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## A transfer matrix approach to the 3D wetting and pinning problems

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**Résumé.** — Cet article traite du comportement d'une interface tracée sur un réseau tridimensionnel en présence d'un potentiel de paroi, en géométrie semi-infinie. Ce problème est une modélisation de la transition de mouillage, observée dans des systèmes de mélanges binaires ou de gaz adsorbés. La méthode de la matrice de transfert nous permet d'accéder à des résultats exacts sur des rubans de largeur finie. Nous proposons une façon de les extrapoler, et d'en déduire le diagramme de phases du système infini. Le mécanisme de la transition change lorsque la température d'accrochage croise la température de transition rugueuse.

**Abstract.** — We consider the pinning of an interface on a 3D lattice by an edge potential (semi-infinite geometry). This situation models the wetting transition occurring in such physical systems as binary fluids or adsorbed gases. The transfer matrix method is used to get exact results on strips of finite width; we propose a way of extrapolating them and of deriving the phase diagram of the infinite system. The mechanism of the transition changes when the pinning and roughening temperatures coincide.

### 1. Introduction.

A wall of a container enclosing a binary mixture cooled below its consolute temperature  $T_c$  can be completely wetted by one of the coexisting phases. The formation of a macroscopic film of one phase on the surface of the wall at a certain well-defined temperature  $T_w$  ( $T_w < T_c$ ) is an example of the *wetting transition*. It has been observed recently in various experiments [1].

A theoretical description of this phenomenon, based upon mean field approximation [2], shows that the wetting transition can be either first-order or continuous, according to the values of several physical parameters characterizing the wall (its geometry and its interaction with the system). The case of a continuous phase transition is usually called the *critical wetting*. It has been proved [3] that the mean-field approximation is valid above three dimensions, that is,  $d_c = 3$  is the upper critical dimension for this transition. In three dimensions one can construct some simple effective models [3, 4], in which the main statistical variable is the displacement of the interface separating the two coexisting phases. In these models, the formation of the macroscopic film in the (critical) wetting transition is simply described as the moving away of the interface from the wall. A renormalization-group analysis of the interface displacement models [4]

shows that the critical exponents at the transition point depend continuously on a certain dimensionless parameter  $\omega$  which characterizes the interface.

The wetting transition in binary fluid mixtures can be well described by such continuous models, because the microscopic structure of the fluids in contact with the wall plays no important role in the transition mechanism. This is not always the case in other physical systems (e.g. crystals [5] or adsorbed gases [6]); one should then introduce a lattice to take into account the discreteness on the microscopic level. The phenomenon analogous to (critical) wetting in *lattice models* is not well understood. The critical dimension is still expected to be  $d_c = 3$ : this coincides precisely with the dimensionality at which the roughening transition occurs at a nontrivial temperature  $T_R$  [7]. At low temperatures the discreteness of the system ensures that the *free* interface in an Ising-like system has a finite intrinsic width; above  $T_R$ , on the other hand, the interface position fluctuates on a logarithmic scale, as if it were a continuous surface. These two situations are separated by an infinite order roughening transition, characterized by an essential singularity [7, 8]. It is important to note that this phenomenon does not occur at other dimensions: an Ising interface is always rough ( $T_R = 0$ ) for  $d < 3$ , and always localized ( $T_R = T_c$ ) for  $d > 3$ .

The roughening transition has been studied mostly

in the so-called S.O.S. (solid-on-solid) approximation [8], which discards disconnected parts and overhangs of the interface. The same simplification of the wetting problem leads to the *pinning problem* [9] of a S.O.S. surface placed in an external potential mimicking the attraction of the wall. The two-dimensional problem has been the subject of much effort [9, 10] : in this case the interface going away from the wall always becomes rough; the lattice structure of the model is in fact unimportant. There exist very few results concerning the three-dimensional pinning problem in lattice models. The existence of the transition can be supported using the duality with the Coulomb gas problem [11]; there also exists a rigorous proof [12] that a S.O.S. model with a particular potential exhibits a transition for every value of the depth  $u$  of the potential well.

The aim of this paper is to study the nature of the 3D pinning transition in a discrete lattice model, and in particular to understand the relation between the wetting and roughening transitions. For this purpose we use the finite-size lattice method (strip geometries). In section 2 we introduce the model and describe the method used to solve it on strips of finite width. In particular we show that, despite the broken translational invariance of the problem (in the direction perpendicular to the wall), we can still leave the boundaries of the interface *free*, and thus easily observe its moving away from the wall. In section 3 we give the numerical results for several thermodynamical quantities, and study their behaviour as a function of temperature  $T$  and pinning potential  $u$ . The analysis of these quantities as a function of the strip width  $N$  allows us to postulate a form of the phase diagram for the pinning transition. We do this in section 4, where the method of extrapolation of the (exact) finite-width results to the  $N \rightarrow \infty$  limit is described, together with its difficulties and limitations. In section 5 we give a summary of the results, and give the physical picture of the transition, as obtained from our calculation.

## 2. The model and the method.

We consider a S.O.S. interface model in an external pinning potential, defined by the following Hamiltonian :

$$H = \sum_{\langle i,j \rangle} V(h_i - h_j) + \sum_i U(h_i). \quad (1)$$

An integer height  $h_i$  is attached to each site  $i$  of a square lattice. The nearest-neighbour potential  $V$  ensures the coherence of the interface;  $U$  describes the attraction of the wall and the semi-infinite geometry of the medium. Our choices for  $V$  and  $U$  read :

$$\left. \begin{aligned} V(0) &= 0 & ; & & V(\pm 1) &= 1 \\ V(n) &= +\infty & \text{for } |n| &\geq 2 \\ U(0) &= -u & ; & & U(h) &= 0 \quad \text{for } h \geq 1 \\ U(h) &= +\infty & \text{for } h < 0. \end{aligned} \right\} \quad (2)$$

This model is very similar to that of [12], except for the fact that we allow only height jumps of  $0, \pm 1$ . It has been called the restricted S.O.S. (R.S.O.S.) model in the first paper cited in [9] in the two-dimensional case. This kind of restriction is known not to affect the 3D roughening singularity, as we know from van Beijeren's exactly soluble model [13]. In a previous work [14], one of us has applied the finite-size lattice method to the pure R.S.O.S. model (i.e. without the potential  $U$ ), and our results are in good agreement with the essential singularity expected from universality. In the following, we present the results of the same method applied to the problem defined by (1). This finite-size lattice method was introduced by Nightingale [15] and successfully adapted to many different problems (see [16] and references therein). It consists in *solving exactly* the theory on strips of width  $N$ , by a transfer matrix approach, and in extrapolating the results to  $N \rightarrow \infty$ , for instance by finite-size scaling laws.

Let us first consider our model on a strip of width 1, i.e., describing the pinning transition in two (bulk) dimensions. This case is well understood (see [9]). The partition function at temperature  $T = \beta^{-1}$  reads :

$$Z = \sum_{\{h_i\}} e^{-\beta H} = \sum_{\{h_i\}} T_{h_1 h_2} T_{h_2 h_3} \dots T_{h_L h_1} = \text{Tr } T^L \quad (3)$$

where we use periodic boundary conditions ( $h_{L+1} \equiv h_1$ ), and we introduce the transfer matrix  $T$  defined by :

$$T_{hh'} = \exp[-\beta V(h - h') - \beta U(h')]. \quad (4)$$

The reduced free energy is therefore :

$$f = \beta F = -\ln \lambda, \quad (5)$$

where  $\lambda$  is the largest eigenvalue of  $T$ . Let  $\varphi_h$  be the associated eigenvector; it satisfies :

$$\left. \begin{aligned} \lambda \varphi_0 &= t^{-u}(\varphi_0 + t\varphi_1) \\ \lambda \varphi_h &= \varphi_h + t(\varphi_{h+1} + \varphi_{h-1}) \quad \text{for } h \geq 1. \end{aligned} \right\} \quad (6)$$

The reduced temperature  $t$  is defined by :

$$t = e^{-\beta} = e^{-1/T} \in [0, 1].$$

According to the values of  $t$  and  $u$ , the largest  $\lambda$  can correspond either to a bound state or to an extended one :

a) *bound state* : the unique normalizable solution of (6) is :  $\varphi_h = z^h$  with  $z$  given by :

$$z = \frac{t^{-u} - 1 + [(t^{-u} - 1)(t^{-u} - 1 + 4t^2)]^{1/2}}{2t(1 - t^{-u})}. \quad (7)$$

The associated eigenvalue is related to  $z$  by :

$$\lambda = 1 + t \left( z + \frac{1}{z} \right). \quad (8)$$

These formulae are valid as long as  $z < 1$ , i.e. for

$t < t_p$ , where the pinning temperature is defined by :

$$t_p^u = \frac{1 + t_p}{1 + 2 t_p}. \tag{9}$$

b) *extended states* : they are characterized by a wavenumber  $p : \varphi_h = e^{iph}$ . The corresponding eigenvalue of  $T$  is :

$$\lambda = 1 + 2 t \cos p. \tag{10}$$

The free energy for  $t \geq t_p$  is therefore :

$$-f = \ln \lambda(p = 0) = \ln (1 + 2 t). \tag{11}$$

Note that there exists a finite  $t_p$  for every (positive) value of the potential parameter  $u$ .

The mean transverse position of the interface is given, for  $t < t_p$ , by :

$$\langle h \rangle = \frac{z^2}{1 - z^2}. \tag{12}$$

When  $t$  goes to  $t_p$  from below,  $z$  goes linearly to unity, and therefore we have :

$$\langle h \rangle \sim (t_p - t)^{-v_\perp} \quad \text{with} \quad v_\perp = 1. \tag{13}$$

At the pinning temperature  $t_p$  itself, the free energy and the internal energy  $E$ , defined as :

$$E = \frac{\partial f}{\partial \beta} \tag{14}$$

are continuous. The specific heat :

$$C = -\beta^2 \frac{\partial^2 f}{\partial \beta^2} \tag{15}$$

has a finite discontinuity at  $t_p$ . For fixed  $t$  below  $t_p$ , the largest eigenvalue  $\lambda$  is given by (8), and the second largest one  $\lambda'$  by (10) with  $p = 0$ . The correlations along the interface are dominated by the gap between these two values. A parallel correlation length can be defined by :

$$-\frac{1}{\xi_\parallel} = \ln \frac{\lambda'}{\lambda}. \tag{16}$$

It diverges therefore according to :

$$\xi_\parallel \sim (t_p - t)^{-v_\parallel} \quad \text{with} \quad v_\parallel = 2. \tag{17}$$

All these results, and particularly (13-17) agree with other 2D edge pinning models, with discrete or continuous heights.

Let us now show how these results can be generalized to a strip of arbitrary width  $N > 1$  with periodic transverse boundary conditions : the square infinite lattice is replaced by a strip :  $S = \{ 1, 2, \dots, N \} \times \mathbb{Z}$ , and we identify  $N + 1$  with 1. The dynamical variables are now  $\{ h_1, \dots, h_N \}$  ( $h_{N+1} \equiv h_1$ ). Let us characterize one such collection in the following way :

$$\{ h_1, \dots, h_N \} \leftrightarrow \{ H, A \} \tag{18}$$

where  $H$  is the *smallest* of the  $h_i$ , and  $A$  is a symbol for the internal structure of the  $h_i$ , i.e. for all differences between them. Since our potential  $V$  is truncated, the number  $D(N)$  of internal configuration indices  $A$  is finite as long as  $N$  is finite. Taking into account symmetries of the Hamiltonian, like cyclic ( $h_i \rightarrow h_{i+1}$ ) and reversal ( $h_i \rightarrow h_{N+1-i}$ ) invariances,  $D(N)$  can be considerably reduced to its optimal value, which is given (up to  $N = 7$ ) in table I.

Table I. — Dimension  $D(N)$  of the matrices  $T_M$  and  $W_M$  as a function of  $N$ , the width of the strip.

$N$	$D(N)$
2	2
3	3
4	6
5	10
6	22
7	42

Although the number of degrees of freedom is still infinite in a nontrivial way ( $H = 0, 1, 2, \dots$ ), we have a rather simple method of computing exactly the free energy for arbitrary finite  $N$ . The transfer matrix element between neighbouring configurations  $\{ h_i \}$  and  $\{ h'_i \}$  reads :

$$T_{\{h_i\} \{h'_i\}} = \exp \left\{ -\beta \sum_i [V(h_i - h'_i) + V(h'_i - h'_{i+1}) + U(h'_i)] \right\}. \tag{19}$$

This nonsymmetric formulation of  $T$  is the most appropriate to the following analysis.

The eigenstate equation, generalizing (6), reads :

$$\begin{cases} \lambda \varphi_H^A = \sum_B \sum_{M=-1,0,+1} (T_M)^{AB} \varphi_{H+M}^B & \text{for } H \geq 1 \\ \lambda \varphi_0^A = \sum_B \sum_{M=0,+1} (W_M)^{AB} \varphi_M^B & (H = 0). \end{cases} \tag{20a}$$

$$\tag{20b}$$

The  $T_M$  are three matrices of size  $D(N)$  whose entries are polynomials in  $t$ ; the two matrices  $W_M$  also involve powers of  $t^{-u}$ .

The resolution of (20) consists in two steps :

a) find a basis of solutions of (20a) of the form  $\varphi_H^A = \chi^A z^H$ . In other words, look for  $z$  and  $\chi^A$  such that the following operator :

$$T(z) = T_1 z + T_0 + T_{-1} \frac{1}{z} \quad (21)$$

admits  $\lambda$  as eigenvalue and that the associated eigenvector is  $\chi^A$ . If  $z$  is a solution, then its reciprocal  $1/z$  is also a solution. Let us call  $z_\alpha$  ( $\alpha = 1, 2, \dots, D(N)$ ) the solutions satisfying  $|z_\alpha| \leq 1$  (then  $|z_\alpha| \geq 1$ ) and  $\chi_\alpha^A$  the associated eigenvectors. Note that  $z_\alpha$  and  $\chi_\alpha^A$  are generally complex.

b) select the particular linear combination of these basis vectors which satisfies the boundary equation 20b. It is necessarily of the form :

$$\varphi_H^A = \sum_\alpha C_\alpha \chi_\alpha^A z_\alpha^H. \quad (22)$$

It contains no  $1/z_\alpha$  terms, because they would make the wavefunction grow at infinity. The linear system in the  $C_\alpha$  obtained by putting (22) into (20b) must have a normalizable, and therefore nonzero, solution. Its rank has therefore to be strictly less than  $D(N)$ . This condition reads :

$$\text{Det}_{\alpha, A} \left[ \lambda \chi_\alpha^A - \sum_B \chi_\alpha^B \{ (W_0)^{AB} + (W_1)^{AB} z_\alpha \} \right] = 0. \quad (23)$$

This last formula solves our problem, giving (implicitly)  $\lambda$  as a function of  $t$  and  $u$ . It reduces a nontrivial problem with infinitely many degrees of freedom to finite-dimensional, and therefore numerically tractable, equations. The transfer matrix approach to this problem has a particular interest by itself, since the model on a strip has a phase transition, although it is one-dimensional. Similar cases exist in polymer or lattice animal problems [17].

### 3. Exact numerical results on strips.

**3.1 TRANSITION TEMPERATURES.** — The first quantity we compute is the pinning temperature  $T_p(u)$  for a strip of width  $N$ , generalizing the analytic result (9). The procedure we choose is the following. For fixed  $N$  and  $t$ , determine the largest eigenvalue  $\lambda$  of the operator  $T(z)$  with  $z = 1$  (see (21)). For that  $\lambda$ , find a basis of solutions of (20a) and solve (23) by Newton's method, considering the potential parameter  $u$ , involved in the entries of the  $W_M$  matrices, as the unknown quantity. The convergence of the method is always good (up to  $N = 6$ ); the  $D(N) - 1$  values of  $z$  which are not forced to be unity lay in a circle which gets smaller and smaller when  $N$  is increased.

The variations of  $T_p$  with  $u$  are represented in figure 1, for widths  $N = 1$  to 6. For fixed small  $u$ , the  $T_p(N)$  seem to converge to some finite value; for large enough  $u$ , they seem to diverge. We shall return to this point in next section.

**3.2 THERMODYNAMICAL QUANTITIES.** — The internal energy  $E$  and the specific heat  $C$  are given through formulae 5, 14, 15 as functions of the largest eigenvalues  $\lambda$  of the transfer operator. The situation is completely analogous to the  $N = 1$  case (see sect. 2) :  $t_p$  is the boundary between a bound state and an extended state regime.

For  $t > t_p(u)$ , we have just to consider the largest eigenvalue of  $T(z = 1)$  (see (21)), that we already considered in the last subsection. Thermodynamical quantities are therefore independent of  $u$  in this phase.

For  $t \leq t_p(u)$ , we have to solve (23), considering  $\lambda$  as the unknown. We use Newton method; for each test value of  $\lambda$ , we have to find all the  $z_\alpha, \chi_\alpha^A$ . These quantities are generally complex, and each  $z_\alpha$  is itself determined by Newton's method on the function  $\text{Det} [T(z) - \lambda 1]$ . We have checked (up to  $N = 6$ ) that the mechanism of the transition is the same as for  $N = 1$ , i.e. the fact that the unique bound state disappears continuously into the continuum of extended states. In particular, we never encountered more than one bound state, nor any anomalous variation of the eigenvalue  $\lambda$ .

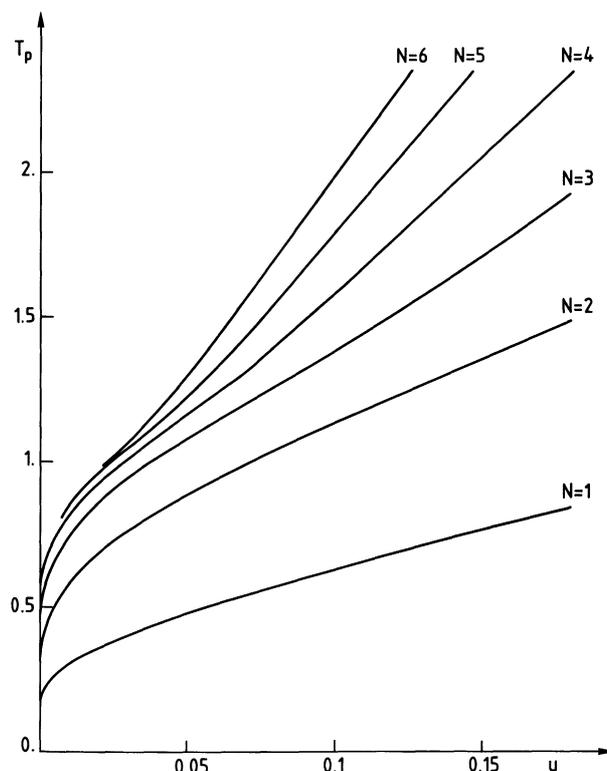


Fig. 1. — Variation of the pinning transition temperature  $T_p$  as a function of the potential parameter  $u$ , on strips of widths  $N = 1$  to 6.

In figures 2, 3 and 4, we present the variations of the specific heat *versus* the reduced temperature  $t$ , for three typical values of the potential parameter  $u$ . The choice of these particular values will be justified in next section, which is devoted to the extrapolation of the data to the 3D system.

In most problems studied by the strip method, the first limitation on the width  $N$  comes from the size of the transfer matrix, which grows exponentially with  $N$ . In our problem, table I shows that the storage of the matrices  $T_M, W_M$  is not at all the first limitation we encounter. The most serious constraint on the

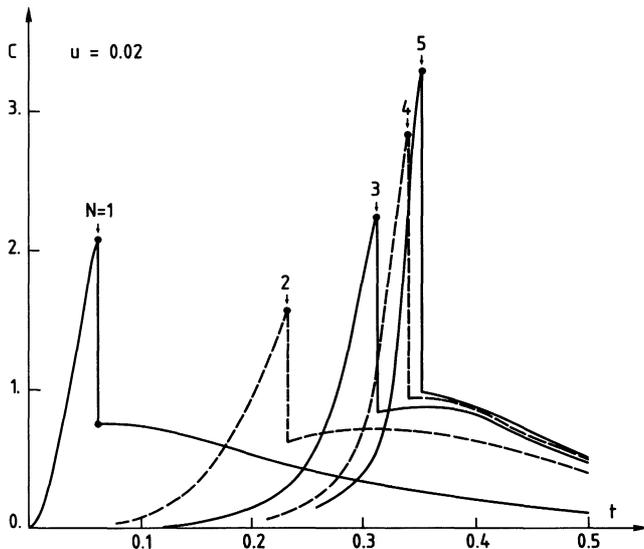


Fig. 2. — Specific heat as a function of  $t$ , for strips of width  $N = 1$  to 5. The potential parameter is  $u = 0.02$ .

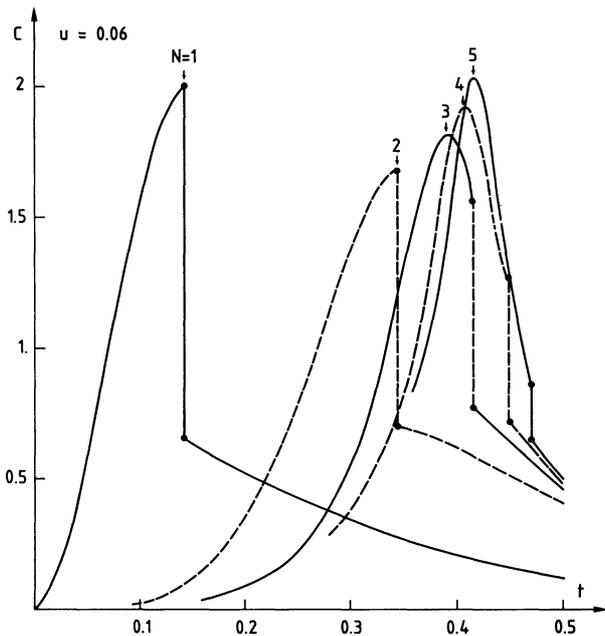


Fig. 3. — Specific heat as a function of  $t$ , for strips of width  $N = 1$  to 5. The potential parameter is  $u = 0.06$ .

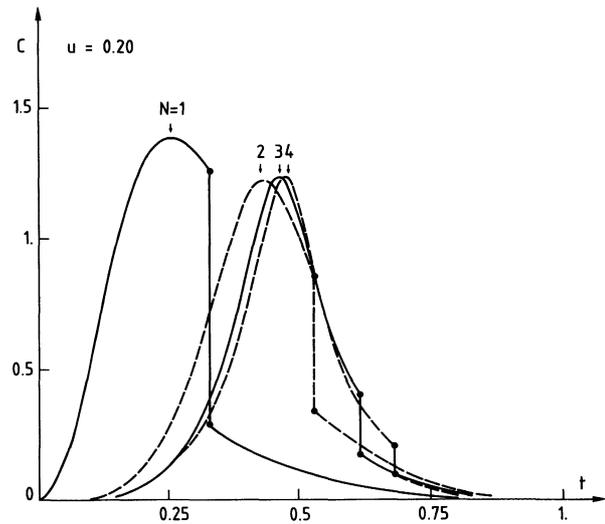


Fig. 4. — Specific heat as a function of  $t$ , for strips of width  $N = 1$  to 4. The potential parameter is  $u = 0.2$ .

values of  $N$  we can correctly deal with is the fact that, for  $N$  larger than 5 or 6, our iterative procedures become very slow, and very unstable with respect to initial conditions on  $\lambda$  and the  $z_n$ , and to convergence to «ghost» states with negative  $\lambda$ . Moreover, we could not guarantee a good enough accuracy of our solutions for  $N \geq 7$ , which could therefore not be used in our extrapolation methods.

#### 4. Extrapolation to the 3D system.

Let us insist upon the fact that the results we report in sections 2 and 3 are exact, whereas the following assertions are numerically and heuristically supported conjectures on what the 3D phase diagram *is likely to be*.

The analysis of the transition temperatures and of the specific heat leads us to a very plausible existence of two critical values of the potential parameter  $u$ , namely  $u_R$  and  $u_S$ , demarcating three regions. Neither the characteristics nor the existence of these three regimes is the result of any proof, but we shall present arguments in favour of the consistency of the strip method with other approaches. Let us describe the phase diagram we predict (Fig. 5).

*Region 1* :  $0 < u < u_R \sim 0.04$ . — The first region is characterized by a fast convergence of the  $T_p(N)$  to a value  $T_p$ , transition temperature of the 3D system. The variations of the specific heat (for  $u = 0.02$  : see Fig. 2) suggest that the transition of the bulk 3D system is a discontinuous one (first order). More precisely, let us define a temperature  $t_i$  ( $t_i < t_p$ ), for fixed  $u$  and  $N$ , as being the intersection point between the curve  $C(t)|_{t < t_p}$  and the continuation of  $C(t)|_{t > t_p}$  (which exists for arbitrary  $t$ , independently of  $u$ ). The width of the specific heat peak is defined by :

$$\Delta t = t_p - t_i \tag{24}$$

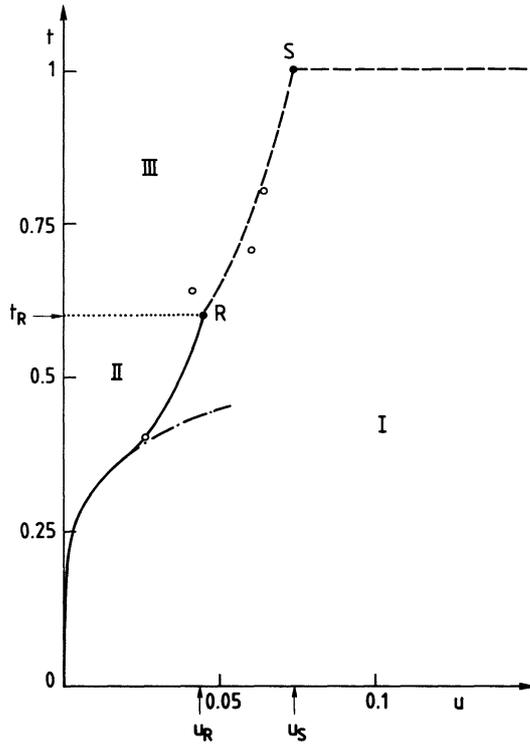


Fig. 5. — Our prediction for the phase diagram of the model : in phase I, the interface is pinned near the wall ; in phase II, it is delocalized and smooth ; in phase III, it is delocalized and rough. The natures of the transition lines are as follows : the solid line between the origin and R is first-order ; the dash-dotted line represents the leading order of the low- $T$  expansion. The dotted line is the infinite-order roughening transition. The dashed line (between points R and S, and along  $t = 1$  above  $u = u_s$ ) is presumably continuous. The white circles are improved Neville approximations to the transition lines.

and the effective latent heat by :

$$\Delta E = E(t_p) - E(t_i). \quad (25)$$

The numerical values of these quantities (see left hand side of table II) are an evidence for a first-order transition (constant  $\Delta E$ ; widths  $\Delta t \rightarrow 0$ ). This prediction is in agreement with the following low-temperature expansion.

Consider first the interface far from the wall. At zero temperature, it is completely flat, and its first excitations are one height difference of ( $\pm 1$ ). We have therefore :

$$Z_1 = 1 + 2At^4 + \dots \quad (26)$$

( $A$  is the area of the sample), and :

$$-f_1 = 2t^4 + \dots \quad (27)$$

In presence of the wall, analogous arguments lead to the following partition function :

$$Z_2 = t^{-4u}(1 + At^{4+u} + \dots) \quad (28)$$

Table II. — Analysis of the specific heat curves for two typical values of  $u$ . A star in the last row indicates that we assume convergence of the data.

N	$u = 0.02$			$u = 0.06$		
	$\Delta t$	$N \cdot \Delta t$	$\Delta E$	$\Delta t$	$N \cdot \Delta t$	$\Delta E$
1	0.034	0.034	0.107	0.084	0.084	0.241
2	0.069	0.137	0.125	0.108	0.217	0.307
3	0.051	0.152	0.153	0.090	0.270	0.377
4	0.038	0.153	0.161	0.088	0.350	0.418
5	0.031	0.153	0.158	0.094	0.471	0.454
$\infty$		*	*	*		

and then :

$$-f_2 = -u \ln t + t^{4+u} + \dots \quad (29)$$

Both free energies are equal along a line in the  $(u, t)$  plane :

$$u = -\frac{t^4}{\ln t} + \dots \quad (30)$$

The corresponding transition is first-order, with a latent heat :

$$\Delta E = \left(4 - \frac{1}{\ln t}\right)t^4 + \dots \quad (31)$$

For  $u = 0.02$ , the analysis reported in table II predicts  $\Delta E = 0.15$ , while formulae 30-31 lead to  $\Delta E = 0.099$ . The discrepancy is only due to higher-order terms in the low temperature expansion and we think that this low-temperature picture is valid up to some value  $u = u_R$ .

*Region 2* :  $u_R < u < u_s \sim 0.075$ . — Let us come back to figure 1 : the pinning temperatures seem to obey two different convergence regimes, separated by a crossover around  $u = 0.04$ . In order to support more precisely this observation, we use the following extrapolation method. Let us remark that we tried other methods without getting stable enough results. Consider the  $u_N$  ( $N = 1$  to 6) at fixed  $t$ . The ordinary Neville method on this suite consists in defining the  $V_N$  by :

$$V_N = u_N - \alpha \frac{(u_{N+1} - u_N)(u_N - u_{N-1})}{u_{N+1} + u_{N-1} - 2u_N}. \quad (32)$$

If  $u_N \sim u_\infty + AN^{-\gamma}$ , then  $V_N$  converges much faster towards  $u_\infty$  for the choice of  $\alpha = 1 + 1/\gamma$ . Since we

do not know the exponent  $\gamma$  for the present problem, we propose to eliminate it between the two equations obtained by setting  $N = 4$  and  $N = 5$  in (32). The corresponding « improved Neville » results lie on figure 5 for some values of particular interest. At very large  $T$  ( $t$  close to 1), the method involves differences of large numbers, and gets unstable. Around  $t = 0.6$ , we get unexpectedly unstable results.

This analysis leads to a transition line ending at a point S ( $T = \infty$ ,  $u = u_s \sim 0.075$ ). A typical point of this line is  $u = 0.06$ , where we observe (Fig. 3) a large peak in the specific heat, but the numerical data (Table II, right hand side) show that the transition is not first-order. The maxima of  $C$  do not seem to diverge rapidly with  $N$ . This fact is compatible with the continuous theory of reference 4, which predicts  $\nu = \nu_{\parallel} > 1$  in all cases, so that the specific heat critical exponent  $\alpha$ , given by the hyperscaling relation :  $\alpha = 2 - 2 \nu_{\parallel}$ , is always negative.

The point  $u_R$  at which the first-order low-temperature transition becomes a continuous one is very likely to correspond to the roughening transition : the low-temperature expansion considers small excitations of a nearly flat surface, while the field theory of [4] is expected to be valid when the interface is rough. This scenario is supported by the following numerical fact : taking the value of  $t_R = 0.60$  from [14], we get from figure 5 :  $u_R \sim 0.04$ , point at which none of the quantities mentioned in table II ( $\Delta t$ ,  $N\Delta t$ ,  $\Delta E$ ) seems to converge. The infinite-order roughening line completes our plausible phase diagram.

*Region 3 :  $u > u_s$ .* — In this last region, we do not see any sign of a phase transition. The values of  $T_p$  diverge quickly ( $\sim$  linearly with  $N$ ); the specific heat (Fig. 4, for  $u = 0.2$ ) seems to converge to a smooth function. We have also observed that the parallel correlation length  $\xi_{\parallel}$  defined in (16) is a *decreasing* function of  $N$  at fixed  $t$  and  $u > u_s$  : in other terms, the interface is more and more bound to the wall and off-critical, when  $N$  is increased.

Although we have no proof of the existence of a finite  $u_s$  in our model, this fact is not very surprising. It has been proved (see [12]) that the (unrestricted) S.O.S. model in the potential we consider has a phase transition for arbitrary  $u$ , but both models (S.O.S. and R.S.O.S.) are very different at very high temperatures. We know that the two-point function of both models, in the absence of a pinning potential, has the following behaviour (for  $T > T_R$ ,  $|\mathbf{R}| \gg 1$ )

$$\langle (h_0 - h_{\mathbf{R}})^2 \rangle \sim \sigma(T) \ln |\mathbf{R}|. \quad (33)$$

In the S.O.S. model, we expect  $\sigma(T)$  to go to infinity with  $T$ , as it does in a continuous field theory; while, in the R.S.O.S. model we consider,  $\sigma(T)$  goes to a constant, we estimated to be 0.37 in [14]. The entropy is therefore much smaller in the restricted model, and the pinning potential may win for arbitrary temperature when it is strong enough ( $u > u_s$ ). Another

similar argument, based on duality, leads to the same possibility. It has been shown in [17] that the interface is unbound for sufficiently small dual temperature  $T^*$ . Assume the transition dual temperature  $T^*$  and the potential parameter  $u$  are related by (once one precise definition of  $T^*$  is chosen) :

$$u = \varphi(T^*) \quad \text{with} \quad \varphi(0) = +\infty. \quad (34)$$

Let us recall that the dual potential is defined (see [8]) by :

$$e^{-V^*(\theta)} = \sum_{h \in \mathbb{Z}} e^{-\beta V(h) - i h \theta}; \quad \theta \in [0, 2\pi]. \quad (35)$$

The dual temperature can be defined by :

$$V^*(\theta) = V^*(0) + \frac{\theta^2}{2 T^*} + O(\theta^4) \quad (\theta \rightarrow 0). \quad (36)$$

These formulae lead to :

$$\begin{aligned} T^* &= \frac{(1-t)^2}{2t} \quad \text{for S.O.S. model} \\ T^* &= \frac{2t+1}{2t} \quad \text{for R.S.O.S. model.} \end{aligned} \quad (37)$$

When  $t$  goes to unity,  $T^*$  goes to zero for the S.O.S. model, and there exist two phases for arbitrary  $u$ . In our R.S.O.S. model,  $T^*$  goes to its lower bound  $\frac{3}{2}$ , and therefore there exist two phases only for :

$$u < u_s \quad \text{with} \quad u_s = \varphi\left(\frac{3}{2}\right). \quad (38)$$

Let us mention that a similar fact is encountered in mean field theory [19], where the true S.O.S. model has a pinning transition, while the discrete gaussian model has only one phase (the interface is bound for every temperature, like in our case for  $u > u_s$ ).

### 5. Conclusions.

In the previous section we have proposed an interpretation of the observed behaviour of physical quantities, which gives rise to a coherent description of what the phase diagram of a 3D edge pinning lattice model is likely to be.

For *weak pinning potentials* the interface, when moving away at  $T = T_p$  from the boundary, still has a finite width. The depinning transition is in this case of first-order. For  $T \geq T_p$  the interface is far away from the wall and in fact does not interact with it. For  $T = T_R > T_p$  it will of course undergo the usual roughening transition of a free model.

For *pinning potentials strong enough* to make  $T_p$  and  $T_R$  coincide, another mechanism takes place. The interface when moving away gets rough. In this case large excursions of the unbound interface play an important role, as they do in continuous models. The depinning transition is now continuous.

For very strong pinning potentials ( $u > u_s$ ), the interface seems to be always bound to the wall. We think that this is a pathology of our model, connected with the truncation of the interactions, as we have explained in section 4.

One should notice that, when defining our model, we have not considered any bulk field or any long-range interactions [18], which are usually present in real systems. Therefore, at  $T_p$ , the interface moves infinitely far from the wall. Neither have we observed the so-called « layering » transitions (see [6]), where the interface is moving away by a series of separate discontinuous « jumps ».

In this paper, we have shown how the transfer matrix method can work in the case of an infinite number of configurations per site. A considerable

advantage of this method is that it leads to exact results on finite strips, the only questionable part of the analysis is the way to extrapolate these results to the infinite system. This approach may certainly be used in other problems, for which a naive formulation of the transfer matrix leads to an infinite dimensional operator, and especially when the 1D system exhibits a phase transition.

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