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LETTER TO THE EDITOR

Wetting in the two-dimensional ANNNI model

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Abstract. We demonstrate the existence of a first-order wetting transition in the (2, 2) phase of the two-dimensional ANNNI model. The position of the wetting line is studied using the interfacial free energy approximation, numerical transfer matrix methods and Monte Carlo techniques. Our theoretical calculations are found to be in reasonable agreement with results obtained from Monte Carlo simulations.

Recently, there has been considerable interest (Sega *et al* 1985, Rujan *et al* 1985, Huse and Fisher 1984, Fisher 1984) in the study of wetting transitions in two-dimensional systems. In particular, a number of general predictions have been made concerning the nature of wetting transitions in $(p \times l)$ systems (Huse and Fisher 1984, Fisher 1984). However, few detailed studies (Sega *et al* 1985, Rujan *et al* 1985, Derrida and Schick 1985) have been carried out for specific systems. In this letter we show the existence of a novel wetting transition which occurs in the ANNNI model (Hornreich *et al* 1979, Selke and Fisher 1980, Villain and Bak 1981, Selke 1981, Beale *et al* 1985) within the (2, 2) phase. We also determine the position of the wetting line by a variety of techniques, all of which are in reasonable agreement. We note that the existence of a wetting transition can among other things affect the kinetics of domain growth (Ala-Nissila *et al* 1985) in different regions of the phase diagram. It should also be noted that a modified version of the ANNNI model in a field (setting $J_1 < 0$ in (1) below) has been studied as a model of the chemisorbed system O/Pd(110) (Rujan *et al* 1983, 1985).

The Hamiltonian for the ANNNI model is given by

$$H = -\sum_{ij} (J_1 s_{i,j} s_{i+1,j} - J_2 s_{i,j} s_{i+2,j} + J_0 s_{i,j} s_{i,j+1}) \tag{1}$$

where J_0, J_1, $J_2 > 0$ and the summation goes over all sites of a square lattice with Ising spins $s_{ij} = \pm 1$. This Hamiltonian has three different ordered states: a commensurate ferromagnetic phase (F), a modulated (2,2) phase and an incommensurate floating (I) phase. In what follows we shall use a standard parametrisation (Selke and Fisher 1980) of J_1 and J_2 in terms of J_0 where $J_1 = (1-\alpha)J_0$ and $J_2 = \alpha J_0$. The corresponding phase diagram for this model (using this parametrisation) is shown in figure 1.

The (2,2) state, which consists of an alternating sequence of two ferromagnetic layers of up and down spins, has a degeneracy $p = 4$. Thus, one expects the maximum number of elementary walls in the x direction between degenerate phases to be equal to $p(p-1) = 12$. However, because our (2,2) phase is a special case of a $(p \times l)$ phase (with $p = 4$). there are only three physically distinct walls corresponding to the three possible 'phase shifts' between the domains (Huse and Fisher 1984, Kaski *et al* 1985).

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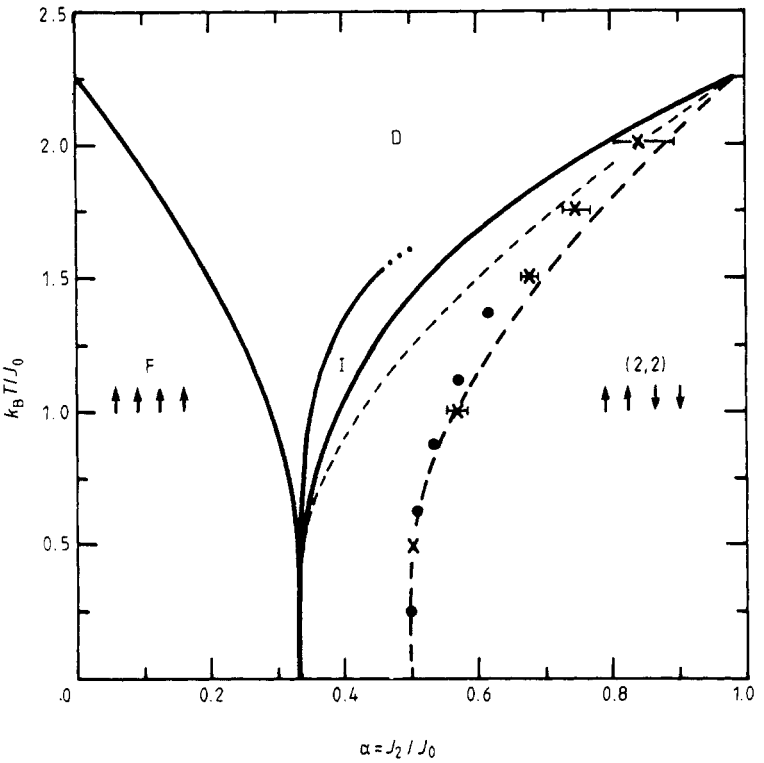

Figure 1. Phase diagram of the ANNNI model showing the disordered (D) phase, the commensurate (2,2) and ferromagnetic (F) phases and the incommensurate (I) phase. Full curves are the phase transition lines from previous MHZ results (the FD line from Hornreich *et al* (1979), the other line from Kroemer and Pesch (1982)). We note that the existence of a Lifshitz point (see the ID line, shown schematically) remains controversial. The light broken curve indicates our results from (4) as discussed in the text. The heavy broken curve shows our theoretical results (6) for the wetting line. The circles are results from numerical transfer matrix calculations at low temperature while the crosses are our MC results. The points at $k_B T/J_0 = 0.5$ and 1.5 are from simulations on the 128×32 system, while the others are from the smaller system. Approximate error bars for the MC data are also shown.

These walls are shown in figures 2(*a*)-(*c*). The ground state energies for these walls are as follows:

$$E_{A|B} = 2J_2 - J_1 = (3\alpha - 1)J_0$$
$$E_{A|D} = 2J_2 + J_1 = (\alpha + 1)J_0 \qquad (2)$$
$$E_{A|C} = 2E_{A|B}.$$

On these grounds we expect the possibility of a wetting transition from a region of the phase diagram favouring a $[p-1]$ wall (dry) to $p-1$ elementary [1] walls (wet region) where $[n]$ denotes the phase shift in the ground state across the wall (Huse and Fisher 1984) (see figure 2).

In our notation this is equivalent to a wetting transition which may be written symbolically as A|D→A|B|C|D where a soft superheavy/light wall becomes wet by

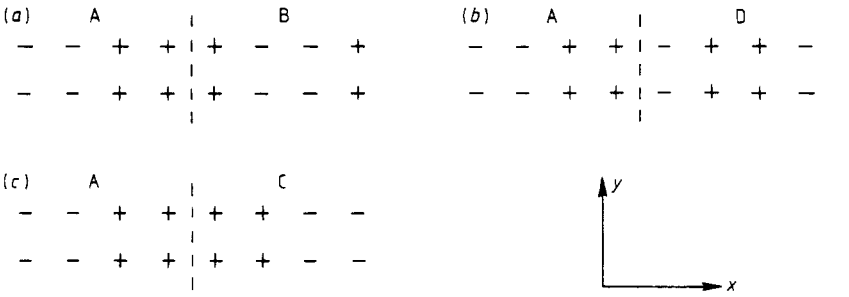

Figure 2. The three physically different walls in the x direction between the degenerate (2,2) phases in the ANNNI model: (*a*) heavy/light or A|B walls, (*b*) soft superheavy/light or A|D walls, (*c*) superheavy/light or A|C walls. Only one type of each wall is shown in each case.

three heavy/light walls. In general this transition will occur when the free energies of the walls satisfy the condition (Huse and Fisher 1984)

$$f_{A|D} = 3f_{A|B}. \tag{3}$$

At $T = 0$, this clearly occurs at $\alpha = \frac{1}{2}$†.

Using the interfacial free energy approximation of Muller-Hartmann and Zittarz (1977) (MHZ) in which the permitted fluctuations of the walls are restricted to kinks with no overhangs (SOS approximation), we have calculated the free energies of the A|B and A|D walls. We note that this approximation is expected to become asymptotically correct at temperatures below the critical temperature (as $T \to 0$) where only the lowest energy excitations are likely‡. In this approximation, the free energies are obtained from the largest eigenvalue of the transfer matrix linking the position of a wall in one column to the next column. Using this approximation we obtain

$$f_{A|B} = J_0(3\alpha - 1) - k_B T \ln(\coth(J_0/k_B T)) \tag{4}$$

and

$$f_{A|D} = J_0(1 + \alpha) - k_B T \ln(\coth(J_0/k_B T)). \tag{5}$$

Inserting these expressions into (3) then gives

$$\alpha = \tfrac{1}{2} + (k_B T/4J_0) \ln \coth(J_0/k_B T). \tag{6}$$

This equation is plotted as the broken curve in figure 1. We note that for $\alpha = 1$, the solution of (6) gives the exact Onsager value ($k_B T/J_0 = 2.269\ldots$), as expected, since for $\alpha = 1$ the model decouples into two uncoupled ($J_1 = 0$, $J_2 = J_0$) layered antiferromagnets. We also note that if we set $f_{A|B} = 0$ we get an estimate for the commensurate-incommensurate transition which is *lower* (see figure 1) than that previously obtained from the MHZ method (Kroemer and Pesch 1982) (for which the walls were taken to

† At zero temperature, another possible wetting transition between the elementary walls which occurs simultaneously is A|D → A|C|D where the wet walls are a superheavy/light (figure 2(*c*)) and a heavy/light wall (figure 2(*a*)). However, at finite temperature, we expect the A|C wall to decay into two walls of type A|B (A|B|C) due to entropy arguments. Thus, this wetting transition is not expected to be observed.

‡ However, for some simple models (such as the Ising model) this approximation gives the exact result for the critical temperature due to an exact cancellation of the neglected fluctuations (see e.g. Muller-Hartmann and Zittartz 1977).

be in the opposite direction). Unlike the previous MHZ calculation, our calculation takes into account the relevant (A|B) walls which appear in the incommensurate phase. (The resulting expression for the commensurate-incommensurate transition, while giving the exact value at $\alpha = 1$ also has the same asymptotic form in the limit of low temperature as the free fermion result (Villain and Bak 1981).) At $\alpha = 1$ the wetting condition (6) becomes true only for $f_{A|B} = f_{A|D} = 0$ since the energy of the two walls is the same, while the entropy contribution for the two is the same in the SOS approximation used. A more accurate determination of the wetting line might be obtained by including the possibility of two wetting phases in addition to the elementary walls, as done by Selke and Pesch (1982) in the calculation of the commensurate-disorder transition line for the 3-state Potts model.

In order to check these results, we have also performed numerical transfer matrix calculations for semi-infinite strips of width $M = 8$ with the strip width running in the x direction (see figure 3). In the limit that the strip width M goes to infinity, the free energy of wall A|B may be written as

$$f_{A|B} = -k_B T \ln(Z_{A|B}/Z_{A|A}) = -k_B T \ln(\lambda_1(A|B)/\lambda_1(A|A)) \tag{7}$$

where λ_1 corresponds to the largest eigenvalue of the transfer matrix with a wall (A|B) and without a wall (A|A). Similarly the free energy of wall A|D may be written as

$$f_{A|D} = -k_B T \ln(\lambda_1(A|D)/\lambda_1(A|A)). \tag{8}$$

Our results from these numerical transfer matrix calculations are shown in figure 1. We note that these calculations are only expected to be valid at low temperatures,

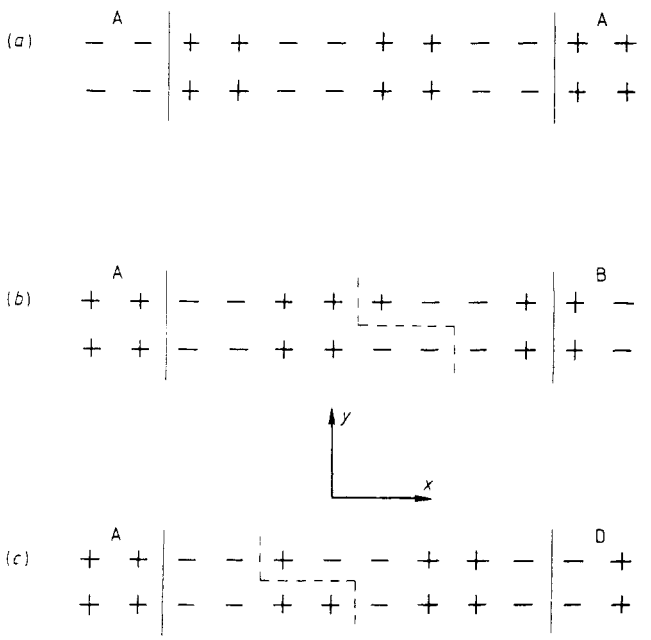

Figure 3. Drawing showing the boundary conditions used in numerical transfer matrix calculations with $M = 8$. The transfer matrix connects successive rows in the infinite y direction. (*a*) Ground state configuration. (*b*) Boundary conditions in the case of an A|B wall. The broken line indicates a wall with a kink for the configuration shown. (*c*) Boundary conditions in the case of an A|D wall. A wall and a kink are also shown by the broken line.

for which the fluctuations of the walls are less than the width of the strip. Nevertheless, they are of interest, since unlike the MHZ method thermal fluctuations other than simple walls are allowed. We note that for large α the transition temperature obtained from the numerical transfer matrix results tend to be high due to the limitation on the size of the wall fluctuations imposed by the finite-size strip width.

In order to check the range of validity of the approximations used above, we have also performed Monte Carlo (MC) simulations with standard Glauber spin-flip dynamics. Two lattices of sizes 64×16 and 128×32 (where the smaller dimension in each case is the y direction) were used to study the effects of finite size. Averages were typically computed by sampling every 100 MC steps per spin over one run of the order of 10^5-10^6 MC steps. The boundaries in the x direction were pinned to the A and D phases (with periodic boundary conditions in the y direction) in order to study the wetting of the A|D wall. Quantities calculated in the MC simulation included the length $L_{A|D}$ of the dry A|D wall

$$L_{A|D}=(1/N)\left\langle\sum_s \delta_{s,A|D}\right\rangle \tag{9}$$

and correspondingly for the wet walls

$$L_{A|B}=(1/3N)\left\langle\sum_s \delta_{s,X|Y}\right\rangle \tag{10}$$

where X|Y = A|B, B|C or C|D. The summations go over the spins s of the N rows of the lattice and $\delta_{s,X|Y}$ is one when a wall X|Y is encountered in a row and is otherwise zero. In the thermodynamic limit one has in the dry region $L_{A|D}=1$, $L_{A|D}=0$ while in the wet region $L_{A|B}=1$ and $L_{A|B}=0$. We have also calculated the net adsorption width of the B and C domains between the A and D phases

$$\langle W\rangle=(1/N)\left\langle\sum_s(\delta_{s,B}+\delta_{s,C})\right\rangle \tag{11}$$

where s denotes a configuration of four consecutive spins along a row which is in either a B or C phase. In the dry region $\langle W\rangle=0$, while in the wet region $\langle W\rangle$ diverges in the thermodynamic limit, i.e. we have complete wetting. In addition, we have calculated the fluctuations of the adsorption width given by

$$(\Delta W)^2=\langle W^2\rangle-\langle W\rangle^2. \tag{12}$$

This exhibits a peak at the transition point.

Our results are summarised in figure 1. Good agreement is apparent between the MHZ results and the MC results up to $k_BT/J_0=1.5$. At higher temperatures the MC results appear to be somewhat above the MHZ results. While finite-size effects were seen to be rather small, a comparison of results (for the two system sizes studied) at $k_BT/J_0=0.5$, 1.0 and 1.5 indicates a slight increase of the wetting temperature (for a given α) with increasing system size. Above $k_BT/J_0\simeq1.5$, the transition rapidly becomes smeared out by increasing temperature and the location of the wetting line (as well as the effects of finite size) become difficult to determine reliably. Figure 4 shows a typical set of data for $L_{A|D}$, $L_{A|B}$ and $(\Delta W)^2$ near the wetting transition at $k_BT/J_0=1.5$.

According to the predictions of Huse and Fisher (1984) the wetting transition in two dimensions should be first order for $p=4$. In order to study this, we have followed

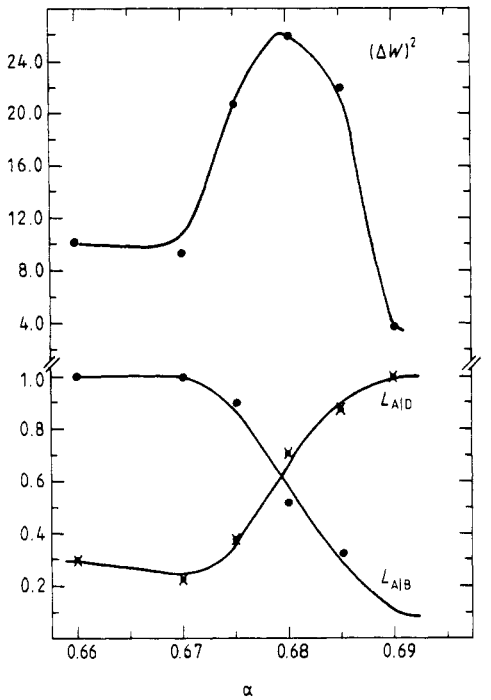

Figure 4. MC results for the 128×32 lattice showing the wetting transition at $k_B T/J_0 = 1.5$. Labels are defined in text.

the scaling of the fluctuations $(\Delta W)^2/M$ (where M is the system width in the x direction) with system size for three different systems at $k_B T/J_0 = 0.5$. While this quantity is expected to diverge with increasing system size for a second-order transition (such as for the case $p = 3$), for the case of $p = 4$ it is expected to vanish in the thermodynamic limit. Our observation of the decrease of $(\Delta W)^2/M$ with increasing system size (the maxima for $(\Delta W)^2/M$ were about 1.0, 0.6 and 0.2 for 64×16, 128×32 and 256×64 systems, respectively) is consistent with this prediction.

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