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Finite-size lattice method and the roughening transition

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Résumé. — La transition rugueuse d'une surface de type SOS à 3 dimensions est étudiée par des méthodes numériques sur des rubans de largeur finie. Les résultats sont compatibles avec une transition d'ordre infini, ce que prévoient des arguments d'universalité.

Abstract. — The roughening transition of an SOS-type surface on a 3-dimensional lattice is studied by numerical methods on strips of finite width. The results are consistent with an infinite-order transition, as expected from universality.

1. Introduction. — It has been shown that the roughening transition, which was introduced in solid state physics, also plays a role in lattice gauge theories [1] for various gauge groups and dimensions. We are using the usual modelization of this phenomenon : a three-dimensional surface where disconnected parts and overhanging configurations are forbidden. This SOS model is related to the well-known $X - Y$ and Coulomb-gas models [2-4]. Its low-temperature phase, where the surface is localized, maps into the plasma phase where the correlation length is finite ; its high-temperature or rough phase corresponds to the dielectric phase where the correlations have a power-law decay. The transition was proved by Kosterlitz to be of an infinite-order [5, 6]. There also exists an exactly solvable version of the model [7].

2. The model and the method. — The surface is defined by an integer height h_i at each site i of a square lattice. The action is then :

$$S = \beta \sum_{(i,j)} V(h_i - h_j) \quad (1)$$

where the sum runs over all pairs of nearest neighbours. We have chosen the potential :

$$V(0) = 0 ; \quad V(\pm 1) = 1 ; \\ V(n) = +\infty \quad \text{for } |n| \geq 2. \quad (2)$$

We define the temperature variable $t = \exp(-\beta)$. We used the transfer matrix method on strips of width N and infinite length. This finite-size lattice method was first used by Nightingale [8], and applied

to different problems : polymers [9], localization [10], and $X - Y$ model [11]. The last model is expected to belong to the same universality class as ours.

In order to study the so-called step energy, a quantity which provides a signature for the transition, and which we studied by low-temperature expansion in a previous paper [12], we introduced the following boundary conditions : $h \equiv 0$ on the left edge ; $h \equiv \Delta$ on the right edge. $\Delta = 0$ corresponds to a flat surface ; $\Delta = 1$ builds a single longitudinal step.

We have computed for $1 \leq N \leq 5$, $\Delta = 0$ and $\Delta = 1$, the following quantities as functions of t : free energy :

$$-\beta F_N = \frac{1}{N} \ln \lambda_1^{(\Delta=0)}$$

correlation lengths :

$$-\frac{1}{\xi_N^{(0)}} = \ln \frac{\lambda_2^{(\Delta=0)}}{\lambda_1^{(\Delta=0)}} \\ -\frac{1}{\xi_N^{(1)}} = \ln \frac{\lambda_2^{(\Delta=1)}}{\lambda_1^{(\Delta=1)}} \quad (3)$$

step energy :

$$-f_N^{\text{st}} = -\beta F_N^{\text{st}} = \ln \frac{\lambda_1^{(\Delta=1)}}{\lambda_1^{(\Delta=0)}}.$$

Where λ_1, λ_2 are the largest (real positive) two eigenvalues of the transfer matrix.

2.1 VARIATIONS OF $\xi_N^{(0)}$ AND $\xi_N^{(1)}$ WITH N . — The results plotted in figures 1 and 2 show the two-phased structure of the model :

The high-temperature regime is characterized in both cases ($\Delta = 0$ and $\Delta = 1$) by a correlation length ξ_N growing linearly with N ; this confirms the existence of a scale invariant phase where ξ_∞ is infinite.

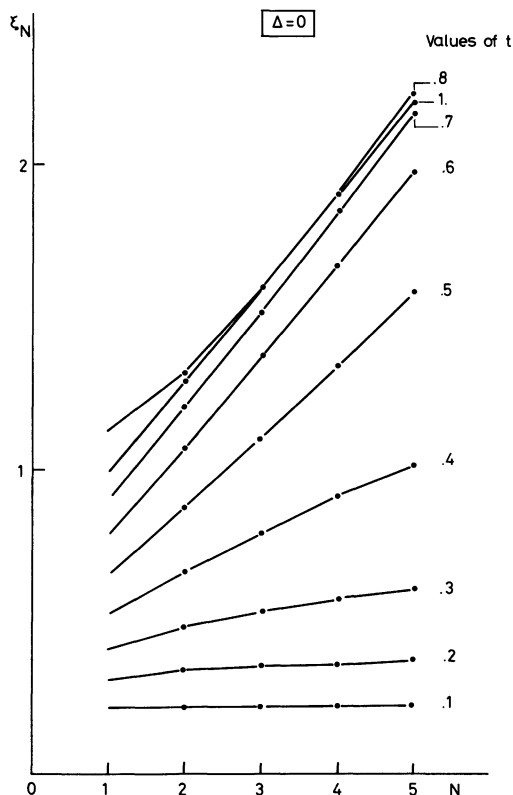


Fig. 1. — Finite-size correlation length ξ_N as a function of the size N for a flat surface ($\Delta = 0$). The low-temperature lines approach a finite ξ_∞ value.

In the low-temperature phase, two distinct behaviours are expected and indeed observed : in the case of figure 1 ($\Delta = 0$), the energy gap between the ground state and the excited ones corresponds to a ξ_N reaching asymptotically its bulk value ξ_∞ ; while for $\Delta = 1$ (Fig. 2) the presence of a mobile step allows the development of soft excitations at low temperatures, and ξ_N grows exponentially with N , as in the ordered phase of the Ising model [8].

A very analogous result was obtained by Pichard and Sarma [10] in the problem of localization in two dimensions. This study gives a rather poor estimate of the transition temperature :

$$t_c \sim 0.5. \quad (4)$$

2.2 EXTRAPOLATION OF THE STEP ENERGIES. — We are specially interested in this quantity : its vanishing is just the mechanism of the roughening transition.

We extrapolated our exact results $f_N^{\text{st}}(t)$ in the following way : by fitting the first j values $f_1^{\text{st}}(t) \dots f_j^{\text{st}}(t)$ with a polynomial function of degree $(j - 1)$ in the

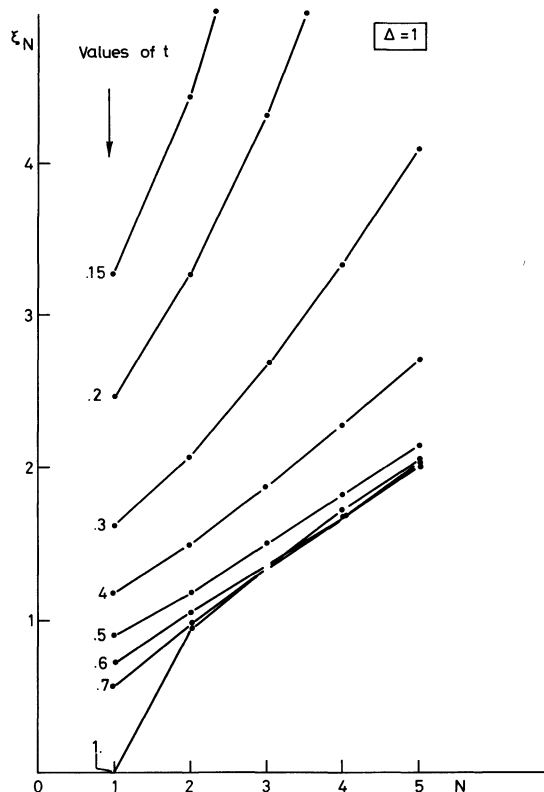


Fig. 2. — The same quantity for $\Delta = 1$, i.e. with a single step. The low-temperature ξ_N now grow exponentially.

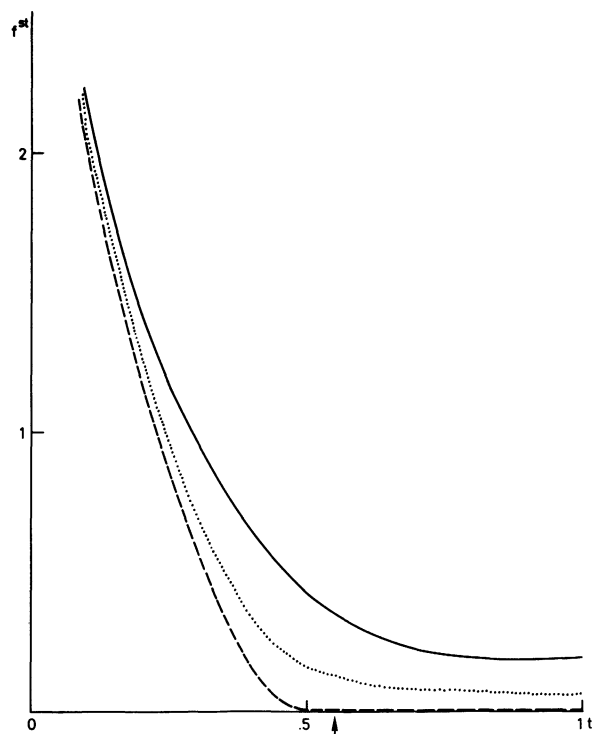


Fig. 3. — The step energy as a function of t . — full line : size $N = 1$; — dotted line : size $N = 5$; — dashed line : extrapolated values for the infinite 2-D system, as explained in part 2.2. The arrow indicates the corresponding value of t_c .

$1/N$ variable, and then by extrapolating the obtained $N = \infty$ polynomial values by assuming a geometrical convergence in the j variable. The accuracy of the final result is expected to be good. In figure 3 we give the finite-size values f_1^{st} and f_5^{st} , and the final extrapolation f_e^{st} .

As evidence of the accuracy of our method, we quote the following : in the rough phase, we obtain as an approximation for the function f_e^{st} , expected to be identical to zero :

$$|f_e^{\text{st}}| < 3 \times 10^{-3} \quad \text{for } 0.6 < t < 1.$$

A log-log plot shows that an ordinary power-law singularity

$$f^{\text{st}} \sim (t_c - t)^{-\nu}, \quad (5)$$

is excluded.

We made the following assumption :

$$f^{\text{st}} \sim \exp[-\text{const.} (t_c - t)^{-\bar{\nu}}]. \quad (6)$$

The presence of an inflexion point in the plot of $(f^{\text{st}})^{1/2}$ as a function of t led us easily to the values for

t_c and $\bar{\nu}$ which fit our results in the best way :

$$\begin{aligned} t_c &= 0.548 \\ \bar{\nu} &= 0.45. \end{aligned} \quad (7)$$

We are not able to estimate honestly the incertitudes. We may reasonably suspect that :

$$\begin{aligned} 0.3 &\leq \bar{\nu} \leq 0.6 \\ 0.53 &\leq t_c \leq 0.57 \end{aligned} \quad (8)$$

but we just mention that the relative difference between (6)-(7) and our extrapolation is less than 2 % in the whole t -interval where it is credible.

3. Conclusion. — Our results are qualitatively (variations of ξ_N) and quantitatively (7) in good agreement with similar finite-lattice works [10, 11], and with the renormalization group [6] and the exactly solvable six-vertex model [7], which both give the value $\bar{\nu} = \frac{1}{2}$. All these models can be said to belong to the same universality class.

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