $H_{sc}(T, \eta)$.

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[27]See, for instance, T. Garel and J. M. Maillard, J. Phys. C **19**, L505 (1986), and references therein.
[28]Since we have chosen a magnetization that points along $\hat{\mathbf{y}}$ (even as $H \rightarrow 0$) the global rotational invariance of the system is broken, allowing all canting angles to be determined.
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