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LETTER TO THE EDITOR

Interface layering transitions in novel geometries

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Abstract. We show that a novel choice of boundary conditions leads to interfaces which unbind from a surface through a series of layering transitions. Even though the models have only nearest-neighbour interactions the transitions take place at zero temperature. Series expansions are used to probe the behaviour of the phase boundaries as the temperature is increased from zero.

There has recently been considerable work on the properties of interfaces (Dietrich 1988, Sullivan and Telo da Gama 1986). In particular it has been known for some time that below the roughening temperature, in the presence of a lattice, interface phase transitions, such as the unbinding from a surface, can take place through a series of layering transitions (de Oliveira and Griffiths 1978, Pandit *et al* 1982). In this letter we consider the behaviour of interfaces on simple lattices in which a novel choice of boundary conditions leads to a sequence of such layering transitions, even at zero temperature. Although such behaviour is well established in models with long-range interactions, we believe that the systems described here are the first to show such an effect with interactions between nearest neighbours only. Because of the simple nature of the Hamiltonians considered it is a relatively straightforward task to use low-temperature series to study the behaviour of the boundaries between the different interface phases as the temperature is increased.

For comparison we first describe the behaviour of an Ising model on a hypercubic lattice with the interface introduced through the most obvious choice of boundary conditions (Duxbury and Yeomans 1985). Letting the subscript i represent the layers and j the spins within a layer an interface is forced into the system by allowing the spins in layer $i=0$ to take the value -1 and those in layer $i=\infty$ to be equal to $+1$ as shown in figure 1(a). The spins then interact according to the Hamiltonian

$$H = -J \sum s_{i,j} s_{i+1,j} - J_0 \sum s_{i,j} s_{i,j'} - H \sum s_{i,j} \tag{1}$$

where j, j' are nearest neighbours within a layer.

The schematic phase diagram of this model for low temperatures is shown in figure 1(b). At zero temperature and zero field the interface can lie in any position parallel to the boundaries of the system. This degeneracy is broken only at finite temperatures by entropic terms in the free energy which tend to favour the unbinding of the interface from the surface at $i=0$ as $H \to 0^+$.

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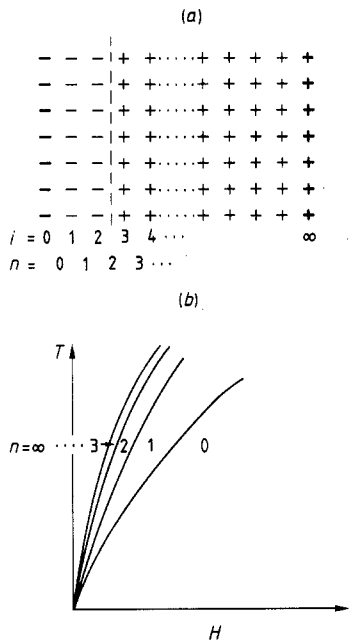

Figure 1. (*a*) A standard interface geometry. Spins depicted in bold type are fixed. (*b*) A schematic representation of the interface layering transitions which result from this choice of boundary conditions.

However, we now show that a qualitatively different behaviour is seen if a novel choice of boundary conditions is considered. The lattice we will study consists of stacked square nets. An interface is introduced by making cuts along intersecting face diagonals and fixing the spins on the resultant boundaries to take the value -1 as shown in figure 2(*a*). The Hamiltonian considered is similar to (1) but with J describing the interactions in planes perpendicular to both boundaries (like that shown in figure 2(*a*)) and J_0 describing interactions between the planes. We define $q_\perp$ as the number of out-of-plane neighbours of each spin.

The field term favours an interface which everywhere lies next to the boundaries whereas the interaction J favours a configuration in which the interface 'cuts the corner'. We shall define the interface position as n, the numbers of rows of $-$ spins at the corner. For example, figure 2(*a*) shows the interface $n=2$. Comparing the ground-state energies for different interface positions shows that there is layering even at zero temperature with the boundary between the phases n and $n+1$ given by

$$(H/J)_{n:n+1} = 2/(2n+1) \tag{2}$$

as shown in figure 2(*b*).

To investigate the effect of finite temperatures on the layering transitions we have performed a low-temperature expansion to second order to obtain the free energy f_n of each phase n. Defining the Boltzmann factors

$$x = \exp(-2\beta J) \qquad \omega = \exp(-2\beta J_0) \qquad h = \exp(-2\beta H) \tag{3}$$

gives, for the difference in reduced free energy per layer between the phases n and $n+1$,

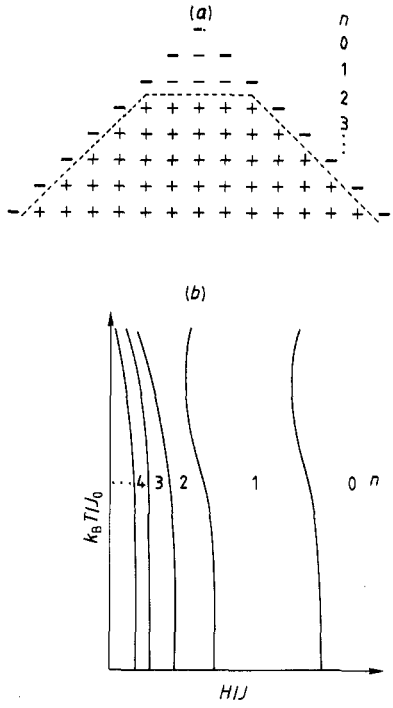

Figure 2. (*a*) An interface geometry which leads to layering transitions at zero temperature. Spins depicted in bold type are fixed and the interface is shown in the position $n=2$. (*b*) The corresponding interface phase diagram.

$$\begin{aligned} F_{n+1}-F_n &= -\beta(f_{n+1}-f_n) \\ &= -2\beta(2n+1)H+4\beta J+(\alpha_1 h+\alpha_2 h^{-1})\omega^{q_\perp}+(\alpha_3 h^2+\alpha_4 h^{-2})\omega^{2q_\perp-2} \\ &\quad +(\alpha_5 h^2+\alpha_6+\alpha_7 h^{-2})\omega^{2q_\perp} \end{aligned} \tag{4}$$

where, for $n>0$,

$$\begin{aligned} \alpha_1 &= -(2n+1)x^4+2x^2-2 \\ \alpha_2 &= (2n-1)x^4+2x^2 \\ \alpha_3 &= -\tfrac{1}{2}(2n+1)q_\perp x^8-q_\perp+q_\perp x^4 \\ \alpha_4 &= \tfrac{1}{2}(2n-1)q_\perp x^8+q_\perp x^4 \\ \alpha_5 &= [(n+\tfrac{1}{2})(q_\perp+1)+4n+1]x^8-(4n+3)x^6-(q_\perp-3)x^4-2x^2+(q_\perp+1) \\ \alpha_6 &= 2x^6-2x^8 \\ \alpha_7 &= [-(n-\tfrac{1}{2})(q_\perp+1)-4n+5]x^8+(4n-7)x^6-(q_\perp+1)x^4+2x^2 \qquad n>1 \\ \alpha_7 &= -\tfrac{1}{2}(q_\perp+1)x^8-x^6-(q_\perp+2)x^4+2x^2 \qquad n=1 \end{aligned} \tag{5}$$

and, for $n=0$,

$$\begin{aligned} &\alpha_1 = -x^4+x^2-x^{-2} \qquad \alpha_2 = x^2 \\ &\alpha_3 = -\tfrac{1}{2}q_\perp x^8+\tfrac{1}{2}q_\perp x^4-\tfrac{1}{2}q_\perp x^{-4} \qquad \alpha_4 = \tfrac{1}{2}q_\perp x^4 \\ &\alpha_5 = \tfrac{1}{2}(q_\perp+3)x^8-2x^6-\tfrac{1}{2}(q_\perp-5)x^4-3x^2+1+\tfrac{1}{2}(q_\perp+1)x^{-4} \\ &\alpha_6 = x^6-x^4 \qquad \alpha_7 = -\tfrac{1}{2}(q_\perp+1)x^4. \end{aligned} \tag{6}$$

The phase boundary is then given by

$$(H/J)_{n:n+1} = 2/(2n+1) + (H_1/J)\omega^{q_\perp} + (H_2/J)\omega^{2q_\perp - 2} + (H_3/J)\omega^{2q_\perp} \tag{7}$$

where the H_i can be expressed in terms of the α_i by

$$\begin{aligned} H_1 &= (\alpha_1 h_0 + \alpha_2 h_0^{-1})/2\beta(2n+1) \\ H_2 &= (\alpha_3 h_0^2 + \alpha_4 h_0^{-2})/2\beta(2n+1) \\ H_3 &= [\alpha_5 h_0^2 + \alpha_6 + \alpha_7 h_0^{-2} + (\alpha_2^2 h_0^{-2} - \alpha_1^2 h_0^2)/(2n+1)]/2\beta(2n+1) \\ h_0 &= \exp[-4\beta J/(2n+1)]. \end{aligned} \tag{8}$$

The phase boundaries are shown schematically in figure 2(b). Note that $(H/J)_{n:n+1}$ initially decreases with increasing temperature. This is becuase the largest entropic contribution to the free energy is from spins which lie next to the boundaries, the number of which is increased as n decreases. Considering the series as an expansion in ω it is apparent that there is only convergence for $q_\perp > 2$. Therefore the situation for the simple cubic lattice is unclear—the layering transitions may be destroyed by roughening.

A similar behaviour is seen when the lattice shown in figure 3(a) is considered. This comprises stacked two-dimensional triangular nets with $q_\perp$ nearest neighbours between spins on neighbouring planes. Let $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\boldsymbol{\chi}$ label the three axes of the

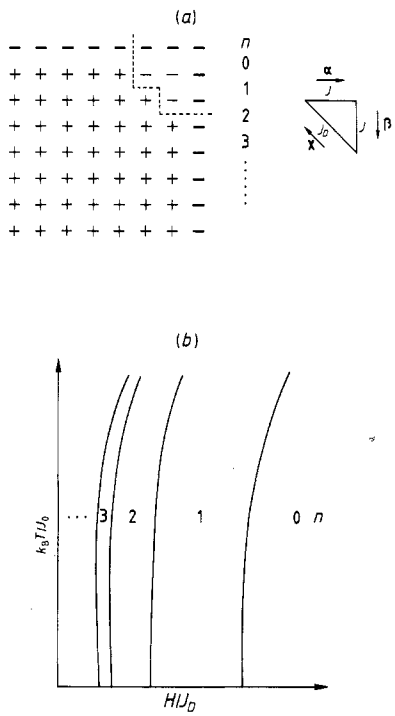

Figure 3. (a) A second choice of lattice and boundary conditions which leads to layering transitions at zero temperature. Spins depicted in bold type are fixed and the interface is shown in the position $n=2$. $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$ and $\boldsymbol{\chi}$ label the axes of the triangular lattice. (b) The corresponding interface phase diagram.

triangular nets. The interface is introduced by fixing spins on intersecting planes parallel to α and β to lie in the state $s_i = -1$. The spins interact through a Hamiltonian

$$H = -J \sum_{\alpha,\beta,j} s_{i,j}s_{i',j} - J_D \sum_{\chi,j} s_{i,j}s_{i',j} - H \sum_{i,j} s_{i,j} - J_0 \sum_{i,j,j'} s_{i,j}s_{i,j'} \tag{9}$$

where j, j' label nearest-neighbour layers and i spins within a layer.

In this case it is the competition between the diagonal interaction, J_D, and the magnetic field, H, that drives the layering transitions. The degenerate interfaces lie diagonally across the corner defined by the boundary spins. We label as n the interface position where n diagonal rows of spins have been flipped to the state $s_i = -1$. For example, $n = 2$ is shown in figure 3(a). A simple comparison of the ground-state energy for interfaces with different values of n gives rise to boundaries

$$(H/J)_{n:n+1} = 2/(n+1) \tag{10}$$

as shown in figure 3(b).

To study the boundaries at finite temperatures we again perform a low-temperature series expansion. Using the definition of the Boltzmann factors given in (3), together with

$$y = \exp(-2\beta J_D) \tag{11}$$

one obtains an expression identical to (7) and (8) for the phase boundaries but with $(2n+1)$ everywhere replaced by $(n+1)$ and the α_i given for $n > 1$ by

$$\begin{aligned}
\alpha_1 &= -nx^4y^2 - 2x^2 + y^2 \\
\alpha_2 &= nx^4y^2 + y^2 \\
\alpha_3 &= -\tfrac{1}{2}nq_\perp x^8y^4 - q_\perp x^4 + \tfrac{1}{2}q_\perp y^4 \\
\alpha_4 &= \tfrac{1}{2}nq_\perp x^8y^4 + \tfrac{1}{2}q_\perp y^4 \\
\alpha_5 &= [\tfrac{1}{2}n(q_\perp+1) + (3n-1)]x^8y^4 + (q_\perp+3)x^4 - \tfrac{1}{2}(q_\perp+3)y^4 - 2x^4y^4 - 2x^6 + y^2 + 4x^6y^2 \\
&\quad - 2nx^6y^4 - 2x^2 - 2x^4y^2 + 2x^2y^4 - (n-1)x^8y^2 \\
\alpha_6 &= 2x^2y^4 - 2y^4 \\
\alpha_7 &= [-\tfrac{1}{2}n(q_\perp+1) - (3n-3)]x^8y^4 - \tfrac{1}{2}(q_\perp+3)y^4 - 2x^4y^4 + 2(n-1)x^6y^4 \\
&\quad + 2x^2y^4 + (n-1)x^8y^2 + y^2
\end{aligned} \tag{12}$$

whereas, for $n = 1$, α_5 is replaced by

$$\begin{aligned}
\alpha_5 &= \tfrac{1}{2}(q_\perp+5)x^8y^4 + (q_\perp+3)x^4 - 2x^2 - y^{-2} + 3 + 2x^6y^2 - 2y^2 - \tfrac{1}{2}(q_\perp+1)y^4 - 2x^6y^4 - 2x^4y^2 \\
&\quad + 2x^2y^4 - 2x^4y^4 - 2x^6 + 2x^6y^2
\end{aligned} \tag{13}$$

and, for $n = 0$,

$$\begin{aligned}
&\alpha_1 = -2x^2 + 2 - y^{-2} \qquad \alpha_2 = y^2 \\
&\alpha_3 = -q_\perp x^4 + q_\perp - \tfrac{1}{2}q_\perp y^{-4} \qquad \alpha_4 = \tfrac{1}{2}q_\perp y^4 \\
&\alpha_5 = (q_\perp+4)x^4 - q_\perp + \tfrac{1}{2}(q_\perp+1)y^{-4} - 4x^2 - 4x^4y^2 + 2x^2y^2 + 2x^6y^2 - y^{-2} + 2x^2y^{-2} - x^4y^{-2} \\
&\alpha_6 = 2x^2y^2 - 2y^2 \qquad \alpha_7 = -\tfrac{1}{2}(q_\perp+1)y^4.
\end{aligned} \tag{14}$$

These are shown schematically in figure 3(b). In this case the boundaries curve towards larger values of (H/J) as the temperaure is increased. This is because the most important entropic contributions to the free energy come from spins lying adjacent to the interface. Hence large values of n are favoured.

In this letter we have shown that interfaces which are constrained to turn a corner can show layering at zero temperature, even in models with only nearest-neighbour interactions. As very little attention has been paid to the interface geometries considered here, further research is likely to uncover other interesting types of behaviour. The interface transitions described are similar to faceting transitions in crystals and it would be of interest to look for layering in such materials.

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