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LETTER TO THE EDITOR

On the surface properties of two-dimensional percolation clusters

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Abstract. The two-dimensional site percolation problem is studied by transfer-matrix methods on finite-width strips with free boundary conditions. The relationship between correlation-length amplitudes and critical indices, predicted by conformal invariance, allows a very precise determination of the surface decay-of-correlations exponent, $\eta_s = 0.6664 \pm 0.0008$, consistent with the analytical value $\eta_s = 2/3$. It is found that a special transition does not occur in the case, corroborating earlier series results. At the ordinary transition, numerical estimates are consistent with the exact value $y_s = -1$ for the irrelevant exponent.

Finite-size scaling concepts are a powerful tool for the determination of critical properties at phase transitions [1], especially when coupled to phenomenological renormalization [2] and conformal invariance [3] ideas. Here we present results from numerical transfer-matrix calculations of the correlation length, and quantities derived therefrom, for site percolation on infinite strips with free boundary conditions (FBC). The use of FBC allows one to assess surface critical properties, including so-called special and surface transitions [4] when they occur.

Our transfer-matrix formulation of the percolation problem relies on the direct application of connectivity concepts [5], as opposed to taking the $s \to 1$ limit of the s-state Potts model [6], which corresponds to bond percolation (and should then, by universality, give the same exponents as for the site problem). While the latter approach benefits from being a systematic expansion in terms of Whitney polynomials, it is devised for general, continuous s and thus carries a high degree of inherent complexity. As shown in earlier work [5, 7, 8] and below, the geometric picture based on cluster connectivity allows a straightforward algorithm to be built, from which a nicely extrapolating sequence of finite-size estimates is extracted.

We use strips of width $L \leqslant 10$ sites, both for square and triangular lattices. This is the same maximum width reached with periodic boundary conditions (PBC) [7, 8], though in the present case lower symmetry implies that the matrices are of considerably larger dimension than on a cylindrical geometry. First, standard phenomenological renormalization (PR) [2] is performed on the site occupation probability p between strips of consecutive widths, from which estimates of the critical concentration p_c, the temperature-like exponent y_p and the surface decay-of-correlations exponent, η_s are obtained. Alternative finite-size sequences

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for η_s are produced by setting p at the exact (or extrapolated) p_c. We then search for a special transition, by introducing a distinct probability p_s for site occupation along the strip boundaries. A two-parameter PR analysis is carried out, by comparing correlation lengths on three strips of consecutive widths [9–11]. Only one non-trivial fixed point, shown to correspond to an ordinary transition, is found upon numerical examination of the recursion relations. No evidence is found for the existence of a multicritical point related to a special, or surface, transition.

The exponent that governs the decay of correlations along the surface of a semi-infinite plane at criticality, η_s, is related to the correlation length on a strip with FBC by

$$\eta_s = \frac{2L}{\pi \xi_L(p_c)} \tag{1}$$

a result from conformal invariance [12, 13]. Note that for a triangular lattice with FBC the strip width $L = N\sqrt{3}/2$, where N is the number of sites across the strip.

Corrections to scaling must be dealt with, since e.g. equation (1) is expected to be valid only asymptotically. Throughout this work, extrapolations toward $L \to \infty$ have been done using the Bulirsch–Stoer (BST) algorithm [14, 15]. As extensively discussed elsewhere [15], whenever the leading correction-to-scaling exponent ω is not known *a priori* BST extrapolations rely on keeping it as a free parameter within an interval guessed to be reasonable. Central estimates and error bars are evaluated self-consistently by selecting the range of ω for which overall fluctuations are minimized. In the following we have allowed $0.45 \leqslant \omega \leqslant 2.4$ for all quantities, as the most likely candidates in the case are $\omega = 1$ and 2 (see below).

We implement standard, one-parameter, PR in the usual way by looking for the fixed point p^* of the implicit recursion relation:

$$\frac{\xi_L(p^*)}{L} = \frac{\xi_{L-1}(p^*)}{L-1} \tag{2}$$

where $\xi_L(p) = -1/\ln \Lambda_L(p)$ is given in terms of the largest eigenvalue $\Lambda_L(p)$ of the column-to-column transfer matrix [5]; p^* is thus a finite-size estimate of p_c. At the fixed point, the temperature-like exponent $y_p = 1/\nu$ is evaluated by taking suitable derivatives [1]. For consistency, η_s is obtained from equation (1) with ξ calculated at p^*.

Our results are shown in table 1, where the values of p^* and y_p for $L = 3$ and 4 on the square lattice have been obtained previously [5]. The amplitude of finite-size corrections is much larger than for the corresponding cases of PBC (see e.g. table 1 in [8]). However, the finite-lattice sequences are generally well-behaved, allowing for smooth extrapolations. Comparing our extrapolated estimates for p_c and y_p with the well-known respective values provides a good overall check of the reliability of our procedures. For the square lattice our p_c agrees very well with, but is less precise than, the best estimate for the percolation threshold $p_c = 0.592\,745 \pm 0.000\,002$ [16]. A similar picture holds for the comparison with the exact $p_c = 1/2$ for the triangular lattice, and $y_p = 3/4$ (both lattices).

Turning now to η_s, table 1 provides a direct test of the prediction $\eta_s = 2/3$ [13], previously confirmed only indirectly via the series result $\gamma_1 = 2.10 \pm 0.02$ [17] which, together with the scaling relation $2\gamma_1 = \gamma + \nu(2 - \eta_s)$ and the exact values $\gamma = 43/18$ and $\nu = 4/3$, gives $\eta_s = 0.64 \pm 0.03$ [13] . Though the agreement is generally very satisfactory, the sequence for the triangular lattice seems to extrapolate towards a region slightly above 2/3.

In order to improve the quality of our estimates [7, 18], we have also generated sequences of finite-size data for η_s by setting p at the best available (or exact) value of p_c. For comparison with the corresponding data in [8] for the bulk exponent η, given by

Table 1. Results from one-parameter PR. Uncertainties in the last quoted digits are shown in parentheses. Extrapolations obtained by the BST algorithm with correction-to-scaling exponent ω in ranges shown. Expected values are exact, unless otherwise noted.

	Square			Triangular		
L	p^*	y_p	η_s	p^*	y_p	η_s
3	0.671 130	0.662 822	0.290 469	0.573 092	0.665 596	0.337 283
4	0.644 177	0.676 427	0.351 082	0.547 377	0.681 787	0.393 936
5	0.629 524	0.686 306	0.394 701	0.533 471	0.692 689	0.434 325
6	0.620 566	0.693 798	0.427 621	0.525 062	0.700 557	0.464 391
7	0.614 644	0.699 685	0.453 367	0.519 561	0.706 500	0.487 600
8	0.610 502	0.704 439	0.474 064	0.515 749	0.711 147	0.506 047
9	0.607 478	0.708 362	0.491 070	0.512 990	0.714 869	0.521 047
10	0.605 197	0.711 655	0.505 297	0.510 928	0.717 880	0.533 458
Expected	0.592 745(2)[a]	3/4	2/3[b]	1/2	3/4	2/3[b]
Extrapolated	0.5925(5)	0.750(2)	0.666(3)	0.5005(2)	0.750(2)	0.676(3)
ω	1.50(50)	1.10(10)	1.00(5)	2.00(10)	1.10(10)	1.05(5)

[a] Monte Carlo [16].
[b] Predicted by conformal invariance [13].

Table 2. Results for η_s and η obtained by setting $p = 0.592745$ (square) or $p = 1/2$ (triangular lattice). Uncertainties in the last quoted digits are shown in parentheses. Extrapolations obtained by the BST algorithm with correction-to-scaling exponent ω in ranges shown. Expected values are exact, unless otherwise noted.

	Square		Triangular	
L	η_s	η	η_s	η
2	0.432 695 188 2	0.216 347 594 1	0.467 384 334 9	0.211 476 582 5
3	0.484 810 173 2	0.213 059 500 8	0.513 592 777 0	0.211 193 304 8
4	0.517 492 502 6	0.212 557 612 8	0.542 352 678 7	0.210 354 950 9
5	0.540 029 183 3	0.211 467 327 6	0.561 983 131 5	0.209 740 964 3
6	0.556 557 680 0	0.210 737 071 4	0.576 242 952 1	0.209 349 267 8
7	0.569 219 447 1	0.210 223 288 6	0.587 074 789 6	0.209 095 612 7
8	0.579 239 953 1	0.209 856 476 8	0.595 584 120 0	0.208 924 559 9
9	0.587 373 373 9	0.209 586 803 3	0.602 447 280 9	0.208 804 513 7
10	0.594 110 246 6	0.209 383 309 9	0.608 102 683 2	0.208 717 300 9
Expected	2/3[a]	5/24	2/3[a]	5/24
Extrapolated	0.6664(4)	0.208 35(2)	0.665(1)	0.208 33(2)
ω	1.00(5)	1.90(10)	1.00(10)	2.00(5)

[a] Predicted by conformal invariance [13].

$\eta = L/\pi\xi_L(p_c)$ [12] (where ξ_L is related to the largest eigenvalue of the transfer matrix with PBC and, in [8], is calculated at the respective p^* as in table 1), we have done the same for PBC. The results are displayed in table 2.

For the square lattice the central estimate of p_c from [16] has been used. Had the respective error bars been taken into account, this would typically give rise to uncertainties in the sixth decimal place of η_s or η. BST extrapolations of the truncated values point essentially towards the same limits exhibited in table 2 (though with error bars roughly doubled), which shows that the corresponding sequences are rather robust.

The amplitude of finite-size corrections is much larger for FBC than for PBC, a trend already noticed in the discussion of table 1. Comparison with the final estimate

$\eta = 0.2088 \pm 0.0008$ of [8] suggests that, for PBC at least, setting $p = p_c$ rather than at the approximate p^* reduces error bars by one order of magnitude. This latter statement assumes that both BST and the extrapolation procedures described in [8] are of comparable intrinsic accuracy, which is reasonable for long ($\simeq$ 10 elements) sequences such as those encountered here (for shorter sequences, BST would be relatively more reliable than other methods [15]). Turning to FBC, one sees a similar improvement in the extrapolated values of η_s relative to those in table 1. Focusing on the remarkably smooth sequence for the square lattice, and taking into account the effect of the uncertainty in p_c on the estimates of η_s as discussed above, we reach the final estimate $\eta_s = 0.6664 \pm 0.0008$. This is entirely in agreement with the prediction $\eta_s = 2/3$ from conformal invariance [13], and $1\frac{1}{2}$ orders of magnitude more accurate than previous numerical results [13, 17].

It is known from the exact solution of the Ising model that finite-size estimates of the critical temperature and exponents converge as $T_c(L) - T_c \sim L^{-3}$; $y(L) - y \sim L^{-2}$ ($y = \nu, \eta$) for PBC [7], while for FBC the corrections are respectively proportional to L^{-2} and L^{-1} [19]. For percolation on strips with PBC, numerical evidence is similarly consistent with $p_c(L) - p_c \sim L^{-3}$ and $y_p(L) - y_p \sim L^{-2}$ [7]. In the present case, the data of tables 1 and 2 point towards the following scenario: $y_p(L) - y_p \sim L^{-1}$, $\eta_s(L) - \eta_s \sim L^{-1}$ (FBC); $\eta(L) - \eta \sim L^{-2}$ (PBC). Though data for the triangular lattice indicate $p_c(L) - p_c \sim L^{-2}$ as expected, for the square lattice one seems to get fits with the same quality either for $\omega = 1$ or 2, or just about any value in between. We have been unable to sort out this apparently discrepant behaviour.

We have investigated the possible existence of a higher-order critical point, related to a surface-assisted transition. Series work indicates that a special transition should not be expected for percolation clusters in two dimensions (though in three-dimensional systems it should occur) [17, 20]. The work described below is a direct test of such results for the two-dimensional case.

As in, for example, studies of polymer adsorption [10, 11], a distinct occupation probability p_s is introduced for sites on either strip boundary. Fixed points (p^*, p_s^*) are obtained by comparing correlation lengths on three strips [9]:

$$\frac{\xi_L(p^*, p_s^*)}{L} = \frac{\xi_{L-1}(p^*, p_s^*)}{L-1} = \frac{\xi_{L-2}(p^*, p_s^*)}{L-2}. \tag{3}$$

By analogy with polymer adsorption, if a special transition occurs it must be at some $p_s^* > p^*$ so that the critical cluster is located predominantly close to the edge. As p^* is a bulk quantity, one expects it to converge to p_c regardless of whether the transition is ordinary or special. By scanning the (p, p_s) space we have ascertained that there is only one non-trivial solution of equation (3), which corresponds to an ordinary transition. This can be seen from the estimates of critical parameters and respective exponents shown in table 3.

Once again, the smooth convergence of the sequences of estimates of p^*, y_p and η_s towards the expected values confirms that our procedures are, on the whole, reliable. That the second exponent, y_s, is negative ensures that we are dealing with an ordinary critical point; our extrapolation is compatible with $y_s = -1$, a result derived on general grounds for the ordinary transition of two-dimensional systems [21]. The non-universal p_s^* converges to values smaller than the respective p_c for each lattice. This resembles the ordinary transition for polymers, at which the fugacity for surface contacts is slightly *de*-enhanced [10, 11].

With the notable exception of the sequence for p_s^* for the square lattice, the leading correction-to-scaling exponent seems to be in the vicinity of 2, or even larger, for all quantities involved. At present it is not clear whether this feature is fortuitous or in some

Table 3. Results from two-parameter PR. Uncertainties in the last quoted digits are shown in parentheses. Extrapolations obtained by the BST algorithm with correction-to-scaling exponent ω in ranges shown. Expected values are exact, unless otherwise noted.

(a) Square

L	p^*	p_s^*	y_p	y_s	η_s
5	0.595 339	0.503 680	0.731 343	−1.033 26	0.634 489
6	0.595 215	0.503 230	0.736 897	−1.049 06	0.635 388
7	0.594 602	0.500 260	0.740 391	−1.043 01	0.640 568
8	0.594 148	0.497 414	0.742 624	−1.036 92	0.644 923
9	0.593 824	0.494 839	0.744 160	−1.031 61	0.648 407
10	0.593 590	0.492 552	0.745 265	−1.027 19	0.651 168
Expected	0.592 745(2)[a]	—	3/4	−1	2/3[b]
Extrapolated	0.5926(1)	0.460(2)	0.750(2)	−1.001(1)	0.666(1)
ω	2.0(4)	0.85(15)	2.0(2)	1.9(1)	2.00(5)

(b) Triangular

L	p^*	p_s^*	y_p	y_s	η_s
5	0.503 487	0.425 365	0.734 458	−1.022 979	0.844 465
6	0.502 259	0.421 150	0.741 249	−1.027 182	0.802 242
7	0.501 519	0.417 782	0.744 379	−1.024 663	0.777 288
8	0.501 064	0.415 120	0.746 081	−1.021 105	0.760 540
9	0.500 776	0.413 005	0.747 086	−1.017 650	0.748 374
10	0.500 595	0.411 374	0.747 618	−1.013 932	0.738 967
Expected	1/2	—	3/4	−1	2/3[b]
Extrapolated	0.497(2)	0.402(1)	0.750(2)	−1.004(3)	0.680(15)
ω	2.0(4)	2.0(1)	2.0(4)	2.0(4)	2.0(4)

[a] Monte Carlo [16].

[b] Predicted by conformal invariance [13].

way related to the structure of the two-parameter PR equations.

We have shown that the exponent that controls the decay of critical correlations along the surface of a semi-infinite percolating plane is $\eta_s = 0.6664 \pm 0.0008$, consistent with the prediction from conformal invariance $\eta_s = 2/3$. By setting the site occupation probability p at its critical value p_c, clean numerical evidence has been provided that the finite-size estimates of η_s and of the bulk exponent η scale respectively as $\eta_s(L) - \eta_s \sim L^{-1}$ (FBC); $\eta(L) - \eta \sim L^{-2}$ (PBC). It has been shown by numerical examination of suitable two-parameter PR recursion relations that no special transition occurs in the case; furthermore, at the ordinary critical point the irrelevant exponent is, with all probability, $y_s = -1$ exactly.

Extensions of the present work to branched polymers (lattice animals) [7] are currently being pursued. Though conformal invariance concepts are not applicable in the case [22], surface critical indices such as the crossover exponent $\phi = y_s/y$ can be calculated and compared, e.g., to series results [23], for which error bars are rather large at present.

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