Disorder-induced first-order wetting transitions in two dimensions

1988 J. Phys. A: Math. Gen. 21 L567

(http://iopscience.iop.org/0305-4470/21/10/007)

J. Phys. A: Math. Gen. **21** (1988) L567-L571. Printed in the UK

LETTER TO THE EDITOR

Disorder-induced first-order wetting transitions in two dimensions

Th M Nieuwenhuizen

Institut für Theoretische Physik A, Rhein.-Westf. Technische Hochschule Aachen, Templergraben 55, 5100 Aachen, Federal Republic of Germany

Received 20 January 1988

Abstract. The wetting transition of a two-dimensional system with short-range forces is studied in the presence of disorder, fully correlated in the direction of the substrate. In a solid-on-solid description the row-to-row transfer matrix is of the same type as in random one-dimensional systems. Therefore the substrate bound state is still localised when it becomes degenerate with a bulk state. This results in an unusual first-order wetting transition. The corresponding wetting temperature varies from sample to sample.

A wetting transition takes place in a binary mixture at coexistence if a macroscopically thick layer of one of the phases coats the wall of a container. This transition may be continuous or first order. In a three-dimensional system with either short-range or long-range forces both types may occur. It is believed, however, that in two-dimensional systems with short-range forces the transition is always continuous (Fisher 1985). Kroll and Lipowsky (1983) have even shown that it remains continuous when the wall potential $V(z)$, apart from an attractive short-range part, has an attractive tail which decays faster than $1/z^2$ for large z; when it decays slower than $1/z^2$ the transition becomes first order when the tail is repulsive and it is continuous when the tail is attractive. The intermediate situation, where $V(z) = -W/z^2 + \text{short-range part}$, has three different regimes: (A) an infinite-order transition for $0 < W_c \leqslant W$; (B) a continuous transition with exponents depending parametrically on W for $W_u \leqslant W < W_c$ with $W_u < 0$; (C) a first-order transition with complete breakdown of scaling for $W < W_u$ (see Lipowsky and Nieuwenhuizen (1988) and references therein).

The presence of uncorrelated randomness in the bulk (Kardar 1985, Lipowsky and Fisher 1986) or in the substrate (Forgacs *et al* 1986, 1988a) affects the critical properties of the transition but keeps it continuous. First-order transitions do occur in two-dimensional systems when the interface may jump to the other wall of the container (Chalker 1981) or to a widely separated line with additional attractions (Forgacs *et al* 1988b). But if this line contains random impurities, the first-order transition may be driven to second order (Forgacs and Nieuwenhuizen 1988).

It is the purpose of the present work to show that first-order transitions also occur in two-dimensional systems with short-range forces, if one assumes the presence of disorder which is fully correlated in the direction of the wall. We shall consider the restricted solid-on-solid (RSOS) model, where the interface is described by its integer height variable $z_i \geqslant 0$ above the wall position labelled by $i = 1, \ldots, N$, and where jumps

larger than unity are forbidden (they cost infinite energy). The most general Hamiltonian that we shall consider is

$$H = \sum_{i=1}^{N} (J|z_i - z_{i+1}| - u\delta_{z_i,0} + v(z_i) + hz_i). \tag{1}$$

Here J describes the surface tension, u is the wall potential, the set $\{v(z);\ z \geqslant 1\}$ describes bulk disorder and h is the difference in chemical potential between the two phases ($h = 0$ in coexistence). We shall consider the situation where disorder is fully correlated in the direction of the wall and uncorrelated in the direction perpendicular to the wall, i.e. we assume that the $v(z)$ are independent random variables. The binary case, $v(z) = 0$ with probability q or $v(z) = v_0 > 0$ with probability $p = 1 - q$, could model a crystal cut under an angle $\vartheta = \tan^{-1} p$, where steps are perfectly straight and have random distances with average $1/p$, the energy cost for the interface to cross a step being v_0. The partition sum of this model involves the Nth power of the tridiagonal transfer matrix

$$\begin{aligned} T_{z,z'} &= \exp(-\beta v(z) - \beta hz)(\delta_{z,z'} + \gamma\delta_{z,z'+1} + \gamma\delta_{z,z'-1}) \qquad (z \geqslant 1) \\ T_{0,z'} &= \exp(\beta u)(\delta_{0,z'} + \gamma\delta_{1,z'}) \end{aligned} \tag{2}$$

with $\gamma \equiv \exp(-\beta J)$. The free energy is $f = -T \ln \lambda_{\max}$ where $\lambda_{\max}$ is the largest eigenvalue of (2). The system (2) actually is similar to a random chain problem, about which a lot is known. For instance, with probability one all eigenfunctions are localised exponentially (Furstenberg 1963). We first consider the system at coexistence, $h \equiv 0$. For any temperature and for any value of the surface potential u there is a surface bound state, with eigenvalue λ_μ. Further there is a continuum of bulk states with eigenvalues $(1-2\gamma)\exp(-\beta v_0) \leqslant \lambda \leqslant 1 + 2\gamma \equiv \lambda_B$. In particular, a state with eigenvalue $\lambda = 1 + 2\gamma\cos\varepsilon$ close to λ_B is localised in a strip of width $n \simeq \pi/\varepsilon$ where all $v(z)$ vanish. Narrower strips cannot yield such a large eigenvalue; wider ones allow eigenvalues closer to λ_B. This phenomenon is nothing but the Lifshitz band-edge singularity (Lifshitz 1964). For recent discussions, see Simon (1985) and Nieuwenhuizen *et al* (1986).

The wetting transition occurs when λ_μ crosses λ_B, at a temperature $T = T_w$. Due to disorder the surface bound state remains localised and thus has a finite average height $\langle z \rangle$ at the transition. The bulk state, however, is infinitely separated. Thus the transition is first order. The parallel correlation length $\xi_\parallel$ is inversely proportional to the energy gap $\lambda_\mu - \lambda_B \sim t = T_w - T$ and thus $\nu_\parallel = 1$. This is typical for first-order transitions in two dimensions but different from the usual higher-dimensional situation where $\xi_\parallel$ stays finite at a first-order transition.

It is a property of our model that the critical point varies from sample to sample. The reason is that the free energy of the surface bound state strongly depends on the realisation of disorder close to the substrate. Because disorder is fully correlated, there is no self-averaging in the direction parallel to the wall, as was the case in the systems studied by Kardar (1985), Lipowsky and Fisher (1986) and Forgacs *et al* (1986, 1988a). The bulk state, on the other hand, always has the same free energy $f_B = -T\ln(\lambda_B)$ when the system is infinitely large. Hence, for a given distribution of random bulk potentials $v(z)$ and for fixed values of the surface tension parameter J and wall attraction strength u, there is a distribution of wetting temperatures. In figure 1 we present a plot of this distribution, obtained by numerically calculating T_w for a large number of configurations. We consider a typical situation, namely binary distributions

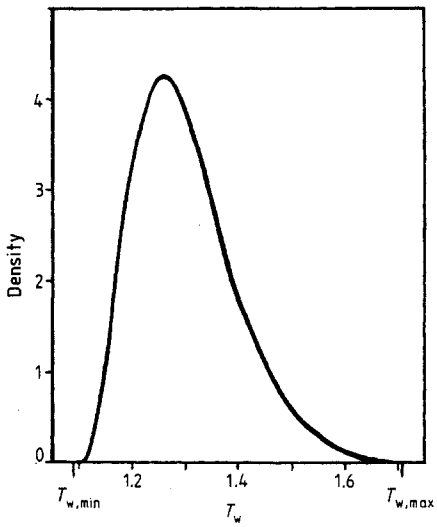

Figure 1. Distribution of possible wetting temperatures, related to different realisations of disorder for different samples of the ensemble of systems with binary disorder. See the text for parameters.

of the $v(z)$ ($v(z)=0$ with probability $q=\frac{3}{4}$ and $v(z)=v_0=0.25$ with probability $p=\frac{1}{4}$) and $J=0.25$, $u=0.4$. The support of the distribution is $T_{w,min}=1.090\,833\leqslant T_w\leqslant T_{w,max}=1.706\,947$, values for systems with all $v(z)$ equal to 0 and v_0, respectively. The density decays exponentially near its lower and upper edges. The reason is that $T_w=T_{w,min}+\Delta T_w$ results for small ΔT_w from realisations of disorder such that the first n rows away from the wall have no disorder ($v(z)=0$ for $1\leqslant z\leqslant n$). The influence of impurities will yield $\Delta T_w\sim\exp(-n\mu)$, where $\mu\sim\Delta T_w$ is the localisation length of the pure system at this temperature. Realising that this situation occurs with probability q^n and eliminating n one finds a behaviour $\exp[-(\text{constant}\times\ln q\ln\Delta T_w)/\Delta T_w]$ for the density near $T_{w,min}$. Near the upper edge one has to replace q by p. Such exponential singularities are typical for Lifshitz singularities.

We next consider the system off coexistence, $h\neq 0$. A bulk state localised in an impurity-free strip of width n at height z will have an additional free energy hz for small h, resulting in $f\approx hz-T\ln(1+2\gamma\cos\pi/n)$. The largest width n of strips without disorder up to height z can be estimated as follows. The probability for occurrence of such a strip involves a factor p^2q^n for finding n successive lines with $v(z)=0$, in between two lines with $v(z)=v_0$, and a degeneracy factor z for the location of its centre. The estimate follows by equating this probability to unity, hence one solves n from $zp^2q^n=1$. Therefore the minimum of f occurs at

$$z\simeq\frac{2\pi^2T\gamma}{(1+2\gamma)(\ln q)^2}\frac{1}{h|\ln h|^3}. \tag{3}$$

This essentially linear behaviour deviates from the mean-field behaviour $z\sim\ln(1/h)$. Note, however, that the width of the interface n is proportional to $\log 1/h$. It thus turns out that this behaviour is dominated by the set of locations z_j of larger and larger widths n_j of impurity-free strips ($n_{j+1}>n_j$ and $z_{j+1}>z_j$). Also this set strongly depends on the actual realisation of disorder in the system.

It is an interesting question whether on changing h the interface changes its average height in a continuous or discontinuous manner, i.e. do layering transitions occur in the system off coexistence? A simple and very general answer to this question can be given if one goes to a continuum description of the eigenvalue equation of the transfer matrix. One thus studies a Schrödinger equation with two degenerate eigenstates, one localised near the substrate and one at infinity. When an arbitrarily small field with potential hz is added, the state at infinity will be lifted to an average height $z_0 \sim 1/h$. But then the Schrödinger particle will *tunnel* from one state to the other. Hence for no value of h there will be non-analytic behaviour, i.e. there will be no layering or prewetting transitions in the system off coexistence. This argument is expected to apply to two-dimensional systems in general. (In systems with uncorrelated disorder one first introduces the replica method for having a site-independent transfer matrix.)

In the model under consideration there will only be real layering transitions in the not very physical limit $v_0 \to \infty$, when it costs infinite energy for the interface to cross an impurity line. For finite v_0 there will still be similar behaviour, but the layers no longer grow in a discontinuous way. However, for small h the transitions will be quite sharp, because the interface makes 'jumps' of the order $1/h$.

The unbound interface is extremely rough. To show this we consider a situation where the starting point of the interface is pinned somewhere in an impurity-free strip of width $n \gg 1$. If the interface stays at this height over a length $2L_\parallel \gg 1$ it will have a free energy $-2TL_\parallel \ln(1+2\gamma \cos \pi/n)$. Another possibility is that it will go to a wider strip (with width $n+\delta n$, $\delta n \ll n$) at distance $L_\perp$ in, say, the first $L_\parallel$ steps, and remain there in the other $L_\parallel$ steps. At finite temperatures the free energy cost can be estimated by the kinetic term $L_\parallel S(L_\perp/L_\parallel)^2$, where S is the stiffness; the free energy gain is $2TL_\parallel \gamma\pi^2 \delta n/n^3$. Thus such a 'kink' is favourable up to a height $L_\perp \sim L_\parallel(\ln L_\parallel)^{-3/2}$. Therefore the interface has a roughness exponent $\zeta \equiv \ln L_\perp/\ln L_\parallel = 1^-$, a result also valid in higher-dimensional systems where disorder is correlated in hyperplanes of constant height above the substrate. (Because $\zeta = 1$ one expects S to vanish slowly with increasing $L_\parallel$; this will not influence the value of ζ, however.) It follows that the interface is much rougher than in the non-disordered situation, where $\zeta = \frac{1}{2}$, and in the problem with uncorrelated randomness, where $\zeta = \frac{2}{3}$ (Huse and Henley 1985). Actually, a similar relation $x \sim t(\ln t)^{-1/2}$ has been discussed for the displacement x as a function of time of a particle diffusing in a random one-dimensional potential (Zel'dovich *et al* 1985, Zhang 1986, Engel and Ebeling 1987, and references therein) resulting in subballistic hopping behaviour as a result of Anderson localisation.

A model as studied here could also describe wetting within monolayers adsorbed on facets of decagonal quasicrystals (see Lipowsky and Henley 1987). The disorder in the bottom layer of such crystals comes from random mismatches of quasiperiodicity and these errors are replicated in higher layers by the growth process. It is necessary, however, that the wetting temperature be low, because we have assumed disorder to be quenched.

Another realisation could apply to crystals of binary alloys, which occur in layers of random thickness. When cut perpendicularly to the direction of the layers, one has crystals with facets consisting of perfectly straight strips of random width. Monolayer wetting transitions on such substrates are expected to be first order, even when the pure compounds would have continuous transitions. The wetting temperature then varies from sample to sample.

We also expect first-order wetting transitions to occur when disorder lines are not perfectly straight, but occur, at least, in two types (this would mean $v = 0$ or v_0 or v_1

in the above model for straight disorder lines). One could think of monolayer wetting on $p * 1$ incommensurate structures (see, e.g., Fisher 1985, Rujan *et al* 1986). In such problems the role of random *positions* of disorder lines in the above model is expected to be played by the random *type* of incommensurability lines.

Our model is closely related to wetting models on pure quasiperiodic structures, such as the Penrose lattice. Henley and Lipowsky (1987) have argued that they may also be described by an equation of the form (2), but now with $v(z)$ being a quasiperiodic function. Two cases have been considered: $v(z)$ is a binary sequence with Fibonacci structure and $v(z)$ is proportional to Harper's potential, $v(z) = -\lambda \cos(2\pi z/\tau)$, where $\tau = (1+\sqrt{5})/2$ is the golden mean. The case $\lambda > \lambda_c$ leads to localised eigenfunctions and a smooth interface. In the presence of an additional short-range wall potential first-order wetting transitions of the same type as discussed above will appear, if λ still exceeds λ_c at T_w. In particular, in such quasiperiodic systems prewetting and layering transitions also do not occur.

In conclusion, we have studied a two-dimensional wetting transition in the presence of disorder which is fully correlated in the direction of the substrate. This leads to a first-order wetting transition. Physical observables, such as the wetting temperature, vary from sample to sample. There are no layering or prewetting transitions. Therefore the phase diagram differs from the possibilities considered by Pandit *et al* (1982).

It is a pleasure to thank Paul Rujan and Reinhard Lipowsky for stimulating discussions, and Reinhard Lipowsky also for a critical reading of the manuscript.

References

Chalker J T 1981 *J. Phys. A: Math. Gen.* **14** 2431
Engel A and Ebeling W 1987 *Phys. Rev. Lett.* **59** 1979
Forgacs G, Luck J M, Nieuwenhuizen Th M and Orland H 1986 *Phys. Rev. Lett.* **57** 2184
—— 1988a *J. Stat. Phys.* to be published
Forgacs G and Nieuwenhuizen Th M 1988 to be published
Forgacs G, Svrakic N M and Privman V 1988b *Phys. Rev.* B **37** 3818
Furstenberg H 1963 *Trans. Am. Math. Soc.* **108** 337
Fisher M E 1985 *Fundamental Problems in Statistical Mechanics VI* (Amsterdam: North-Holland)
Henley C L and Lipowsky R 1987 *Phys. Rev. Lett.* **59** 1679
Huse D A and Henley C L 1985 *Phys. Rev. Lett.* **54** 2708
Kardar M 1985 *Phys. Rev. Lett.* **55** 2235
Kroll D M and Lipowsky R 1983 *Phys. Rev.* B **28** 5273
Kroll D M, Lipowsky R and Zia R K P 1985 *Phys. Rev.* B **32** 1862
Lifshitz I M 1964 *Adv. Phys.* **13** 483
Lipowsky R and Fisher M E 1986 *Phys. Rev. Lett.* **56** 472
Lipowsky R and Henley C L 1987 to be published
Lipowsky R and Nieuwenhuizen Th M 1988 *J. Phys. A: Math. Gen.* **21** 89
Nieuwenhuizen Th M, Luck J M, Canisius J, van Hemmen J L and Ventevogel W J 1986 *J. Stat. Phys.* **45** 395
Pandit R, Schick M and Wortis M 1982 *Phys. Rev.* B **26** 5112
Rujan P, Selke W and Uimin G 1986 *Z. Phys.* B **65** 235
Simon B 1985 *J. Stat. Phys.* **38** 65
Zel'dovich Ya B, Molchanov S A, Ruzmaikin A A and Sokolov D D 1985 *Sov. Phys.-JETP* **62** 1188
Zhang Y C 1986 *Phys. Rev. Lett.* **56** 2113