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Layering transitions at an interface in the Blume-Capel model

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Abstract. An interface in the three-dimensional Blume-Capel model is studied using low-temperature series and mean-field theory. By calculating the leading-order diagrams in the low-temperature series expansion to all orders using a transfer matrix technique, we are able to show that the interface wets through an infinite sequence of layering transitions which become quasicontinuous as the bulk phase boundary is approached. The mean-field approximation agrees well with the low-temperature series results.

1. Introduction

Much research has recently been devoted to the statistical mechanics of surfaces and interfaces (Pandit *et al* 1982, Binder 1983, Fisher 1986). In particular, de Olivera and Griffiths (1978) and Pandit *et al* (1982) used mean-field theory to show that there can be an infinite sequence of first-order layering transitions when an interface in a lattice-gas model unbinds from a surface. Since then it has been shown (Duxbury and Yeomans 1985) that low-temperature series expansions provide a powerful tool to analyse the layering transitions.

Duxbury and Yeomans (1985) used this method to show that at low temperatures an interface in an Ising model on a cubic lattice, pinned to a surface by a bulk magnetic field, depins through an infinite sequence of first-order layering transitions. More recently Armitstead *et al* (1986) showed that the wetting of an interface in a threedimensional three-state chiral clock model is mediated by a similar sequence of transitions. In both cases the low-temperature series expansions were taken to general order by selecting the important graphs at each step. In this paper we apply the same methods to analyse wetting at an interface in a three-dimensional Blume-Capel model (Blume 1966, Capel 1966).

The wetting transitions in the Blume-Capel model occur in the vicinity of the bulk transition between states $S_i = \pm 1$ and $S_i = 0$. The transition line is a line of triple points and thus this is an instance of triple-point wetting. The general phenomenology of wetting near bulk triple points has been discussed by Pandit and Fisher (1983). Bricmont *et al* (1986) have predicted that wetting occurs in a similar model.

Interfacial adsorption in the two-dimensional Blume-Capel model has been studied by Selke and Yeomans (1983) and Selke *et al* (1984), who investigate scaling behaviour when close to the tricritical point using Monte Carlo methods and scaling arguments. In two-dimensional systems, however, there are no first-order layering transitions because the interface is always rough. The outline of this paper is as follows: in §§ 2 and 3 the model is introduced and its ground states are elucidated. In § 4 the results obtained from the low-temperature series expansion are described. The calculation is taken to general order using a transfer matrix method described in the appendix. The results of the mean-field approximation for the model are presented in § 5.

2. The model

We consider a lattice of spin-1 Ising spins, $S_i = -1, 0, 1$, situated on the sites *i* of a cubic lattice. The spins interact through the Blume-Capel Hamiltonian (Blume 1966, Capel 1966)

$$\mathcal{H} = -J_0 \sum_{\langle ij \rangle}^{\perp} S_i S_j - J \sum_{\langle ij \rangle}^{\parallel} S_i S_j + D \sum_i S_i^2$$
(2.1)

where J_0 , J and D are all positive. $\langle ij \rangle$ represents a sum over nearest-neighbour pairs and we distinguish couplings in the axial direction, \parallel , which will lie normal to the interface, from the two perpendicular directions, \perp .

An interface is introduced by fixing opposite ends of the system along the axial direction in states +1 and -1 by infinite surface fields, as shown in figure 1. Periodic boundary conditions are assumed in the other two directions.



Figure 1. The geometry of the interface model considered.

3. Ground states

Clearly at zero temperature the spins in the layers are ferromagnetically ordered and the interface is smooth. To specify the ordering along the axial direction it is helpful to define n to be the number of layers of spin $S_i = 0$ which appear at the interface. The ground-state value of n then depends on D as follows:

$$0 < D < \frac{1}{2} q_{\perp} J_0; n = 0; 1 1 \dots 1 1 - 1 - 1 \dots - 1 - 1$$
(3.1a)

$$\frac{1}{2}q_{\perp}J_{0} < D < \frac{1}{2}q_{\perp}J_{0} + J : n = 1; 1 1 \dots 1 1 0 - 1 - 1 \dots - 1 - 1$$
(3.1b)

$$\frac{1}{2}q_{\perp}J_0 + J < D: n = \infty; \ 1 \ 0 \ 0 \ \dots \ 0 \ 0 \ 0 \ -1$$
 (3.1c)

where q_{\perp} is the coordination number of the layers parallel to the interface ($q_{\perp} = 4$ for the cubic lattice considered here).

Note that at $D = \frac{1}{2}q_{\perp}J_0 + J$ where the interface wets, the ground state is infinitely degenerate, with any state with $n \ge 1$ having the same energy. Our aim is to study the phase diagram in the region close to this multiphase point (Fisher and Selke 1980, 1981).

Defining δ as

$$\delta = D - \left(\frac{1}{2}q_{\perp}J_0 + J\right) \tag{3.2}$$

it follows immediately from (2.1) that

$$E_n - E_1 = (1 - n)\delta \tag{3.3}$$

where E_n is the ground-state energy per interface spin of the state with an interface width of n.

4. Low-temperature series expansion

4.1. Method

Our aim is to perform a low-temperature series expansion about all the states stable at the multiphase point. By picking out the important terms at each order of the series expansion we can calculate which of the degenerate phases has the lowest free energy at finite temperatures. The argument is an inductive one with a new stable phase being identified at each order of the expansion. The method is described in detail in Armitstead *et al* (1986) and therefore we limit ourselves here to defining the notation we shall need and presenting results for first, second and then general order.

If F_n is the free energy of the state with interface width *n* then the reduced free energy per interface spin f_n is given by

$$f_n = \frac{-\beta F_n}{N} = -\beta E_n + \sum_{m=1}^{\infty} \frac{\Delta Z_n(m, N)}{N}$$

$$\tag{4.1}$$

where $\beta = 1/kT$, N is the number of sites on each layer and $\Delta Z_n(m, N)$ is the contribution to the free energy from configurations obtained from the ground state by flipping m spins which, by the linked cluster theorem, will be linear in N.

The free energy will be written in terms of the following Boltzmann factors:

$$\omega = \exp(-\beta J_0) \qquad x = \exp(-\beta J) \qquad y = \exp(-\beta D). \tag{4.2}$$

4.2. First order

Contributions to the reduced free energy, f_n , from first-order (single spin-flip) terms are listed in table 1 for different values of n. From (3.3), (4.1) and table 1 one obtains $f_n - f_1 = (n-1)\beta\delta + 2(xy + x^{-1}y) + 2(n-3)y - (n-1)x^2y^{-1}\omega^{q_-} + O(y^{-2}\omega^{2q_--1}).$ (4.3)

Table 1. One-spin-flip contributions to $f_n - f_1$. A hat denotes the flipped spin.

Configuration	Count	Boltzmann weight	
100	2	$xy + x^{-1}y$	
000	n-2	2.	
$-1 - \hat{1} - 1$	-(n-1)	$x^2y^{-1}\omega^{q} + x^4\omega^{2q}$	
10-1	-1	2y	

Using (3.2) we can write

$$v = e^{-\beta\delta} x \omega^{q_2/2} \tag{4.4}$$

and since we are only interested in the region close to $\delta = 0$ we assume

$$3\delta \sim \mathcal{O}(\omega^{q_{\perp}/2}). \tag{4.5}$$

(This assumption will be shown later to be self-consistent.) Hence to first order we can substitute $y = x\omega^{q_{\perp}/2}$ into (4.3) to obtain

$$f_n - f_1 = (n-1)\beta\delta + [2(x^2+1) + (n-5)x]\omega^{q_2/2} + O(\omega^{q_2-1})$$
(4.6)

from which it immediately follows that

$$f_2 - f_1 = \beta \delta + (2 - 3x + 2x^2) \omega^{q_\perp/2} + O(\omega^{q_\perp})$$
(4.7)

$$f_n - f_m = (n - m)\beta\delta + (n - m)x\omega^{q_2/2} + O(\omega^{q_2-1}) \qquad (n, m \ge 2).$$
(4.8)

A given phase will become stable when its reduced free energy is the largest. So if we define $\delta_{12}(T)$ and $\delta_{2\infty}(T)$ by

$$f_{2}\{\delta_{12}(T)\} - f_{1}\{\delta_{12}(T)\} = 0$$

$$f_{2}\{\delta_{2\infty}(T)\} - f_{\infty}\{\delta_{2\infty}(T)\} = 0$$
(4.9)

we find that the n = 2 phase is stable for $\delta_{12}(T) < \delta < \delta_{2\infty}(T)$ where

$$\beta \delta_{12} = -(2 - 3x + 2x^2) \omega^{q_2/2} + O(\omega^{q_2-1})$$
(4.10)

$$\beta \delta_{2\infty} = -x \omega^{q_{2}/2} + O(\omega^{q_{2}-1}).$$
(4.11)

To see this it may be helpful to look at figure 2(a) where the free-energy differences,



Figure 2. Schematic comparisons of the reduced free energy differences per site $(f_n - f_1)$ plotted as functions of δ at (a) first order and (b) second order of the low-temperature series expansion.

 $f_n - f_1$, are plotted schematically as a function of δ . Note that (4.10) and (4.11) are consistent with (4.5).

So to first order we can conclude that a layering transition occurs from the n = 1 phase to the n = 2 phase. However, to this order phases with $n \ge 2$ remain degenerate along the phase boundary $\delta_{2\infty}$. To break this degeneracy we need to look at higher-order terms in the series expansion.

4.3. Second order

To second order we must consider the contributions to $f_2 - f_1$ and $f_n - f_2$ from flipping two spins. But since $q_{\perp} = 4$ there will also be contributions to the same power of ω from some three and four spin-flip diagrams. All the diagrams contributing to second order are listed in tables 2(a) and 2(b). Summing all the contributions and using (4.3)-(4.5) we find that

$$f_{2}-f_{1} = \beta\delta + (2-3x+2x^{2})\omega^{q_{-}/2} - (2-x+2x^{2})\beta\delta\omega^{q_{-}/2} + 2(2-3x^{2}+2x^{4})\omega^{q_{-}-1} + (4+10x - \frac{5}{2}x^{2} - 18x^{3} - 9x^{4} + x^{5} + 12x^{6} + 2x^{8})\omega^{q_{-}} + O(\omega^{q_{-}+1})$$
(4.12)
$$f_{n}-f_{2} = (n-2)\beta\delta + (n-2)x\omega^{q_{-}/2} - 3(n-2)x\beta\delta\omega^{q_{-}/2} + 2(n-2)x^{2}\omega^{q_{-}-1} + [3+(n-11)x + (31 - \frac{21}{2}n)x^{2} + (8n-22)x^{3} + (n+1)x^{4} - x^{5}]\omega^{q_{-}} + O(\omega^{q_{-}+1}).$$
(4.13)

From (4.13) we can find $f_3 - f_2$ and $f_n - f_m$ (for $n, m \ge 3$) and hence arrive at the following phase boundaries:

$$\beta \delta_{12} = -(2 - 3x + 2x^2) \omega^{q_2/2} - 2(2 - 3x^2 + 2x^4) \omega^{q_2-1} - (8 + 2x + \frac{17}{2}x^2 - 26x^3 - 5x^4) + x^5 + 12x^6 + 2x^8) \omega^{q_2} + O(\omega^{q_2+1})$$
(4.14)

$$\beta \delta_{23} = -x \omega^{q_{-}/2} - 2x^2 \omega^{q_{-}-1} - (3 - 8x + \frac{5}{2}x^2 + 2x^3 + 4x^4 - x^5) \omega^{q_{+}} + \mathcal{O}(\omega^{q_{-}+1})$$
(4.15)

$$\beta \delta_{3\infty} = -x \omega^{q_{-}/2} - 2x^2 \omega^{q_{-}-1} - (x - \frac{15}{2}x^2 + 8x^3 + x^4) \omega^{q_{-}} + O(\omega^{q_{-}+1}).$$
(4.16)

Therefore n = 3 appears as a stable phase for $\delta_{23} < \delta < \delta_{3\infty}$ with the n = 2 phase remaining stable for $\delta_{12} < \delta < \delta_{23}$. Figure 2(b) gives a schematic representation of the free-energy differences and the phase boundaries are shown in figure 3.

Note that, to this order, phases with $n \ge 3$ remain degenerate along the phase boundary $\delta_{3\infty}$. As before, higher-order terms are needed to break this degeneracy but the series expansion rapidly becomes very complicated. However, we can infer that an infinite sequence of layering transitions occurs through inductive arguments based on considering the leading term at successive orders.

4.4. General order

Suppose that after considering the (n-1)th order of the expansion all phases with interface width $\leq n$ are found to be stable and non-degenerate in particular regions of the phase diagram and that all phases with interface width $\geq n$ are degenerate along the phase boundary $\delta_{n,x}$ (cf § 4.2 and 4.3 where n = 2 and 3, respectively).

In order to break this degeneracy we need to look at the leading-order contribution to the free-energy difference between phases n' and n, where n' > n. This will arise at the *n*th order of the expansion. Some thought shows that the important graphs will be axial chains of *n* flipped spins that span the interface, together with their associated **Table 2.** Graphs which need to be considered to obtain the second order contribution to (a) $f_2 - f_1$ and (b) $f_n - f_2$. The notation used to define the flipped configurations is a: 100, b: 000, c: -1 - 1 - 1, d: 10 - 1, e: 110.

(<i>a</i>)				
Configuration	Count	Boltzmann weight		
In-layer connected				
spin nips		(2, 2, 2), (-2, 2), -1, 2, 2		
aa		$(x^{-}y^{-} + x^{-}y^{-})\omega^{-} + 2y^{-}\omega^{-}$		
cc	$-\frac{1}{2}q_{-}$	$x^{+}y^{-}\omega^{-}y^{-} + 2x^{+}y^{-}\omega^{-}y^{-} + x^{+}\omega^{-}y^{-} +$		
dd	$-\frac{1}{2}q_{-}$	$2y^2\omega^{-1} + 2y^2\omega^{-1}$		
aaa	$q_{\perp}(q_{\perp}-1)$	$(1+x^3)\omega^{(3/2)q} = 2 + O(\omega^{(3/2)q})$		
ccc	$-\frac{1}{2}q_{\perp}(q_{\perp}-1)$	$x^{3}\omega^{(3/2)q_{-2}^{-2}} + O(\omega^{3q_{-4}^{-4}})$		
ddd	$-\frac{1}{2}q_{\perp}(q_{\perp}-1)$	$2x^{3}\omega^{(3/2)q} + O(\omega^{(3/2)q})$		
aaaa	2	$(1+x^8)\omega^{2q4} + O(\omega^{2q})$		
cccc {forming square	-1	$x^4 \omega^{2q} - 4 + O(\omega^{(7/2)q} - 6)$		
dddd	-1	$2x^4\omega^{2q} + O(\omega^{2q})$		
Axially connected spin flips				
e, a	2	$2x\omega^{q} + xy\omega^{2q} + x^{3}y\omega^{2q}$		
a, a	1	$3x^{-1}y^2 + x^3y^2$		
e, d	-2	$(1+x^2)\omega^{q} + (1+x^4)\psi^{2q}$		
c, c	-1	$x^{3}y^{-2}\omega^{2q} + 2x^{4}y^{-1}\omega^{3q} + x^{4}\omega^{4q}$		
Separated spin flips				
a; e	-2	$(1+x^2)\omega^{q} + (x+x^3)\psi^{2q}$		
a; a	$-(q_1+2)$	$2y^2 + x^2y^2 + x^{-2}y^2$		
d; e	2	$2x\omega^{q} + 2x^{2}\gamma\omega^{2q}$		
d; d	$\frac{1}{2}(q + 1)$	$4v^2$		
c; c	$\frac{1}{2}(q_{\perp}+3)$	$x^4y^{-2}\omega^{2q} + 2x^6y^{-1}\omega^{3q} + x^8\omega^{4q}$		
(b)				
Configuration	Count	Boltzmann weight		
In-layer connected				
bb	$\frac{1}{n-2}a$	$2w^2 + \frac{-1}{2} + 2w^2 + \frac{-1}{2}$		
00	$\frac{1}{2}(n-2)q_{\perp}$	$2y \omega + 2y \omega$ $4u^{-2} \cdot 2a^{-1} + 2u^{-6} \cdot -1 3a^{-2} + 8 4a^{-4}$		
66 666	$-\frac{1}{2}(n-2)q_{\pm}$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$		
0000	$\frac{1}{2}(n-2)q_{-}(q_{+}-1)$	$2x \omega + 0 (\omega + 4)$		
bbbb)	$-\frac{1}{2}(n-2)q_{-}(q_{+}-1)$	$x \omega^{-1} + O(\omega^{-4} - 1)$		
forming square	n-2 -(n-2)	$2x \omega^{-4} + O(\omega^{-4})$ $x^4 \omega^{2q} + O(\omega^{(7/2)q} - 6)$		
Axially connected	(n 2)	x w - + O(w)		
spin flips				
a, b	2	$2y^2 + x^2y^2 + x^{-2}y^2$		
D, D	n-3	$2xy^2 + 2x^{-1}y^2$		
a, a	-1	$3x^{-1}y^{-1} + x^{-2}y^{-1}$		
с, с	-(n-2)	$x^{5}y^{-2}\omega^{2q} + 2x^{4}y^{-1}\omega^{3q} + x^{4}\omega^{4q}$		
Separated spin flips				
a; a	1	$2y^2 + x^2y^2 + x^{-2}y^2$		
a; b	-2	$2xy^2 + 2x^{-1}y^2$		
D; D	$-(q_+2)$	$4y^2$		
c; c	$\frac{-\frac{1}{2}(n-4)(q_{\perp}+3)}{\frac{1}{2}(n-2)(q_{\perp}+3)}$	$x^4 y^{-2} \omega^{2q} + 2x^6 y^{-1} \omega^{3q} + x^8 \omega^{4q}$		



Figure 3. Phase diagram for the layering transitions in the Blume-Capel model. The full curves are the phase boundaries obtained from the low-temperature series expansion taken to second order. The broken curves are those found from the mean-field approximation. In both cases we have taken $J_0 = J$.

decompositions (Fisher and Selke 1981). (It is perhaps intuitively obvious that these will be the first fluctuations to differentiate between the phases n and n+1; a simpler model which behaves in the same way is described in Duxbury and Yeomans (1985).) Other diagrams will contribute to $f_n - f_n$ to leading order (for example connected and disconnected configurations of n flipped spins running in the layers) but these shift the boundaries $\delta_{n,n+1}$ and $\delta_{n+1,\infty}$ by the same amount and hence drop out when the phase width of the n+1 phase

$$\Delta \delta_{n+1} = \delta_{n,n+1} - \delta_{n+1,\infty} = -\beta^{-1} [(f_{n+1}^{(n)} - f_n^{(n)})$$
(4.17)

$$-(f_{n'}^{(n)} - f_{m'}^{(n)})/(n' - m')] \qquad n', m' \ge n + 1$$
(4.18)

is calculated. The superscript on f denotes the number of flipped spins.

Because of the one-dimensional nature of the graphs corresponding to axial chains of flipped spins, the corresponding Boltzmann factor can be evaluated using a transfer matrix method, the details of which are described in the appendix, to give

$$\tilde{f}_{n+1}^{(n)} - \tilde{f}_{n}^{(n)} = \frac{1}{2} x^{-1} (1-x)^{n+1} [(1+x)^{n+1} - (1-x)^{n+1}] \omega^{nq_{\perp}/2} + x(1-x)^{n-1} [2(1-x)^{n-1} - 1] \omega^{nq_{\perp}/2} + O(\omega^{(n+3)q_{\perp}/2})$$

$$\tilde{f}_{n'}^{(n)} - \tilde{f}_{m'}^{(n)} = (n'-m') x(1-x)^{n-1} [2(1-x)^{n-1} - 1] \omega^{nq_{\perp}/2}$$
(4.19)

The tilde on f is used to emphasise that only axial chains are included as opposed to all configurations of n flipped spins.

It follows immediately from (4.17)-(4.20) that

$$\beta \Delta \delta_{n+1} = -\frac{1}{2} x^{-1} (1-x)^{n+1} [(1+x)^{n+1} - (1-x)^{n+1}] \omega^{nq_{-}/2} + O(\omega^{nq_{-}/2+1})$$
(4.21)

showing that the n+1 phase has a finite phase width and is stabilised at the *n*th order of the expansion. From (4.20) phases of width $\ge n+1$ remain degenerate on $\delta_{n+1,\infty}$ to this order. Hence, by an inductive argument, considering each order of the series expansion in turn, an infinite series of layering transitions can be established. The factor $\omega^{nq_{-}/2}$ in (4.21) shows that the phase widths decrease exponentially with increasing *n*, so that the layering transitions effectively become quasicontinuous as $n \to \infty$.

4.5. Low-temperature bulk phase boundary

It is of interest to compare the position of the phase boundary in a system with no interface to those obtained for the interface transitions. Expanding around a ground state with $S_i = 1$ for all *i* one obtains a reduced free energy

$$f_{\alpha} = -\beta \delta(1 - x\omega^{q_{-}/2}) + x\omega^{q_{-}/2} + 2x^{2}\omega^{q_{-}-1} + (x - \frac{7}{2}x^{2} + 6x^{3} + x^{4})\omega^{q_{-}} + O(\omega^{q_{-}+1})$$
(4.22)

whereas an expansion around the state with $S_i = 0$ for all *i* gives

$$f_{\beta} = 2x\omega^{q_{-}/2}(1-\beta\delta) + 4x^{2}\omega^{q_{-}-1} + (2x-14x^{2}+14x^{3}+2x^{4})\omega^{q_{-}} + O(\omega^{q_{-}+1}).$$
(4.23)

Equating (4.22) and (4.23) gives a bulk phase boundary

$$\beta \delta_{\alpha\beta} = -x \omega^{q_{-}/2} - 2x^{2} \omega^{q_{-}-1} - (x - \frac{15}{2}x^{2} + 8x^{3} + x^{4}) \omega^{q_{-}} + \mathcal{O}(\omega^{q_{-}+1})$$
(4.24)

which coincides with the interface boundary $\delta_{3\infty}$. Indeed, this is what we would expect at this order as indicated in the next section.

4.6. Domain wall interaction free energy

Some insight into the nature of the layering transitions is gained by considering the contribution to the free energy of the state n due to the interaction between the domain walls $(\ldots 1 \ 1 \ 0 \ 0 \ \ldots \ and \ \ldots \ 0 \ 0 \ -1 \ -1 \ \ldots)$. This can be expressed to leading order as

$$F_{\rm dw}(n) = -kT \lim_{n' \to \infty} \{f_n^{(n)} - f_{n'}^{(n)} - (n'-n)[f_{\alpha}^{(n)} - f_{\beta}^{(n)}]\}.$$
(4.25)

Subtracting $f_{n'}^{(n)}$ and taking $n' \rightarrow \infty$ removes the contributions to the free energy from isolated domain walls. The leading-order surviving terms in $F_{dw}(n)$ are again those occurring from flipping axial chains of *n* spins. (4.25) is easily evaluated using results derived in the appendix to yield

$$F_{\rm dw}(n) = -\Delta \delta_{n+1}. \tag{4.26}$$

Comparing with (4.21) we see that $F_{dw}(n)$ is always positive and decreases monotonically ($\sim \omega^{nq_{1}/2}$) with *n*, and is therefore repulsive at all distances. This is an example of entropic repulsion (Bricmont *et al* 1986) where the domain walls want to move further apart so as to have more freedom to fluctuate.

We can now argue that complete wetting occurs at the bulk phase boundary. As $\delta(T)$ approaches $\delta_{\alpha\beta}(T)$ from below, repulsion between the domain walls increases the value of *n*. But because there is a bulk term in the free energy favouring $S_i = \pm 1$

spins, equilibrium must correspond to the domain walls being at a finite separation. Only at $\delta(T) = \delta_{\alpha\beta}(T)$, when the bulk free energies of the $S_i = \pm 1$ and $S_i = 0$ states become equal, can the domain walls wet the interface completely. This agrees with the result found by Bricmont *et al* (1986).

5. Mean-field theory

We now compare our results to those obtained using the mean-field approximation. The mean-field equations follow as usual from a variational principle (Blume *et al* 1971) except that the lack of translational invariance means that the mean field, h_j , on a given layer, *j*, must be allowed to vary with *j*. The expectation value of the spin in layer *j* with respect to the mean-field Hamiltonian, $\langle S_i \rangle$, is then

$$\langle S_j \rangle = \frac{\sinh \beta h_j}{\cosh \beta h_i + \frac{1}{2} e^{\beta D}}$$
(5.1)

where

$$h_j = 4J_0(S_j) + J(\langle S_{j+1} \rangle + \langle S_{j-1} \rangle)$$
(5.2)

and the mean-field free energy per spin, $F_{\rm mf}$, is given by

$$F_{\rm mf} = L^{-1} \sum_{j=1}^{L} \{ -kT \ln(2 \cosh \beta h_j + e^{\beta D}) + D + \frac{1}{2} h_j \langle S_j \rangle \}$$
(5.3)

where L is the number of layers.

These equations were solved for phases with various values of n by numerical iteration of equations (5.1) and (5.2). The mean-field phase diagram was then constructed by comparing $F_{\rm mf}$ for the different phases. The resulting phase boundaries are shown by the broken curves in figure 3. We were able to find stable phases with $n \le 7$ although for clarity only phases with $n \le 4$ are shown in figure 3. Note the close qualitative similarity to the results obtained from the low-temperature series expansion.

6. Summary

We have shown that an interface in the Blume-Capel model wets from a state with a single layer of zeros at the interface through an infinite sequence of first-order layering transitions at each of which the number of zero layers increases by one. The phase widths decrease exponentially as the number of zero layers increases. This process is a result of competition between the entropic repulsive interaction between the 10 and 0-1 domain walls and the effects of the bulk transition from the phase where all $S_i = 1$ (or all $S_i = -1$) to the phase where all $S_i = 0$. It is therefore an example of triple-point wetting. The results of a mean-field approximation agree qualitatively with the low-temperature series results.

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Appendix. Calculation to general order using a transfer matrix method

We require the contribution to the reduced free energies from axial chains of n flipped spins and their associated decompositions. For this we use a transfer matrix method which was first developed by Yeomans and Fisher (1984) and whose application to interface problems has been described by Armitstead *et al* (1986).

The method relies on sequentially building up the contribution to the free energy, bond by bond, using a transfer matrix to record the Boltzmann weights for each broken bond in turn. For example, if the initial configuration is a $\dots 00\dots$ bond, both spins must flip giving a total of four final states whose Boltzmann weights are recorded in the matrix

second spin

$$-1 \quad 1$$
first spin

$$1 \quad x \quad x^{-1} \quad y$$

We must also include contributions due to the flipped spins being separated. This gives a factor of -1 in addition to the Boltzmann weights (Yeomans and Fisher 1984):

second spin

$$-1$$
 1
 -1 -1 -1
first spin 1 -1 -1 y

Therefore the total transfer matrix is

...
$$\hat{0} \hat{0} \dots$$
 $\mathbf{B} = \begin{pmatrix} x^{-1} - 1 & x - 1 \\ x - 1 & x^{-1} - 1 \end{pmatrix} y.$ (A1)

Similarly, for a ... 1 1... bond we have the following transfer matrix:

...
$$\hat{1} \hat{1} \dots = \begin{pmatrix} x(1-x)y^{-1}\omega^{q_{\perp}} & x(1-x^{2})\omega^{2q_{\perp}} \\ x(1-x^{2})y^{-1}\omega^{q_{\perp}} & (1-x^{4})\omega^{2q_{\perp}} \end{pmatrix}.$$
 (A2)

There must also be contributions from the bond preceding the first flipped spin (initial bond) and the bond following the last flipped spin (final bond). These are given by row and column vectors, respectively. We obtain the following row vectors for the indicated initial bonds:

$$1 \hat{0} \dots \qquad \mathbf{b}_{i}^{T} = (x \ x^{-1})y$$
 (A3)

$$0 \hat{0} \dots \qquad \mathbf{c}_{i}^{\mathsf{T}} = (1 \quad 1) y \tag{A4}$$

1 î ...
$$\mathbf{d}_{i}^{\mathsf{T}} = (xy^{-1}\omega^{q_{\perp}} \ x^{2}\omega^{2q_{\perp}})$$
 (A5)

and the following column vectors for the final bonds:

$$\dots \hat{0} - 1 \qquad \mathbf{b}_{\mathbf{f}} = \begin{pmatrix} x^{-1} \\ x \end{pmatrix} \tag{A6}$$

$$\dots \hat{0} 0 \qquad \mathbf{c}_{\mathrm{f}} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \tag{A7}$$

$$\dots \hat{1} 1 \qquad \mathbf{d}_{\mathrm{f}} = \begin{pmatrix} x \\ x^2 \end{pmatrix}. \tag{A8}$$

Recall that we seek to calculate $\tilde{f}_{n}^{(n)} - \tilde{f}_{n}^{(n)}$ (see § 4.4). The following configurations contribute to this free-energy difference:

Configuration	Count	Weight
$\dots 1 \hat{0} \hat{0} \dots \hat{0} \hat{0} - 1 \dots$	-1	$\mathbf{b}_{i}^{\mathrm{T}}\mathbf{B}^{n-1}\mathbf{b}_{\mathrm{f}}$
1 ô ô ô ô o	2	$\mathbf{b}_{i}^{T}\mathbf{B}^{n-1}\mathbf{c}_{f}$
0 ô ô ô ô o	n' - n - 1	$\mathbf{c}_{i}^{T} \mathbf{B}^{n-1} \mathbf{c}_{f}$
111	-(n'-n)	$\mathbf{d}_{i}^{\mathrm{T}}\mathbf{D}^{n-1}\mathbf{d}_{f}$.

Hence

$$\tilde{f}_{n'}^{(n)} - \tilde{f}_{n}^{(n)} = \mathbf{b}_{i}^{\mathsf{T}} \mathbf{B}^{n-1} (2\mathbf{c}_{f} - \mathbf{b}_{f}) + (n' - n - 1) \mathbf{c}_{i}^{\mathsf{T}} \mathbf{B}^{n-1} \mathbf{c}_{f} - (n' - n) \mathbf{d}_{i}^{\mathsf{T}} \mathbf{D}^{n-1} \mathbf{d}_{f}.$$
(A9)

To evaluate (A9) we diagonalise **B**. Its eigenvalues λ_1, λ_2 and corresponding eigenvectors $\boldsymbol{u}_1, \boldsymbol{u}_2$ are

$$\lambda_1 = (x^{-1} - x)y$$
 $\lambda_2 = (x^{-1} - x - 2)y$ (A10)

$$u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
 $u_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ (A11)

from which it follows immediately that

$$\mathbf{B}^{n-1} = \frac{1}{2} \begin{pmatrix} \lambda_1^{n-1} + \lambda_2^{n-1} & -\lambda_1^{n-1} + \lambda_2^{n-1} \\ -\lambda_1^{n-1} + \lambda_2^{n-1} & \lambda_1^{n-1} + \lambda_2^{n-1} \end{pmatrix}.$$
 (A12)

 \mathbf{D}^{n-1} can easily be evaluated to leading order:

$$\mathbf{D}^{n-1} = \begin{pmatrix} [x(1-x)y^{-1}\omega^{q}_{-}]^{n-1} + \mathcal{O}(y^{2-n}\omega^{nq}_{-}) & \mathcal{O}(y^{2-n}\omega^{nq}_{-}) \\ (1+x)[x(1-x)y^{-1}\omega^{q}_{-}]^{n-1} + \mathcal{O}(y^{2-n}\omega^{nq}_{-}) & \mathcal{O}(y^{2-n}\omega^{nq}_{-}) \end{pmatrix}.$$
 (A13)

Finally, substituting (A3)-(A8), (A10), (A12) and (A13) into (A9) and putting $y = x\omega^{q_2/2}$ yields

$$\tilde{f}_{n'}^{(n)} - \tilde{f}_{n}^{(n)} = \frac{1}{2}x^{-1}(1-x)^{n+1}[(1+x)^{n+1} - (1-x)^{n+1}]\omega^{nq_{\perp}/2} + (n'-n)x(1-x)^{n-1}[2(1-x)^{n-1} - 1]\omega^{nq_{\perp}/2} + O(\omega^{(n+3)q_{\perp}/2}).$$
(A14)

(4.19) and (4.20) follow immediately from (A14).

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