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 $\phi = 1/2$ exactly for all space dimensionalities.

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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 $\phi = 1/2$. 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 $d \geq 8$; and (iv) perturbation theory in $d = 8 - \epsilon$ dimensions, all four of which yield $\phi = 1/2$.

In the present work we use finite-size scaling [6] and phenomenological renormalisation [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 numerically calculated by diagonalisation of the corresponding transfer matrix [8]. By imposing FBC one is enabled to assess surface critical behaviour, in particular the adsorption transition. Our main goal is to check on the proposed hyperuniversal value $\phi = 1/2$ at the adsorption point. Accordingly, only impenetrable surfaces are considered throughout this paper. We start by applying standard one-parameter phenomenological renormalisation (PR) [7], reobtaining bulk quantities such as the critical fugacity $x_c$ and the temperature-like exponent $y = 1/\nu$ which are very accurately known [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, 11, 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 \( \phi = 1/2 \) 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:

\[
Z = \sum_{N,N_s} C_{N,N_s} x^N x_s^{N_s},
\]

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 \((x_0^c, x_0^s)\) on the critical line in \((x,x_s)\) space, the bulk correlation length \( \xi \) diverges as \( \xi \sim \delta^{-\nu} \) where the scaling field \( \delta \) is a suitable linear combination of \( \delta x \equiv x - x_0^c \) and \( \delta x_s \equiv x_s - x_s^c \). Close to the adsorption point, a second length \( \xi_s \) diverges with a different exponent \( \nu_s \equiv 1/y_s \) (and a different combination \( \delta_s \) of the variables \( \delta x \) and \( \delta x_s \)). Physically, \( \xi_s \) measures the thickness of the adsorbed polymer layer. Thus the average number of surface contacts \( < N_s > \) scales asymptotically with the average number of sites \( < N > \) as \[13\]

\[
< N_s > \sim < N >^\phi, \quad \phi \equiv y_s/y.
\]

Below the adsorption threshold one has \( \phi = 0 \), while in the adsorbed phase \( \phi = 1 \). At the threshold \( \phi \) 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 \( \delta \) and \( \delta_s \) defined above, as \[6\]

\[
L^{-1} \xi_L(\delta, \delta_s) = F(L^y \delta, L^{y_s} \delta_s).
\]

Upon rescaling of \( \xi_L \), one expects two non-trivial fixed points \[11, 12, 13\]: (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 \( L \leq 10 \) 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 \[14, 13, 16\]. In the present work, extrapolations toward \(L \to \infty\) have been done using the Bulirsch-Stoer (BST) algorithm \[17, 18\]. As extensively discussed elsewhere \[18\], whenever the leading correction-to-scaling exponent \(\omega\) is not known \textit{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 \(\omega\) for which overall fluctuations are minimised.

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:

\[
\xi_L(x^*_L) = \frac{\xi_{L-1}(x^*_L)}{L - 1},
\]

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

\[
y_L = \frac{\ln \left\{ (d\xi_L/dx)_{x^*_L} / (d\xi_{L-1}/dx)_{x^*_L} \right\} }{\ln (L/L - 1)} - 1.
\]

In order to check on universality of critical amplitudes \[19\], we also calculate the quantity \(A_L \equiv 2L/\pi \xi_L(x^*_L)\). 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. 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, \(\eta_s\).

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 e.g. table I of reference \[9\]). 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 \(\omega\) in table 1. Though some degree of subjectivity is inevitable when dealing with error estimation within the BST scheme, our results for \(\omega\) reflect
the fact that, roughly for $\omega$ between 1 and 2 the fluctuation estimates for fixed $\omega$ (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 e.g. to similar extrapolations for percolation with FBC [14] where usually one can pinpoint a much narrower band of values of $\omega$ within which fluctuations are minimised.

### 3.2. Two-parameter renormalisation

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

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

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, 11, 12]. Again we calculate the quantity

| $L$ | $x_L^*$ | $y_L$ | $A_L$ | $x_L^*$ | $y_L$ | $A_L$ |
|-----|---------|-------|-------|---------|-------|-------|
| 3   | 0.298906| 1.43406| 1.02271| 0.247186| 1.39519| 0.998368|
| 4   | 0.274596| 1.45806| 1.27009| 0.221892| 1.42363| 1.25590 |
| 5   | 0.263725| 1.47490| 1.44619| 0.210650| 1.44332| 1.43950 |
| 6   | 0.257947| 1.48691| 1.57871| 0.204743| 1.45791| 1.57633|
| 7   | 0.254533| 1.49588| 1.68219| 0.201287| 1.46922| 1.68213|
| 8   | 0.252364| 1.50284| 1.76528| 0.199107| 1.47828| 1.76637|
| 9   | 0.250909| 1.50841| 1.83350| 0.197652| 1.48570| 1.83506|
| 10  | 0.249890| 1.51296| 1.89052| 0.196638| 1.49190| 1.89217|
| Expected | 0.246150(10) | 1.5607(4) | — | 0.192925(10) | 1.5607(4) | — |
| Extrapolated | 0.2460(2) | 1.55(1) | 2.4(4) | 0.1928(2) | 1.55(1) | 2.4(1) |
| $\omega$ | 1.5(4) | 1.5(5) | 1.45(20) | 1.5(4) | 1.5(5) | 1.5(5) |

\[ \text{Table 1. Results from one-parameter PR. Uncertainties in last quoted digits are shown in parentheses. Extrapolations obtained by BST algorithm with correction-to-scaling exponent } \omega \text{ in ranges shown. Expected values from Ref. [9].} \]
\[ A_L \equiv 2L/\pi \xi_L (x^*, x_s^*). \]

Our results for the ordinary and special fixed points are displayed respectively in tables 2 and 3.

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 \(\omega\) is increased from 0.45 to, say, 6: (i) fluctuation estimates at fixed \(\omega\) always decrease, and (ii) last-order approximants \(Q(\omega)\) vary monotonically, and seem to be converging towards fixed points (that is, \(dQ(\omega)/d\omega \to 0\)). This is consistent with what is found from three-point extrapolations adjusting \(\omega\) for the best straight-line fit of data against \(L^{-\omega}\) [9]: as a rule, \(\omega\) tends to converge to unrealistically high values. Thus, although strictly speaking there are no regions where the BST algorithm is stable with respect to \(\omega\) [18] in such cases, one can produce reasonably reliable estimates by looking at trends followed upon increasing \(\omega\). 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 \(\omega \geq \omega_{\min}\), with \(\omega_{\min}\) 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 \(L \geq 6\). 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 of magnitude. For the non-universal \(x_s^*\) on the triangular lattice, we have found neither an optimal range for \(\omega\), nor the smooth decrease of error as \(\omega\) increases, described above. Thus we quote for \(x_s^*\) an average of last-order estimates for \(1.0 \leq \omega \leq 4.0\). In general, the final results for the ordinary fixed point show agreement to within less than 0.5\% with those of Ref. [18]; for the exact result \(y_s = -1\) [20] fluctuations are higher, but still kept smaller than 2\%. Universality of the amplitude \(A\) 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 \(A_L\) 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 \(\omega\) explored, so we quote an average of last-order estimates for \(1.0 \leq \omega \leq 4.0\). 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
Table 2. Results from two-parameter PR at the ordinary fixed point. Uncertainties in last quoted digits are shown in parentheses. Extrapolations obtained by BST algorithm with correction-to-scaling exponent $\omega$ in ranges shown.

| $L$ | $x^*$  | $x^*_s$ | $y$ | $y_s$ | $A_L$ |
|-----|--------|--------|-----|------|-------|
| 6   | 0.246282 | 0.223963 | 1.57916 | –1.02151 | 2.49768 |
| 7   | 0.246420 | 0.232356 | 1.57746 | –1.05163 | 2.48955 |
| 8   | 0.246352 | 0.225924 | 1.57451 | –1.04907 | 2.49477 |
| 9   | 0.246294 | 0.225924 | 1.57451 | –1.04907 | 2.49477 |
| 10  | 0.246254 | 0.209961 | 1.57057 | –1.03480 | 2.50516 |

(a) Square

Expected 0.246150(10)$^a$ — 1.5607(4)$^a$ – 1$^b$ —

Extrapolated 0.24617(3) 0.18(1) 1.566(1) 1.104(6) 2.519(4)

$\omega > 3.0$ $> 3.0$ $> 3.0$ $> 3.0$ $> 3.0$

| $L$ | $x^*$  | $x^*_s$ | $y$ | $y_s$ | $A_L$ |
|-----|--------|--------|-----|------|-------|
| 6   | 0.194510 | 0.352877 | 1.53424 | –0.836625 | 2.381520 |
| 7   | 0.193555 | 0.289360 | 1.54238 | –0.804216 | 2.445904 |
| 8   | 0.193238 | 0.257802 | 1.54615 | –0.841891 | 2.472772 |
| 9   | 0.193115 | 0.240468 | 1.54833 | –0.880553 | 2.485607 |
| 10  | 0.193056 | 0.229288 | 1.54982 | –0.910094 | 2.492939 |

(b) Triangular

Expected 0.192925(10)$^a$ — 1.5607(4)$^a$ – 1$^b$ —

Extrapolated 0.19296(1) 0.185(15) 1.555(2) 1.00(1) 2.512(2)

$\omega > 3.0$ — $> 3.0$ $> 3.0$ $> 3.0$ $> 3.0$

$^a$Ref. [9] $^b$Ref. [20] $^c$No optimal $\omega$ found (see text).

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 Ref. [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 e.g. from exact results.

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

| \( L \) | \( x^* \) | \( x^*_s \) | \( y \) | \( y_s \) | \( A_L \) |
|-------|--------|--------|-----|-----|------|
| 5     | 0.244202 | 2.34075 | 1.54294 | 0.717355 | – 0.0980272 |
| 6     | 0.246045 | 2.28235 | 1.55829 | 0.796012 | – 0.0579771 |
| 7     | 0.246033 | 2.28278 | 1.56222 | 0.796973 | – 0.0583358 |
| 8     | 0.246088 | 2.28049 | 1.56514 | 0.801618 | – 0.0551068 |
| 9     | 0.246108 | 2.27951 | 1.56697 | 0.802352 | – 0.0542317 |
| 10    | 0.246123 | 2.27877 | 1.56825 | 0.802352 | – 0.0542317 |
|       | Expected |        |       |       |       |
|       | 0.246150(10)^a | – | 1.5607(4)^a | – | – |
|       | Extrapolated | 2.277(1) | 1.571(2) | 0.804(1) | – 0.054(2) |
| \( \omega \) | > 3.0 | > 3.0 | > 3.9 | \( \_b \) | > 3.0 |

| \( L \) | \( x^* \) | \( x^*_s \) | \( y \) | \( y_s \) | \( A_L \) |
|-------|--------|--------|-----|-----|------|
| 5     | 0.190915 | 2.85122 | 1.53472 | 0.701013 | – 0.117316 |
| 6     | 0.192174 | 2.78810 | 1.54574 | 0.745358 | – 0.087032 |
| 7     | 0.192573 | 2.76501 | 1.55200 | 0.764248 | – 0.0761753 |
| 8     | 0.192735 | 2.75442 | 1.55608 | 0.773683 | – 0.0695443 |
| 9     | 0.192813 | 2.74873 | 1.55889 | 0.778886 | – 0.0655337 |
| 10    | 0.192856 | 2.74527 | 1.56086 | 0.781982 | – 0.0628311 |
|       | Expected |        |       |       |       |
|       | 0.192925(10)^a | – | 1.5607(4)^a | – | – |
|       | Extrapolated | 2.745(5) | 1.5663(5) | 0.7888(5) | – 0.054(3) |
| \( \omega \) | 3.5(6) | 2.7(4) | 3.6(6) | 3.5(7) | 2.0(4) |

^aRef. [9]
^bNo optimal \( \omega \) found (see text).

is similar to that of the corresponding \( \eta \) of linear polymers. For PBC \( \mathcal{A} \approx 0.68 \) [8, 9]; with FBC, at the ordinary transition \( \mathcal{A} \approx 2.51 \); at the special transition \( \mathcal{A} \approx -0.054 \). For linear polymers \( \eta_{\text{bulk}} = 5/24 \); \( \eta_{\text{Ord}}^{\text{ord}} = 5/4 \); \( \eta_{\text{Sp}}^{\text{sp}} = -1/12 \) [11, 12]. Unfortunately the analogy does not seem to go beyond this level.

The result \( x^c_s = 2.277(1) \) 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 \( x^c_s \) 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 $y = 4/3$ and $y_s = 2/3$, thus $\phi = 1/2$ exactly; two-parameter PR sequences for a locally directed (but globally isotropic) square lattice extrapolate respectively to $y \simeq 1.339$ and $y_s \simeq 0.679 \ [12]$, 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 $4/3 \ [11]$, 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 $0.50 \pm 0.01$ (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 $\phi = 1/2 \ [1]$, and 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 $\phi$ at the adsorption point satisfies, within error bars, the recent hyperuniversality conjecture $\phi = 1/2 \ [3]$.

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