Wetting of a Disordered Substrate: Exact Critical Behavior in Two Dimensions

G. Forgacs[a]
Service de Physique du Solide et de Résonance Magnétique, Centre d'Etudes Nucléaires de Saclay, 91191 Gif-sur-Yvette Cedex, France

and

J. M. Luck, Th. M. Nieuwenhuizen,[b] and H. Orland
Service de Physique Théorique, Centre d'Etudes Nucléaires de Saclay, 91191 Gif-sur-Yvette Cedex, France
(Received 30 July 1986)

The critical behavior of the wetting transition of a two-dimensional solid-on-solid model with a random substrate is calculated exactly. By resumming of the most divergent diagrams of a field-theoretical version of the model, the disorder is found to be marginal and to lead to logarithmic corrections to the critical behavior of the pure system.

PACS numbers: 68.45.Gd, 64.60.Cn

Under suitable conditions, one of the phases of a multiphase system at coexistence enclosed in a container can form a macroscopically thick film on the wall of the container. When this occurs in a continuous way, a critical wetting transition is said to take place.[1]

The effect of randomness on this transition is the subject of great current interest. Two kinds of randomness have been considered. (i) Impurities in the bulk can change the universality class of wetting in two dimensions, as shown by Kardar[2] and by Lipowsky and Fisher.[3] (ii) Disorder in the short-ranged wall-adatom interaction, i.e., on the substrate, has been considered with use of the Harris criterion[4] and mean-field calculations.[5] It was shown that disorder is irrelevant for more dimensions than two, and marginal in two dimensions (because of the vanishing of the specific-heat exponent α). However, since the specific heat does not diverge at the pure critical point, the effect of the disorder is expected to be quite weak.

The purpose of this paper is to investigate this two-dimensional marginal case and calculate the corrections due to disorder. We are able to find exactly the critical singularities of the restricted solid-on-solid (SOS) model[6] of the wetting problem. The main results of this paper are that (i) the critical temperature of the quenched system is the same as that of the annealed system and (ii) the specific heat develops logarithmic corrections, possibly related to Griffiths singularities,[7] while other observables such as the average distance between the substrate and the interface do not exhibit such singularities.

The method used is the replica trick and an exact resummation of the most divergent diagrams of the weak disorder expansion. The validity of the replica trick has been checked numerically with a very high accuracy.

In the following, we will briefly describe our calculations. A detailed version will be published elsewhere.[8] Our starting point is a discrete SOS[6] model, where a configuration of the interface is characterized by a set of variables h_i, the index $i=1,\ldots,N$ numbers the columns, and h_i is the height of the interface at the ith column with respect to the substrate level $h=0$. The height variables are positive integers, and we further assume that the system is enclosed in a box of height L, so that $h_i=\{0,1,2,\ldots,L\}$.

The SOS model is known not to take into account certain effects such as overhangs or bubbles of one phase inside another. However, it is reasonable to use it to model the wetting transition, especially when the wetting temperature is not too close to the critical temperature.[6]

We use a restricted SOS model in which the interface can wander only by zero or one step between two adjacent columns. The energy of the interface is thus given by

$$E(\{h_i\})=J\sum_{i=1}^{N}|h_{i+1}-h_i|^{\infty}-\sum_{i=1}^{N}u_i\delta(h_i). \qquad (1)$$

The first term accounts for the surface tension in bending of the interface, and the second term represents the effect of the substrate random field. We assume the random field $\{u_i\}$ to be a set of independent random Gaussian variables with mean value u_0 and variance v. It can be shown[8] that the random-field distribution is irrelevant to the critical behavior.

The quenched average of observables is performed by use of the replica trick,[9] which amounts to introducing an additional index $\alpha=1,\ldots,n$ to the height variables. It is a simple matter to show that in the thermodynamic limit, $\overline{Z^n}\approx\Lambda_n^N$, where Z is the partition function, the bar stands for the average over the disorder, and Λ_n denotes the largest eigenvalue of the transfer matrix M_n, which acts in the space of n-

dimensional vectors $(h_1, \ldots, h_n)$:

$$M_n(\{h_\alpha\},\{h'_\alpha\}) = \exp\left[-\beta J \sum_{\alpha=1}^{n} |h_\alpha - h'_\alpha|^\infty + \beta \bar{u} \sum_{\alpha=1}^{n} \delta(h_\alpha) + v\beta^2 \sum_{1\le\alpha<\beta\le n} \delta(h_\alpha)\delta(h_\beta)\right], \tag{2}$$

where $\bar{u} = u_u + \beta v/2$. The quenched free energy is given by $-\beta F = \partial \bar{Z}_n/\partial n|_{n=0}$.

In order to evaluate the largest eigenvalue Λ_n, let us recall how things work in the annealed case, i.e., when the partition function is averaged over the disorder.

This amounts to setting $n=1$ in (2) and it is formally equivalent to the nonrandom case. The matrix M_1 has two sets of eigenstates, namely, a localized one, denoted by $\phi_0(h)$, and a set of nonlocalized ones, denoted by $\phi_q(h)$. The wetting transition takes place at $T = T_w$, where the localization length $\xi = \mu^{-1} \approx (T_w - T)^{-1}$ of the state ϕ_0 diverges. This occurs when $y = (1+2t)/(1+t)$, where $y = \exp(\beta\bar{u})$ and $t = \exp(-\beta J)$.

In the critical region ($\mu \to 0$), on the dry side ($\mu > 0$), the localized eigenstate reads

$$\phi_0(h) = (2\mu)^{1/2} \epsilon_h e^{-\mu h}, \tag{3}$$

where $\epsilon_h = 1$ except for $\epsilon_0 = y^{-1/2}$. The corresponding eigenvalue is given by $\lambda_0 = 1 + 2t + t\mu^2$ and the value of the wave function at the origin is denoted by f_0.

The set of nonlocalized eigenstates is given by

$$\phi_q(h) = (2/L)^{1/2} \epsilon_h \sin q(h - L), \tag{4}$$

with eigenvalue $\lambda_q = 1 + 2t - tq^2$ (for small q).

Equation (4) applied at $h = 0$ implies a quantization condition on the q's, which reads

$$\tan qL = \frac{yt \sin q}{y(1 + t\cos q) - (1 + 2t\cos q)} \tag{5}$$

This equation has $L+1$ positive solutions q, in the interval $[0, \pi]$, and in the thermodynamic limit, we use $L^{-1}\sum_q = \pi^{-1}\int_0 dq$. The wave function at the origin is given (for small q) by

$$f_q = \phi_q(0) = \left[\frac{2}{yL}\,\frac{q^2}{q^2+\mu^2}\right]^{1/2}. \tag{6}$$

These results imply a discontinuous specific heat and that the average distance $\langle h \rangle$ between the substrate and the interface diverges as $1/(T_w - T)$.

It will be useful for the quenched case to define an effective Hamiltonian H_0 by the relation $M_1 = (1+2t)\exp(-H_0)$. In terms of the eigenstates and eigenvalues of M_1, the Hamiltonian reads (for small q and small μ)

$$H_0 = -\gamma\mu^2 |\phi_0\rangle\langle\phi_0| + \gamma \textstyle\sum_q q^2 |\phi_q\rangle\langle\phi_q|, \tag{7}$$

where $\gamma = t/(1+2t)$.

It will be shown in a forthcoming paper[8] that the exact critical behavior of the quenched system is given by the largest eigenvalue of the many-body Hamiltonian

$$H = \sum_\alpha H_{0\alpha} - \sum_{\alpha<\beta} V_{\alpha\beta}, \tag{8}$$

where $H_{0\alpha}$ is the same Hamiltonian as (7), with an additional replica index α, and $V_{\alpha\beta}$ is the interaction term in Eq. (2). The n particles labeled by α are to be considered as distinguishable particles, since they are not constrained to any symmetrization condition *a priori*. However, since the Hamiltonian H is totally symmetric, it is well known that its ground state has the same property, i.e., it is a bosonic state.

We may thus consider the bosonic second-quantized representation of H, denoted by H_b:

$$H_b = -\gamma\mu^2 \Psi_0^\dagger \Psi_0 + \sum_q \gamma q^2 \Psi_q^\dagger \Psi_q - \frac{1}{2} \sum_{\lambda\mu\nu\rho} (\lambda\mu|V|\nu\rho) \Psi_\lambda^\dagger \Psi_\mu^\dagger \Psi_\nu \Psi_\rho, \tag{9}$$

where $\Psi_\lambda^\dagger$ and Ψ_λ denote the creation and annihilation operators of a particle in $|\phi_\lambda\rangle$. It is easy to check that the matrix element of the two-body interaction V (which is a diagonal two-body interaction) is given by

$$(\lambda\mu|V|\nu\rho) = g f_\lambda f_\mu f_\nu f_\rho, \tag{10}$$

where $g = 2v\beta^2$.

In order to calculate the ground state energy of H_b, we shall perform a perturbation expansion in powers of g. This is most simply done by using the high-spin trick.[10] The idea is to replace the n-boson system by a system of n fermions which have the same quantum numbers, but have an additional color degree of freedom denoted by σ, which ranges from 1 to n.

Let us consider the fermion Hamiltonian

$$H_f = \sum_{\sigma=1}^{n} \left(-\gamma\mu^2 \Psi_{0\sigma}^\dagger \Psi_{0\sigma} + \sum_q \gamma q^2 \Psi_{q\sigma}^\dagger \Psi_{q\sigma}\right) - \frac{g}{2} \sum_{\sigma,\sigma'=1}^{n} \sum_{\lambda\mu\nu\rho} f_\lambda f_\mu f_\rho f_\nu \Psi_{\lambda\sigma}^\dagger \Psi_{\mu\sigma'}^\dagger \Psi_{\nu\sigma'} \Psi_{\rho\sigma}. \tag{11}$$

It is very easy to show that the Hamiltonians H_f and H_b have the same ground-state energies and wave functions. We treat the interaction in perturbation theory using the Goldstone[11] time-oriented diagrams.

The unperturbed ground state is a Slater determinant where the n particles are in the state $|\phi_{0\sigma}\rangle$, with color $\sigma = 1, \ldots, n$. The ground-state energy is the sum of all vacuum Goldstone diagrams, evaluated with the following rules: (a) A diagram is a set of time-ordered vertices connected by oriented downgoing and upgoing lines. (b) Each downgoing line represents a hole state $|\phi_{0\sigma}\rangle$, with energy $-\gamma\mu^2$, and each upgoing line represents a particle state $|\phi_{q\sigma}\rangle$, with energy γq^2. A line connecting the same vertex is a hole line. (c) Each interaction is represented by a vertex [Fig. 1(a)], with a contribution of $-g$. Each hole line carries a factor f_0^2 and each particle line carries a factor f_q^2. (d) Between any pair of consecutive vertices, there is an energy denominator, equal to the sum of the energies of the upgoing lines minus the sum of the energies of the downgoing lines. (e) Finally, one must sum over all states λ and color labels σ, and there is a factor -1 for each fermion loop and a factor $\frac{1}{2}$ for each pair of equivalent lines.

In the thermodynamic limit, all sums are replaced by integrals, and, for example, the diagram of Fig. 1(b) is given by

FIG. 1. (a) Diagram for the vertex. (b) A typical vacuum Goldstone diagram.

$$g^2(-1)^2 n^2 f_0^4 \frac{L^2}{\pi^2}\int_0^{\pi} dq_1 \int_0^{\pi} dq_2 \frac{f_{q_1}^2 f_{q_2}^2}{2\mu^2 + q_1^2 + q_2^2}.$$

From rule (e), it is obvious that in the limit $n=0$, only diagrams with a single loop survive, as in the case of polymers.[12]

Let us consider a generic diagram contributing to the ground-state energy E_n. Let us denote the numbers of its hole lines, particle lines, and vertices, respectively, by N_h, N_p, V. There is an obvious topological relation $N_p + N_h = 2V$, and after rescaling of the momenta $q_i = \mu x_i$, the contribution of the graph has the form

$$\Gamma = -(-g)^V \frac{\mu^2}{(2\pi)^{N_p}} \int_0^{\pi/\mu} \prod_{i=1}^{N_p} dx_i \left(\frac{2}{y}\right)^{N_p+N_h} \prod_{i=1}^{N_p} \frac{x_i^2}{x_i^2+1} \prod_{j=1}^{V-1} \left(\alpha \sum_i x_i^2 + \alpha \sum 1\right)^{-1}. \tag{12}$$

When $\mu \to 0$, we see that the critical behavior is determined by the most ultraviolet-divergent diagrams. The superficial degree of divergence of Γ is given by $\delta_\Gamma = N_p - 2(V-1) = 2 - N_h$. If $\delta_\Gamma < 0$, the diagram converges, whereas it diverges if $\delta_\Gamma > 0$. Thus, since for any diagram one has $N_h > 2$, the only divergent diagrams are those with $N_h = 2$, and since they have $\delta_\Gamma = 0$, they are logarithmically divergent. We have thus

$$E_n = -n\gamma\mu^2 + (\text{sum of all ladder graphs of Fig. 2}). \tag{13}$$

Because of the factorized nature of V, these diagrams can be resummed in a geometric series, leading to

$$E_n = -n\gamma\mu^2 - ng\mu^2(2/y)^2(1-gI)^{-1}, \tag{14}$$

where

$$I = \frac{4}{y^2}\frac{1+2t}{t}\frac{1}{\pi^2}\int_0^{\pi} dq_1 \int_0^{\pi} dq_2 \frac{q_1^2}{\mu^2+q_1^2}\frac{q_2^2}{\mu^2+q_2^2}\frac{1}{2\mu^2+q_1^2+q_2^2}. \tag{15}$$

This integral can be evaluated for small μ and yields $I = [2(1+2t)/ty^2\pi]\ln(\mu^{-1})$. Hence, the free energy is given by

$$-\beta F = \ln(1+2t) + [\mu^2 t/(1+2t)][S + 2\pi/\ln(\mu^{-1})], \tag{16}$$

where S is the sum of all nondivergent diagrams.

The $\ln(\mu^{-1})$ singularity also shows up in the specific heat. It is remarkable to note that the nonsingular part depends on g, whereas the logarithmic correction which involves only divergent diagrams is universal and independent of the disorder. Also, the condition of criticality of the quenched system is identical to that of the annealed system, for arbitrary disorder.

The same kind of power counting can be done to show that the average distance $\langle h \rangle$ between the substrate and the interface is not affected by the disorder. In particular, it is not corrected by logarithms.[8]

We have checked our results numerically, by an exact enumeration of disorder configurations of an infinite strip of finite width $N = 1, \ldots, 8$. Indeed, our analysis could be invalidated if the replica trick should

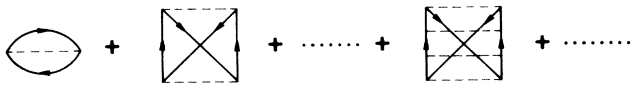

FIG. 2. Sum of ladder diagrams giving the most divergent contribution to the ground-state energy.

fail. We used a two-valued random field, and calculated numerically the largest eigenvalue of the transfer matrix of a strip of width N. This eigenvalue is related to the free energy of a periodic strip of infinite width with period N, and it is obtained by our representing the eigenstate by a mixture of N plane waves and solving for the matching conditions. Observables are then averaged over the 2^N configurations of disorder. The fact that the critical temperature of the quenched system is identical to that of the annealed system is verified with a very high accuracy ($\approx 1/1000$). The logarithmic corrections are not seen, but this is because the region where they are sizable is exponentially small with the disorder.

One of us (Th.M.N.) was supported by the Netherlands Organization for the Advancement of Pure Research (ZWO).

---

[a]Present address: Department of Physics, Clarkson University, Potsdam, NY 13676.

[b]Present address: Institut für Theoretische Physik, Rheinisch-Westfälischen Technische Hochschule, 5100 Aachen, Federal Republic of Germany.

[1]For recent reviews, see D. Sullivan and M. M. Telo de Gama, in *Fluid Interfacial Phenomena,* edited by C. A. Croxton (Wiley, New York, 1985); P. G. de Gennes, Rev. Mod. Phys. **57**, 827 (1985).

[2]M. Kardar, Phys. Rev. Lett. **56**, 2235 (1985).

[3]R. Lipowsky and M. E. Fisher, Phys. Rev. Lett. **56**, 472 (1986).

[4]A. B. Harris, J. Phys. C **7**, 1671 (1974).

[5]G. Forgacs, H. Orland, and M. Schick, Phys. Rev. B **32**, 4683 (1985).

[6]J. M. J. van Leeuwen and H. J. Hilhorst, Physica (Amsterdam) **107A**, 319 (1981).

[7]R. B. Griffiths, Phys. Rev. Lett. **23**, 17 (1969).

[8]G. Forgacs, J. M. Luck, Th. M. Nieuwenhuizen, and H. Orland, to be published.

[9]S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

[10]G. Gentile, Nuovo Cimento **17**, 493 (1940), and **19**, 109 (1942); G. Schubert, Z. Naturforsch. **1**, 113 (1946); B. H. Brandow, Ann. Phys. (N.Y.) **64**, 21 (1971).

[11]See, for example, A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw-Hill, New York, 1971).

[12]P. G. de Gennes, Phys. Lett. **38A**, 339 (1972).