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Surface deconstruction and roughening in the multiziggurat model of wetting

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We relate a random surface model appropriate for wetting in three dimensions to first-passage percolation for the planar Ising model. This establishes that the macroscopic drop, sitting on a rectangular substrate in the completely wet phase, adopts the shape of a pitched roof. It also suggests that fluctuations about this mean shape are not logarithmic, but rather have a roughness exponent $\chi=\frac{1}{3}$.

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Burton, Cabrera, and Frank [1] (hereafter BCF) suggested that an interface established between coexisting, oppositely magnetized, phases in a $d=3$ Ising ferromagnet should undergo a phase transition at $T_c(2)$, the $d=2$ critical temperature, because the interfacial spins would be acted on by equal and opposite Curie-Weiss mean fields coming from the remaining spins above and below the interface respectively, thereby removing the bulk influence entirely at this level of approximation. Thus the interfacial free energy would be expected to display a logarithmic specific heat divergence. Extremely compelling evidence has accrued [2] for an interfacial *roughening* phase transition at, or above [3] the $d=2$ critical temperature, but since the free energy should then have an isolated essential singularity as a function of temperature, this would place the Ising interface in a different universality class from that of the BCF transition. It is therefore of considerable interest to find that an interface model [4–6], of potential relevance to wetting as it happens, does exist which has BCF behavior for some range of values of substrate interaction parameter.

BCF made few geometrical claims about their transition. A number of results have been established for our model in the low-temperature phase and wetting has been proved above the transition, but without obtaining detailed geometric behavior of the wetting film. In this communication, we shall show that our random surface, suspended over a rectangular substrate of length scale L, adopts the shape of a pitched roof with volume of order L^3 unlike the usual wetting case, with volume of order $L^2\ln L$ [2]. In addition, the square of the height difference fluctuations about their mean shape value for points in the same roof facet, but separated by a distance r, diverges; furthermore, we give good reasons why this divergence is a power law in r rather than the Kosterlitz-Thouless logarithmic behavior. These results are obtained by an association of the *static* geometry of a random surface with the stochastic process of first-passage percolation [7,8].

A brief review of our model will now be given, followed by some facts gleaned for the most part from the probability literature about first-passage percolation. The volume bounded by our random surface is assembled out of unit cubes (representing molecules and following Kossel and Stransky [9]); these are stacked up vertically over cells of a unit-sided quadratic lattice to form a planar histogram. Thus we have a solid-on-solid (SOS) model with non-negative integer-valued heights $h(x)$ for $x\in\mathbb{Z}^2$. Such a surface can also be described in terrace-ledge-kink (TLK) [1] terminology by specifying the surfaces of constant height as terraces which are bounded by closed polygonal paths on crossing which the height must jump. These closed paths are the ledges which must contain bends (in order to close); these are kinks.

We obtain a mapping from the three-dimensional (3D) surfaces to a 2D classical statistical mechanical model by specifying suitable energetics and by restricting the height variables as follows: (i) Whenever $|x-y|=1$, $h(x)-h(y)=0,\pm 1$. (ii) The extent of the random surface model on the substrate is denoted $\Lambda\subset\mathbb{Z}^2$; it is defined by requiring $h(x)=0$ for all $x\notin\Lambda$. We shall usually take $\Lambda=\Lambda_L$, an $a_1L\times a_2L$ rectangle centered on the origin and parallel to the coordinate axes with a_1,a_2 fixed as $L\to\infty$. (iii) From any $x\in\Lambda$, there is a path to the boundary $\partial\Lambda$ along which the height does not increase. Thus local height minima are excluded and, with this, the "fingering" often considered crucial for wetting [10]. In particular, we allow adatoms on the terraces, but not vacancies; this asymmetry establishes a crucial distinction from the usual SOS models. However, more than one height local maximum is permitted, in a way which is essential for a correct description of partial wetting. We shall call this the multiziggurat (MZ) model. For a more physical, but lengthier definition in terms of molecular rafts, see [4] or Appendix B of [5]. Antecedents of the MZ model are discussed at the end of the paper. We explain next how the MZ model can be mapped into the planar Ising model.

Consider an auxiliary planar Ising model with spins $\sigma(y)=\pm 1$ located at the sites of $\mathbb{Z}^2$. With Λ defined as above, we take $\sigma(y)=+1$ for all $y\notin\Lambda$. The crucial result of the configurational restrictions is that the terraces become parallel-spin clusters of the Ising model and the ledges become Peierls contours. The relationship is completed by specifying the energy $E_\Lambda(\Gamma)$ of a configuration Γ:

$$E_\Lambda(\Gamma)=\tau L(\Gamma)+(\tau-\varepsilon)A_0(\Gamma). \tag{1}$$

Here τ is the surface tension of the upper surface defined by the histogram. Its area has a contribution from plaquettes with normals parallel to the substrate. Because of restriction (i) above, this is the total length $L(\Gamma)$ of the ledges. The term $A_0(\Gamma)$ is the area of plaquettes in the surface with normals perpendicular to the substrate. By virtue of the model, this is the contact area with the substrate; $-\varepsilon A_0(\Gamma)$ is a contact interaction of the droplets with the substrate. Equation (1) goes over into the Ising expression

$$E_\Lambda(\Gamma)=\tau\sum_{|x-y|=1}[1-\sigma(x)\sigma(y)]/2+b\sum_{x\in\Lambda}[\mu(x)-1]. \tag{2}$$

In the last term on the right-hand side, $b=\varepsilon-\tau$ and $\mu(x)=1$ if there is a path from x to some y outside of Λ along which there are no spin flips [if there is no such path, $\mu(x)=0$]. In spin terminology, the last term is a magnetic field applied only to spins in the plus cluster of the boundary.

Elsewhere [4–6], we have described results about the phase transitions in this model which follow from Ising model percolation theory. They are summarized in Fig. 1. Here we focus on recent developments in first-passage percolation [11–13].

The first-passage problem will be described here for percolation in the plane. A non-negative random variable $\tau(e)$, called a passage time, is assigned to each unit-length edge e, equivalently nearest-neighbor bond, in $\mathbb{Z}^2$. The passage time for a contiguous collection, or path p, of bonds $e_1,\dots,e_n$ is defined by

$$T(p)=\sum_1^n \tau(e_j). \tag{3}$$

The travel time between vertices u and v is then appropriately given by

$$T(u,v)=\min\{T(p):\ p \text{ is a path from } u \text{ to } v\}. \tag{4}$$

We mention immediately the connection with the random surface problem: suppose we take its Ising equivalent and for $e=\langle x,y\rangle$ define

$$\tau(\langle x,y\rangle)=[1-\sigma(x)\sigma(y)]/2. \tag{5}$$

Then $T(u,v)$ is the minimum number of Peierls contours crossed in going from u to v and

$$h_\Lambda(x)=\min\nolimits_{y\in\partial\Lambda}T(x,y), \tag{6}$$

where the Ising model has $\sigma(y)=+1$ for all $y\notin\Lambda$.

Returning to the general model, define the region $B(t)$ attainable from the origin in time t or less in terms of

$$\tilde{B}(t)=\{x\in\mathbb{Z}^2:\ T(0,x)\le t\} \tag{7}$$

and fill in for convenience between the quadratic lattice points to get

$$B(t)=\{x+y:\ x\in\tilde{B}(t),\ y\in U\}, \tag{8}$$

where $U=\{(x_1,x_2):\ |x_j|\le 1/2\}$.

Richardson's theorem and its extensions [14] relate the existence of an asymptotic shape for $B(t)$ to the strict positivity of the time constant μ defined by

$$\mu=\lim_{n\to\infty}T(0,(n,0))/n. \tag{9}$$

It has been shown [11] that $\mu>0$ (strictly) is guaranteed if $\langle|C_0|^{4+\delta}\rangle$ is finite for some $\delta>0$, where $|C_0|$ is the number of sites in C_0, the parallel-spin cluster containing the origin. Higuchi [15] has proved that this condition is satisfied whenever $T>T_c(2)$. An alternate proof (also based on [15]) that $\mu>0$ appears in [16]. The shape theorem in a version of Derrienic [17] asserts that if $\mu>0$, there exists a nonrandom, bounded, convex set $B_0\subset\mathbb{R}^2$ such that with probability 1, given any $\epsilon>0$,

$$(1-\epsilon)B_0\subset t^{-1}B(t)\subset(1+\epsilon)B_0 \tag{10}$$

for all large enough t. If $\mu=0$, $B(t)$ grows faster than linearly. The asymptotic scaled shape B_0 has a boundary ∂B_0 compatible with convexity lying between a square S_1 with vertices at $(0,\pm\mu^{-1})$ and $(\pm\mu^{-1},0)$ and a square S_2 with vertices at $\sqrt{2}\mu^{-1}(\pm1,\pm1)$. Evidently S_1 is inscribed in S_2. It is intuitively clear, and even correct, that to construct an asymptotic shape function for the surface height $h_L(x)$ above the large rectangular substrate Λ_L with x far from $\partial\Lambda_L$, we dilate a B_0 centered on a fixed x' in the fixed rectangle Λ_L/L until it just touches the boundary. As (7)–

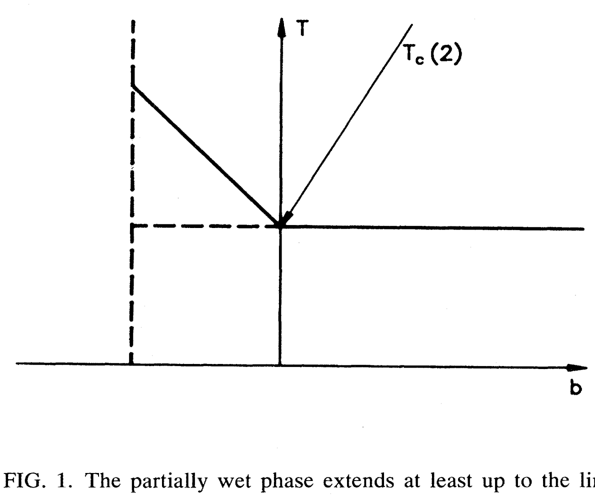

FIG. 1. The partially wet phase extends at least up to the line $\{T=T_c(2)(1-b/[4\tau]),\ b<0\}$ and the wet phase extends strictly into the region $\{T>T_c(2),\ b<0\}$. The free energy approaches the wetting transition curve analytically from the wet side. It has a discontinuous b derivative at the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

(10) indicate, the dilation factor $H(x')$ is then the limit of $h_L(Lx')/L$, and a simple roof shape follows. The roof has four facets, corresponding to the four boundaries of the rectangle. The facets are triangular pieces of linear height functions with gradients $(0,\pm\mu)$ and $(\pm\mu,0)$.

We have been reticent on two points: firstly, the first-passage Ising percolation of Refs. [11,12] refers to an infinite lattice, not to Λ with all boundary spins up. This cannot be easily dismissed by configurationwise consideration of spin states; a stochastic domination argument is simpler. After discussing this briefly, we shall then look into the second point, namely what happens if $b\neq 0$, but we are still in the wet region.

Going back to (6), let $h_\Lambda^\infty(x)$ be the minimum number of Peierls contours crossed to reach $\partial\Lambda$ from x, within the infinite area Ising system. In a distributional sense, $h_\Lambda(x)$ is bounded between $h_\Lambda^\infty(x)-2$ and $h_\Lambda^\infty(x)+1$. To justify this [13], first note that two distinct roles are played by the $+$ boundary conditions on $h_\Lambda(x)$: (a) they determine the distribution of spins inside Λ; and (b) they determine whether a change in height occurs on the last edge of a path from Λ to $\partial\Lambda$. Suppose in replacing $h_\Lambda(x)$ by $h_\Lambda^\infty(x)$ we first do this in respect of (a). By the Fortuin-Kasteleyn-Ginibre (FKG) inequalities, this decreases the zero-height region and hence increases the heights [5]. If we consider role (b), this can decrease the height by at most 1. The lower bound for $h_\Lambda(x)$ is obtained similarly. The $O(1)$ effects which we get are irrelevant for the shape theorem.

Going back to the second point, if $b>0$ there is a monolayer squeezing out the plus cluster of $\partial\Lambda$. The shape theorem is unchanged. For $b<0$, we expect this to be true as well in the wet phase, but the free-energy result [6] is not strong enough to prove this. More information would be needed about the nature of the zero-height region in Λ hugging the boundary.

Our result shows that the wetting transition in the multiziggurat model is accompanied by a kind of surface reconstruction [18,19] to the roof shape discussed above. Note, however, that the slope of the facets of the roof is μ, which is temperature dependent. Hence we call this a surface deconstruction to distinguish it from the usual case where the slope is determined by boundary conditions. For $b\geqslant 0$ (but *not* for $b<0$ [6]), the specific heat diverges on the high-temperature side (an exact result). It has been suggested that this divergence is associated with a roughening transition [20]. By adapting recent results for first-passage percolation, we see that this is indeed true. The inequalities relating $h_\Lambda(x)$ and $h_\Lambda^\infty(x)$, that allowed us to replace $h_L(x)$ by its counterpart $h_L^\infty(x)$ and obtain the roof shape, also show [13] that the mean square fluctuations, $\mathrm{var}(h_L(x))=\langle[h_L(x)-\langle h_L(x)\rangle]^2\rangle$ and $\mathrm{var}(h_L^\infty(x))$, diverge comparably. But $\mathrm{var}(h_L^\infty(x))$ can be proved to diverge *at least* logarithmically in $\tilde{L}=d(x,\partial\Lambda)$, the distance from x to the boundary of Λ, by essentially the same arguments used for Theorem 4 of [12]:

$$\mathrm{var}(h_L(x))\geqslant A(T)\ln\tilde{L}, \tag{11}$$

where $A(T)>0$ for $T>T_c(2)$.

We suspect strongly, however, that the transition is *not* of Kosterlitz-Thouless type [21,19], for which (11) would be an asymptotic equality. Firstly, at a thermodynamic level, for $b\geqslant 0$ we have a logarithmically divergent specific heat as mentioned above, rather than the essential singularity as found exactly in the body-centered SOS (BCSOS) model [22], which is an example of the Kosterlitz-Thouless (KT) universality class. Secondly, although lacking a complete proof, we argue that $\mathrm{var}(h_L(x))$ should diverge as a power $\tilde{L}^{2\chi}$ with a strictly positive exponent $\chi=\frac{1}{3}$.

To simplify the argument, we suppose that as $L\to\infty$, $x=x(L)$ stays well within one of the four facets (say the eastern one) of the roof. Replacing, as we did above, h_L by h_L^∞, we note that the shape theorem implies that the paths from x to $\partial\Lambda_L$ which cross the minimum number (i.e., h_L^∞) of Peierls contours (we shall call these minimizing paths) end up (with high probability) on the eastern boundary. Let ξ denote the exponent for transverse fluctuations of these minimizing paths, i.e., the smallest value such that the minimizing paths are (with high probability) contained within a strip of width $\tilde{L}^\xi$ about the horizontal straight line from x to the eastern boundary. A simple heuristic argument [23] gives $\xi=(1+\chi)/2$ [24]. It is generally believed [24,23] but not proved, that $2\chi=\xi$. This would follow if, locally, the boundary of $B(t)$ behaved like an ordinary random walk. These two identities yield the well-known values $\chi=1/3$ and $\xi=2/3$ for growing interfaces, polymers in random environments, etc. [24,23]. We see no reason why the replacement of an independent random environment by an Ising environment should change the universality class. Hence we expect that $\chi=1/3$ is also the correct value for height fluctuations in the MZ model.

In the absence of a rigorous proof that $\chi=\frac{1}{3}$, it would still be of interest to prove that $\chi>0$ since that would differentiate from the KT class logarithmic divergence. The current status is as follows. An extension of Theorem 5 of [12] yields the inequality, $\chi\geqslant(1-\xi)/2$, of Wehr-Aizenman type [25]. To show that $\xi\leqslant\frac{3}{4}$ and thus $\chi\geqslant\frac{1}{8}$, as in the independent random environment case [12], one would need to verify in the Ising case two things. First (and somewhat stronger than what has been proved for the independent case), that the boundary of the asymptotic shape B_0 has finite radius of curvature at its intersection with the coordinate axes; second, that $B(t)\sim tB_0+O(t^{(1/2)+\epsilon})$, as was previously shown for independent environments [26].

We conclude the paper with a brief discussion of antecedent models. There appears to be some confusion in the literature between the MZ model described here (as introduced in [4]) and the "wedding cake" model [27] (see Ref. 42 of [28] and also [16]) which is a natural development of the SOS tube model of correlations [29] as follows: Let the normal to the substrate be (0,0,1). We form a pile of cubes as for the SOS model, but with constraints. Let the intersection of the surface of the pile with the plane $z=n+\frac{1}{2}$ (n a nonnegative integer) be P_n (these are the ledges); then (like SOS tubes) each P_n must be a simple closed path which (unlike SOS tubes) encloses the next closed path P_{n+1} (disregarding the z coordinates) with P_0 arbitrary. Thus the wedding cake model of [27] has a surface with a single maximum, which can be a plateau (since the ultimate P_n has no further constraints), and no other local maxima; we therefore suggest that it be renamed the single-ziggurat (SZ) model. As explained above, the MZ model can be mapped into the planar Ising model and hence is largely soluble. The SZ model, however, has no mapping to the Ising model and the nodal analysis techniques employed for SOS tubes are inappropriate; thus the SZ model, in addition to being less physically relevant, has only meager results to date.

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