A series approach to wetting and layering transitions. II. Solid-on-solid models

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A series approach to wetting and layering transitions: II. Solid-on-solid models

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Abstract. This is the second of three papers in which we discuss the applicability of series methods to interface wetting and layering transitions. Here we study the behaviour of a solid-on-solid interface, which is attracted to a surface by a local pinning potential. We find that, both for the standard and the restricted solid-on-solid models, the interface depins from the surface through an infinite sequence of layering transitions as the potential tends to zero. The applicability of our results to previous work on the Abraham model in three dimensions is discussed.

1. Introduction

This paper is the second in a series of three papers on the application of low-temperature expansions to wetting and layering transitions. Previously (Armitstead and Yeomans 1987) we have shown that the unbinding of an interface from a wall in the q-state Potts model takes place through a sequence of first-order layering transitions as the bulk field pinning the interface to the wall tends to zero. We now use extensions of the same techniques to study various solid-on-solids models, which are interface Hamiltonians that neglect bulk fluctuations and overhangs (Temperley 1952). We shall consider the case in which a two-dimensional interface is attracted to a substrate by a pinning potential. Entropy causes the interface to be repelled by the surface, and it has been proved (Chalker 1982a) that for all values of pinning potential there is a temperature below which the interface is bound, and another, higher one, above which it is unbound. Moreover, Bricmont *et al* (1986) have shown that, in the case when the surface potential equals zero, the distance of the interface from the wall diverges as the thermodynamic limit is taken. Our aim is to investigate the nature of this wetting transition as the potential tends to zero; in particular, whether layering occurs or whether there is just a single unbinding transition.

The solid-on-solid Hamiltonian we shall consider is

$$H_{\mathrm{SOS}} = \tfrac{1}{2}J \sum_{i,j} |h_i - h_j|^{\nu} + \sum_i U(h_i) \tag{1.1}$$

where the h_i can take integer values. As we are interested in a two-dimensional interface the sums are taken over the sites, i, of a square lattice and restricted to nearest neighbours.

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The solid-on-solid model was first proposed in connection with the theory of crystal growth (Temperley 1952, Weeks *et al* 1973) and has been applied extensively to the roughening transition of an interface in the three-dimensional Ising model. It is believed to be a good approximation to the Ising model (Burton and Cabrera 1949, Weeks *et al* 1973, Swendsen 1977), at least up to the roughening temperature, where the bulk is almost (98%) saturated. Indeed, the solid-on-solid approximation becomes exact in the highly anisotropic limit. If an Ising model has interactions $J_{\parallel}$ and $J_{\perp}$ parallel and perpendicular, respectively, to the normal to the wall then the limit $J_{\parallel} \to \infty$ with $J_{\perp}$ fixed, and with the boundary conditions which force an interface into the system, gives the solid-on-solid model.

The $U(h_i)$ may also be easily related to the interactions and fields in an Ising model (Nightingale *et al* 1984). However, it need not be, and may describe interactions which cannot arise in a rigid Ising model such as those introduced by strain in a solid film.

Various special cases the Hamiltonian (1.1) which have been considered in the literature (see, for example, Chui and Weeks 1981, Chalker 1982b) are distinguished by their values of y: for the 'standard' solid-on-solid model, $y = 1$; for the discrete Gaussian model, $y = 2$; and for the restricted solid-on-solid model ($|h_i - h_j| = 0, 1$), $y = \infty$. The importance of the value of y will depend on whether excitations with $|h_i - h_j| \geq 2$ contribute significantly. There is considerable evidence that the roughening transitions in models with different values of y all belong to the same universality class (Chui and Weeks 1976, 1981, Weeks *et al* 1973, van Beijeren 1977, Emery and Swendsen 1977). We consider two values of y, $y = 1$ and $y = \infty$, to see whether they give qualitatively the same phase diagram at low temperatures.

In § 2 we consider the case $y = 1$. Diagrams in the low-temperature series which are important in driving the transition are identified, and we show that the interface unbinds from the surface through an infinite sequence of layering transitions. The model is shown to correspond to the extreme anisotropic limit of the Abraham model (Abraham 1980), which has been studied using similar techniques by Duxbury and Yeomans (1985), and hence the accuracy of the solid-on-solid model as an approximation to the Abraham model can be tested. Moreover, Duxbury and Yeomans (1985) were unable to establish an infinite sequence of layering transitions and the solid-on-solid result suggests that such a sequence does in fact exist in the Abraham model.

In § 3 we take $y = \infty$ and obtain a qualitatively similar phase diagram. In this limit it is easier to identify the important fluctuations. Our results are in disagreement with previous work by Luck *et al* (1983) and we suggest why they were unable to identify any layering transitions. Finally, in § 4, the results are discussed and compared to those obtained numerically within a mean-field approximation, which has to date been the most extensively used method of studying layering transitions.

The technique used throughout is low-temperature series, expanding about all possible degenerate ground states in terms of a small, temperature-dependent variable. This method was explained in detail in the previous paper (Armitstead and Yeomans 1987), and we shall therefore just quote the lowest-order results before showing how to evaluate the leading terms to general order.

2. The standard solid-on-solid model, $y = 1$

We consider the Hamiltonian (1.1) with $y = 1$ and

$$U(h) = \infty, h < 0 \qquad U(0) = -u \qquad U(h) = 0, h \geq 1. \tag{2.1}$$

At zero temperature, $T=0$, the interface will lie flat and parallel to the surface. When $u=0$ all possible positions of the interface are degenerate—for convenience these will be labelled by $h=h_i(T=0)$. For $u>0$, the interface will lie next to the surface, $h=0$.

At non-zero temperature entropic fluctuations repel the interface, and hence, for $u=0$, $h=\infty$ is stable. For small u at finite T the interface must unbind from the surface because of the competition between the energetic attraction and entropic repulsion. To determine the nature of the transition we performed an expansion about the multiphase point, $u=0$, $T=0$.

2.1. Low-order calculations

The low-temperature variable used was $w=\exp(-\beta J)$, the Boltzmann factor for introducing a one-step height difference between neighbouring sites. As usual, $\beta=1/k_B T$ and k_B is Boltzmann's constant. Single excitations of the interface lead to expressions for the reduced free energy per interface site, F_h, which are $O(w^4)$. To this order, F_0 and F_1 contain Boltzmann factors which depend on the magnitude of u, whilst F_h, $h\geq 2$, remain degenerate. The free-energy differences are given by

$$F_1-F_0=-\beta u+(1+v-v^{-1})w^4+O(w^6) \tag{2.2}$$

$$F_h-F_0=-\beta u+(2-v^{-1})w^4+O(w^6) \qquad h\geq 2 \tag{2.3}$$

where $v=\exp(\beta u)$. Equations (2.2) and (2.3) show that for a transition between the phases with $h=0$ and $h>0$ βu must be $O(w^4)$. Using this approximation to expand the factor associated with the pinning potential

$$\exp(\beta u)=1+O(w^4) \tag{2.4}$$

leads to

$$F_h-F_0=-\beta u+w^4+O(w^6) \qquad h\geq 1. \tag{2.5}$$

Note that all phases with $h\geq 1$ are degenerate in this region. Hence there is a phase boundary between phases with $h=0$ and $h\geq 1$ given by

$$(\beta u)_{0:h}=w^4+O(w^6) \qquad h\geq 1. \tag{2.6}$$

To determine which interface position, h, becomes stable in the vicinity of this boundary requires higher-order terms in the expansion. Taking terms $O(w^{12})$ in the reduced free-energy differences where necessary gives

$$F_1-F_0=-\beta u+(1+v-v^{-1})w^4+2(1+v^2-v^{-2}]w^6 + [\tfrac{11}{2}-(v+v^{-1})-\tfrac{5}{2}(v^2-v^{-2})+6(v^3-v^{-3})+(v^4-v^{-4})]w^8+O(w^{10}) \tag{2.7}$$

$$F_2-F_1=(1-v)w^4+2(1-v^2)w^6+(\tfrac{7}{2}+2v+\tfrac{5}{2}v^2-6v^3-v^4)w^8+4w^{10}+18w^{12}+O(w^{14}) \tag{2.8}$$

$$F_h-F_1=(1-v)w^4+2(1-v^2)w^6+(\tfrac{9}{2}+v+\tfrac{5}{2}v^2-6v^3-v^4)w^8 + 4w^{10}+19w^{12}+O(w^{14}) \qquad h\geq 3 \tag{2.9}$$

where we have expanded $\exp(\beta u)$ as in (2.4) to simplify the higher-order terms. As an example, we list the diagrams which give rise to (2.8) to $O(w^8)$, along with their

counts per lattice site and their Boltzmann weights, in table 1. Equations (2.7)-(2.9) lead to the boundary

$$(\beta u)_{0;1} = w^4 + 2w^6 + \tfrac{11}{2}w^8 + O(w^{10}). \tag{2.10}$$

Evaluating $F_h - F_1$, $h \geq 2$, along (2.10) gives

$$F_h - F_1 = -2w^{10} + O(w^{12}) \qquad h \geq 2. \tag{2.11}$$

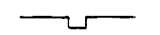
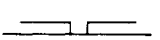
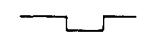
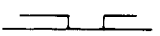
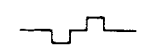
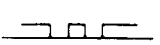
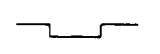
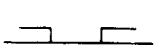
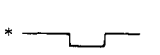
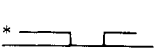
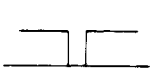
This is negative. Hence $h = 1$ is a stable phase and there is a phase boundary

$$(\beta u)_{1;h} = w^4 + \tfrac{5}{2}w^8 + O(w^{10}) \qquad h \geq 2. \tag{2.12}$$

To find the next stable phase we calculate $F_h - F_2$, $h \geq 3$. To $O(w^{16})$

$$F_h - F_2 = [-\beta u(1 + 4w^2) + w^4 + 4w^6 + \tfrac{1}{2}w^8]w^8 + O(w^{18}) \qquad h \geq 3. \tag{2.13}$$

Table 1. Contributions to $F_2 - F_1$ for the $y = 1$ solid-on-solid model to $O(w^8)$. The lower line in each diagram denotes the wall. In the diagrams marked by * the interface fluctuates at four lattice sites which form a square.

Diagram	Count per lattice site	Boltzmann weight
	1	w^4
	-1	vw^4
	2	w^6
	-2	v^2w^6
	-1	w^8
	1	vw^8
	$-\frac{5}{2}$	w^8
	$\frac{5}{2}$	v^2w^8
	6	w^8
	-6	v^3w^8
* 	1	w^8
* 	-1	v^4w^8
	1	vw^8

Along the $1:h$ boundary given by (2.12)

$$F_h - F_2 = -2w^{16} + O(w^{18}) \qquad h \geq 3 \tag{2.14}$$

showing that $h = 2$ is stable. There is a $2:h$ phase boundary at

$$(\beta u)_{2:h} = w^4 + \tfrac{1}{2}w^8 + 2w^{10} + O(w^{12}) \qquad h \geq 3. \tag{2.15}$$

Similar calculations taken to $O(w^{22})$ show that the phase with $h = 3$ becomes stable along the boundary given by (2.15). The $3:h$, $h \geq 4$, boundary is given by

$$(\beta u)_{3:h} = w^4 + \tfrac{1}{2}w^8 + \tfrac{7}{3}w^{12} + O(w^{14}) \qquad h \geq 4. \tag{2.16}$$

Notice that the boundaries between higher-order phases differ from those between lower-order phases by successively higher-order terms in w. By considering terms in the free energy $O(w^{28})$ we may show that all boundaries $(\beta u)_{h:h'}$, $h' > h \geq 4$, have the first few terms

$$(\beta u)_{h:h'} = w^4 + \tfrac{1}{2}w^8 + \tfrac{1}{3}w^{12} + O(w^{14}) \qquad h' > h \geq 4. \tag{2.17}$$

In order to establish the phase sequence we have needed to consider diagrams of sufficiently high order that the interface touches the surface at two lattice sites, as may be seen for the particular case listed in table 1. This is also true when the interface is at some general position, and means that the number of the terms in the expansion which are needed to demonstrate a possible layering transition increases rapidly as the interface moves away from the wall.

2.2. General-order calculations

In order to perform a general-order calculation it is necessary to identify the lowest-order fluctuations which are important in distinguishing between the free energies of different interface phases. The diagrams with different Boltzmann weights between phases at height h and h', $h' > h$, at lowest order are axial chains of length h, as shown in figure 1. Their contribution is

$$F_{h'} - F_h = (1 - v)w^{4h} + O(w^{4h+2}) \qquad h' > h \geq 1. \tag{2.18}$$

However, these diagrams do not give any information about the sequence of phases, and lead to a phase boundary

$$(\beta u)_{h:h'} = 0 + O(w^2) \qquad h' > h \geq 1. \tag{2.19}$$

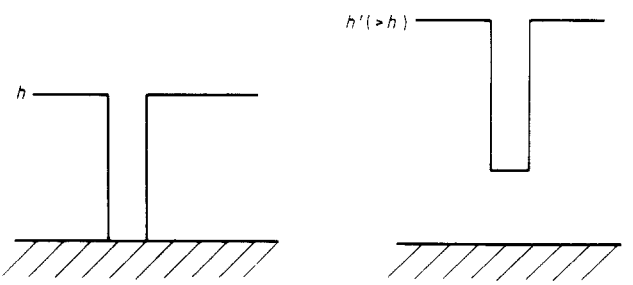


Figure 1. The lowest-order graphs, for the unrestricted model, which have different Boltzmann weights for interface phases h and h', $h' > h$.

To obtain a non-zero phase boundary requires terms in the expansion $O(w^{4h+4})$

$$F_{h'} - F_h = [1 - v + 4(1-v)w^2 + 20(1-v)w^4 + v^{\delta(h',h+1)}w^4]w^{4h} + O(w^{4h+6}) \qquad h' > h \geq 3 \tag{2.20}$$

where δ is the Kronecker delta. This gives

$$(\beta u)_{h:h'} = w^4 + O(w^6) \qquad h' > h \geq 3. \tag{2.21}$$

This boundary is independent of h and all interface phases remain degenerate along (2.21). To lift this degeneracy we would need the coefficient of w^{4h} in equation (2.20) to depend on h in the vicinity of a phase boundary. In fact, the lowest-order diagrams which do give a non-degenerate phase boundary touch the surface at two lattice sites, as noted in the explicit lowest-order calculations in § 2.1. This situation should be compared to the Potts model in a bulk field (Armitstead and Yeomans 1987) where this complication does not arise. In that case simple chains, such as those shown in figure 1, are sufficient to establish the phase sequence, because the bulk field contributes to an energy difference between the two phases.

The numbers of ways of obtaining the diagrams contributing to $F_{h'} - F_h$, $h' > h$, for orders greater than w^{4h} increases rapidly with the order. However, it is shown in the appendix that to establish a sequence of layering transitions, it is not necessary to count them explicitly. The necessary inductive argument is explained here, leaving the mathematical expressions to the appendix.

Assume that the phase h has been shown to be stable, and that there is a phase boundary between h and h', $h' > h$. In the low-temperature series approximation, the reduced free-energy difference may be written as

$$F_{h'} - F_h = \sum_{i=0}^{m} f(i)w^i + O(w^{m+1}) \qquad h' > h \tag{2.22}$$

where we terminate the series at $O(w^m)$, and assume, as usual, that higher orders do not affect the qualitative nature of the phase diagram. The boundary $(\beta u)_{h:h+1}$ is determined by the condition

$$F_{h+1} - F_h = 0 = \sum_{i=0}^{m} f(i)w^i + O(w^{m+1}). \tag{2.23}$$

Substitution of (2.23) into (2.22) for $h' > h+1$ determines the sign of $F_{h'} - F_h$ (or equivalently, $F_{h'} - F_{h+1}$) along the $h : h+1$ boundary. If

$$F_{h'} - F_h < 0 + O(w^{m+1}) \qquad h' > h+1 \tag{2.24}$$

$h+1$ appears as the adjacent stable phase. It is shown in the appendix that (2.24) holds for general h. Therefore, having demonstrated that the phase $h+1$ is stable, we may repeat the argument, replacing h by $h+1$, to show that $h+2$ is stable along the $h+1 : h'$, $h' > h+1$, boundary. As $h = 3$ has explicitly been shown to be stable, iterating the argument leads to a sequence of layering transitions.

Recall that, for the Potts model described by Armitstead and Yeomans (1987), it is not possible to predict an infinite sequence of layering transitions because of correction terms $O(hw^2)$ arising from axial diagrams with side bumps which may dominate for large h. The exclusion of interfacial overhangs and bulk flucutations in the solid-on-solid model removes this difficulty, and allows us to predict that the sequence is infinite.

Note that the boundary between two phases may be written as a power series in w. All phase boundaries have the same lowest-order terms, and boundaries between phases with larger h have more terms in common. Chalker (1982a) has derived a lower limit on βu, $(\beta u)_c$, below which the surface will be completely wet:

$$(\beta u)_c = -\ln(1-w^4). \tag{2.25}$$

An expansion of $(\beta u)_c$ to $O(w^{12})$ is in agreement with equation (2.17), which describes the boundary along which all phases $h \geqslant 4$ are degenerate.

3. The restricted solid-on-solid model, $y = \infty$

We now study the restricted solid-on-solid model, taking $|h_i - h_j| = 0, 1$ in (1.1), with the same choice (2.1) for $U(h_i)$. This proves to be much more tractable mathematically, and we are more easily able to demonstrate a full layering sequence at sufficiently low temperatures.

The first two boundaries obtained from the expansion, including ground-state terms are

$$(\beta u)_{0:1} = w^4 + 2w^6 + \tfrac{3}{2}w^8 + O(w^{10}) \tag{3.1}$$

$$(\beta u)_{1:h} = 16w^{12} + O(w^{14}) \qquad h \geqslant 2. \tag{3.2}$$

The diagrams which contribute to the expression for the phase boundaries to lowest order are shown in figure 2. The restriction on $|h_i - h_j|$ forces the diagrams to have a three-dimensional 'staircase' structure and, in contrast to the unrestricted case, the differences in Boltzmann weights and counting factors between lowest-order diagrams of heights h and $h+1$ depend explicitly on h. Therefore these diagrams are already sufficient to determine the phase sequence. It is for this reason that the calculations are much easier for the case $y = \infty$.

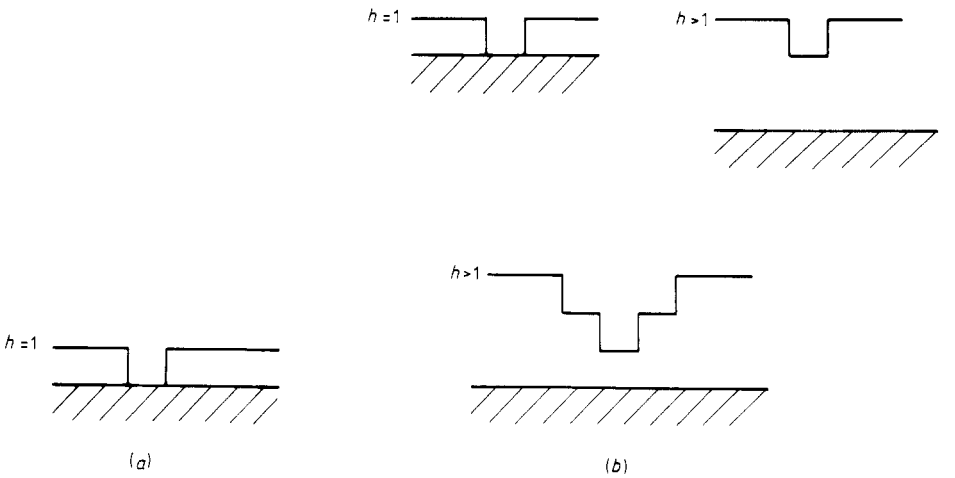


Figure 2. Lowest-order three-dimensional graphs for the restricted solid-on-solid model which give rise to a non-zero value of βu along (*a*) the 0 : 1 boundary, (*b*) the 1 : h boundary, $h > 1$.

To show that there is an infinite sequence of layering transitions we use the usual inductive argument (Duxbury and Yeomans 1985). Assume first that the phase h has been shown to be stable and that there is a phase boundary between the phases h and $h' > h$. The reduced free-energy difference between interface positions h and h' is needed. A typical lowest-order 'staircase' diagram which has different Boltzmann weights for interface positions h and h' is shown in figure 3(a). There will be several such diagrams of height h at this order: counting them as $A(h)$ gives

$$F_{h'} - F_h = A(h)w^a(1 - e^{\beta u}) + O(w^{a+2}) \qquad h' > h \tag{3.3}$$

where $a = 4h^2$. Expanding $e^{\beta u}$ as a power series gives

$$(\beta u)_{h;h'} = 0 + O(w^2) \qquad h' > h. \tag{3.4}$$

Inclusion of other diagrams of height h, such as that shown in figure 3(b), will also lead to a zero value for $\beta u_{h;h'}$. The diagrams which give the leading-order non-zero expression for this phase boundary are of height $h+1$ and $O(w^{a'})$, where $a' = 4(h+1)^2$. There will be $A(h+1)$ such diagrams and hence to leading order near the phase boundary

$$F_{h'} - F_h = A(h+1)\exp[\beta u \delta(h', h+1)]w^{a'} + A(h)w^a(1 - e^{\beta u}) + O(w^{a'+2}) \qquad h' > h. \tag{3.5}$$

The phase boundary between h and h' is therefore given by

$$(\beta u)_{h;h'} = A(h+1)w^{8h+4}/A(h) + O(w^{8h+6}) \qquad h' > h. \tag{3.6}$$

To establish whether a new phase is stable along the boundary (3.6) we examine the sign of $F_{h'} - F_{h+1}$, $h' > h+1$. The lowest-order contribution follows from (3.3) and

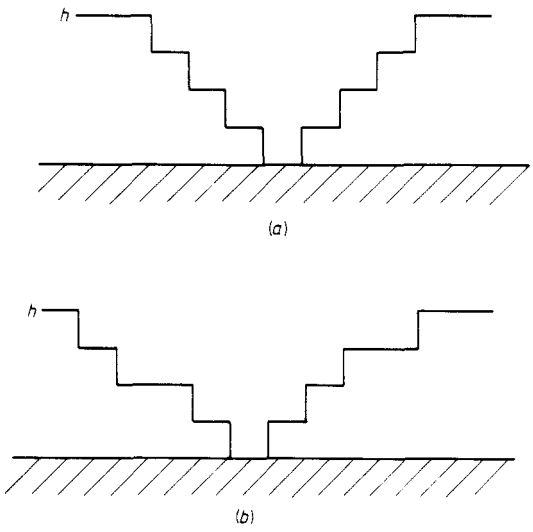


Figure 3. (a) Lowest-order graph with different Boltzmann weights for the restricted solid-on-solid model for interface phases h and h', $h' > h$. (b) Graphs of height h which have the same counts for h and h', and hence do not break the degeneracy between h and h' at $\beta u = 0$.

is given by

$$F_{h'} - F_{h+1} = -(\beta u)_{h:h'} A(h+1) w^{a'} + O(w^{2a'-a+2}) \qquad h' > h+1 \tag{3.7}$$

$$= -[A(h+1)]^2 w^{2a'-a} / A(h) + O(w^{2a'-a+2}). \tag{3.8}$$

As this is negative $h+1$ is stable and we may expect a $h+1:h'$, $h' > h+1$, boundary to exist. Explicit calculations have already demonstrated a $0:1$ and $1:h$ boundary. Therefore, using an inductive argument, a sequence of layering transitions is obtained.

The qualitative form of the phase diagram is the same as the $y = 1$ model. However, the quantitative values are very different as one would expect. The phase diagrams are compared in figure 4, which is exaggerated for clarity. In the $y = \infty$ model the effects of thermal fluctuations are suppressed. Hence for a given potential the phase boundaries are at a higher temperature.

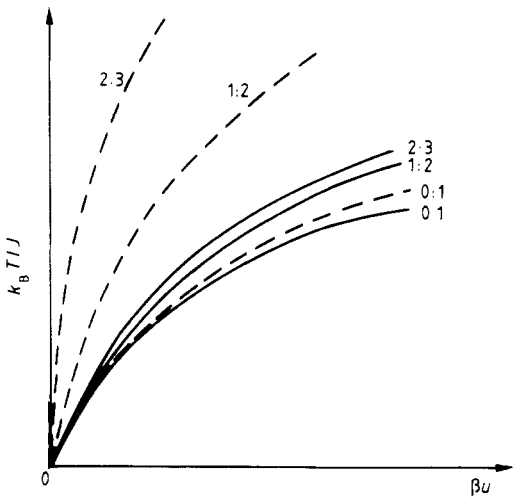


Figure 4. Qualitative comparison of the first three phase boundaries for the standard, $y = 1$, solid-on-solid model (full curves) and the restricted, $y = \infty$, solid-on-solid model (broken curves).

Luck *et al* (1983) have studied the restricted solid-on-solid model using numerical solutions for strips of finite width, extrapolating the results to an infinite system. At low temperatures they obtain a single first-order transition from $h = 0$ to $h = \infty$, and they support their results by a first-order low-temperature expansion. We believe that they do not observe layering because the numerical method is not sufficiently discerning to pick up the narrow layering transitions. Moreover, in the low-temperature expansion they do not appear to have considered the stability of phases other than $h = 0$ and $h = \infty$.

4. Conclusion

Although the solid-on-solid model is of interest in its own right we can also regard it as a simplification of similar models which are otherwise intractable. Duxbury and

Yeomans (1985) studied the three-dimensional Abraham Hamiltonian (Abraham 1980)

$$H = -\tfrac{1}{2}J_0^* \sum_{ijj'} S_{i,j}S_{i,j'} - aJ^* \sum_j S_{0,j}S_{1,j} - J^* \sum_{ij} S_{i,j}S_{i+1,j} \tag{4.1}$$

with infinite surface fields on $i = 0$ and ∞ forcing $S_0 = -1$ and $S_\infty = +1$ respectively. Taking the anisotropic limit

$$J_0^* \to \tfrac{1}{2}J \qquad 2(1-a)J^* \to u \qquad J^* \to \infty \tag{4.2}$$

(4.1) becomes equivalent to the $y = 1$ solid-on-solid model. Taking this limit in the equations given by Duxbury and Yeomans (1985) reduces them, as would be hoped, to our results. The most important terms which occur in the analysis of the Ising model and which disappear in the solid-on-solid limit are $O(w^6)$. Therefore the phase transitions in the Ising model differ noticeably from those of the solid-on-solid model when w^2 becomes significant compared with $O(1)$, which is not within the region of validity of the low-temperature series. For temperatures below roughening there should be good agreement (within 20%) between the models.

Duxbury and Yeomans (1985) were able to establish the existence of only two transitions in the Abraham model with, to the order to which they were able to take the expansion, all phases with $h \geq 2$ (using a notation consistent with the calculations in this paper) remaining degenerate on the $2{:}\infty$ boundary. It is now obvious from our calculations that the problem which they experienced in obtaining further phase boundaries arose because the pinning potential is a surface field as opposed to a bulk one. To obtain a non-degenerate phase boundary, the expansion must be taken to sufficiently high order that the relative change in succcessive terms depends upon h. Therefore consideration of just the contribution from axial chains of flipped spins, which is easily calculable using a matrix method (Armitstead and Yeomans 1987) is not sufficient. Although it is possible to go to sufficiently high orders for the solid-on-solid limit, a similar calculation for the full Abraham model appears intractable at the moment.

Pandit *et al* (1982) have performed a mean-field theory for the Hamiltonian (4.1) with the inclusion of a bulk field term. Although a detailed comparison is not possible, as the calculations presented here correspond to an examination of a small region of their parameter space, the qualitative results are in agreement.

As was discussed in Armitstead and Yeomans (1987), when using low-temperature series to expand about a multiphase point one should be aware that the expansion is about metastable states for, in this case, finite u. Therefore the exact meaning or convergence of the reduced free energies is not obvious.

In this paper we have shown that both the unrestricted and the restricted solid-on-solid models depin from a local surface potential through an infinite sequence of layering transitions. The lowest-order diagrams which are required to demonstrate a layering transition between h and $h+1$ are $O(w^{6h+10})$ and $O(w^{4(h+1)(h+1)})$ respectively. Hence it is more difficult to establish the phase boundaries than in cases where there is a bulk field in the Hamiltonian (Duxbury and Yeomans 1985, Armitstead and Yeomans 1987), where chains of spins, $O(w^{4h})$, which link the surface to the interface drive the transition. This analysis has enabled us to explain the difficulty experienced by Duxbury and Yeomans (1985) in trying to establish an infinite sequence of layering transitions for the Abraham model.

Having demonstrated the applicability of the solid-on-solid approximation to the study of wetting transitions, the method explained in this paper could now be extended

to more realistic, long-ranged, surface potentials which would allow comparison with experiment.

Appendix

In this appendix we demonstrate the existence of a sequence of layering transitions for the unrestricted, $y = 1$, solid-on-solid model.

The lowest-order excitation of the interface of height h' is $O(w^{4h'})$ and has a count per interface site of 1: this simple excitation is shown in figure 5(a). There are four possible diagrams of height h' per interface site at $O(w^{4h'+2})$, as shown in figure 5(b). At $O(w^{4h'+4})$, however, there are many possible diagrams of height h', some examples of which are shown in figure 5(c). At order $O(w^{4h'+j})$ we shall count the number of diagrams of height h', with $2h' > j$, as a_j, for example, $a_0 = 1$ and $a_2 = 4$. Notice that we have imposed $2h' > j$ on the a_j. The number of diagrams $O(w^{4h'+2h})$, $h' > h$, is a_{2h}; however, the number of diagrams $O(w^{4h+2h})$ is not a_{2h}, but $a_{2h} - 2$. The diagrams which cause this difference are shown in figures 6(a) and (b). There are four possible orientations of the diagram shown in figure 6(a) but only two of the type shown in figure 6(b). It is these differences which ultimately lead to the layering transitions.

To $O(w^{6h-2})$, that is considering diagrams which can only touch the surface once,

$$F_{h+1} - F_h = (1 - e^{\beta u}) w^{4h} \sum_{i=0}^{h-1} a_{2i} w^{2i} + w^{4h+4} e^{\beta u} \sum_{i=0}^{h-3} a_{2i} w^{2i}. \tag{A1}$$

The first summation arises from fluctuations of height h, whilst the second is from those of height $h+1$. To the same order

$$F_\infty - F_h = (1 - e^{\beta u}) w^{4h} \sum_{i=0}^{h-1} a_{2i} w^{2i} + w^{4h+4} \sum_{i=0}^{h-3} a_{2i} w^{2i} + \ldots + w^{6h-6} \sum_{i=0}^{2} a_{2i} w^{2i} + w^{6h-2} \tag{A2}$$

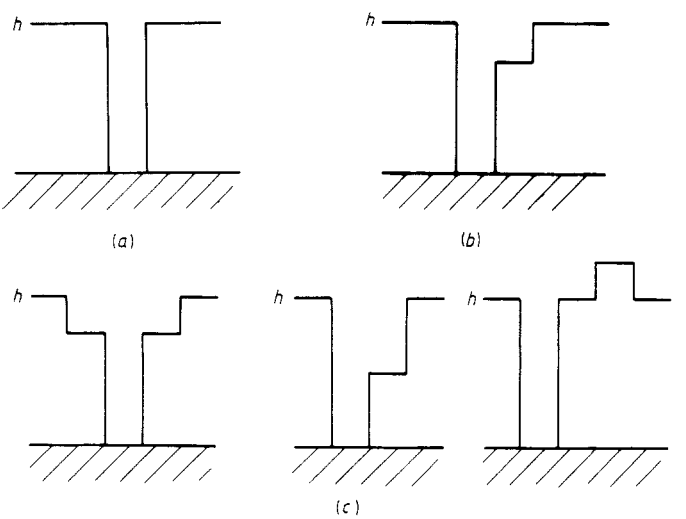


Figure 5. Examples of graphs which must be considered to establish an infinite phase sequence in the unrestricted solid-on-solid model. (a) The lowest-order excitation of the interface of height h. (b) Graphs of height h and $O(w^{4h+2})$. There are four possible orientations of the graph. (c) Examples of graphs of height h and $O(w^{4h+4})$.

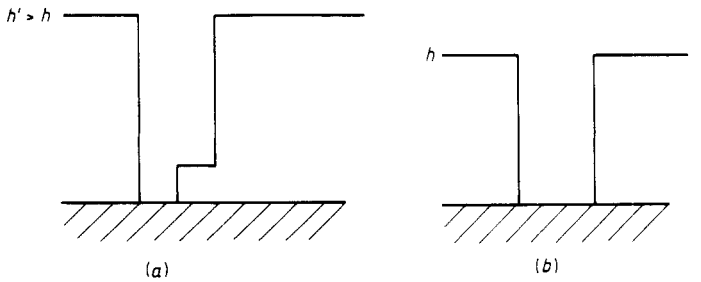


Figure 6. Graphs which show that for the unrestricted solid-on-solid model there are a_{2h} possible graphs $O(w^{4h'-2h})$, $h'>h$, but only $a_{2h}-2$ $O(w^{4h+2h})$: (a) has a count of four per site whereas (b) has a count of only two per site.

for h odd. Similar expressions follow easily for h even and for $F_{h'}-F_h$, $h'>h+1$.

Along the $h:h+1$ boundary (A1) is zero and so we may use

$$(1-e^{\beta u})w^{4h}\sum_{i=0}^{h-1}a_{2i}w^{2i}=-w^{4h+4}e^{\beta u}\sum_{i=0}^{h-3}a_{2i}w^{2i} \tag{A3}$$

in equation (A2) to show that

$$F_{h'}-F_h=0+O(w^{5h}) \qquad h'>h+1. \tag{A4}$$

Hence we must go to higher order to establish the phase sequence.

To $O(w^{6h+2})$, i.e. including diagrams which touch the surface at two lattice sites,

$$F_{h+1}-F_h=(1-e^{\beta u})w^{4h}\sum_{i=0}^{h+1}a_{2i}w^{2i}-4(1-e^{\beta u})w^{6h}+2(1-e^{2\beta u})w^{6h}$$

$$-36(1-e^{\beta u})w^{6h+2}+16(1-e^{2\beta u})w^{6h+2}+4^{4h+4}e^{\beta u}\sum_{i=0}^{h-1}a_{2i}w^{2i} \tag{A5}$$

where the first two modifications, $O(w^{6h})$, to the summation are due to the diagrams shown in figure 6, and the second two, $O(w^{6h+2})$, are due to those shown in figure 7. Figure 7(a) shows the diagrams which are counted in a_{2h+2} in which two of the fluctuations are of at least height h which should not be included in (A5), whereas figure 7(b) shows the diagrams which actually occur when the interface is a distance h from the wall.

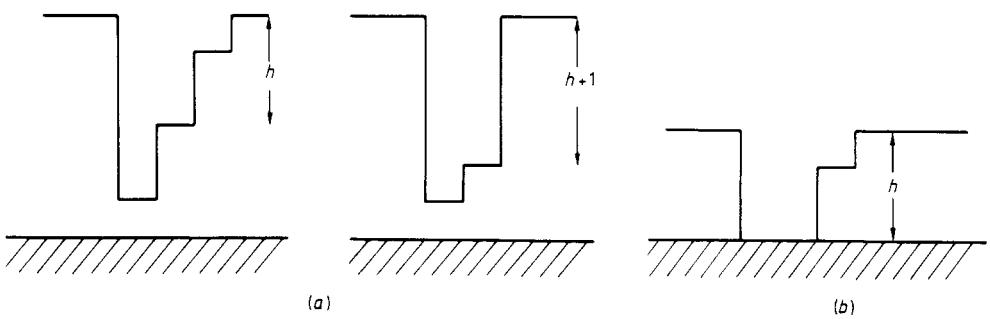


Figure 7. (a) Graphs for the unrestricted solid-on-solid model which are counted in a_{2h+2} which should not be included when the interface is a distance h from the wall, but must be replaced by those shown in (b).

Also $O(w^{6h+2})$

$$F_\infty - F_h = (1-e^{\beta u})w^{4h}\sum_{i=0}^{h+1} a_{2i}w^{2i} - 4(1-e^{\beta u})w^{6h} + 2(1-e^{2\beta u})w^{6h} - 36(1-e^{\beta u})w^{6h+2}$$

$$+16(1-e^{2\beta u})w^{6h+2} + w^{4h+4}\sum_{i=0}^{h-1} a_{2i}w^{2i} + \ldots + w^{6h+2} \qquad h \text{ odd.} \qquad \text{(A6)}$$

However, putting equation (A5) equal to zero to define the $h:h+1$ boundary, and inserting the resultant expression into (A6), again leads to

$$F_{h'} - F_h = 0 + O(w^{6h+4}) \qquad h' > h+1. \qquad \text{(A7)}$$

Indeed terms to $O(w^{6h+10})$ are needed in $F_{h+1} - F_h$ to obtain the non-zero result necessary to check if layering occurs. However, one can show that the higher-order diagrams do not contribute to this difference (Armitstead 1987) and it is the expansion of $e^{\beta u}$ in the terms already shown in (A5) and (A6) which eventually leads to

$$F_{h'} - F_h = -2w^{6h+10} + O(w^{6h+12}) \qquad h' > h+1. \qquad \text{(A8)}$$

This free-energy difference is negative and hence, following the inductive argument given in § 3.2, a sequence of layering transitions can be established.

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