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Surface crossover exponent for branched polymers in two dimensions

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Abstract. Transfer-matrix methods on finite-width strips with free boundary conditions are applied to lattice site animals, which provide a model for randomly branched polymers in a good solvent. By assigning a distinct fugacity to sites along the strip edges, critical properties at the special (adsorption) and ordinary transitions are assessed. The crossover exponent at the adsorption point is estimated as $\phi = 0.505 \pm 0.015$, consistent with recent predictions that $\phi = \frac{1}{2}$ exactly for all space dimensionalities.

1. Introduction

The conformational properties of linear polymers near an attractive wall are well understood by now [1]. The fact that conformal invariance concepts [2] are applicable to the problem has been extremely helpful, especially in two dimensions (in which case the 'wall' is a line) where these tools provide a number of exact values for critical exponents. In contrast, for branched polymers it has been shown that the underlying field theory is *not* conformal [3]. Exact results on bulk properties of randomly branched polymers have, however, been obtained through a connection with the theory of Yang–Lee edge singularities [4]. The corresponding extension towards surface properties has been accomplished only recently [5] yielding, among others, the interesting prediction that the crossover exponent at the adsorption point has the hyperuniversal (dimension-independent) value $\phi = \frac{1}{2}$. This result applies for an impenetrable wall; penetrable surfaces have not been considered [5]. The case in favour of hyperuniversality is built from the following elements [5]: (i) an exact calculation in $d = 3$, by means of a correspondence between branched polymers and an epidemic process plus a supersymmetric mapping of the latter onto a semi-infinite one-dimensional Yang–Lee edge problem; (ii) conformal invariance properties of the two-dimensional Yang–Lee problem leading to information on four-dimensional branched polymers near a surface; (iii) mean-field theory, expected to be valid for $d \geqslant 8$; and (iv) perturbation theory in $d = 8 - \epsilon$ dimensions, all four of which yield $\phi = \frac{1}{2}$.

In the present work we use finite-size scaling [6] and phenomenological renormalization [7] ideas to study surface properties of site lattice animals (which provide a model for randomly branched polymers in a good solvent) in two dimensions. To this end, the correlation length for animals on infinite strips with free boundary conditions (FBC) is calculated numerically by diagonalization of the corresponding transfer matrix [8]. By

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imposing FBC one is able to assess surface critical behaviour, in particular, the adsorption transition. Our main goal is to check on the proposed hyperuniversal value $\phi = \frac{1}{2}$ at the adsorption point. Accordingly, only impenetrable surfaces are considered throughout this paper. We start by applying standard one-parameter phenomenological renormalization (PR) [7], reobtaining bulk quantities such as the critical fugacity x_c and the temperature-like exponent $y = 1/\nu$ which are known very accurately [8,9]. This is important as a check of the overall reliability of our procedures. We then search for a surface-driven transition, by introducing a distinct fugacity for occupied sites along the strip boundaries. A two-parameter PR analysis is carried out, by comparing correlation lengths on three strips of consecutive widths [10–12]. Two non-trivial fixed points are found, which are respectively related to the ordinary (bulk-dominated) and adsorption transitions. The corresponding finite-size estimates of critical parameters and exponents are extrapolated. Our main final result is $\phi = 0.505 \pm 0.015$, providing support to the hyperuniversality conjecture [5] $\phi = \frac{1}{2}$, at least in two dimensions.

2. Model and calculational procedure

The generating function of the model, defined on a semi-infinite lattice, can be written as

$$\mathcal{Z} = \sum_{N,N_s} C_{N,N_s} x^N x_s^{N_s} \tag{1}$$

where C_{N,N_s} is the number of different configurations that can be built with a total of N sites constrained to form one cluster, of which N_s are at the surface; x is the fugacity for site occupation and $x_s = \exp \epsilon_s / k_B T$ where $-\epsilon_s$ is the extra energy assigned to each site at the surface. It is expected on general grounds [13] that the critical fugacity x_c will be a constant as a function of x_s, from small x_s up to the adsorption threshold given by some $x_s^c > 1$. Upon approach to a point (x_c^0, x_s^0) on the critical line in (x, x_s) space, the bulk correlation length ξ diverges as $\xi \sim \delta^{-\nu}$ where the scaling field δ is a suitable linear combination of $\delta x \equiv x - x_c^0$ and $\delta x_s \equiv x_s - x_s^0$. Close to the adsorption point, a second length ξ_s diverges with a different exponent $\nu_s \equiv 1/y_s$ (and a different combination δ_s of the variables δx and δx_s). Physically, ξ_s measures the thickness of the adsorbed polymer layer. Thus the average number of surface contacts $\langle N_s \rangle$ scales asymptotically with the average number of sites $\langle N \rangle$ as [13]

$$\langle N_s \rangle \sim \langle N \rangle^{\phi} \qquad \phi \equiv y_s / y \,. \tag{2}$$

Below the adsorption threshold one has $\phi = 0$, while in the adsorbed phase $\phi = 1$. At the threshold ϕ is expected to take on a non-trivial value.

The correlation length $\xi_L(x, x_s)$ along a strip depends on the largest eigenvalue $\Lambda_L^0(x, x_s)$ of the transfer matrix via [8]: $\xi_L(x, x_s) = -1/\ln \Lambda_L^0(x, x_s)$. For large L and close enough to criticality of the corresponding (semi-)infinite system, the correlation length must scale, in terms of δ and δ_s defined above, as [6]

$$L^{-1} \xi_L(\delta, \delta_s) = F(L^{y}\delta, L^{y_s}\delta_s) \,. \tag{3}$$

Upon rescaling of ξ_L, one expects two non-trivial fixed points [11–13]: (i) the ordinary fixed point, which governs the critical behaviour of the unbound (bulk) phase, at which the surface interactions are irrelevant and thus exhibits $y_s < 0$; and (ii) the special fixed point, corresponding to the adsorption transition, with $y_s > 0$.

We use strips of width $L \leqslant 10$ sites, both for square and triangular lattices. Building up the transfer matrix involves the analysis of connectivity properties of adjacent columns of occupied and empty sites. For the present case of animals on strips with FBC, this is a straightforward extension of earlier work on percolation and animals with periodic boundary conditions (PBC) [8, 9] and percolation with FBC [14]. The resulting matrix is rather sparse, owing to restrictions imposed by connectivity [8]: for $L = 10$ on the square lattice, for instance, only 4.2% of the possible combinations of adjacent column states are allowed.

Extrapolation of finite-width results must be dealt with carefully, especially as convergence of estimates produced with FBC is usually slower than that of their counterparts generated with use of PBC [14–16]. In the present work, extrapolations toward $L \to \infty$ have been done using the Bulirsch–Stoer (BST) algorithm [17, 18]. As discussed extensively elsewhere [18], 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.

3. Results

3.1. One-parameter renormalization

We first consider no surface binding ($x_s \equiv 1$). We can then implement standard one-parameter PR in the usual way by looking for a finite-size estimate of x_c given by the fixed point x_L^* of the implicit recursion relation

$$\frac{\xi_L(x_L^*)}{L} = \frac{\xi_{L-1}(x_L^*)}{L-1}\,. \tag{4}$$

At the fixed point, an approximation to the bulk exponent $y = 1/\nu$ is evaluated by [6]

$$y_L = \frac{\ln\{(\mathrm{d}\xi_L/\mathrm{d}x)_{x_L^*}/(\mathrm{d}\xi_{L-1}/\mathrm{d}x)_{x_L^*}\}}{\ln(L/L-1)} - 1\,. \tag{5}$$

In order to check on universality of critical amplitudes [19], we also calculate the quantity $\mathcal{A}_L \equiv 2L/\pi\xi_L(x_L^*)$. Note that for a triangular lattice with FBC the strip width is $L = N\sqrt{3}/2$, where N is the number of sites across the strip. If the underlying field theory were conformal at the critical point, this would be an estimate of the exponent describing the decay of critical correlations along the surface, η_s.

Our results are shown in table 1. Overall agreement with expected values, where these are available, is rather good. Universality of critical correlation-length amplitudes is satisfied within error bars. However, finite-size data show that the amplitude of corrections is much larger than for the corresponding cases of PBC (see, for example, table 1 of [9]). Partially as a consequence of this, our extrapolated estimates for x_c and y are somewhat less accurate than those obtained with PBC [9]. A second source of imprecision emerges when one considers the broad ranges allowed for the correction-to-scaling exponent ω in table 1. Though some degree of subjectivity is inevitable when dealing with error estimation within the BST scheme, our results for ω reflect the fact that, roughly for ω between 1 and 2 the fluctuation estimates for fixed ω (based on the spread between next-to-highest order estimates [18]) keep to the same order of magnitude. On the other hand, outside this interval fluctuations increase, and estimates deteriorate, quickly. This is to be compared, for example, to similar extrapolations for percolation with FBC [14] where usually one can pinpoint a much narrower band of values of ω within which fluctuations are minimized.

3.2. Two-parameter renormalization

We next allow the surface interaction to vary. Similarly, for example, to studies of linear polymer adsorption [11, 12], an extra energy $-\epsilon_s$ is introduced for sites on either strip

Table 1. Results from one-parameter PR. Uncertainties in last quoted digits are shown in parentheses. Extrapolations obtained by the BST algorithm with correction-to-scaling exponent ω in ranges shown. Expected values from [9].

	Square			Triangular		
L	x_L^*	y_L	A_L	x_L^*	y_L	A_L
3	0.298 906	1.434 06	1.022 71	0.247 186	1.395 19	0.998 368
4	0.274 596	1.458 06	1.270 09	0.221 892	1.423 63	1.255 90
5	0.263 725	1.474 90	1.446 19	0.210 650	1.443 32	1.439 50
6	0.257 947	1.486 91	1.578 71	0.204 743	1.457 91	1.576 33
7	0.254 533	1.495 88	1.682 19	0.201 287	1.469 22	1.682 13
8	0.252 364	1.502 84	1.765 28	0.199 107	1.478 28	1.766 37
9	0.250 909	1.508 41	1.833 50	0.197 652	1.485 70	1.835 06
10	0.249 890	1.512 96	1.890 52	0.196 638	1.491 90	1.892 17
Expected	0.246 150(10)	1.560 7(4)	—	0.192 925(10)	1.560 7(4)	—
Extrapolated	0.246 0(2)	1.55(1)	2.45(4)	0.192 8(2)	1.55(1)	2.4(1)
ω	1.5(4)	1.5(5)	1.45(20)	1.5(4)	1.5(5)	1.5(5)

boundary, so that $x_s = \exp \epsilon_s/k_B T$. L-dependent fixed points (x^*, x_s^*) are obtained by comparing correlation lengths on three strips [10]:

$$\frac{\xi_L(x^*, x_s^*)}{L} = \frac{\xi_{L-1}(x^*, x_s^*)}{L-1} = \frac{\xi_{L-2}(x^*, x_s^*)}{L-2} . \tag{6}$$

In the present case these equations give two fixed points: the ordinary fixed point, which describes the behaviour of the unbound animal and the special fixed point which describes the animal's behaviour at the binding transition. Linearizing around the fixed points, the exponents y and y_s can be found from suitable partial derivatives evaluated at the fixed point in question [10–12]. Again we calculate the quantity $\mathcal{A}_L \equiv 2L/\pi\xi_L(x^*, x_s^*)$. Our results for the ordinary and special fixed points are displayed in tables 2 and 3, respectively.

As a general rule, finite-size estimates differ from their limiting ($L \to \infty$) values by much smaller amounts than was the case in one-parameter PR. In several instances, though, convergence turns out not to be monotonic. Further, within the BST scheme we frequently find the following as the trial value of ω is increased from 0.45 to, say, 6: (i) fluctuation estimates at fixed ω always decrease, and (ii) last-order approximants $\mathcal{Q}(\omega)$ vary monotonically, and seem to be converging towards fixed points (that is, $\mathrm{d}\mathcal{Q}(\omega)/\mathrm{d}\omega \to 0$). This is consistent with what is found from three-point extrapolations adjusting ω for the best straight-line fit of data against $L^{-\omega}$ [9]: as a rule, ω tends to converge to unrealistically high values. Thus, although strictly speaking there are no regions where the BST algorithm is stable with respect to ω [18] in such cases, one can produce reasonably reliable estimates by looking at trends followed upon increasing ω. For the entries in tables 2 and 3 to which this picture applies we display the ranges of variation of last-order approximants corresponding to $\omega \geqslant \omega_{\rm min}$, with $\omega_{\rm min}$ as given in the respective entry.

3.2.1. The ordinary transition. For the ordinary transition, the corresponding fixed point can be found only for $L \geqslant 6$. The exact result $y_s = -1$ is expected to hold, as it is based on general properties of the ordinary transition of two-dimensional systems [20]. For both square and triangular lattices, extrapolations were performed discarding data for $L = 6$. Though, for the latter, these do not usually imply non-monotonic variation along the sequence, their inclusion would increase the scatter of extrapolates by at least one order

Table 2. Results from two-parameter PR at the ordinary fixed point. Uncertainties in last quoted digits are shown in parentheses. Extrapolations obtained by the BST algorithm with correction-to-scaling exponent ω in ranges shown.

L	x^*	x_s^*	y	y_s	$\mathcal{A}_L$
(a) Square					
6	0.246 282	0.223 963	1.579 16	−1.021 51	2.497 68
7	0.246 420	0.232 356	1.577 46	−1.051 63	2.489 55
8	0.246 352	0.225 924	1.574 51	−1.049 07	2.494 77
9	0.246 294	0.217 824	1.572 23	−1.041 72	2.500 40
10	0.246 254	0.209 961	1.570 57	−1.034 80	2.505 16
Expected	0.246 150(10)[a]	—	1.5607(4)[a]	−1[b]	—
Extrapolated	0.246 17(3)	0.18(1)	1.566(1)	−1.014(6)	2.519(4)
ω	> 3.0	> 3.0	> 3.0	> 3.0	> 3.0
(b) Triangular					
6	0.194 510	0.352 877	1.534 24	−0.836 625	2.381 520
7	0.193 555	0.289 360	1.542 38	−0.804 216	2.445 904
8	0.193 238	0.257 802	1.546 15	−0.841 891	2.472 772
9	0.193 115	0.240 468	1.548 33	−0.880 553	2.485 607
10	0.193 056	0.229 288	1.549 82	−0.910 094	2.492 939
Expected	0.192 925(10)[a]	—	1.5607(4)[a]	−1[b]	—
Extrapolated	0.192 96(1)	0.185(15)	1.555(2)	−1.00(1)	2.512(2)
ω	> 3.0	—[c]	2.4(9)	3.3(5)	2.4(6)

[a] Reference [9].
[b] Reference [20].
[c] No optimal ω found (see text).

of magnitude. For the non-universal x_s^c on the triangular lattice, we have found neither an optimal range for ω, nor the smooth decrease of error as ω increases, described above. Thus we quote for x_s^c an average of last-order estimates for $1.0 \leqslant \omega \leqslant 4.0$. In general, the final results for the ordinary fixed point show agreement to within less than 0.5% with those of [9]; for the exact result $y_s = -1$ [20] fluctuations are higher, but still kept smaller than 2%. Universality of the amplitude $\mathcal{A}$ is satisfied within 0.05%.

3.2.2. The special transition. For the special fixed point on the square lattice we have discarded $L = 5$ and 6 data for x^*, x_s^* and $\mathcal{A}_L$ on account of non-uniform convergence; otherwise, all data in table 3 have been used in extrapolations. For y_s on the square lattice, fluctuations were approximately constant and small throughout the range of ω explored, so we quote an average of last-order estimates for $1.0 \leqslant \omega \leqslant 4.0$. While extrapolates from square-lattice results undoubtedly suffer as a result of the above-mentioned difficulties, application of the BST algorithm nevertheless gives a fairly accurate numerical picture.

On the other hand, results for the triangular lattice fall into smooth, well behaved sequences from which we have extracted a set of very precise extrapolates. Our central estimate for y is higher by 0.4% than that of [9], with non-overlapping error bars. Recalling that our error bars reflect uncertainties in the extrapolation procedure itself, and do not take into account systematic errors in the original sequence of finite-size results, we do not take this fact as necessarily meaning that our estimates conflict. Indeed, other instances are known [11, 12] in which extrapolates from two-parameter PR differ slightly, for example, from exact results.

Table 3. Results from two-parameter PR at the special fixed point. Uncertainties in last quoted digits are shown in parentheses. Extrapolations obtained by the BST algorithm with correction-to-scaling exponent ω in ranges shown.

L	x^*	x_s^*	y	y_s	$\mathcal{A}_L$
(a) Square					
5	0.244 202	2.340 75	1.542 94	0.717 355	−0.098 027 2
6	0.246 045	2.282 35	1.558 29	0.796 012	−0.057 977 1
7	0.246 033	2.282 78	1.562 22	0.796 973	−0.058 335 8
8	0.246 088	2.280 49	1.565 14	0.800 373	−0.056 153 8
9	0.246 108	2.279 51	1.566 97	0.801 618	−0.055 106 8
10	0.246 123	2.278 77	1.568 25	0.802 352	−0.054 231 7
Expected	0.246 150(10)[a]	—	1.560 7(4)[a]	—	—
Extrapolated	0.246 15(1)	2.277(1)	1.571(2)	0.804(1)	−0.054(2)
ω	> 3.0	> 3.0	> 3.9	—[b]	> 3.0
(b) Triangular					
5	0.190 915	2.851 22	1.534 72	0.701 013	−0.117 316
6	0.192 174	2.788 10	1.545 74	0.745 358	−0.088 703 2
7	0.192 573	2.765 01	1.552 00	0.764 248	−0.076 175 3
8	0.192 735	2.754 42	1.556 08	0.773 683	−0.069 544 3
9	0.192 813	2.748 73	1.558 89	0.778 886	−0.065 533 7
10	0.192 856	2.745 27	1.560 86	0.781 982	−0.062 831 1
Expected	0.192 925(10)[a]	—	1.560 7(4)[a]	—	—
Extrapolated	0.192 92(1)	2.745(5)	1.566 3(5)	0.788 8(5)	−0.054(3)
ω	3.5(6)	2.7(4)	3.6(6)	3.5(7)	2.0(4)

[a] Reference [9].
[b] No optimal ω found (see the text).

4. Discussion and conclusions

It can be seen from tables 2 and 3 that universality of critical amplitudes [19] is satisfied to within error bars. The qualitative behaviour as one spans the distinct possibilities is similar to that of the corresponding η of linear polymers. For PBC $\mathcal{A} \simeq 0.68$ [8, 9]; with FBC, at the ordinary transition $\mathcal{A} \simeq 2.51$; at the special transition $\mathcal{A} \simeq -0.054$. For linear polymers $\eta_{\text{bulk}} = \frac{5}{24}$; $\eta_s^{\text{Ord}} = \frac{5}{4}$; $\eta_s^{\text{Sp}} = -\frac{1}{12}$ [11, 12]. Unfortunately, the analogy does not seem to go beyond this level.

The result $x_s^c = 2.277(1)$ for the adsorption threshold on the square lattice compares well with, and is more precise than, the series estimate 2.25(5) [21]. It would be interesting to check whether using our value of x_s^c in the series analysis would improve other results.

Turning now to the crossover exponent $\phi = y_s/y$, the safest course seems to be separately extrapolating the sequences for y_s and y, and then calculating the ratio of final estimates. From the square-lattice data of table 2 one would get $\phi = 0.511 \pm 0.002$, while for the triangular lattice of table 3 one gets $\phi = 0.5035 \pm 0.0005$. Though, as mentioned earlier, the above error bars do not take into account systematic errors, it is desirable to have an estimate of these. In order to do so, we refer to the similar case of adsorption of two-dimensional linear polymers, where conformal invariance asserts that $y = \frac{4}{3}$ and $y_s = \frac{2}{3}$, thus $\phi = \frac{1}{2}$ exactly; two-parameter PR sequences for a locally directed (but globally isotropic) square lattice extrapolate to $y \simeq 1.339$ and $y_s \simeq 0.679$, respectively [12], which gives $\phi \simeq 0.507$, just under 2% off the exact value. For fully isotropic lattices, the extrapolation for y_s overshoots the exact value by 4% [11]. In this latter case the corresponding extrapolations of y have not been published; however, finite-lattice data point towards a value somewhat larger than $\frac{4}{3}$ [11], thus one expects at least a partial compensation of errors for the ratio y_s/y. Assuming systematic errors of order 2% in the extrapolated exponents also for the present case, one gets $\phi = 0.51 \pm 0.01$ (square lattice) and 0.50 ± 0.01 (triangular). Systematic deviations are thus estimated to increase uncertainties by at least one order of magnitude over those coming from extrapolation procedures. Our final result must encompass both the latter central estimates and allow for the spread between them, plus their own inherent uncertainties. Thus we have $\phi = 0.505 \pm 0.015$. This is consistent with the hyperuniversality conjecture $\phi = \frac{1}{2}$ [5], and is to be compared with the series result $\phi = 0.6 \pm 0.1$ [21].

We have studied surface properties of randomly branched polymers in two dimensions. Our estimates of bulk quantities such as critical fugacity x_c and critical exponent y are in very good agreement with results obtained with PBC [8, 9]. We have checked that universality of critical amplitudes [19] holds in all instances investigated. The adsorption threshold for the square lattice has been located with greater accuracy than previously available [21]. The crossover exponent ϕ at the adsorption point satisfies, within error bars, the recent hyperuniversality conjecture $\phi = \frac{1}{2}$ [5].

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