

Antiferromagnetic planar-rotator model under h_n fields

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The antiferromagnetic planar-rotator model in a uniform magnetic field is considered. In addition to the usual Hamiltonian, a crystal field is added. The analysis is set up in mean-field theory for the general case. The specific case of the triangular lattice is solved in the small crystal-field limit.

I. INTRODUCTION

Although the planar-rotator model (also known as the classical XY model) with ferromagnetic interactions has been well understood¹⁻⁴ for some years now, it has only recently been observed that there are significant new effects in the antiferromagnetic planar-rotator (APR) models.⁵⁻⁸ In particular, the APR on a triangular lattice has attracted much attention because of the existence of long-range order associated with a helicity⁹ symmetry breaking. This is supported by a variety of calculations including exact ground-state analysis,⁷ Monte Carlo,^{6,8} and mean-field theory (MFT).⁷

Besides these interesting phase-transition properties, models such as this have been suggested to describe such diverse systems as two-dimensional arrays of coupled Josephson junctions⁵ and graphite intercalation compounds^{10,11} (GIC's). These comparisons will not be elaborated on here.

The previously mentioned calculations⁶⁻⁸ start out with a reduced Hamiltonian of the form

$$H_0 = K \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j - \mathbf{h} \cdot \sum_i \mathbf{s}_i, \quad (1.1)$$

where $K \equiv J/(k_B T) > 0$ and $\mathbf{h} \equiv \mathbf{H}/(k_B T)$. The sum is over a lattice of N spins with coordination number z , and $\langle i,j \rangle$ denotes nearest neighbors. The \mathbf{s}_i is a two-component unit vector making an angle θ_i relative to the direction of the field \mathbf{h} . Only the component of the field \mathbf{h} in the plane of the two-component spins has any effect, and thus \mathbf{h} will be assumed to be totally in this plane.

In this paper the MFT analysis of Ref. 7 is extended to the case where an additional term

$$- h_n \sum_i \cos(n\theta_i - n\sigma)$$

is included (n is an integer). This term may be produced by the crystal structure in which the spins lie. The angle

σ is allowed because the field might not be aligned with the crystal axes.

The significance of such terms is due to the fact that most of the APR models possess a phase or phases in which a continuum of solutions exist which have no free-energy barrier between them. The presence of a modulation as described above breaks the continuous symmetry, but may still leave a degeneracy associated with the periodicity of the lattice. This will be expounded in detail for the most interesting case, the triangular (or more generally the tripartite) lattice. In the ferromagnetic planar rotator model with $\mathbf{h} = 0$ such terms produce a degeneracy associated with rotations by $2\pi/n$, which is distinct from the structural ordering found here.

In Sec. II, I will set up the most general form of the MFT equations. In Sec. III, I will describe the solution of the theory in several limiting cases. In Sec. IV, I draw general conclusions.

II. FORMALISM

Consider the reduced Hamiltonian:

$$H = K \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) - h \sum_i \cos\theta_i - h_n \sum_i \cos(n\theta_i - n\sigma). \quad (2.1)$$

MFT is performed by minimizing a free-energy functional¹² of the form

$$\Psi[\rho] \equiv \text{Tr}(\rho H + \rho \ln \rho) \quad (2.2)$$

under the constraints

$$\rho = \prod_i \rho_i, \quad \text{Tr}_{\theta_i} \rho_i = 1 \quad \text{for all } i, \quad (2.3)$$

where Tr and Tr_{θ_i} represent the traces over all states of the system and over all states of site i , respectively. Here ρ_i is the density matrix of site i . Define

$$C_i \equiv \text{Tr}(\rho_i \cos\theta_i), \quad S_i \equiv \text{Tr}(\rho_i \sin\theta_i), \quad M_i \equiv C_i + iS_i, \quad C_{n,i} \equiv \text{Tr}[\rho_i \cos(n\theta_i - n\sigma)] \quad \text{for all } i. \quad (2.4)$$

M_i is the (complex) magnetization of the site i . Representing the spins θ_i by the real and imaginary parts of the complex number $e^{i\theta_i}$ is done to reduce the number of equations and simplify the notation. Then

$$\Psi[\rho] = K \sum_{\langle i,j \rangle} (C_i C_j + S_i S_j) - h \sum_i C_i - h_n \sum_i C_{n,i} + \sum_i \text{Tr}(\rho_i \ln \rho_i), \quad (2.5)$$

which gives the variational equations

$$-K \sum_j' (C_j \cos \theta_i + S_j \sin \theta_i) + h \cos \theta_i + h_n \cos(n\theta_i - n\sigma) + \lambda_i - 1 = \ln \rho_i(\theta_i) \quad \text{for all } i. \quad (2.6)$$

In Eq. (2.6) λ_i is the Lagrange multiplier introduced to preserve the normalization of ρ_i . Here, and throughout the paper, the prime on the sum represents a restriction of the index to only the nearest neighbors of i . Thus

$$\rho_i(\theta_i) = A_i^{-1} \exp[a_i \cos(\theta_i - \phi_i) + h_n \cos(n\theta_i - n\sigma)] \quad \text{for all } i, \quad (2.7)$$

where A_i is a normalization constant,

$$a_i e^{i\phi_i} \equiv h - K \sum_j' M_j, \quad (2.8)$$

and $a_i (\geq 0)$ and ϕ_i are both real. The normalization of ρ_i requires

$$A_i \equiv \text{Tr}_{\theta_i} \exp[a_i \cos(\theta_i - \phi_i) + h_n \cos(n\theta_i - n\sigma)] = \text{Tr}_{\theta_i} \exp\{a_i \cos(\theta_i) + h_n \cos[n(\theta_i + \phi_i - \sigma)]\}. \quad (2.9)$$

A Fourier transformation gives

$$\begin{aligned} e^{h_n \cos[n(\theta_i + \phi_i - \sigma)]} &= \sum_{k=-\infty}^{\infty} \cos(k\theta_i) \cos(k\phi_i - k\sigma) \sum_{m=-\infty}^{\infty} \delta_{k-mn} I_m(h_n) + [\sin \theta_i]_{\text{odd}} \\ &= \sum_{m=-\infty}^{\infty} I_m(h_n) \cos[mn(\phi_i - \sigma)] \cos(mn\theta_i) + [\sin \theta_i]_{\text{odd}}, \end{aligned} \quad (2.10)$$

where $[\]_{\text{odd}}$ represents terms odd in $\sin \theta_i$, so that

$$A_i = \sum_{m=-\infty}^{\infty} 2\pi I_m(h_n) I_{mn}(a_i) \cos[mn(\phi_i - \sigma)], \quad (2.11)$$

where $I_\nu(x)$ is the modified Bessel function of the first kind¹³ of order ν . Similarly,

$$\begin{aligned} M_i &= A_i^{-1} \text{Tr}_{\theta_i} \exp[a_i \cos(\theta_i - \phi_i) + h_n \cos(n\theta_i - n\sigma) + i\theta_i] \\ &= A_i^{-1} \text{Tr}_{\theta_i} \exp\{a_i \cos(\theta_i) + h_n \cos[n(\theta_i + \phi_i - \sigma)] + i(\theta_i + \phi_i)\}, \end{aligned} \quad (2.12)$$

$$\begin{aligned} e^{h_n \cos[n(\theta_i + \phi_i - \sigma)] + i(\theta_i + \phi_i)} &= \sum_{k=-\infty}^{\infty} \cos(k\theta_i) \sum_{m=-\infty}^{\infty} I_m(h_n) \frac{1}{2} (e^{ik(\phi_i - \sigma)} \delta_{k-1-mn} + e^{-ik(\phi_i - \sigma)} \delta_{k+1-mn}) e^{i\sigma} + [\sin \theta_i]_{\text{odd}} \\ &= e^{i\phi_i \frac{1}{2}} \sum_{m=-\infty}^{\infty} I_m(h_n) \{ \cos[(mn+1)\theta_i] e^{imn(\phi_i - \sigma)} + \cos[(mn-1)\theta_i] e^{-imn(\phi_i - \sigma)} \} + [\sin \theta_i]_{\text{odd}} \\ &= e^{i\phi_i} \sum_{m=-\infty}^{\infty} I_m(h_n) \cos[(mn+1)\theta_i] e^{imn(\phi_i - \sigma)} + [\sin \theta_i]_{\text{odd}}, \end{aligned} \quad (2.13)$$

so that

$$M_j = A_j^{-1} e^{i\phi_j} \sum_{m=-\infty}^{\infty} 2\pi I_m(h_n) I_{mn+1}(a_j) e^{imn(\phi_j - \sigma)} \quad \text{for all } j. \quad (2.14)$$

Inserting Eqs. (2.14) in Eqs. (2.8) gives the self-consistent MFT equations (SCMFE):

$$a_i e^{i\phi_i} = h - K \sum_j' A_j^{-1} e^{i\phi_j} \sum_{m=-\infty}^{\infty} 2\pi I_m(h_n) I_{mn+1}(a_j) e^{imn(\phi_j - \sigma)} \quad \text{for all } i. \quad (2.15)$$

The SCMFE describe the state of the entire lattice, which requires solving for $2N$ variables. As is illustrated in the appendix, for the triangular lattice it is possible to reduce the number of independent spin variables to finitely many. This type of argument easily generalizes to a p -partite lattice. (A lattice is p -partite if there are p equivalent sublattices for which spins on the same sublattice do not interact.) Thus, throughout the remainder of the paper I will deal exclusively with the case of a p -partite lattice for which the SCMFE reduce to

$$e^{i\phi_i} \left[a_i - K \frac{z}{p-1} \frac{\sum_{m=-\infty}^{\infty} I_m(h_n) I_{mn+1}(a_i) e^{imn(\phi_i - \sigma)}}{\sum_{m=-\infty}^{\infty} I_m(h_n) I_{mn}(a_i) \cos[mn(\phi_i - \sigma)]} \right] = h - \frac{Kzp}{p-1} M \quad \text{for } i = 1, \dots, p, \quad (2.16)$$

where the magnetization per site of the system is

$$M \equiv p^{-1} \sum_{j=1}^p M_j . \quad (2.17)$$

Summing Eq. (2.8) over the sites give the simple relation

$$\sum_{j=1}^p (a_j e^{i\phi_j} - h) = -KzpM . \quad (2.18)$$

The free energy can now be obtained by inserting these expressions into Eq. (2.5):

$$\Psi[\rho] = - \sum_i \ln A_i - K \sum_{\langle i,j \rangle} (C_i C_j + S_i S_j) , \quad (2.19a)$$

$$p\Psi[\rho]/N = \sum_{j=1}^p \left[-\ln A_j - \frac{Kz}{2(p-1)} \sum_{i(\neq j)=1}^p (C_i C_j + S_i S_j) \right] \quad (2.19b)$$

$$= \sum_{j=1}^p -\ln A_j - \frac{Kz}{2(p-1)} \left[\left| \sum_{j=1}^p M_j \right|^2 - \sum_{j=1}^p |M_j|^2 \right] \quad (2.19c)$$

$$= \sum_{j=1}^p -\ln A_j - \frac{Kz}{2(p-1)} \left[p^2 |M|^2 - \left(\frac{Kz}{p-1} \right)^{-2} \sum_{j=1}^p \left| a_j e^{i\phi_j} - h + \frac{Kzp}{p-1} M \right|^2 \right] \quad (2.19d)$$

$$= \sum_{j=1}^p -\ln A_j + \frac{p-1}{2Kz} \sum_{j=1}^p \left[|a_j e^{i\phi_j} - h|^2 + (a_j e^{i\phi_j} - h) \frac{Kzp}{p-1} M^* + (a_j e^{-i\phi_j} - h) \frac{Kzp}{p-1} M \right] \quad (2.19e)$$

$$= \sum_{j=1}^p -\ln A_j + \frac{p-1}{2Kz} \left[\sum_{j=1}^p |a_j e^{i\phi_j} - h|^2 - \frac{2}{p-1} \left| \sum_{j=1}^p (a_j e^{i\phi_j} - h) \right|^2 \right] . \quad (2.19f)$$

It will be useful to define the function $R_n(x) \equiv I_n(x)/I_0(x)$. It should be pointed out as a check that when $h_n=0$ the results of Ref. 7 are obtained.

III. ANALYSIS

With the formalism described in the previous section it is possible to numerically determine any part of the full $(K, h, h_n, n, \sigma, p)$ phase diagram by solving the SCMFE and comparing the free energies of the roots. However, in this paper I will look at the simplest cases only, which I believe indicate the behavior in at least a large portion of the phase diagram.

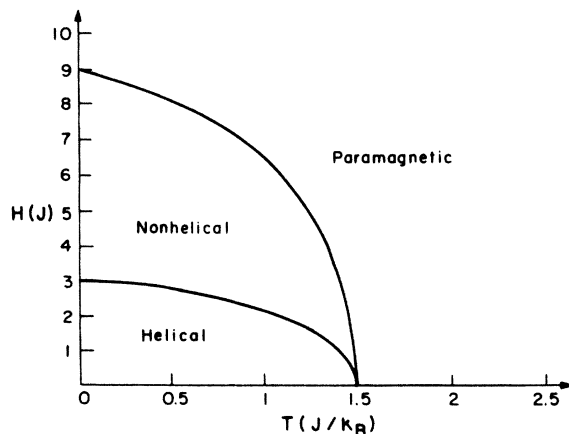


FIG. 1. The phase diagram [from Ref. 7] of the triangular antiferromagnetic planar-rotator model with $h_n=0$.

A. The unperturbed case ($h_n=0$): review

As explained in detail in Ref. 7 the unperturbed case has both paramagnetic and ordered phases. In the paramagnetic phase $\phi_i=0$ and $a_i=a_0$, where $a_0 + KzR_1(a_0) = h$ which has a unique solution. The or-

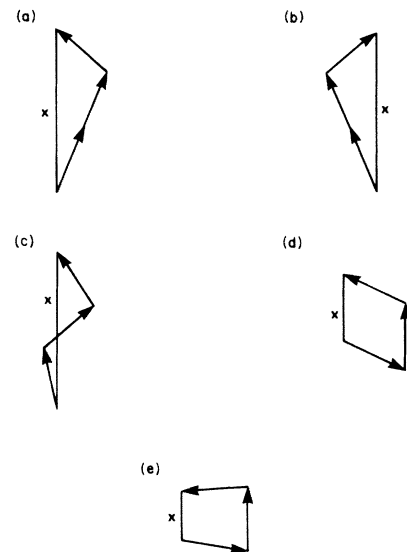


FIG. 2. The structure of the different phases. At any point in the phase diagram three unit vectors (or equivalently three complex phases) with the directions ϕ_i , $i=1,2,3$ relative to the field \mathbf{h} must add up to \mathbf{h}/a'_0 (or equivalently the real number $x \equiv h/a'_0$). (a) L phase: Two spins are equal and point to the right (helicity=0). (b) R phase: Two spins are equal and point to the left (helicity=0). (c) B_1 and B_2 phases: No spins are equal (helicity=0). (d) The helicity transition ($x=1$). (e) Helical phase: Helicity $= \pm 1$.

dered phase or phases satisfy $pM = h/a'_0$ with

$$a'_0 = \frac{Kz}{p-1} R_1(a'_0).$$

For $p > 3$ there is a $(p-2)$ -dimensional continuum of solutions with the same free energy. For $p=3$, there is either one such continuum (in the nonhelical phase) or two such continua (in the helical phase) with opposite helicity. For $p=2$ there are only two solutions (except when $h=0$).

The $p=3$ phase diagram (from Ref. 7) is shown in Fig. 1. In Fig. 2, (e) is in the helical phase, (d) is at the helicity transition, and (a), (b), and (c) are in the nonhelical (ordered) phase.

B. $h=0$

In the paramagnetic phase the solution can rotate (without cost to the pair interactions) to optimize the h_n term, i.e., $\phi_i = \sigma$, and a_i is independent of i with

$$a_i + Kz \frac{\sum_{m=-\infty}^{\infty} I_m(h_n) I_{m+1}(a_i)}{\sum_{m=-\infty}^{\infty} I_m(h_n) I_{mn}(a_i)} = 0. \quad (3.1)$$

Such a free rotation is also possible in the ordered phase, though it may be true here that for appropriate p, n it is impossible to fully satisfy all the h_n terms and, thus, a transition might still take place by varying h_n . However, for the triangular lattice the relative angles of $2\pi/3$ between the sublattices does fully satisfy the h_n terms, and hence no additional transition should take place. This argument can be generalized somewhat more. The unperturbed solution satisfies $\sum_{i=1}^p e^{i\phi_i} = 0$ which certainly has (among others) the solutions $\phi_j = mj2\pi/p + \eta$, where m is an integer ($0 < m < p$) and η is anything. If n is an integer multiple of p then the h_n terms will be satisfied by $\eta = \sigma$. This holds for the simplest cases but is not obviously general. In fact the coordination number of a p -partite lattice is proportional to $p-1$ but not necessarily proportional to p . It does hold for the triangular and square lattices. Such solutions will in fact be seen in the next section where the small h_n limit is treated.

C. Small h_n

The paramagnetic phase was already discretized to a unique solution in the unperturbed case, and thus is not going to be qualitatively changed by a small h_n . The only effect will be a slight rotation of the magnetization towards the angle σ .

However, the small h_n limit is probably the most interesting limit because it shows how the continua in the ordered phases become discretized. In this limit I assume that variation of the a_i 's and ϕ_i 's out of the continuum is much more costly in free energy than is a variation along the continuum, and thus that the solution still satisfies the conditions $a_j = a'_0$, where

$$a'_0 = R_1(a'_0) \frac{Kz}{p-1}$$

and

$$a'_0 \sum_{j=1}^p e^{i\phi_j} = h.$$

With this constraint then Eq. (2.19f) becomes

$$p\Psi[\rho]/N = - \sum_{i=1}^p \ln A_i - \frac{p(p-1)}{2Kz} [(a'_0)^2 - h^2] \quad (3.2a)$$

$$= - \sum_{i=1}^p \ln \left[2\pi \sum_{m=-\infty}^{\infty} I_m(h_n) I_{mn}(a'_0) \cos[mn(\phi_i - \sigma)] \right] + [\phi_j]_{\text{ind}} \quad (3.2b)$$

$$= - \sum_{i=1}^p h_n R_n(a'_0) \cos[n(\phi_i - \sigma)] + [\phi_j]_{\text{ind}} + O(h_n^2) \quad (3.2c)$$

$$= - h_n R_n(a'_0) \sum_{i=1}^p \cos[n(\phi_i - \sigma)] + [\phi_j]_{\text{ind}} + O(h_n^2), \quad (3.2d)$$

where $[\phi_j]_{\text{ind}}$ represents terms independent of the ϕ_j 's. Therefore, for $h_n > 0$ one should maximize $\Omega \equiv \sum_{i=1}^p \cos[n(\phi_i - \sigma)]$. It should be pointed out here that although this looks like the additional energy, the prefactor $R_n(a'_0)$ contained the temperature dependence of the free energy.

After including Lagrange multipliers for the constraints on the real and imaginary parts of the magnetization and then algebraically eliminating them, I obtain the minimization conditions

$$h \{ \sin\phi_j \sin[n(\phi_j - \sigma)] - \sin\phi_j \sin[n(\phi_i - \sigma)] \} = a'_0 \sin(\phi_i - \phi_j) \sum_{k=1}^p \sin[n(\phi_k - \sigma)] + O(h_n), \quad (3.3)$$

which constitutes $p-2$ independent constraints.

The case of prime interest, of course, is the triangular lattice for which $p=3$ and $n=6$. This case is obtained by first setting $\phi_2 = \phi_+$ and $\phi_3 = \phi_-$ (or vice versa) where

$$e^{i\phi_{\pm}} = (x - e^{i\phi_1})^{1/2} (1 \pm i\alpha), \quad (3.4)$$

$$|x - e^{i\phi_1}|^2 (1 + \alpha^2) / 4 = 1, \quad (3.5)$$

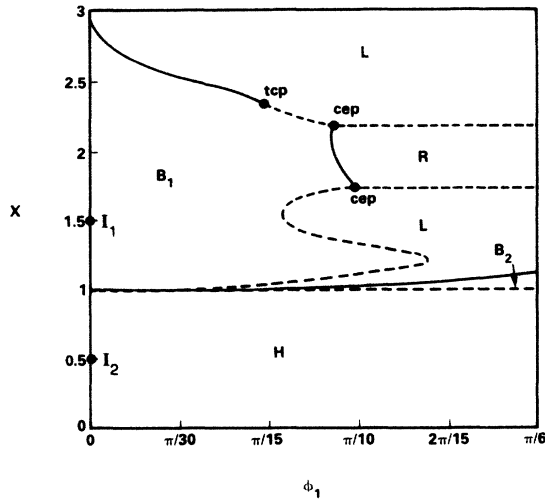


FIG. 3. The ordered region of the phase diagram for the triangular lattice; $x \equiv h/a'_0$. The helicity transition is at $x=1$. Solid lines are critical. Dashed lines are first order. cep indicates critical endpoint, tcp indicates tricritical point. I_1 and I_2 are upper and lower Ising critical points, respectively. H is the helical phase, B_1 , B_2 , L , and R are (nonhelical) ordered phases described in the text.

$x \equiv h/a'_0$, and then minimizing with respect to ϕ_1 .

The phase diagram is shown in Fig. 3. To illustrate this, Fig. 4 shows a plot of Ω as a function of ϕ_1 for many values of x and σ . Most of the results shown in Fig. 3 are the result of automated numerical searches. It should be pointed out that (for $n=6, p=3$) Eq. (3.3) can be reduced to a polynomial of degree 20 in $\cos\phi_1$ with coefficients depending only on x and σ . This polynomial allows sufficiently few roots (many of which are grouped together by the permutation symmetry) that Ω stays well behaved. Furthermore, it appears from Fig. 4 that the phase is easily determined in most of the phase diagram.

As described in Sec. III B, at $x=0$ there is no competition of the h field with the h_n term, and thus $|\phi_1 - \phi_2| = |\phi_3 - \phi_1| = 2\pi/3, \phi_1 = \sigma + m\pi/3$ for integer m , which is 12 states.

At $x=1, \sigma \neq 0$ the solution is $\phi_1=0, \phi_2 = \phi_3 - \pi = \sigma + m\pi/3$ (or permutations of the indices). It is thus essentially a six-state clock model whose angles ϕ_2 and ϕ_3 completely satisfy the h_n term. This is 18 states, and is a first-order line. The sharp spike near $\phi_1=0$ in the figures near $x=1$ is produced by the rotational symmetry of the unperturbed model at $x=1: \phi_1=0, \phi_2 = \phi_3 + \pi = \text{anything}$ (i.e., totally degenerate), or permutations of the indices.

For $\sigma=0$ and $x > 1.49827685\dots$ the solutions have the form $\phi_1=0, \phi_2 = -\phi_3$, with $x = 1 + 2\cos\phi_2$. At $\sigma=0, x = 1.49827685\dots (x = 0.51367508\dots)$ there is an upper (lower) Ising critical point terminating a line of first-order transitions. The upper Ising critical point must be present because $x \leq 3$ has three peaks and $x=1$ has six peaks, requiring a splitting of the peaks for some value of x . However, as σ becomes nonzero one peak from each split pair becomes greater and the phase B (described below) is obtained.

In the nonhelical phase there are four phases, denoted L, R, B_1 , and B_2 (see Figs. 2 and 3). The L and R phases both have $\phi_2 = \phi_3$, (i.e., $\alpha=0$),

$$\cos\phi_1 = \frac{x^2 - 3}{2x}$$

or a permutation of the indices 1,2,3. This feature can be identified in Fig. 4 by the fact that the extremum of Ω occurs at the left end (for L) or at the right end (for R) of the curve. The necessary degeneracy at these points follows from the permutation symmetry of the indices which would otherwise require the number of roots to be divisible by 3. When x is near 3 the angles are constrained near 0 and cannot relax to the vicinity of σ . The two angles which become equal are thus pulled as far towards σ as possible producing the L phase. At the larger values of σ as x is reduced these extrema move relative to σ and it becomes better to bring the third spin close to sigma rather than the two degenerate spins. This produces a first-order phase transition at $x = 2.1867313\dots$. Similarly there is first-order transition at $x = \sqrt{3} [(\phi_1, \phi_2, \phi_3) = (\pi/2, -\pi/3, -\pi/3)$ or $(-\pi/2, \pi/3, \pi/3)]$ which reverses the process. Because the L and R phases are known exactly, the value of Ω can be compared and these are known to be the only transitions between L and R .

The phases B_1 and B_2 are broken-symmetry phases. In

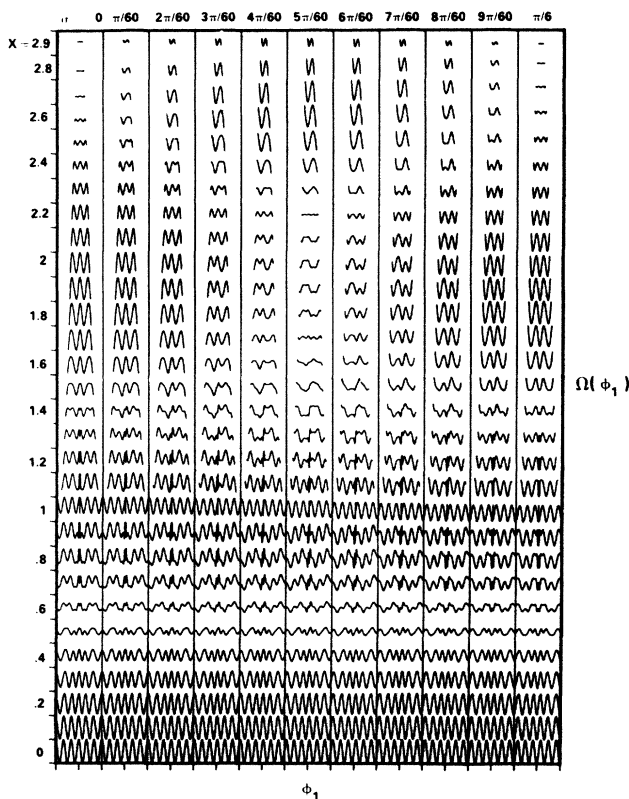


FIG. 4. $\Omega(\phi_1)$ for $x=0, 0.1, 0.2, \dots, 2.9$ and $\sigma=0, \pi/60, 2\pi/60, \dots, \pi/6$.

these regions the system can relax enough to partially satisfy both σ and x with a nonextreme value of ϕ_1 . Since $\alpha \neq 0$ there are now six states.

Since the phases which coexist at $x=1$, $\sigma \neq 0$ are known to be neither L nor R , then this broken symmetry phase (B_2) must cover the entire range of σ for x directly above $x=1$. However the angles turn very quickly in this region, so that the L phase is obtained very near $x=1$ as x is increased. The numerical calculations suggest that this is always critical. Criticality requires that $(d\Omega/d\phi_1)=0$ at $\alpha=0^+$, i.e., when the end of the Ω curve becomes horizontal. This is in fact the case at $x=1$, $\sigma=0$, so that the transition reaches this point.

In the B_1 phase the aforementioned competition between x and σ is weak enough that an intermediate (symmetry-broken) phase exists which largely satisfies both interactions. The transition from B_1 to R appears to be critical. The transition from B_1 to L is critical for large x and first order for smaller x with a tricritical point at ~ 2.3 . In addition, there are thus two critical endpoints terminating the R to B_1 transition.

The B_1 and B_2 phases do not meet, but have a narrow region of R phase separating them.

Since $\sigma = \pi/6 + \epsilon$ is equivalent to $\sigma = \pi/6 + \epsilon - \pi/3 = -(\pi/6 - \epsilon)$ the unshown portion of the phase diagram is easily obtained. As one crosses $\sigma = \pi/6$ there is a first-order transition either from L to R or from R to L , as is appropriate.

There appears to be only one phase, H , in the helical region. As in the nonhelical B phase, there is a first-order transition at $\sigma=0$ and at $\sigma=\pi/6$. When these values of σ are crossed, the state changes to a totally equivalent but reflected ($\phi_i \rightarrow -\phi_i$) state.

The point $x=1$, $\sigma=0$ is a very complicated point because B_1 , B_2 , R , H and the equivalent phases for negative sigma all meet there with the above mentioned transitions.

IV. DISCUSSIONS

In this paper I have shown that the APR models can be described in MFT even in the presence of a crystal field of the form $h_n \cos[n(\theta - \sigma)]$. Although the equations can be numerically handled in rather general circumstances, the problem was analyzed mostly in the limit of small h_n . The presence of h_n terms discretizes the solutions, but leaves a symmetry break associated with permutations of the sublattices in a periodic state. Furthermore the specific case of the triangular lattice (which is known to have interesting properties even in the absence of such fields)

was elaborated on. In this case a variety of phase transitions was observed, both first-order and critical. There were also observed a tricritical point, two critical endpoints and two Ising critical points. There are first-order transitions associated with a free energy crossing of the two extrema of the continuum (from the $h_n=0$ case). Because these extrema have a degeneracy in the angles, it then followed that there is (sometimes) an Ising transition breaking this symmetry as one moves to values of σ and h which are not so strongly in competition with each other.

It is appropriate to discuss the validity of these calculations. The MFT approximation reduces to a ground-state analysis at $T=0$. The equations set up in Sec. II are exact (for the MFT). The assumption in Sec. III C, that the state stays in the continuum of the unperturbed model should be correct for $T=0$ (with fixed, small h_n). Thus at the very least we have done an exact ground-state analysis. The fact that the previous MFT (for the $h_n=0$ case) is in reasonable agreement with the Monte Carlo studies suggest that the calculations presented here should reflect much of the phenomena present even at finite temperature. To date no other analysis (Monte Carlo, renormalization-group, etc.) has been done on this model (with $h_n \neq 0$) with which to compare. Extensive studies have been made on the ferromagnetic versions with $h=0$, but the phenomena involved are distinct from most of those seen here. Since such terms in the Hamiltonian are quite likely based on crystal symmetry, it seems very reasonable to look further at this question.

ACKNOWLEDGMENT

I would like to thank D.-H. Lee for discussions of these results.

APPENDIX

The arguments concerning the periodicity of the ground state of this model on a triangular lattice can be easily generalized to a much broader class of Hamiltonians of the form

$$H \equiv \sum_{\langle i,j \rangle} V(\theta_i, \theta_j) + \sum_i U(\theta_i), \quad (\text{A1})$$

where $V(\theta_i, \theta_j) = V(\theta_j, \theta_i)$. This can be rewritten as

$$H = \sum_k W(\theta_{k,1}, \theta_{k,2}, \theta_{k,3}), \quad (\text{A2})$$

where k runs over a $\sqrt{3} \times \sqrt{3}$ sublattice, $\theta_{k,1}$, $\theta_{k,2}$, and $\theta_{k,3}$ are the spins of three nearest neighbors, and

$$W(\theta_{k,1}, \theta_{k,2}, \theta_{k,3}) \equiv V(\theta_{k,1}, \theta_{k,2}) + V(\theta_{k,2}, \theta_{k,3}) + V(\theta_{k,1}, \theta_{k,3}) + [U(\theta_{k,1}) + U(\theta_{k,2}) + U(\theta_{k,3})]/3. \quad (\text{A3})$$

(Note: Each θ_i must be included in three such trios and thus the variables for different k 's are not all independent.) Because of the structure of the triangular lattice it thus follows that the ground state of the entire system is precisely the set of states for which W is minimized on each trio of nearest-neighbor sites. As is typically the case, assume that the set of minima for W is such that if two of the spins are known then so is the third. (This as-

sumption is true for the case actually considered in this paper.) If this assumption is true, then knowing any two nearest-neighbor spins in the triangular lattice allows the state of the entire lattice to be determined, resulting in a $\sqrt{3} \times \sqrt{3}$ periodicity.

It should be pointed out that the MFT free energy also has this form and thus the arguments still apply at finite temperature (in MFT).

- ¹J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **5**, 124 (1972).
- ²J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **6**, 1181 (1973).
- ³J. M. Kosterlitz, *J. Phys. C* **7**, 1046 (1974).
- ⁴J. V. Jose, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, *Phys. Rev. B* **16**, 1217 (1977).
- ⁵S. Teitel and C. Jayaprakash, *Phys. Rev. B* **27**, 598 (1983).
- ⁶D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, *Phys. Rev. Lett* **52**, 433 (1984).
- ⁷D. H. Lee, R. G. Caflisch, J. D. Joannopoulos, and F. Y. Wu, *Phys. Rev. B* **29**, 2680 (1984).
- ⁸D. H. Lee, J. D. Joannopoulos, J. W. Negele, and D. P. Landau, *Phys. Rev. B* **33**, 450 (1986).
- ⁹The helicity is defined as $\Delta\theta/2\pi$, where $\Delta\theta$ is the change in angle as a given triangle of nearest-neighbor spins is traversed in a clockwise direction. At each individual step the smallest possible change is chosen. The possible values are +1, 0, -1.
- ¹⁰Y. Kimishima, A. Furukawa, H. Nagano, P. Chow, D. Wiesler, H. Zabel, and M. Suzuki, Proceedings of the International Symposium of Graphite Intercalation Compounds, Tsukuba, Japan, 1985 [*Synth. Met.* **12**, 455 (1985)].
- ¹¹In Ref. 10 it is asserted that a Hamiltonian much like this is responsible for the production of a $2\sqrt{3}\times 2\sqrt{3}$ phase in a MnCl_2 GIC. They add a ferromagnetic interlayer coupling, which produces an important difference in the ordering properties. However, the important point here is that such a description is valid independent of the precise values of the couplings, and related GIC's might indeed have a Hamiltonian with the correct sign of the interactions.
- ¹²H. Falk, *Am. J. Phys.* **38**, 858 (1970).
- ¹³For all the properties of $I_\nu(x)$ used here, see, for example, M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, (National Bureau of Standards, Washington, D.C., 1964).