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Asymmetric phases in the mean-field theory of the axial next-nearest-neighbor Ising model

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We study the effect of the weakening of the intraplane interactions on the mean-field theory of the axial next-nearest-neighbor Ising model and show that commensurate phases, which lack the usual reflection or inversion symmetries, may be stabilized. These asymmetric phases separate commensurate phases with the same period but different symmetries, and the phase-locking angle changes continuously as a function of the temperature. We also compute the phase boundaries numerically and by a continuum approximation, and show that they have a characteristic bottleneck shape.

During the past decade there have been many studies of the axial next-nearest-neighbor Ising (ANNNI) model.[1,2] In this model the spins interact with nearest-neighbor coupling J_1 and next-nearest-neighbor coupling J_2 along a single spatial direction, and with nearest-neighbor ferromagnetic coupling $J_0>0$ within the planes perpendicular to this direction. The ANNNI model exhibits a complex series of commensurate and incommensurate structures, and it has been applied to the description of a variety of experimental systems, including binary alloys, ferroelectrics, polytypism, and magnetic systems. A survey of theoretical work on the ANNNI model and its application to experimental systems can be found in recent review articles by Selke[3] and Yeomans.[4]

Among the variety of methods used to study the ANNNI model, much insight has been provided by the mean-field theory.[1,5,6] Many aspects of the mean-field calculations have been confirmed by low-temperature series analysis.[2,7] The mean-field studies have, however, been largely limited to the situation $J_0=J_1$. In this paper we report some interesting implications that the weakening of the intralayer coupling J_0 relative to the interlayer coupling J_1 has on the mean-field theory of the model. Of particular interest are the possibilities of commensurate phases with disordered planes (zero magnetization), and asymmetric commensurate phases which lack the usual reflection or inversion symmetries. Recently Nakanishi has carried out a similar study,[8] but he did not consider the possibility of asymmetric phases. We note, however, that asymmetric phases have already been observed in Frenkel-Kontorova-type models[9] and also in competing spin models on Cayley trees.[10]

The mean-field theory of the model is based on the following free-energy functional:[1]

$$N^{-2}F=-J_1\sum_n(2\rho M_n^2+M_nM_{n+1}-\kappa M_nM_{n+2})-k_BT\sum_n\int_{M_n}^{1}\tanh^{-1}m\,dm\ , \quad (1)$$

where $\rho=J_0/J_1$, $\kappa=-J_2/J_1$, M_n is the magnetization per spin in the nth layer, and N^3 is the number of spins in the system. In what follows we will set $J_1=1$ and $k_B=1$ throughout. The condition for an extremum $\partial F/\partial M_n=0$ gives the mean-field equations

$$M_n=\tanh\frac{1}{T}\left[4\rho M_n+M_{n-1}+M_{n+1}-\kappa(M_{n-2}+M_{n+2})\right] . \quad (2)$$

For a given value of the parameters ρ, κ, and T there are in general many solutions to the above equations. The condition for a given solution with period Q to be at least a local minimum is that the matrix

$$\mathbf{M}=\prod_{n=1}^{Q}\begin{bmatrix}0&1&0&0\\0&0&1&0\\0&0&0&1\\-1&\frac{1}{\kappa}&B_n&\frac{1}{\kappa}\end{bmatrix}, \quad (3)$$

where

$$B_n=\frac{1}{\kappa}\left[4\rho-\frac{T}{1-M_n^2}\right] \quad (4)$$

has no complex eigenvalues of unit modulus.[5,11] The sought-for solution corresponds to the absolute minimum of the free-energy functional.

Let us consider the commensurate phase with wave number $q=\frac{1}{6}$. Near the phase boundary at $\kappa=\frac{1}{2}$ and $T_c=4\rho+\frac{3}{2}$ the modulated phase is given approximately by a sinusoidal magnetization $M_n=A_1\cos[2\pi q(n+\phi)]$. Some time ago we observed (Ref. 12, Appendix A 2) that due to the Umklapp terms the phase-locking angle ϕ is 0 for $\rho>\frac{3}{10}$ and $\frac{1}{2}$ for $\rho<\frac{3}{10}$. The magnetization structure corresponding to $\phi=0$ and $\frac{1}{2}$, to be denoted A and B, respectively, are shown in Figs. 1(a) and 1(b). Phase B is characterized by the presence of disordered planes with zero magnetization. Due to the high entropy associated with the disordered planes, we expect this phase to be stabilized only at high temperatures. Figure 1(c) shows an intermediate situation between A and B, to be denoted C, in which $0<\phi<\frac{1}{2}$. Phase C is asymmetric, without the reflection or inversion symmetries present in phases A

and B. We have found that for $\rho < \frac{3}{10}$ the commensurate phase changes from B to A as the temperature is decreased. Inbetween these phases there is a narrow strip of phase C where the locking angle ϕ varies continuously, as shown in Fig. 2. The transition to the C phase was determined by monitoring the eigenvalues of the matrix $\mathbf{M}$ given in Eq. (3). The B phase is locally stable at high temperatures, but as the temperature is lowered it eventually becomes unstable at a temperature $T_B(\kappa)$. Analogously, the A phase is stable at low temperatures but it becomes unstable at a higher temperature $T_A(\kappa)$. For $T_A(\kappa) < T < T_B(\kappa)$ phase C is the locally stable one, as depicted in the inset of Fig. 3.

The local stability is a necessary condition for the existence of the $q=\frac{1}{6}$ phase, but it is not sufficient because other commensurate phase may have lower free energy. Thus it is necessary to investigate the stability against the creation of domain walls.[1,5,6,7] Let us represent the magnetization in the $q=\frac{1}{6}$ phase by the Fourier series

$$M_n = A_1 \cos 2\pi q(n+\phi) + A_3(-1)^n . \tag{5}$$

In the neighborhood of T_c we can make the constant amplitude approximation[1] by assuming that A_1 has the same value of the commensurate phase and that $\phi(n)$ and $A_3(n)$ are slowly varying functions of n. Then we obtain for $\phi(n)$ a sine-Gordon soliton solution, from which we get the asymptotic form of the commensurate-incommensurate transition line of the $q=\frac{1}{6}$ phase close to T_c:

$$T = T_c - \frac{3\pi}{4}|1-2\kappa| \left[\frac{5(3+8\rho)}{6} \right]^{1/2} \left\{ \tfrac{3}{2} \left|1-\tfrac{10}{3}\rho\right|^{-1/2} \right\} . \tag{6}$$

The above equation differs from the result of Ref. 1 by the factor between the curly brackets because in their work the third harmonic term A_3 was not taken into account. Fortunately for $\rho=1$ this factor is nearly equal to 1, being 0.981 98. . ., but for other values of ρ this term makes a significant difference.

Equation (6) is valid only asymptotically close to T_c. For lower temperatures we have compared numerically the free-energy densities of the $\frac{1}{6}$ phase and phases $(j+1)/2(3j+2)$ or $\langle 2\ 3^j \rangle$, in the notation of Ref. 2, for $\kappa > 0.5$ and phases $(j+1)/2(3j+4)$ or $\langle 4\ 3^j \rangle$ for $\kappa < 0.5$. These phases can be interpreted as describing regularly spaced walls in the $\frac{1}{6}$ commensurate matrix. In Fig. 4 we show the structures of the phase $\langle 2\ 3^{59} \rangle$ in different regions of the phase diagram. The arrows indicate the location of the walls. In Fig. 4(a), which corresponds to the region $T < T_A(\kappa)$, we observe that the core of the walls have structures similar to the B phase. On the other hand, in Fig. 4(c) corresponding to the region $T > T_B(\kappa)$, the core of the walls have structures similar to the A phase. These walls are spaced by $3j+2$ lattice spacings. The situation is rather different in Fig. 4(b) corresponding to the region $T_A(\kappa) < T < T_B(\kappa)$ where we observe two different types of walls, one with the structure resembling the A phase and the other the B phase. The two different types of walls occur alternately and they are separated by $(3j+2)/2$ lattice spacings.

The transition from phase $\frac{1}{6}$ to phase $\langle 2\ 3^j \rangle$ will be of first order for any finite j. For the case $J_0 = J_1$ the transitions are of first order up to the accumulation point of

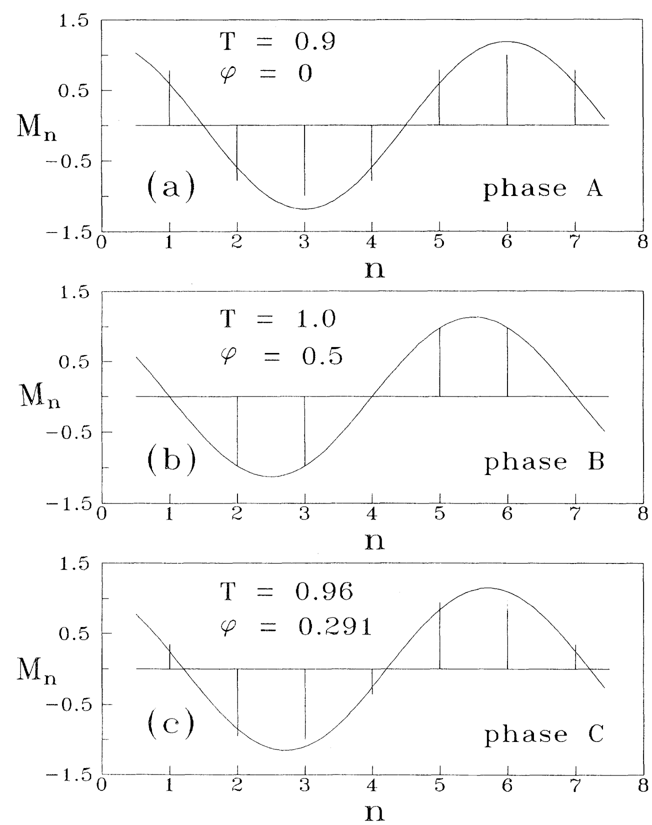

FIG. 1. Magnetization per spin in phase $\frac{1}{6}$ as a function of the layer coordinate for $\rho=0.2$, $\kappa=0.5$, and different temperatures. The solid curve represents the main harmonic.

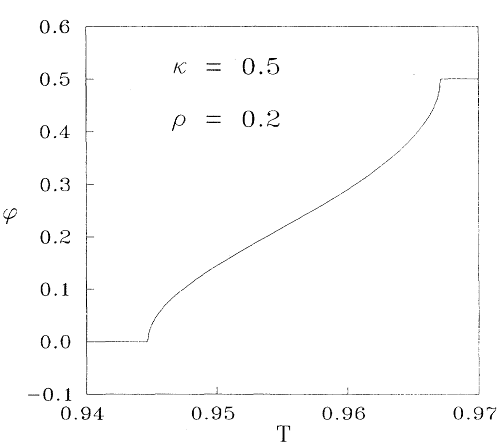

FIG. 2. Graph of the phase angle ϕ of the main harmonic as a function of the temperature T.

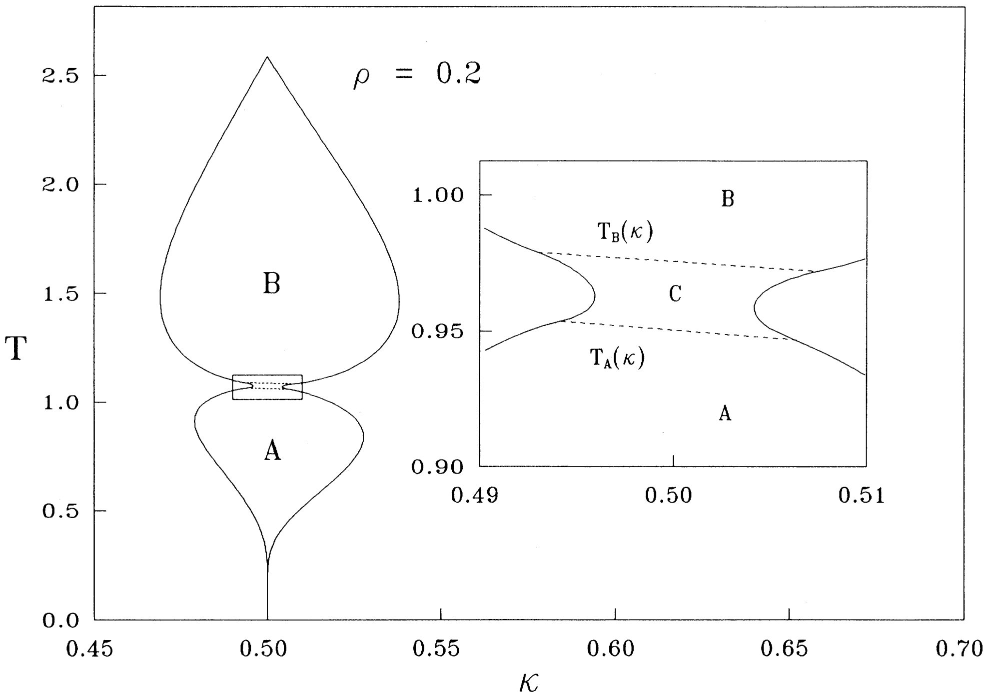

FIG. 3. Phase diagram of the $\frac{1}{6}$ phase with phases A and B separated by a bottleneck-shaped region where phase C is stable. The inset shows the detail around the bottleneck.

the branching points that occur at a temperature $T_b^{(\infty)}$.[6] The temperature $T_b^{(\infty)}$ can be determined by studying the interaction of the walls at a large distance of separation, which can be related to the eigenvalues of the matrix (3).[13,14] This kind of analysis indicates that for $\rho < \frac{3}{10}$ most of the phase boundary is a second-order commensurate-incommensurate type, except perhaps at very low temperatures. To determine the phase boundary in practice we have compared the free-energy density of phase $\frac{1}{6}$ with the free-energy densities of phases $\langle 2\ 3^j \rangle$ for increasing values of j, up to $j=300$, until we reach a value of j such that the wall-wall interaction energy becomes negligible within the numerical precision employed. The main problem we had to face in this calculation was the slow decay of the wall-wall interaction in the neighborhood of $T_A(\kappa)$, $T_B(\kappa)$, and T_c. This implies not only that we have to solve the system of Eq. (2) for a very large number of equations but also that the convergence of the straightforward iterative process to solve this set of equations becomes prohibitively slow. We overcame this difficulty by observing that phases $\langle 2\ 3^j \rangle$ present either symmetries by reflection or by inversion, which halves the number of equations to be solved. Moreover, the application of the Newton method to this new set of equations involves only the inversion of a band diagonal matrix of bandwidth five, a process in which the computation time only increases (roughly) linearly with the dimension of the matrix. The efficiency of this procedure can be gauged by the fact that all the computations reported here were performed on a microcomputer PC-XT. The transition to the phase $\langle 4\ 3^j \rangle$ can be studied analogously except that the possibility of first-order transition to the ferromagnetic phase should be taken into account.

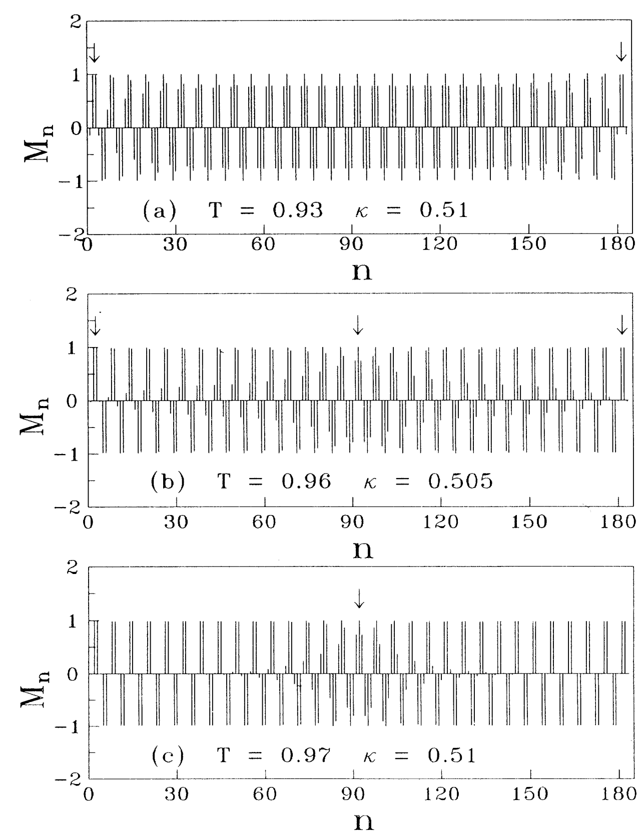

FIG. 4. Magnetization per spin of phase $\langle 2\ 3^{59} \rangle$ as a function of the layer coordinate for $\rho=0.2$ in different regions of the phase diagram. The arrows indicate the location of the domain walls.

To conclude we mention that there are other commensurate phases, e.g., $\frac{1}{8}$, $\frac{1}{10}$, and $\frac{3}{14}$, which show behavior similar to the $\frac{1}{6}$ phase for small values of ρ.[8] It would be interesting to investigate the effect of the pinning energy of the walls which may have interesting implications on the phase diagram.[9] Also it would be quite interesting to know whether type-B or -C phases are present in the real ANNNI model, in contradistinction to its mean-field version.

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