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LETTER TO THE EDITOR

Surface roughening for two-dimensional percolation at $p = 1$

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Abstract. We introduce [10] and [11] interface models for percolation on the square lattice and on the triangular lattice. In the case of $p = 1$ (p probability) only the [10] models show surface roughening. An analytic calculation gives a square-root divergence for the interface width in the thermodynamic limit.

Surface roughening, especially the occurrence of a roughening transition, is not only a well known phenomenon of critical behaviour physics as observed for interfaces of the 3D Ising model (Weeks *et al* 1973, Gilmer *et al* 1974), crystal growth models (see Weeks 1980), liquid-vapour systems or binary fluids (see Wallace 1980). It appears also in gauge theory models (Drouffe and Zuber 1981, Lüscher 1981, Münster and Weisz 1981, Hasenfratz *et al* 1981), and experimentalists have detected a possible roughening transition in helium too (see Balibar and Castaing 1980).

Our interest is concentrated on surfaces of percolation clusters. Concerning the square lattice, we found a rough surface for all p above p_c, but no roughening transition, by Monte Carlo simulations (Franke 1980). In analogy with the 2D Ising model, a square-root divergence in the interface width was found to be quite probable. The purpose of this Letter is to remove the remaining uncertainty on this point, at least in the case of $p = 1$.

In site percolation perimeters are unoccupied next-neighbour sites of occupied sites. Their number t corresponds to the energy E for thermal phenomena (Stauffer 1979). At $p = 1$ there are only perimeters at the surface of the cluster. They separate its interior from the outside region and can be identified with the surface energy. As the case $p = 1$ corresponds thermally to $T = 0$ we are speaking of the ground state and its degeneracy. If a variety of configurations with minimal perimeter $t_{\min}$ exists for an interface system, we have a degenerate ground state and surface roughening may occur. We deal first with the square lattice, and then with the triangular lattice. A calculation is sketched which confirms the presumed square-root divergence in the thermodynamic limit.

We consider first the square lattice in the high-density limit. Figure 1 shows types of interface configurations of the square lattice. In (*a*) and (*b*) the direction perpendicular to the interface is given by [10], in (*c*) and (*d*) by [11]. As can be seen, variations of the straight configuration are possible without changing the perimeter number, but this is

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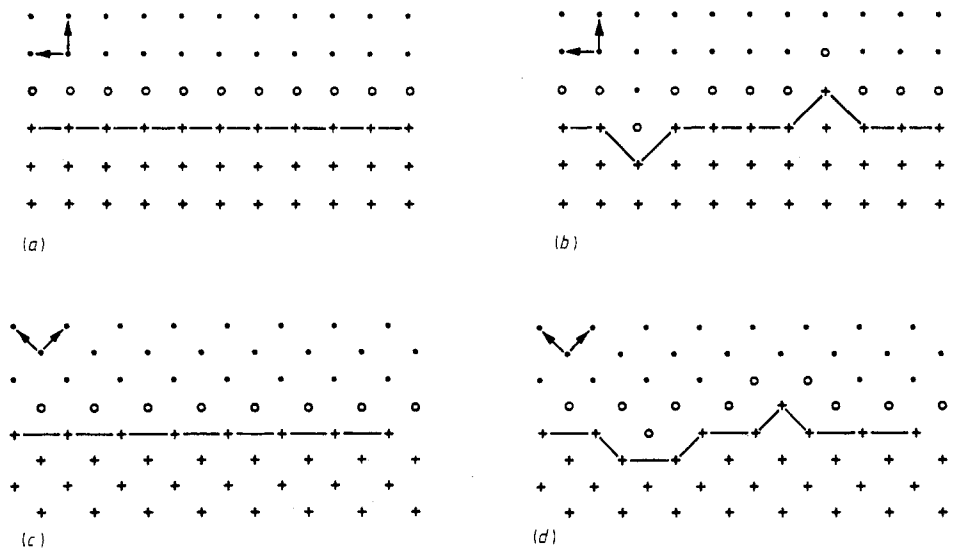

Figure 1. Interface configurations of the square lattice, indicated by crosses (occupied sites), circles (perimeters) and dots (empty sites). Straight configuration of the [10] model: length of the system $L = 11$, number of perimeters $t = 11$ (a), another [10] configuration $L = 11$, $t = 11$ (b), straight [11] configuration $L = 16$, $t = 8$ (c), another [11] configuration $L = 16$, $t = 10$ (d).

valid only for the [10] interface model. In the case of the [11] model the straight configuration (figure 1(c)) is the only possible one for $p = 1$ (if one neglects some configurations due to boundary effects with interface width less than or equal to unity). The ground state of this model is not degenerate and there is no surface roughening. This, however, is not true for $p < 1$, as shown by our Monte Carlo simulations (figure 2). Even for $p = 0.99$ we found a clear $\sqrt{L}$-law for the interface width and so far there exists no difference from the [10] model†.

Concerning this [10] model, it is our intention to confirm analytically the $\sqrt{L}$-law in the case of $p = 1$, which was suggested by our previous Monte Carlo work (Franke 1980). In figure 3(a) all interface configurations with minimal perimeter number are listed for systems of length $L = 2$ and $L = 3$, where free edges are applied as boundary conditions. It is obvious that every configuration of the L-system generates three configurations of the $L + 1$-system by enlarging the L-configuration on the right in the manner illustrated (figure 3(b)).

We define the interface width of a configuration as the difference in height between the highest and lowest surface sites. (For example the configurations in figure 1(a) and (b) have widths 0 and 2, respectively.) Let N_L be the sum of the interface widths of all 3^{L-1} configurations of an L-system with minimal perimeter number $t = L$. Then we obtain for the mean interface width‡

$$W_L = N_L / 3^{L-1}. \tag{1}$$

† The situation is quite similar to the square Ising model: the antiferromagnetic [10] model, for example, corresponds to the [11] percolation model and is not degenerate; surface roughening occurs only for $T > 0$ (Weeks *et al* 1973), whereas the [11] model shows surface roughening already for $T = 0$.

‡ Note that this definition differs from that in our Monte Carlo simulations, where the mean square distance from the surface centre of the density profile was taken.

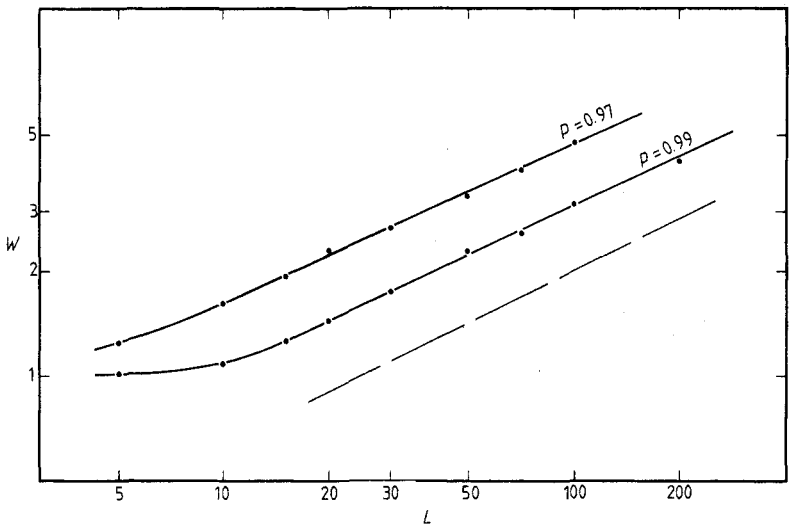

Figure 2. Monte Carlo data of the square-lattice [11] model: log–log plots of interface width W against system length L at fixed concentration p. The broken line gives a square root law. Data for [10] surfaces were published before (Franke 1980).

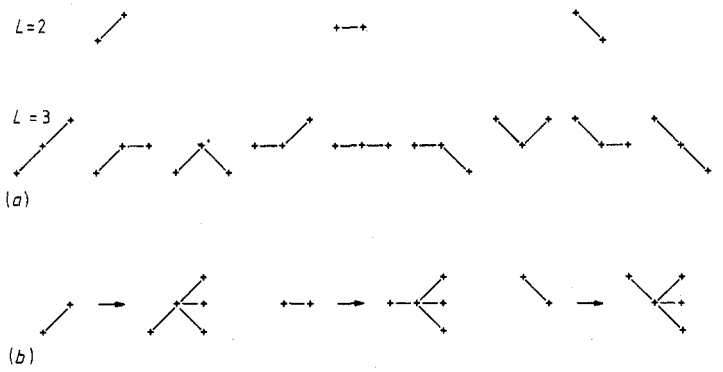

Figure 3. Complete set of [10] interface configurations with minimal perimeters for the $L=2$ and $L=3$ square-lattice system with free edges (a). Generation of $L+1$-configurations by L-configurations (b).

Consider configurations which have the last site on the right at the highest or lowest level. If J_L is the number of these configurations, then (setting $N_1=0$, $J_1=2$, counting the straight-line configuration always twice in the enumeration of J_L) it follows that

$$N_{L+1}=3N_L+J_L \qquad (L=1,2,3,\ldots). \tag{2}$$

Moreover, we define numbers B_L by the additional recursion relations

$$J_{L+1}=3J_L-2B_{L-1} \qquad (L=1,2,3,\ldots). \tag{3}$$

Formulating the problem in terms of infinite matrices and by applying some graphic

techniques it can be shown that

$$B_0 = B_1 = 1,$$

$$B_L = B_{L-1} + \sum_{l=0}^{L-2} B_l B_{L-2-l} \qquad (L = 2, 3, \ldots). \tag{4}$$

An equation for the generating function $B(x) = \Sigma_{L=0}^{\infty} B_L x^L$ can be derived by (4),

$$x^2(B(x))^2 - (1-x)B(x) + 1 = 0, \tag{5}$$

which is known to determine the generating function of the generalised Ballot numbers (Sloane 1973, Motzkin 1948). The solution of (5), satisfying the condition $B(0) = B_0 = 1$, is

$$B(x) = [1 - x - (1 - 2x - 3x^2)^{1/2}]/(2x^2). \tag{6}$$

To obtain the Ballot numbers we expand (6) into powers of x,

$$B_L = 2^{-(L+2)} \sum_{l=0}^{[L/2]+1} C_{L+1-l} \binom{L+2-l}{l} 3^l \qquad (L = 0, 1, 2, \ldots), \tag{7}$$

where C_L are the Catalan numbers (Sloane 1973),

$$C_L = \binom{2L}{L} \Big/ (L+1) = \frac{(2L)!}{(L!)^2(L+1)} \qquad (L = 0, 1, 2, \ldots), \tag{8}$$

and $[L/2]$ means the integer part of $L/2$. By some simple but tedious mathematical arguments, based on Stirling's formula, one can show that the asymptotic behaviour of the Ballot numbers is

$$B_L \propto 3^L L^{-3/2} \qquad \text{as } L \to \infty. \tag{9}$$

Solving the recursion relations (3) for J_L in terms of B_L and using $\Sigma_{L=0}^{\infty} B_L/(3^L) = B(\frac{1}{3}) = 3$ (following from (6)) it may be shown that $J_L \propto 3^L L^{-1/2}$. A similar procedure due to (2) yields $N_L \propto 3^L L^{1/2}$. Hence, from the definition (1) we find the presumed square-root divergence

$$W_L \propto L^{1/2} \qquad \text{as } L \to \infty \tag{10}$$

for the interface width of the square lattice in the thermodynamic limit.

We now consider the triangular lattice for $p = 1$. Figure 4 gives corresponding configurations for the triangular lattice. Obviously, the [10] model is degenerate again (figure 4(*a*), (*b*)) and thus yields the only candidate for surface roughening, if $p = 1$ is assumed. An analogous analysis can be performed. Instead of equations (1), (2), (3), (7) we find in this case

$$W_L = N_L / 2^{L-1}, \tag{11}$$

$$N_{L+1} = 2N_L + J_L \qquad (\text{with } N_1 = 0, J_1 = 2), \tag{12}$$

$$J_{L+1} = 2J_L - 2B_{L-1}, \tag{13}$$

$$B_L = \begin{cases} C_\lambda & \text{for } L = 2\lambda, \\ 0 & \text{for } L = 2\lambda + 1 \end{cases} \qquad (\lambda = 0, 1, 2, \ldots), \tag{14}$$

where C_λ are the Catalan Numbers (8). Applying Stirling's formula, we obtain immediately $C_\lambda \propto 4^\lambda \lambda^{-3/2}$, whence $B_L \propto 2^L L^{-3/2}$ as L (even) $\to \infty$, and we are led to (10) again.

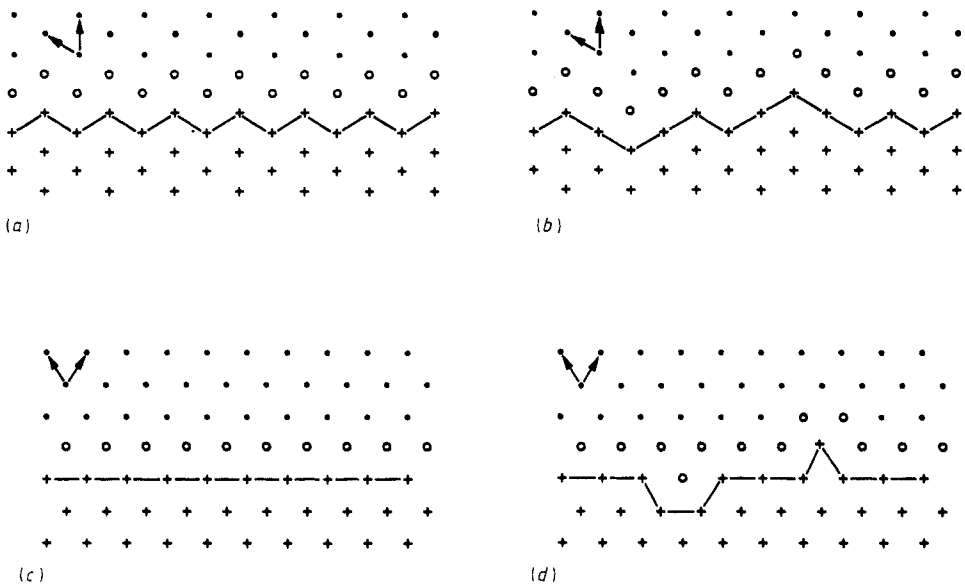

Figure 4. Interface configurations of the triangular lattice. 'Straight' [10] configuration $L = 14$, $t = 14$ (a), another [10] configuration $L = 14$, $t = 14$ (b), straight [11] configuration $L = 20$, $t = 10$ (c), another [11] configuration $L = 20$, $t = 12$ (d).

To make these results more obvious we add two plots of $\mathrm{d}\ln W_L/\mathrm{d}\ln L \simeq \ln(W_L/W_{L-1})/\ln[L/(L-1)]$ as functions of L, which clearly tend to 0.5 as $L \to \infty$ (figure 5). The data up to $L = 500$ were produced by simple computer algorithms executed in a time less than one second.

For both the square lattice and the triangular lattice we have introduced a [10] and [11] interface model. We pointed out that only the [10] models are degenerate and

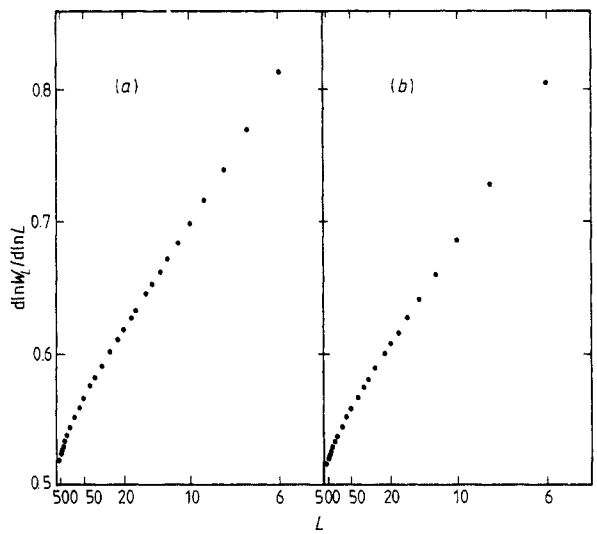

Figure 5. Plots of $\mathrm{d}\ln W_L/\mathrm{d}\ln L$ as a function of $1/L$ for the square lattice (a) and the triangular lattice (b).

therefore only these models can show surface roughening if we assume $p = 1$. Using a different definition of the interface width W_L we found again a square-root divergence $W_L \propto \sqrt{L}$ in the thermodynamic limit. Thus our analytic calculation at $p = 1$ agrees with the Monte Carlo results for $p \leqslant 1$. Moreover, for intermediate L the deviations from the asymptotic result could be studied.

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