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The Wetting Transition in a Random Surface Model

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We continue our analysis of the phase diagram of a discrete random surface, with no "downward fingers," lying above a flat two-dimensional substrate. The surface is closely related to the 2D Ising model and its free energy is exactly solvable in much (but not all) of the phase diagram. There is a transition at temperature T_w from a high-T infinite height or wet phase to a low-T finite height or partially wet phase. Previously it was shown that when a parameter b, related to the contact interaction, is positive, T_w is independent of b and there is a logarithmic specific heat divergence as T_w is approached from *either* side. Here we show that for $b<0$, T_w does depend on b and there is *no* thermodynamic singularity from the wet phase. The partially wet phases for $b \leqslant 0$ and $b>0$ differ in the absence or presence of a monolayer covering the entire substrate; this results in a first-order transition across the line $b=0$, $T<T_w$.

KEY WORDS: Wetting; random surface; Ising model; monolayer.

1. INTRODUCTION

In this paper, we derive further rigorous results on the phase diagram of a statistical mechanical model[1,2] of a random, two-dimensional surface embedded in three-dimensional space. The surface is formed by joining together along their edges plaquettes from $\mathbb{Z}^3$. The fluctuations of the surface are controlled by surface tension in a statistical mechanical canonical treatment with inverse temperature β. The surface is further restricted by suspending it over a flat substrate with which it interacts. If we think of the surface as separating two coexistent but immiscible phases, then we are dealing with a model which could be relevant to the wetting phenomenon. It is generally felt on the basis of renormalization group arguments that the

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location and nature of the phase transition ought to depend on the nature of the substrate interaction.[3] In our earlier results, we obtained a phase transition for the three-dimensional system precisely at the transition of a related planar Ising model, and with the same type of singularity for the free energy. Fortunately, this was only for part of the phase diagram. Although we have not been able to obtain critical exponents in the other part, we have proved that our model has an interaction-dependent transition curve there and furthermore that the free energy is nonsingular as that curve is approached from the wet region.

Our model is unlike others to discuss wetting which feature the entropic repulsion idea of Fisher.[4,5] This repulsion comes from fingers which project below the surface and intercept the substrate. Our model does not have this feature, but entropic wandering enters in another way, at least implicitly.

We would like to dedicate this work to J. K. Percus on the occasion of his 65th birthday. As well as making many contributions to the statistical mechanics of inhomogeneous systems, he established some inequalities[6] which enabled van Beiejeren[7] to make an important contribution to the theory of roughening in Ising models.

2. MODEL AND RESULTS

We have described the background to our model at length elsewhere.[1,2] Here we will just describe its construction and discuss other new exact results on the phase diagram. In the following sections, precise statements of these results will be given along with their derivation.

Let Λ be a finite subset of $\mathbb{Z}^2$, e.g., $\{(x, y)\colon -n \leqslant x, y \leqslant n\}$. For each $\mathbf{r} \in \Lambda$ define a height function $h(\mathbf{r}) \in \mathbb{Z}$. The fact that a phase-separating surface is described uniquely by such a height function is of course a restriction which eliminates overhangs and reentrants. (i) We set

$$h(\mathbf{r}) = 0 \qquad \text{on} \quad \mathbb{Z}^2 \backslash \Lambda \tag{2.1}$$

and (ii) since the surface is suspended over a flat substrate, we require

$$h(\mathbf{r}) \geqslant 0 \qquad \text{on} \quad \mathbb{Z}^2 \tag{2.2}$$

The energy of such a surface is a sum of two parts: first there is the surface tension τ for each plaquette, which gives a contribution

$$\tau \sum_{\langle \mathbf{r}, \mathbf{s} \rangle} |h(\mathbf{r}) - h(\mathbf{s})| + \tau A_1 \tag{2.3}$$

where $\langle \mathbf{r}, \mathbf{s} \rangle$ denotes any nearest neighbor bond on $\mathbb{Z}^2$. Here A_1 is the number of plaquettes or faces of the surface which are parallel to the substrate; it is also the area of substrate in contact with molecules. The second contribution to the energy is simply a term

$$-\varepsilon_1 A_1 = -\varepsilon_1 \sum_{\mathbf{r}: h(\mathbf{r}) \neq 0} 1 \tag{2.4}$$

where ε_1 is the binding energy per molecule. The total Hamiltonian is thus

$$H = \tau \sum_{\langle \mathbf{r}, \mathbf{s} \rangle} |h(\mathbf{r}) - h(\mathbf{s})| + (\tau - \varepsilon_1) A_1 \tag{2.5}$$

(iii) To make progress, we further restrict the surface:

$$h(\mathbf{r}) - h(\mathbf{s}) = 0, \pm 1 \qquad \text{for each} \quad \langle \mathbf{r}, \mathbf{s} \rangle \tag{2.6}$$

and a final restriction which disallows downward-pointing fingers:

(iv) For every $\mathbf{r} \in \Lambda$ there is some nearest neighbor path to an $\mathbf{r}' \in \mathbb{Z}^2 \backslash \Lambda$ along which $h(\mathbf{r})$ *never increases.*

There is an alternative way of looking at this construction as a "raft" model given in Appendix B of ref. 2, which may help in visualizing the model.

The point behind the restrictions is that the configuration space is isomorphic to that of the planar Ising model as expressed in the following result.

Proposition 2.1.[1,2] For a finite $\Lambda \subset \mathbb{Z}^2$, the height configurations $h(\mathbf{r})$ [or $h_\Lambda(\mathbf{r})$] satisfying (i)–(iv) are in one-to-one correspondence with the Ising model configurations $\{\sigma_\Lambda(\mathbf{r}) = \pm 1 : \mathbf{r} \in \mathbb{Z}^2\}$ with $\sigma_\Lambda(\mathbf{r}) = +1$ for all $\mathbf{r} \in \mathbb{Z}^2 \backslash \Lambda$; $h_\Lambda(\mathbf{r})$ is identified as the minimum number of Peierls contours crossed, among all possible nearest-neighbor paths from $\mathbf{r}$ to $\mathbb{Z}^2 \backslash \Lambda$. With this identification, and putting $b = \varepsilon_1 - \tau$, we have

$$H = -b|\Lambda| - \frac{\tau}{2} \sum_{\langle \mathbf{r}, \mathbf{s} \rangle} [\sigma_\Lambda(\mathbf{r})\, \sigma_\Lambda(\mathbf{s}) - 1] + \frac{b}{2} \sum_{\mathbf{r} \in C_+(\partial \Lambda)} [\sigma_\Lambda(\mathbf{r}) + 1] \tag{2.7}$$

where $|\Lambda|$ denotes the number of sites in Λ and $C_+(\partial \Lambda)$ denotes the plus spin cluster of $\partial \Lambda$, the boundary of Λ; i.e., $C_+(\partial \Lambda) = \Lambda \backslash \Lambda_1$, where $\Lambda_1 = \{\mathbf{r} : h_\Lambda(\mathbf{r}) \neq 0\}$.

Evidently level sets of the surface are parallel spin clusters, establishing a useful connection with percolation ideas.[8]

The previously known results for this model are sketched in Fig. 1. For $b \geqslant 0$ and $T \geqslant T_c(2)$, the system is wet because the surface wanders

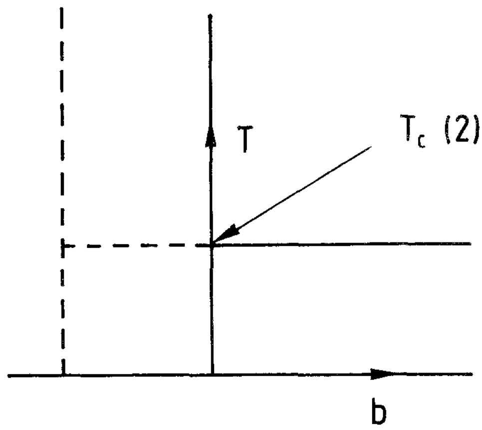

Fig. 1. Previously known results for the phase diagram. For $b \geqslant 0$ there is a transition at $T = T_c(2)$ from a partially wet to a wet phase. $T_c(2)$, the solution of $\sinh[\tau/T_c(2)] = 1$, is independent of b. As $T \to T_c(2) \pm$, there is a logarithmic specific heat divergence. For $b > 0$ and $T < T_c(2)$, the partially wet phase has a monolayer covering the entire substrate. For $b \leqslant 0$ and $T < T_c(2)$, the system is partially wet with no monolayer. The physically relevant portion of the plane is $b > -2\tau$, to ensure stability against detachment from the substrate.

away from the substrate: $h_\Lambda(\mathbf{r})$ diverges as $\Lambda \to \mathbb{Z}^2$. For any b and $T < T_c(2)$, there is partial wetting since $\langle h_\Lambda(\mathbf{r}) \rangle$ remains finite as $\Lambda \to \mathbb{Z}^2$. The partially wet phase for $b > 0$ involves the presence of a monolayer. For $b \geqslant 0$ and all T, the free energy is given by

$$f(T, b) = f(T, 0) - b \tag{2.8}$$

where $f(T, 0)$ is the Onsager free energy. [Note: In ref. 2, there is a missing minus sign in the equations for f numbered (2.7) and (2.8) there.] Thus, for $b \geqslant 0$, the phase transition has a logarithmic specific heat singularity which is independent of b as the line $T = T_c(2)$ is approached from *either* side.

Our new results are sketched in Fig. 2. It was known previously that for $b < 0$, the phase transition curve must lie above or on $T = T_c(2)$. One new result (see Propositions 3.6 and 4.4) is that this curve lies strictly above $T = T_c(2)$ and strictly within the $b < 0$ region (at least for T high enough). Thus the dependence on b is nontrivial in the $b \leqslant 0$ half-plane of the phase diagram. This is an important extension to previous results on this model since it is generally felt that a satisfactory theory of wetting ought to have an interaction-dependent transition and, moreover, interaction-dependent critical exponents.[3] Unfortunately, we are unable yet to shed any light on the latter point.

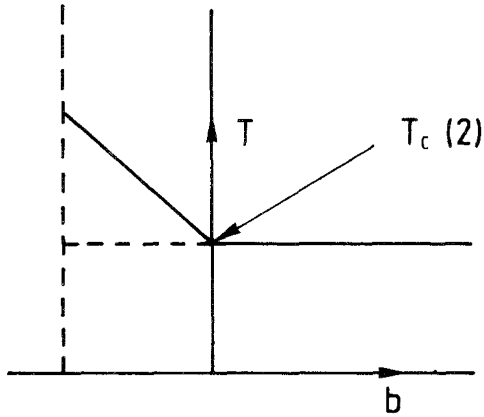

Fig. 2. New results for the phase diagram. The partially wet phase extends at least up to the line $\{T = T_c(2)(1 - b/[4\tau]),\ b < 0\}$ and the wet phase extends strictly into the region $\{T > T_c(2),\ b < 0\}$. The free energy approaches the wetting transition curve analytically from the wet side. It has a discontinuous b-derivative at the line $\{T < T_c(2),\ b = 0\}$ due to the appearance of a monolayer.

A second new result (see Proposition 5.1) is that (2.8) remains valid in the entire wet regime for $b < 0$. This, combined with the fact that the wetting temperature is strictly above $T_c(2)$, has the important consequence that for $b < 0$, there is no singular behavior of the free energy as the wetting transition curve is approached from the wet regime. The free energy is *not* given by (2.8) in the partially wet, $b < 0$ regime; indeed, we show (see Proposition 5.2) that there is a first-order transition, corresponding to the appearance of a monolayer as the line $b = 0$, $T < T_c(2)$ is crossed. As a byproduct of our main results, we also obtain an inequality relating two critical exponents at the point $b = 0$, $T = T_c(2)$ (see Proposition 5.3).

3. PARTIALLY WET PHASE

In this section, we give results for the partially wet phase with $b < 0$. First we state a result of Jogdeo[9] about FKG inequalities. A collection of random variables (or their joint probability distribution) is said to have the FKG property[10] (or, equivalently, is called associated[11]) if increasing functions of the variables are always positively correlated.

Proposition 3.1.[9] Consider discrete random variables N_i and M_j and express the probability of the joint configuration $(\mathbf{n}, \mathbf{m})$ in the usual way as $\mu(\mathbf{n})\,\nu(\mathbf{m}\,|\,\mathbf{n})$, the product of a marginal and a conditional probability. Suppose that:

1. μ has the FKG property (in $\mathbf{n}$).
2. For each $\mathbf{n}$, $\nu(\mathbf{m}\,|\,\mathbf{n})$ has the FKG property (in $\mathbf{m}$).
3. As $\mathbf{n}$ increases, $\nu(\cdot\,|\,\mathbf{n})$ is stochastically increasing; i.e., the ν-average of an increasing function of $\mathbf{m}$ increases as $\mathbf{n}$ increases.

Then $\{\mathbf{N}, \mathbf{M}\}$ has (jointly) the FKG property.

Proposition 3.2. Take the plus-boundary-condition Ising model as defined in Proposition 2.1 of the previous section, but with the Hamiltonian (2.7) replaced by

$$H = -\frac{\tau}{2} \sum_{\langle \mathbf{r}, \mathbf{s} \rangle} [\sigma(\mathbf{r})\,\sigma(\mathbf{s}) - 1] - h \sum_{\mathbf{r} \in \Lambda} [\sigma(\mathbf{r}) + 1] \tag{3.1}$$

with any real h. Define

$$N_{\mathbf{r}} = \begin{cases} 1 & \text{for} \quad \mathbf{r} \in C_+(\partial\Lambda) \\ 0 & \text{otherwise} \end{cases} \tag{3.2}$$

$$M_{\mathbf{r}} = \begin{cases} -1 & \text{if} \quad \sigma(\mathbf{r}) = +1, \quad \mathbf{r} \in \Lambda \backslash C_+(\partial\Lambda) \\ 0 & \text{otherwise} \end{cases} \tag{3.3}$$

Then $(\mathbf{M}, \mathbf{N})$ satisfy the hypotheses of Proposition 3.1.

Proof. Condition 1 is true because each $N_{\mathbf{r}}$ is an increasing function of $\{\sigma(\mathbf{s}): \mathbf{s} \in \Lambda\}$. Thus the condition follows from the usual FKG inequalities for the spins.[10] Condition 2 is true because given any $\mathbf{n}$ and hence given $\Lambda_1 = \Lambda \backslash C_+(\partial\Lambda)$ and its interior $L_\Lambda = \Lambda_1 \backslash \{\mathbf{r} \in \Lambda_1 : \mathbf{r}$ is a nearest neighbor of some $\mathbf{s}$ in $\mathbb{Z}^2 \backslash \Lambda_1\}$, the conditional distribution of $\{\sigma(\mathbf{s}): \mathbf{s} \in L_\Lambda\}$ is that of a minus-boundary-condition Ising model. Each $M_{\mathbf{r}}$ is a decreasing function of these minus-boundary-condition spin variables and hence they have the FKG property. (See Appendix A of ref. 2 for more details in similar arguments.) To prove the validity of condition 3, we must show that the $M_{\mathbf{r}}$ increase stochastically if $\mathbf{n}$ increases. First, increasing $\mathbf{n}$ decreases L_Λ deterministically, which forces certain $M_{\mathbf{r}}$, not formerly zero, to vanish. Now consider $M_{\mathbf{r}}$ for $\mathbf{r}$ in the *new* (and smaller) L_Λ. These are functions of a minus-b.c. Ising model in a *smaller* region than before. But a minus-b.c. Ising model in a region L_Λ stochastically decreases as L_Λ decreases by the FKG property of the spins (since some fields must have been reduced to $-\infty$). Since the $M_{\mathbf{r}}$'s are decreasing functions of these spin variables, they are stochastically increasing as L_Λ decreases, which completes the proof.

Proposition 3.3. For a given Λ and inverse temperature $\beta = 1/T$, let $\langle \cdot \rangle_{\beta,b}$ and $\langle \cdot \rangle^*_{\beta,h}$ denote the thermal averages for the two plus-b.c. Ising models with respective Hamiltonians given by (2.7) and (3.1). For both cases define $M_{\mathbf{r}}$ and $N_{\mathbf{r}}$ as in (3.2)–(3.3). If $h \geqslant 0$, then

$$\langle f_1 \rangle^*_{\beta,h} \leqslant \langle f_1 \rangle_{\beta,-2h} \tag{3.4}$$

for any increasing function f_1 of $(\mathbf{M}, \mathbf{N})$.

Proof. Let us denote by $P_{\beta,b}$ and $P^*_{\beta,h}$ the Gibbs distributions for the spin variables with these two Hamiltonians. When $h = 0 = b$, $P_{\beta,0}$ and $P^*_{\beta,0}$ are both just the zero-field Ising-model Gibbs distribution. We have

$$P_{\beta,-2h} = C_1 \exp\left(2\beta h \sum_{\mathbf{r}\in\Lambda} N_{\mathbf{r}}\right) P^*_{\beta,0} \tag{3.5}$$

$$P^*_{\beta,h} = C_2 \exp\left[2\beta h \sum_{\mathbf{r}\in\Lambda} (N_{\mathbf{r}} - M_{\mathbf{r}})\right] P^*_{\beta,0} \tag{3.6}$$

and so

$$\langle f_1 \rangle_{\beta,-2h} = \left\langle f_1 \exp\left(2\beta h \sum M_{\mathbf{r}}\right)\right\rangle^*_{\beta,h} \Big/ \left\langle \exp\left(2\beta h \sum M_{\mathbf{r}}\right)\right\rangle^*_{\beta,h} \tag{3.7}$$

By Propositions 3.1 and 3.2, we have for $h \geqslant 0$ that

$$\left\langle f_1 \exp\left(2\beta h \sum M_{\mathbf{r}}\right)\right\rangle^*_{\beta,h} \geqslant \langle f_1 \rangle^*_{\beta,h} \left\langle \exp\left(2\beta h \sum M_{\mathbf{r}}\right)\right\rangle^*_{\beta,h} \tag{3.8}$$

from which (3.4) follows.

Proposition 3.4.[12,13] If $h \geqslant 0$, then

$$\langle f_2 \rangle^*_{\beta,0} \leqslant \langle f_2 \rangle^*_{2\tau\beta/(2\tau+h),h} \tag{3.9}$$

for any increasing function f_2 of $\{\sigma(\mathbf{r}) : \mathbf{r} \in \Lambda\}$.

Proof.

$$P^*_{2\tau\beta/(2\tau+h),h} = \frac{(\exp\{\theta \sum_{\langle \mathbf{r},\mathbf{s}\rangle} [\sigma(\mathbf{r}) + \sigma(\mathbf{s}) - \sigma(\mathbf{r})\,\sigma(\mathbf{s})]\})P^*_{\beta,0}}{\langle \exp\{\theta \sum_{\langle \mathbf{r},\mathbf{s}\rangle} [\sigma(\mathbf{r}) + \sigma(\mathbf{s}) - \sigma(\mathbf{r})\,\sigma(\mathbf{s})]\}\rangle_{\beta,0}} \tag{3.10}$$

with $\theta = \beta h\tau/2(2\tau + h)$. Now $\sigma(\mathbf{r}) + \sigma(\mathbf{s}) - \sigma(\mathbf{r})\,\sigma(\mathbf{s})$ is increasing in the $\{\sigma(\mathbf{r}')\}$. So is $\exp\{\theta \sum_{\langle \mathbf{r},\mathbf{s}\rangle} [\sigma(\mathbf{r}) + \sigma(\mathbf{s}) - \sigma(\mathbf{r})\,\sigma(\mathbf{s})]\}$ because $\theta \geqslant 0$. Hence the desired result follows from the FKG property of $P^*_{\beta,0}$.

Proposition 3.5. If $b \leqslant 0$, then

$$\langle g \rangle_{\beta,0} \geqslant \langle g \rangle_{4\tau\beta/(4\tau-b),b} \tag{3.11}$$

for any increasing function g of $\{h_\Lambda(\mathbf{r})\}$.

Proof. The only difficulty arises through having a function of $\{h_\Lambda(\mathbf{r})\}$ rather than one which depends only on $\{N_\mathbf{r}\}$. From Proposition 3.4, the zero-height region is stochastically bigger for $P_{4\tau\beta/(4\tau-b),b}$ than for $P_{\beta,0}$. But given the zero-height region $C_+(\partial\Lambda) = \Lambda \backslash \Lambda_1$, the *conditional* distribution of the $\{\sigma(\mathbf{r}): \mathbf{r} \in \Lambda_1\}$ and thus of $\{h_\Lambda(\mathbf{r}): \mathbf{r} \in \Lambda_1\}$, the heights in the nonzero height region, is the *same* for the two measures; this distribution of heights is that of $\{1 + h_{\Lambda_1}(\mathbf{r}): \mathbf{r} \in \Lambda_1\}$ from the Λ_1 version of $P_{\beta,0}$. But from Proposition A1 of ref. 2, these heights stochastically decrease as Λ_1 decreases. Thus the heights for all $\mathbf{r} \in \Lambda$ from $P_{4\tau\beta(4\tau-\beta),b}$ are stochastically smaller than those from $P_{\beta,0}$ as desired.

We use the last proposition to compare a point (β, b) in the left half-plane with $\beta < \beta c$ and $|b|$ sufficiently large to a partially-wet point $(\beta, 0)$ with $\beta > \beta_c$. This immediately yields the following result.

Proposition 3.6. The wetting transition curve in the left half-plane must lie above the curve

$$\beta = 4\beta_c \tau/(4\tau - b) \tag{3.12}$$

i.e., the heights $h_\Lambda(\mathbf{r})$ remain bounded as $\Lambda \to \mathbb{Z}^2$ if $b < 0$ and

$$T < T_c(2)\left(1 - \frac{b}{4\tau}\right) \tag{3.13}$$

4. WET PHASE

In this section, we give results for the wet phase with $b < 0$.

Proposition 4.1. For any $\beta \leqslant \beta_c$, real b, and $\Lambda_n \to \mathbb{Z}^2$: if for every $\mathbf{r}$,

$$P_{\beta,b}(h_{\Lambda_n}(\mathbf{r}) = 0) \to 0 \quad \text{as} \quad n \to \infty \tag{4.1}$$

then for any $\mathbf{s}$ and any k

$$P_{\beta,b}(h_{\Lambda_n}(\mathbf{s}) \geqslant k) \to 1 \quad \text{as} \quad n \to \infty \tag{4.2}$$

i.e., $h_{\Lambda_n}(\mathbf{s}) \to +\infty$ as $n \to \infty$.

Proof. Let $L_n = L_{\Lambda_n}$ denote the interior of the positive height region for $\{h_{\Lambda_n}(\mathbf{r})\}$ [as in Eq. (A.2) of ref. 2]. Limit (4.1) implies that $L_n \to \mathbb{Z}^2$ as

$n \to \infty$. But conditional on L_n, $\{h_{\Lambda_n}(\mathbf{s}): \mathbf{s} \in L_n\}$ for the given β and b has the same distribution as $\{1 + h_{L_n}(\mathbf{s}): \mathbf{s} \in L_n\}$ for some β and $b = 0$. The proof is completed by noting that Theorem II-3 of ref. 2 with $b = 0$ states that $h_{L_n}(\mathbf{s}) \to +\infty$ as $L_n \to \mathbb{Z}^2$.

In the next proposition, we compare the $P_{\beta,b}$ distribution to the distribution P_p for *independent* spin variables $\{\sigma(\mathbf{r})\}$ with $P_p(\sigma(\mathbf{r}) = +1) = p$ for each $\mathbf{r}$. The average for these variables is denoted $\langle \cdot \rangle_p$. The P_p is the same as $P^*_{\beta,h}$ in the limit $\beta = 0$ and $p = (1 + e^{-2\beta h})^{-1}$.

Proposition 4.2. For any β, $b \leqslant 0$, finite $\Lambda \subset \mathbb{Z}^2$, and $\mathbf{r} \in \Lambda$,

$$\langle e^{-\beta b |C_+|} \rangle^*_{\beta,0} \leqslant \langle e^{-\beta b |C_+|} \rangle_p \tag{4.3}$$

and

$$P_{\beta,b}(h_\Lambda(\mathbf{r}) = 0) \leqslant \langle e^{-\beta b |C_+|} 1_{\mathbf{r} \in C_+} \rangle_p \tag{4.4}$$

where $C_+ = C_+(\partial\Lambda)$ as usual denotes the plus-spin cluster within Λ which reaches the boundary of Λ, and

$$P_p(\sigma(\mathbf{r}) = +1) = p = 1/(1 + e^{-4\beta\tau}) \tag{4.5}$$

Remark. The critical value for independent-site percolation in $\mathbb{Z}^2$ is strictly greater[14] than 1/2. Thus, for sufficiently small β, the p given by (4.5) is below the threshold for plus-spin percolation.

Proof of Proposition 4.2:

$$P_{\beta,b}(h_\Lambda(\mathbf{r}) = 0) = \frac{\langle e^{-\beta b |C_+|} 1_{\mathbf{r} \in C_+} \rangle^*_{\beta,0}}{\langle e^{-\beta b |C_+|} \rangle^*_{\beta,0}} \leqslant \langle e^{-\beta b |C_+|} 1_{\mathbf{r} \in C_+} \rangle^*_{\beta,0} \tag{4.6}$$

for $b \leqslant 0$. But, for f any increasing function of the spin variables in Λ,

$$\langle f \rangle^*_{\beta,0} \leqslant \langle f \rangle_p \tag{4.7}$$

with p given by (4.5). This can be obtained as a limiting case of Proposition 3.4 of the last section; it was also derived as Eq. (5.12) of ref. 2 [except that an incorrect version of (4.5) is given there]. Since for $b \leqslant 0$, $e^{-b|C_+|}$ and $e^{-b|C_+|} 1_{\mathbf{r} \in C_+}$ are increasing functions of the spins, we obtain (4.3) and (4.4), as desired.

Proposition 4.3. Let Λ_n denote the square $\{-n, -n+1, ..., n\} \times \{-n, -n+1, ..., n\}$; let $C_n = C_+(\partial\Lambda_n)$ and let p_c denote the critical value for independent-site percolation in $\mathbb{Z}^2$. For any $p < p_c$, there is some positive $\bar{B}(p)$ so that for $-\bar{B}(p) < \bar{b} \leqslant 0$,

$$|\Lambda_n|^{-1} \log \langle e^{-\bar{b}|C_n|} \rangle_p \to 0 \qquad \text{as} \quad n \to \infty \tag{4.8}$$

and for any fixed **r**,

$$\langle e^{-\bar{b}|C_n|} 1_{\mathbf{r} \in C_n} \rangle_p \to 0 \qquad \text{as} \quad n \to \infty \tag{4.9}$$

Remarks. Since the averages in (4.8) and (4.9) are clearly increasing in p, it follows that $\bar{B}(p)$ can be chosen to be decreasing. The proposition and proof remain valid if Λ_n is replaced by a sequence of regions tending to $\mathbb{Z}^2$ such that $|\partial\Lambda_n| = O(\text{dist}(\mathbf{0}, \partial\Lambda_n))$. For the validity of (4.8), one only needs $|\partial\Lambda_n|/|\Lambda_n| \to 0$.

Proof of Proposition 4.3. Our argument will be based on the fact[15,16] that $C(\mathbf{0})$, the plus cluster at the origin (in all of $\mathbb{Z}^2$), has

$$P_p(|C(\mathbf{0})| \geqslant k) \leqslant e^{-\alpha k} \tag{4.10}$$

for some $\alpha = \alpha(p) > 0$ when $p < p_c$. We begin with the bounds

$$\begin{aligned} \langle e^{-\bar{b}|C_n|} 1_{\mathbf{r} \in C_n} \rangle &\leqslant e^{|\bar{b}|un} P_p(\mathbf{r} \in C_n) + \langle e^{-\bar{b}|C_n|} 1_{|C_n| > un} \rangle_p \\ P_p(\mathbf{r} \in C_n) &\leqslant P_p(|C(\mathbf{r})| \geqslant n - |\mathbf{r}|) \\ \langle e^{-\bar{b}|C_n|} 1_{|C_n| > un} \rangle_p &\leqslant e^{-tun} \langle e^{(|\bar{b}| + t)|C_n|} \rangle_p \end{aligned} \tag{4.11}$$

where $u > 0$ will be specified later. To control $|C_n|$, we note that by expressing it as a union of distinct clusters in Λ_n which reach $\partial\Lambda_n$, each of which is smaller than $C(\mathbf{r})$ for some $\mathbf{r}$ in $\partial\Lambda_n$, it is easily seen that one has the stochastic inequality

$$|C_n| \prec \sum_{i=1}^{|\partial\Lambda_n|} Y_i \tag{4.12}$$

where $Y_1, Y_2,...$ are independent random variables with the same distribution as $|C(\mathbf{0})|$. Thus, by (4.10),

$$\langle e^{-\bar{b}|C_n|} \rangle_p \leqslant e^{8nf(|\bar{b}|)} \tag{4.13}$$

and

$$\langle e^{-\bar{b}|C_n|} 1_{\mathbf{r} \in C_n} \rangle_p = O(e^{(|\bar{b}|u - \alpha)n} + e^{[8f(|\bar{b}| + t) - tu]n}) \tag{4.14}$$

where

$$e^{f(t)} = \langle e^{t|C(\mathbf{0})|} \rangle_p < \infty \qquad \text{for} \quad t < \alpha \tag{4.15}$$

Clearly (4.8) follows if $|\bar{b}| < \alpha$. Since $f(t) = 0 + f'(0)t + O(t^2)$, we may choose

$$u > 8f'(0) = 8E(|C(\mathbf{0})|) \tag{4.16}$$

and then t sufficiently small to that $8f(t) - tu < 0$. Then we have for small enough $|\bar{b}|$ that both $|\bar{b}|u - \alpha$ and $8f(|\bar{b}| + t) - tu$ are negative. This yields (4.9) as desired.

Combining the three last propositions, we have the following result.

Proposition 4.4. Let Λ_n be as in Proposition 4.3. There is a function $B(T)$ which is strictly positive for large T; in particular, if

$$T > 4\tau/\log\left[\frac{p_c}{1-p_c}\right] \tag{4.17}$$

such that for $\beta = 1/T$ and $-B(T) < b < 0$, the following are valid as $n \to \infty$:

$$|\Lambda_n|^{-1} \log\langle e^{-\beta b|C_+|}\rangle^*_{\beta,0} \to 0 \tag{4.18}$$

$$\langle |C_+|/|\Lambda_n|\rangle_{\beta,b} \to 0 \tag{4.19}$$

and for any fixed site $\mathbf{s}$,

$$h_{\Lambda_n}(\mathbf{s}) \to +\infty \tag{4.20}$$

in the sense of (4.2).

Proof. We take

$$B(T) = T\bar{B}\left(\frac{1}{1+e^{-4\tau/T}}\right) \tag{4.21}$$

where $\bar{B}(p)$ is as in Proposition 4.3. Then (4.18) and (4.20) follow immediately from the pevious propositions. To obtain (4.19), we note that the left-hand side of (4.18) is a convex function of b which converges to zero on $(-B, 0)$. It follows that its derivative, which is $-\beta$ times the right-hand side of (4.19), also converges to zero on $(-B, 0)$.

Remark. The proof of Proposition 4.3 shows that for the validity of (4.8) [but not necessarily of (4.9)] it suffices to take $\bar{b}$ in $(-\alpha, 0]$, where $\alpha = \alpha(p)$ is given in (4.10). Thus (4.18) and (4.19) will be valid if

$$-b < T\alpha\left(\frac{1}{1+e^{-4\tau/T}}\right) \tag{4.22}$$

This gives an upper bound for the wetting temperature for $b < 0$. From (4.17) and the numerical value[17] $p_c \approx 0.59$, we see that this yields the rather weak bound

$$T_w \leqslant \frac{4\tau}{\log[p_c/(1-p_c)]} \approx 11.0\tau \qquad \text{as} \quad b \to 0- \tag{4.23}$$

This may be contrasted with the lower bound from (3.13),

$$T_w \geqslant T_c(2) \approx 1.13\tau \qquad \text{as} \quad b \to 0- \tag{4.24}$$

Presumably $T_c(2)$ is the correct limiting value, but this has not been rigorously proved. It is not physically meaningful to compare the upper and lower bounds of (4.22) and (3.13) for very large negative b, since there is a physical requirement that $b > -2\tau$ (to ensure stability against detachment from the substrate; see ref. 1).

5. CONCLUSIONS

In our wetting model with Hamiltonian (2.5) or equivalently (2.7), the free energy as a function of $T = 1/\beta$ and $b = \varepsilon_1 - \tau$ is

$$f(T, b) = f(T, 0) - b - T \lim_{n \to \infty} |\Lambda_n|^{-1} \log\langle e^{-\beta b |C_n|}\rangle^*_{\beta,0} \tag{5.1}$$

Here $f(T, 0)$ is the Onsager free energy for the Hamiltonian (2.7) with $b = 0$, $\langle \cdot \rangle^*_{\beta,0}$ is the thermal average for this zero field plus b.c. Ising model in the region $\Lambda_n \subset \mathbb{Z}^2$, $C_n = C_+(\partial\Lambda_n)$ is the zero height (or dry) portion of Λ_n and we take Λ_n to be the sequence of squares $\{-n,..., n\} \times \{-n,..., n\}$.

In ref. 2, it was shown that

$$f(T, b) = f(T, 0) - b \qquad \text{for} \quad b \geqslant 0 \tag{5.2}$$

Thus, as the wetting transition curve

$$T_w(b) = T_c(2) \qquad \text{for} \quad b \geqslant 0 \tag{5.3}$$

is approached from *either* the partially wet phase $[T < T_c(2)]$ or from the interior of the wet phase $[T > T_c(2)]$, there is a thermodynamic singularity in the free energy behavior. Both the independence of T_w on b and the singularity from the high-temperature side are not expected for ordinary wetting transitions.[3] The results from the last two sections show that neither of these phenomena occurs for $b < 0$. In order to state this conclusion as a formal proposition, we first define (for $b < 0$)

$$T_w(b) = \inf\{T' \colon \lim_{n \to \infty} \langle A_1/|\Lambda_n|\rangle_{\beta,b} = 1 \qquad \text{for all} \quad \beta < 1/T'\} \tag{5.4}$$

Proposition 5.1. For $b < 0$,

$$T_c(2) < T_c(2)\left(1 - \frac{b}{4\tau}\right) \leqslant T_w(b) < \infty \tag{5.5}$$

Furthermore,

$$f(T, b) = f(T, 0) - b \qquad \text{for} \quad b < 0 \quad \text{and} \quad T \geqslant T_w(b) \tag{5.6}$$

Proof. (5.4) follows immediately from the results of Sections 3 and 4 and the fact[2] that for $b = 0$ and $T < T_c(2)$,

$$\lim_{n \to \infty} \langle A_1/|A_n|\rangle_{\beta,b} = 1 - \lim_{n \to \infty} \langle |C_n|/|A_n|\rangle_{\beta,b} = 1 - P_{\beta,0}(H(\mathbf{0}) = 0) < 1 \tag{5.7}$$

[here $H(\mathbf{0}) = \lim h_{A_n}(\mathbf{0})$]. To obtain (5.6), we claim that it suffices to show that if β and $b_0 < 0$ are such that

$$\lim_{n \to \infty} \langle |C_n|/A_n\rangle_{\beta,b_0} = 0 \tag{5.8}$$

it follows that

$$\lim_{n \to \infty} |A_n|^{-1} \log\langle e^{-\bar{b}|C_n|}\rangle^*_{\beta,0} = 0 \qquad \text{for} \quad \beta b_0 < \bar{b} < 0 \tag{5.9}$$

To see why this suffices, note first that it would imply that $T_w(b)$ is a nondecreasing function of $-b$ and second that, by continuity of f, we then need only prove (5.6) in the interior of $\{b < 0,\ T \geqslant T_w(b)\}$. By convexity, for $\beta b_0 < \bar{b} < 0$,

$$0 \leqslant \log\langle e^{-\bar{b}|C_n|}\rangle^*_{\beta,0} \leqslant |\bar{b}| \left.\frac{d}{dt} \log\langle e^{t|C_n|}\rangle^*_{\beta,0}\right|_{t = \beta|b_0|} = |\bar{b}| \langle |C_n|\rangle_{\beta,b_0} \tag{5.10}$$

Thus, (5.8) implies (5.9), as desired, which completes the proof.

The formula (5.6) for the free energy ceases to be valid in the $b < 0$, partially wet region of the phase diagram. This is because, by standard convexity arguents, $\lim\langle A_1/|A_n|\rangle_{\beta,b}$ must fall in between the two one-sided derivatives, $-(\partial f/\partial b)(T, b-)$ and $-(\partial f/\partial b)(T, b+)$; hence the limit cannot be strictly below 1 if (5.6) is valid. The next proposition points out in particular that $\partial f/\partial b$ has a jump discontinuity along the line $b = 0$, $T < T_c(2)$. On the $b > 0$ side of this line, even though the surface heights remain finite (and we thus have called this region partially wet), it differs from the $b \leqslant 0$ side of the line by the presence of a monolayer covering the entire substrate.

Proposition 5.2. Along the line $b = 0$, $T < T_c(2)$,

$$-\frac{\partial f}{\partial b}(T, 0+) = 1, \qquad -\frac{\partial f}{\partial b}(T, 0-) < 1 \tag{5.11}$$

Proof. The derivative at 0+ follows from (5.2). By our previous discussion and the results of Section 3 of ref. 2, we have

$$-\frac{\partial f}{\partial b} T(0, -) \leqslant \lim_{n\to\infty} \langle A_1/|A_n| \rangle_{\beta,0} = 1 - P_{\beta,0}(H(\mathbf{0}) = 0) \tag{5.12}$$

where $H(\mathbf{0})$ denotes $\lim h_{A_n}(\mathbf{0})$. The probability of zero height, $P_{\beta,0}(H(\mathbf{0}) = 0)$, is just the plus-cluster percolation density, which is strictly positive[8] for $T < T_c(2)$.

We conclude this section with a critical exponent inequality which follows from Proposition 3.5. We define the surface height order parameter,

$$\theta(T, b) = \sup_{A} \langle h_A(\mathbf{0}) \rangle_{\beta,b} \tag{5.13}$$

and then critical exponents q and q' by assuming

$$\theta(T, 0) \sim (T_c(2) - T)^{-q} \qquad \text{as} \quad T \uparrow T_c(2) \tag{5.14}$$

$$\theta(T_c(2), b) \sim |b|^{-q'} \qquad \text{as} \quad b \uparrow 0 \tag{5.15}$$

In ref. 2, it was shown that $q \leqslant 1/8$, or more precisely,

$$\theta(T, 0) \leqslant \text{const} \cdot (T_c(2) - T)^{-1/8} \qquad \text{for} \quad T < T_c(2) \tag{5.16}$$

Proposition 5.3. $q' \leqslant q \leqslant 1/8$, or more precisely,

$$\theta(T_c(2), b) \leqslant \theta\left(\frac{T_c(2)}{1 - b/(4\tau)}, 0\right) \leqslant \text{const} \cdot \left(\frac{|b|}{4\tau + |b|}\right)^{-1/8} \qquad \text{for} \quad b < 0 \tag{5.17}$$

Proof. This is an immediate consequence of Proposition 3.5 by taking

$$4\tau\beta/(4\tau - \beta) = 1/T_c(2) \qquad \text{and} \qquad g = h_A(\mathbf{0})$$

Remark. One should consider exponents $q(b)$ and $q'(b)$ defined all along the transition curve $T_w(b)$ by

$$\theta(T, b) \sim (T_w(b) - T)^{-q(b)} \qquad \text{as} \quad T \uparrow T_w(b) \tag{5.18}$$

$$\theta(T_w(b), b') \sim (b - b')^{-q'(b)} \qquad \text{as} \quad b' \uparrow b \tag{5.19}$$

Our previously defined q and q' are of course just $q(0)$ and $q'(0)$. For $b, b' > 0$, $\theta(T, b) = 1 + \theta(T, 0)$, while $\theta(T_c(2), b') = \infty$.[2] Hence, for $b > 0$, $q'(b)$ is undefined (or else it is $+\infty$), while $q(b) = q(0)$. Unfortunately, we have no results to report on these critical exponents for $b < 0$.

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