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LETTER TO THE EDITOR

Lattice gas model with competing interactions: hard walls, dimerisation and a new melting mechanism

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Abstract. We study the low temperature phases of the two-dimensional ANNNI model in an external field. A new type of melting mechanism due to hard walls is found and special Lifshitz-type multicritical points are predicted. For strong attraction between elementary units of different periodicity the dimerisation process leads to a phase diagram typical for an *XXZ* chain.

Recently much attention has been paid to the study of lattice gas models with anisotropic competing interactions (Kinzel *et al* 1982, Selke *et al* 1983). In two dimensions this interest is motivated by different experimental realisations of such simple models, most noticeably H/Pd(100), O/W(110), H/Fe(110) and O/Pd(110).

In this letter we consider the low temperature region of the 2D axial next-nearest-neighbour Ising (ANNNI) model in a field (Rujan *et al* 1983). For antiferromagnetic competing first and second neighbour interactions in the x direction and ferromagnetic interactions in the y direction, this model describes reasonably well the structures observed in the system O/Pd(110) (Ruján *et al* 1983). Moreover, we believe that our analysis is also valid for the more general problem of commensurate (C)–incommensurate (IC) phase transitions in two dimensions. In the following we shall pursue the line of thought of Villain and Bak (1981) and interested readers are referred to their work for technical details. The Hamiltonian under consideration has the form

$$-\beta E = \sum_{i,j} (-K_1 s_{ij} s_{i+1,j} - K_2 s_{ij} s_{i+2,j} + K_0 s_{ij} s_{i,j+1} + H s_{ij})$$

where $K_i = J_i / k_B T$, $H = \mu_B B / k_B T$ and $s_{ij} = \pm 1$.

The $T = 0$ phase diagram of this model consists of the different layered structures shown in figure 1 (Oguchi 1965). The notation $\langle 2, \bar{1} \rangle$ refers to a periodic structure of two columns of up-spins followed by one column of down-spins, etc. The ferromagnetic phase ($F_\uparrow$) is uniquely fixed by the external field.

At low temperatures and near the multicritical lines AC, AB and BD (see figure 1) the dominant low temperature excitations are line defects (walls) and their thermal motion represented by short wall excursions (kinks) to the left or to the right. In simple cases the problem of thermalised walls can be solved exactly (Villain and Bak 1981), while the effect of higher excitations, mainly dislocations, is assessed using renormalisation group arguments (Coppersmith *et al* 1981).

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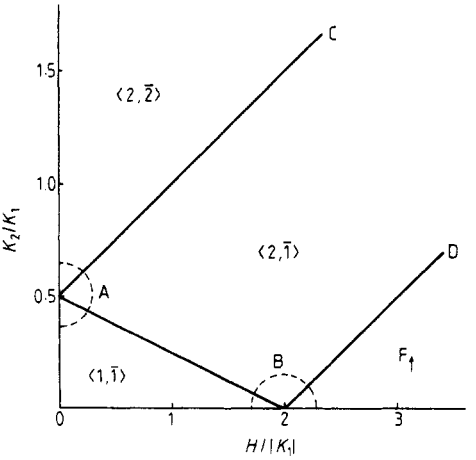

Figure 1. Ground state phase diagram of the ANNNI model in a field at $T=0$ as a function of $\kappa = K_2/K_1$ and $h = H/|K_1|$.

We generalise this approach in two different directions. First, we consider a typical situation where one has an additional competition between two different types of walls (near point A in figure 1). Our approach is exact in second order in the 'temperature' variable $\gamma = e^{-2K_0} \simeq K_0^* = -0.5 \ln \tanh K_0$.

A quite different situation is encountered near point B in figure 1, where the strong attraction between two types of elementary units cannot be neglected even in first order in γ and leads to a dimerised phase. Some questions related to our analysis had been studied previously in a different context by Howe *et al* (1983) and Kardar and Shankar (1983).

Let us consider first the encircled region near point A (figure 1). All layered ground state (GS) structures ($T=0$) may be formed as an alternating sequence of A-type units (++ or +) and B-type units (−− and −). At low temperatures and near the multicritical lines the ABAB... ground state structure is altered by a few line defects (walls or solitons) corresponding to the change of an A(B)-type GS unit into an 'excited' unit of the same type, a(b). The a(b) units have different excitation energies and 'easy' ('hard') wall denote a light (heavy) excitation, respectively. Following Villain and Bak (1981) the a(b) units are considered as particles and the GS units A and B as holes. A fictitious lattice is introduced whose length M equals twice the total number of A-type or B-type units. Note that the length of M in original lattice constants depends on the present number of particles.

In the usual approach one uses the transfer matrix formalism to calculate the partition function of thermalised walls at *fixed M*. Then the free energy is obtained by minimising with respect to M.

Writing the row-to-row transfer operator in the fictitious space as

$$T = \exp(-H) \qquad (M \text{ fixed}) \tag{1}$$

we construct H through a low temperature expansion valid in second order in γ. The cases A = ++, a = +, B = −−, b = − and A = +, a = ++, B = −, b = −− lead to H operators of similar structure. The processes involved in the construction of the Hamiltonian are shown in table 1 together with the corresponding sums written in terms of the fermion operators $\{c_m\}(n_m = c_m^+ c_m)$. The counterterms arise because of

Table 1. Typical processes leading to the Hamiltonian (3). For the $\langle 2, \bar{2}\rangle$ GS $\varepsilon_1 = -K_1 + 2K_2$ while for the $\langle 1, \bar{1}\rangle$ GS $\varepsilon_1 = 2K_1 - 4K_2$. In both cases $\varepsilon_2 = H$.

Process		Contribution to H
Ground state		
1, A = ++, B = −−		$E_{GS} = -K_2 N_0$
2, A = +, B = −		$E_{GS} = -(K_1 - K_2)N_0$
Straight walls		
ABABaBab	○○○○●○●●	$\varepsilon_1 \sum n_m + \varepsilon_2 \sum e^{i\pi m} n_m$
Thermal fluctuations of walls		
ABaBA	○○●○○	$-\gamma \sum (c_m^+ c_{m+1} + c_{m+1}^+ c_m)$
AbABA	○●○○○	
ABaBA	○○●○○	$-\gamma^2 \sum (c_m^+ c_{m+2} + c_{m+2}^+ c_m)$
aBABA	●○○○○	
Counterterms		
ABaBA	○○●○○	
AbABA	○●○○○	$\frac{1}{2}\gamma^2 \sum (c_m^+ c_{m+2} + c_{m+2}^+ c_m)$
aBABA	●○○○○	
ABaBA	○○●○○	
AbABA	○●○○○	$\frac{1}{2}\gamma^2 \sum [n_m(1 - n_{m+1}) + n_{m+1}(1 - n_m)]$
ABaBA	○○●○○	

the exponentiation of the low temperature series. Terms of order $\gamma^2 n_m n_{m+1}$ are neglected because near the C-IC boundary $\bar{n}$ is small.

After a Fourier transformation one folds the Brillouin zone into the $-\pi/2 \leq k \leq \pi/2$ interval and one has

$$H = \sum_{-\pi/2 \leq k \leq \pi/2} H_k, \qquad H_k = h_1^{(+)}(a_k^+ a_k) + h_1^{(-)} b_k^+ b_k + h_2(b_k^+ a_k + a_k^+ b_k), \tag{2}$$

where $a_k = c_k$, $b_k = c_{k+\pi}$ and

$$h_1^{(\pm)} = -K_1 + 2K_2 \mp 2\gamma \cos k + 2\gamma^2 \sin^2 k, \qquad h_2 = -H,$$

for the $\langle 2, \bar{2}\rangle$ structure, while for the $\langle 1, \bar{1}\rangle$ GS structure $(-K_1 + 2K_2) \to (2K_1 - 4K_2)$. The diagonalisation of (2) is standard and one obtains the C-IC boundaries as

$$\begin{aligned} H^2 &= (-K_1 + 2K_2)^2 - 4\gamma^2 \qquad \text{for } \langle 2, \bar{2}\rangle - \text{IC}, \\ H^2 &= (2K_1 - 4K_2)^2 - 4\gamma^2 \qquad \text{for } \langle 1, \bar{1}\rangle - \text{IC}. \end{aligned} \tag{3}$$

The incommensurate (floating) phase near the $\langle 1, \bar{1}\rangle$ boundary is not stable against dislocations (Coppersmith *et al* 1981, Villain and Bak 1981) and (3) represents the boundary between the $\langle 1, \bar{1}\rangle$ phase and the ferro-paramagnetic (liquid) phase. This transition is of Ising type. The 'four-leg' easy wall dislocations, however, are not relevant near the $\langle 2, \bar{2}\rangle$ boundary. If

$$H = 2K_1 - 4K_2 + 2\gamma^2 \tag{4}$$

the IC phase melts into the liquid phase through a C-IC type phase transition ($\alpha = \frac{1}{2}$ and the misfit parameter obeys the square root law on the IC side; $\nu = 1$ and the specific heat is regular on the liquid side).

The situation is even more interesting for the $\langle 2, \bar{1}\rangle$ GS structure, A = ++, B = −, a = +, b = −−. The low temperature processes are illustrated in table 2. Note that the dominant term in γ order is the creation (absorption) of a pair of easy(hard) walls.

Table 2. Typical processes leading to the Hamiltonian (6), $\varepsilon_1 = H$, $\varepsilon_2 = \frac{1}{3}(4K_1 - 8K_2 + H)$.

Process		Contribution to H
Ground state A = ++, B = −		$E_{GS} = -\frac{1}{3}(K_1 + K_2 + H)$
Straight walls a = +, b = −−		
ABaBabA	○○●○●●○	$\varepsilon_1 \sum n_m + \varepsilon_2 \sum e^{im\pi} n_m$
Thermal fluctuations of walls		
ABABA	○○○○○	$-\gamma \sum (c_m^+ c_{m+1}^+ + c_{m+1} c_m)$
ABabA	○○●●○	
ABaBA	○○●○○	$-\gamma^2 \sum (c_m^+ c_{m+2} + c_{m+2}^+ c_m)$
aBABA	●○○○○	
Counterterms		
ABaBA	○○●○○	
abaBA	●●●○○	$\frac{1}{2}\gamma^2 \sum (c_m^+ c_{m+2} + c_{m+2}^+ c_m)$
aBABA	●○○○○	
ABabA	○○●●○	
ABABA	○○○○○	$\frac{1}{2}\gamma^2 \sum (n_m n_{m+1} + (1 - n_m)(1 - n_{m+1}))$
ABabA	○○●●○	

Neglecting again the $\gamma^2 n_m n_{m+1}$ terms and after the Fourier transformation the Brillouin zone is folded into the $0 \leq k \leq \pi/2$ interval:

$$H = \sum_{0 \leq k \leq \pi/2} H_k,$$

$$H_k = h_1(a_k^+ a_k + a_{-k}^+ a_{-k} + b_k^+ b_k + b_{-k}^+ b_{-k}) + h_2(b_k^+ a_k + b_{-k}^+ a_{-k} + a_k^+ b_k + a_{-k}^+ b_{-k}) + h_3(a_k a_{-k} + b_{-k} b_k + a_{-k}^+ a_k^+ + b_k^+ b_{-k}^+), \tag{5}$$

where

$$h_1 = H - \gamma^2(1 + \cos 2k), \qquad h_2 = (H - 8K_2 + 4K_1 - \gamma^2)/3, \qquad h_3 = 2\gamma \sin k.$$

The diagonalisation of this Hamiltonian is more involved but is still feasible analytically. The lowest two energy levels are, except for identical constants, given by

$$E_1 = -h_2, \qquad E_2 = -(h_1^2 + h_3^2)^{1/2}. \tag{6}$$

A careful study of the ground state structure of (5) reveals the following phase diagram. A C–IC phase transition takes place at

$$H = 2K_1 - 4K_2 + 5/2\gamma^2 \tag{7a}$$

on the $\langle 1, \bar{1}\rangle$ side and at

$$H = -K_1 + 2K_2 + 7/4\gamma^2 \tag{7b}$$

on the $\langle 2, \bar{2}\rangle$ side of the $\langle 2, \bar{1}\rangle$ phase. This incommensurate phase melts through a second IC–C type transition mediated by hard walls (here point defects become relevant) at

$$H = -K_1 + 2K_2 + 7/4\gamma^2 \tag{8a}$$

on the $\langle 1, \bar{1}\rangle$ side and at

$$H = 2K_1 - 4K_2 + 5/2\gamma^2 \tag{8b}$$

on the $\langle 2, \bar{2}\rangle$ side. There is a direct, Ising type transition from the $\langle 2, \bar{1}\rangle$ phase into the disordered phase at a special Lifshitz-type multicritical point at the intersection of (6*b*)–(7*b*)

$$\gamma^2 = 8K_2 - 4K_1 \geqslant 0. \tag{9}$$

Since the 'three-leg' dislocations of easy walls are not relevant near the $\langle 2, \bar{1}\rangle$ boundary this type of behaviour should be seen around point A ($\kappa \geqslant \frac{1}{2}$, H small in figure 1).

The situation near point B (H finite, κ small) is quite different. The layered structures encountered here can be described in terms of only two elementary units, A = +− and B=+. Considering +− as a hole and + as a particle the low temperature form of the transfer matrix Hamiltonian (1) is

$$H = \text{constant} + \sum_m [\varepsilon n_m + \omega n_m n_{m+1} - \gamma^2(c_m^+ c_{m+1} + c_{m+1}^+ c_m)] \tag{10}$$

where

$$\varepsilon = \varepsilon^{\mathrm{B}} - \varepsilon^{\mathrm{A}} + \varepsilon^{\mathrm{AB}} + \varepsilon^{\mathrm{BA}} - 2\varepsilon^{\mathrm{AA}} + (1 - l_{\mathrm{A}}/l_{\mathrm{B}})(\varepsilon^{\mathrm{A}} + \varepsilon^{\mathrm{AA}}),$$

$$\omega = \varepsilon^{\mathrm{AA}} + \varepsilon^{\mathrm{BB}} - \varepsilon^{\mathrm{AB}} - \varepsilon^{\mathrm{BA}},$$

$\varepsilon^{\mathrm{A,B}}$ is the energy of a single particle A(B), while $\varepsilon^{\mathrm{AA}}$, etc are particle–particle interaction energies, $l_{\mathrm{A}}(l_{\mathrm{B}})$ being the length of unit A(B). A simple calculation yields $\varepsilon = -H + 2K_1 - 4K_2$, $\omega = 4K_2$. Note that the interaction term $n_m n_{m+1}$ is now proportional to K_2 and is not necessarily small. Using the Jordan–Wigner transformation it can be shown that (10) corresponds to an XXZ-chain Hamiltonian:

$$H_{XXZ} = \text{constant}' + \sum_m [\tfrac{4}{3}(H - H_{\mathrm{c}})\sigma_m^z + 2K_2\sigma_m^z\sigma_{m+1}^z - \gamma^2(\sigma_m^x\sigma_{m+1}^x + \sigma_m^y\sigma_{m+1}^y)] \tag{11}$$

where $\sigma^{x,y,z}$ are the usual Pauli matrices and $H_{\mathrm{c}} = 2K_1 - \frac{1}{2}K_2$. As pointed out recently (Uimin and Pokrovsky 1983) the $\langle 2, \bar{1}\rangle$ phase can be considered as a dimerised phase of A = +− and B = + particles. The phase boundary of the $\langle 2, \bar{1}\rangle$ phase can be calculated using the results of Yang and Yang (1966). Along the line $H = H_{\mathrm{c}}$ the $\langle 2, \bar{1}\rangle$ phase changes into an IC phase at $(\gamma^2)_{\mathrm{c}} = 2K_2$ temperature. The C–IC phase boundary has a strong cusp-like behaviour around $H = H_{\mathrm{c}}$, $\gamma^2 = (\gamma^2)_{\mathrm{c}}$:

$$H - H_{\mathrm{c}} \simeq \tfrac{3}{2}\pi\{[(\gamma^2)^2 - (\gamma^2)_{\mathrm{c}}^2]^{1/2}/\lambda\} \exp(-\pi^2/2\lambda) \tag{12}$$

where $\lambda^2 - 2\gamma^2[\gamma^2 - (\gamma^2)_{\mathrm{c}}]$.

At low temperature the phase diagram has the form

$$H - H_{\mathrm{c}} = \tfrac{3}{4}\gamma^2 \sinh\lambda[\tfrac{1}{2} - (\cosh\lambda)^{-1} + (\cosh 2\lambda)^{-1} \mp \ldots] \tag{13}$$

where $\cosh\lambda = |2K_2/\gamma^2|$, γ^2 is small. The first-order result in γ^2 reproduces the free fermion result (Ruján *et al* 1983).

In conclusion we have demonstrated that—at least in special regions of the parameter space—the ANNNI model in a field exhibits a new type of hard wall mediated melting transition which is not of the Kosterlitz–Thouless type. A special type of Lifshitz point emerges as a result of the competition between line and point defects. At small κ we also find a typical dimerisation process appropriately described by an XXZ Hamiltonian. Detailed calculations will be published elsewhere.

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