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Chaotic Behavior and Incommensurate Phases in the Anisotropic Ising Model with Competing Interactions

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The mean-field equations of the Ising model with competing interactions are studied by means of an iteration procedure. It is found that the phase diagram consists of regimes with stochastic behavior, indicating a complete "devil's staircase" with pinned configurations only, and analytic regimes where commensurate pinned phases are separated by incommensurate phases with Goldstone modes.

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The anisotropic Ising model with competing nearest-neighbor interaction, $J_1 > 0$, and next-nearest-neighbor interaction, $J_2 < 0$, in one particular direction only was originally constructed by Elliott[1] in order to describe modulated structures in rare-earth systems. Recently the interest in the model was renewed when von Boehm and Bak[2-4] investigated it numerically by solving the mean-field equations approximately and analytically by mapping the model onto a continuum soliton theory describing commensurate-incommensurate transitions. An infinity of commensurate phases was found. This discovery was subsequently confirmed at *low* temperatures by Villain and Gordon[5] using a different phenomenological mean-field theory, and by Fisher and Selke[6] using a low-temperature expansion technique. No incommensurate phases with Goldstone modes (phasons) were found, but all phases are "pinned" to the lattice.

In this paper, the model is studied by means of a recursion procedure which does not involve the continuum approximation. It will be shown that the phase diagram consists of chaotic regimes where all states are pinned, and "analytic" regimes including incommensurate phases with sliding modes.

Within the mean-field theory the free energy can be written[3,4]

$$F = \sum_{ij} J_{ij} M_i M_j - T \sum_i \int_0^{M_i} \tanh^{-1}\sigma \, d\sigma. \tag{1}$$

Here, J_{ij} is the interaction between spins at sites i and j, and M_i is the thermodynamical average of the spin at site i. The previous calculations[2-6] showed that a large fraction of the phase diagram is formed by the "$++--++$" phase consisting of two "up" layers followed by two "down" layers and so on. This phase has a period of four lattice units and a wave vector $q = 2\pi/4$. To study the stability of the phase diagram in its neighborhood I introduce the *discrete* phases φ_i:

$$M_i = A\cos(\varphi_i + 2\pi i/4). \tag{2}$$

As usual, one assumes that A is a constant in the region of interest,[7] but φ_i may depend on the coordinate i along the direction with competing interactions. A constant $\varphi(=\frac{1}{4}\pi)$ describes the $q = 2\pi/4$ commensurate phase. $\varphi_i = \frac{1}{2}\pi \bar{q} i$ is a phase with $q = \frac{1}{2}\pi(1+\bar{q})$. The amplitude, A, can be calculated by solving the mean-field equations in the commensurate phase:

$$(4J_0 - 2J_2)A = T\tanh^{-1}A. \qquad (3)$$

Here J_0 is the interaction between spins perpendicular to the anisotropy direction. Now (2) is inserted into (1), and F is expanded in terms of the phase differences $(\varphi_i - \varphi_{i-1})$. Terms up to second order are kept. Apart from a constant, the free energy becomes

$$F/N^2 = 2A^2J_2\sum_i\left[\tfrac{1}{2}(\varphi_{i+1} - \varphi_i - \delta)^2 + aV(\varphi_i)\right], \qquad (4)$$

where N is the length of the system, $\delta = J_1/4J_2$,

$$V(\varphi_i) = \tfrac{1}{2}\left[\int_0^{A\cos\varphi_i}\tanh^{-1}\sigma\,d\sigma + \int_0^{A\sin\varphi_i}\tanh^{-1}\sigma\,d\sigma\right], \qquad (5)$$

and

$$a = T/2A^2J_2.$$

$V(\varphi_i)$ is an effective potential for the phase at layer i. The shape of the potential depends on T and J_0 through A. Near T_c, $V(\varphi_i)$ may be expanded in A:

$$V(\varphi_i) \simeq A^4/96\cos(4\varphi_i) \qquad (6)$$

and (4) becomes identical to the Frenkel-Kontorowa model used to discuss commensurate-incommensurate transitions.[7] When A increases, as the temperature is lowered, the shape deviates from the form (6). The configurations minimizing F are found among the solutions to an infinity of difference equations

$$(\varphi_{i+1} - \varphi_i) - (\varphi_i - \varphi_{i-1}) + aV'(\varphi_i) = 0. \qquad (7)$$

The Eqs. (7) may be considered as recursion relations or "mappings" of the quantities φ_i and $w_i = \varphi_i - \varphi_{i-1}$

$$w_{i+1} = w_i - aV'(\varphi_i) \qquad (8)$$
$$\varphi_{i+1} = \varphi_i + w_i.$$

Solutions to (8) can be generated by starting at one point (φ_1, w_1) in (φ, w) space and iterating the equations. Despite its simplicity, (8) cannot be solved analytically (which can be proven) but various mathematical theorems give information on the nature of the solutions. In the continuum approximation the first two terms in (7) are replaced by the second derivative and the problem becomes solvable. My goal, however, is to describe the effects of the lattice.

Figure 1 shows the results of computer iterations of (8) for $A = 0.71$ and (1) $a = 3.86$ and (2) $a = 8$. The diagrams show w_i as a function of $\varphi_i(\mathrm{mod}\,\tfrac{1}{2}\pi)$. Points $(0, w_1)$, $-0.35 < w_1 < 0.35$ and $(\varphi_1, 0)$, $\tfrac{1}{4}\pi < \varphi_1 < 3\pi/4$ were generally chosen as starting points, and typically 2000 iterations were performed.

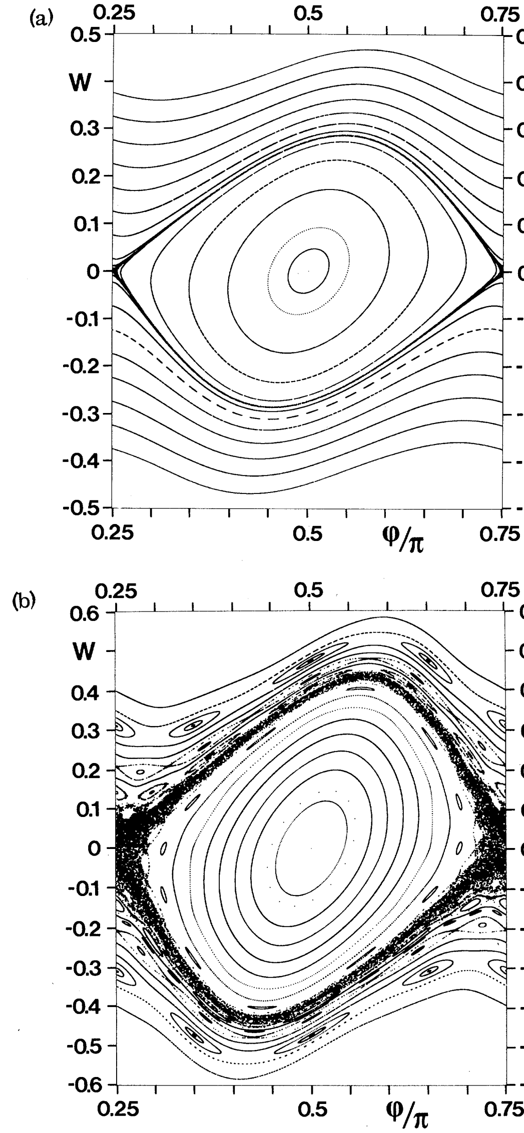

FIG. 1. Solutions to difference equations (7). (a) $a = 3.68$ corresponding approximately to $J_1 = J_0$, $T = 7.36 \times J_0$. At the CI transition $J_2 \sim -2J_0$. (b) $a = 8$ corresponding to $J_1 = 0.341J_0$, $T = 3J_0$, $J_2 \simeq -0.375J_0$ at the CI transition.

Case (1) corresponds to a "relatively" weak potential (temperature not too far from T_c and $J_2 \sim -2J_1$). Several types of trajectories are seen.

(i) Fixed point (FP) at $\varphi_i = \tfrac{1}{4}\pi$, $w_i = 0$. This is the commensurate (C) phase. There is another

FP at $(\frac{1}{2}\pi, 0)$ describing the phase $+0-0+$ which maximizes F.

(ii) Smooth invariant trajectories. Starting at $(\frac{1}{4}\pi,\ w_1 > 0.01)$ the points eventually form continuous curves, despite the discreteness of the steps. These curves describe *incommensurate* (I) states with

$$\varphi_i = (\tfrac{1}{2}\pi\bar{q}i + \alpha) + f(\tfrac{1}{2}\pi\bar{q}i + \alpha),$$
$$f(x) = f(x + \tfrac{1}{2}\pi), \tag{9}$$

where f is a unique function, and α is an arbitrary phase. The existence of such curves can be proven by means of the Kolmagorov, Arnold, Moser theorem.[8,9] A diffraction experiment on the system would produce Bragg satellites at $q = \frac{1}{2}\pi(1+\bar{q})$. Some of the curves appear to be dashed lines. This is because, for illustration, the iterations were stopped before the curves were traced out. An infinitesimal shift of α shifts the starting point, but the curve (and the energy) remain invariant. This is the Goldstone mode (phason) of the I phase. A gapless sliding mode exists despite the discreteness of the Ising model! In the continuum version of (7), all the solutions are of the form (9). At large values of w_1, w_i does not fluctuate much, indicating a relatively small content of higher harmonics. When w_1 becomes smaller (but still > 0.01) the trajectories describe a soliton lattice with a large density of points near $(\frac{1}{4}\pi, 0)$ and a smaller density near the phase kinks at $(\frac{1}{2}\pi, \sim 0.3)$. The width of the solitons is ~ 5 in this case. The closed orbits around the unphysical FP are energetically unfavorable commensurate phases with an incommensurate modulation.

(iii) Chaotic trajectories. When the initial configuration is chosen sufficiently close to $(\frac{1}{4}\pi, 0)$ the trajectories change in a dramatic way. The points do *not* form a curve but tend to fill out completely a finite (but small) area in the phase space. This area is mainly concentrated near $(\frac{1}{4}\pi, 0)$, but the irregular grainy curve connecting this point with the equivalent area around $3\pi/4$ belongs to this "chaotic" trajectory. The recursion relations act as an information source[10] in a way very similar to a random number generator in a digital computer. An infinitesimal shift of the (w_1, φ_1) changes the flow dramatically. Physically, these solutions describe a random combination of pinned solitons and antisolitons. Depending on the sign of δ *either* a series of solitons or antisolitons will be favored. The solutions in this area eventually form the devil's staircase

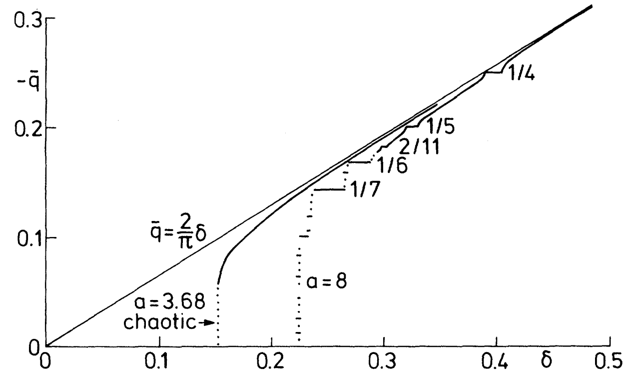

FIG. 2. Wave vector vs $\delta = (J_1/4J_2)$ near the CI transition.

with *no* commensurate phases as discussed in Refs. 2 and 8. The solutions found by Villain and Gordon[5] and by Fisher and Selke[6] can all be classified as pinned domain-wall states. There is no Goldstone mode in this phase, but an infinity of metastable states. A diffraction experiment would show smeared peaks corresponding to some random (metastable) distribution of walls.

Among all these solutions the stable one is the one with lowest energy at a given value of $\delta(=J_1/4J_2)$. Figure 2 shows the wave vector $\bar{q}$ defined by Eq. (9) as a function of δ. At large δ the I phase is stable. When the distance between solitons (at decreasing δ) becomes sufficiently large the repulsive interaction between the solitons cannot overcome the pinning to the lattice, and the soliton lattice breaks up to form the chaotic phase. The critical distance between solitons in case (1) is ~ 18.2 corresponding to a misfit of $\sim 5.5\%$ $(q/2\pi = 0.236)$. At some point, the natural misfit δ becomes small enough to stabilize the C phase (the soliton energy becomes positive).

In summary, the effect of discreteness of (7) is to squeeze in a relatively narrow chaotic regime between the C and I phases. Apart from this, the continuum approach is qualitatively and quantitatively correct.

In case (2) [Fig. 1(b)] the value of the potential is increased. This corresponds to lowering the temperature, or increasing the perpendicular coupling J_0, while keeping A constant. The width of the chaotic regime increases dramatically. However, invariant trajectories describing incommensurate phases still exist. The maximum distance between solitons in the unpinned I phase is only 5.7, yielding a misfit of $\sim 17.7\%$ and $q/2\pi \simeq 0.206$. This trajectory (which borders the chaotic regime) passes through the point $(\varphi, w) \simeq(\frac{1}{4}\pi, 0.17)$ and, as can be seen, follows a quite complicated orbit in (φ, w) space. At larger values of w_i the behavior becomes more regular.

Additional features become evident. In the chaotic regime there are bubbles with no chaotic points inside. They describe higher-order commensurate phases, which eventually form the main steps of the devil's staircase. Also, in the incommensurate regime there are bubbles between the invariant trajectories describing higher-order commensurate phases. For example, between the trajectories through $(\frac{1}{4}\pi, 0.28)$ and $(\frac{1}{4}\pi, 0.35)$ there are four bubbles giving a C phase with $q/2\pi = \frac{1}{4}(1-\frac{1}{4}) = \frac{3}{16}$. The C phase is given by a limit cycle sequence between $(0.286\pi, 0.295)$ and three other points. For w_1 closer to the $\frac{1}{4}$ phase a commensurate phase indicated by a series of five bubbles is evident, and $q/2\pi = \frac{1}{4}(1-\frac{1}{5}) = \frac{1}{5}$. This (and the other) high-order C phases are surrounded by narrow chaotic phases of their own. Consider the sequence of points generated starting from $(\frac{1}{4}\pi, 0.21)$. The behavior is clearly chaotic: Sometimes the points are below the bubble, sometimes they are above. In fact, the regime around $(0.28\pi, 0.2)$ is a miniature reproduction of Fig. 1(a)! The incommensurate phase is thus penetrated by high-order commensurate phases (as is expected[4,5]), each surrounded by its own chaotic phase. This forms the incomplete devil's staircase. It is never possible to go from an incommensurate phase to a commensurate phase without passing a chaotic phase. For very large values of a ($\gtrsim 12$) *no* incommensurate phases exist, and the staircase is believed to be everywhere complete.[8]

Although the results presented here have been derived for a specific model, the picture which emerges may well apply to many different systems in statistical mechanics, magnetism, and other areas of solid state physics where modulated structures occur. In the magnetic system CeSb several commensurate phases have been observed,[2,11] and no "smooth" behavior exists. This would correspond to the chaotic regime in Fig. 1 with pinned phases only. In the epitaxial system, krypton on graphite, a destruction of the Bragg peak has been observed in the "incommensurate" phase near the C phase.[12] This could indicate a chaotic phase, existing even at the lowest temperatures.

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