

# Branched Polymers on the Two-Dimensional Square Lattice with Attractive Surfaces

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Using the renormalization group approach, an analysis is given of the asymptotic properties of branched polymers situated on the two-dimensional square lattice with attractive impenetrable surfaces. We modeled branched polymers as site lattice animals with loops and site lattice animals without loops on the simple square lattice. We found the gyration radius critical exponent  $\nu = 0.6511 \pm 0.0003$  and  $\nu = 0.6513 \pm 0.0003$  for branched polymers with and without loops, respectively. Our results for the crossover exponent  $\phi = 0.502 \pm 0.003$  for branched polymers with loops and  $\phi = 0.503 \pm 0.003$  for branched polymers without loops satisfy the recent hyperuniversality conjecture  $\phi = \frac{1}{2}$ . In addition, we have studied partially directed site lattice animals.

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**KEY WORDS:** Polymer adsorption; crossover exponents; lattice animals.

## 1. INTRODUCTION

Polymer adsorption on a substrate is of experimental and theoretical interest so the statistical mechanics of surface critical phenomena in polymer physics has been the subject of intensive research activity for a long time. The case of randomly branched polymers can be of interest for the understanding of surface properties of some interesting physical systems (sol-gel transition near a wall, for example). Although the renormalization group methods have had widespread use in studying critical properties of lattice animals,<sup>(1-4)</sup> to our knowledge it has never before been used for studying adsorption phenomena of branched polymers on square lattice. Of course, the renormalization group method can be applied only approximately, but it gave very good result for critical exponent of gyration radius for the site lattice

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animals<sup>(4)</sup> by extrapolation in the asymptotic scaling limit when the number of sites in an animal tends to infinity. Therefore, it is interesting to see results which this method gives in the case of branched polymers situated on square lattice with adsorbed walls.

Recently, surface critical behavior of several models of branched polymers has been analyzed. In particular, there is an exact value of the crossover exponent ( $\phi = 1/2$ ) for the adsorption problem.<sup>(5,6)</sup> It has been argued, moreover, that this value should be hyperuniversal, i.e., independent of the dimension of embedding space. This is in good agreement with transfer-matrix<sup>(7)</sup> and series expansion<sup>(8)</sup> results in  $d=2$ , but it does not agree well with Monte-Carlo simulations<sup>(9)</sup> in  $d=3$ .

The paper is organized as follows. In Section 2 we have presented our model of branched polymers on the simple square lattice and corresponding renormalization group method. In Section 3, we have determined the critical exponents and extrapolate data to the case of large systems. Some final remarks and an overall discussion is given in Section 4.

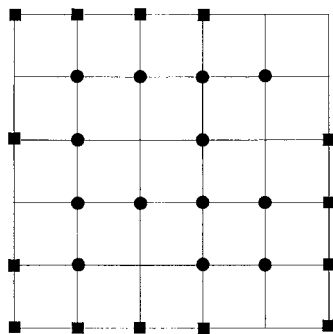
## 2. MODEL AND METHOD

We have modeled branched polymers as site lattice animals with loops, without loops and partially directed ones (see Fig. 1) situated on the simple square lattice with adsorbed surfaces. In the lattice animal problem we are interested in the statistics of all distinct clusters starting at the origin of an infinite lattice and we rescale a cell if it contains a single cluster originating at a fixed origin on the cell.<sup>(4)</sup> But, in order to study branched polymers with attractive surfaces we have investigated branched polymers situated on a finite lattice of  $b \times b$  sites with all four attractive walls, and then we have extrapolated results to the case of an infinite system.

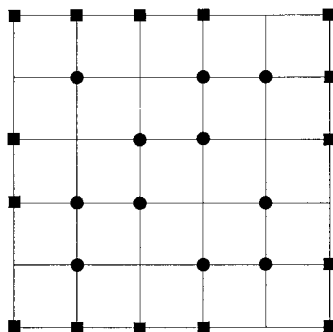
The surface generating function of this model can be written in the form

$$\mathcal{E}^s(x, z) = \sum \omega(M, K) x^M z^K \quad (1)$$

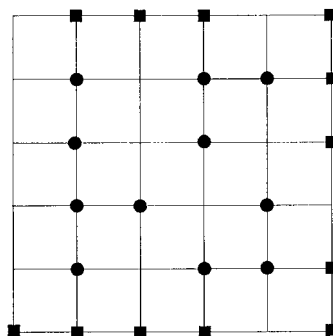
Here, interaction with surfaces is modeled by assigning a coupling  $z$  for every monomer lying on any wall, which may be considered as a short-range force between monomers and the wall while the others have the normal bulk monomer fugacity  $x$ ;  $\omega(M, K)$  denotes the number of all different connected clusters where each cluster starts from a fixed origin (which we have chosen to be the lower left-hand corner, as shown in Fig. 1), and extends to the opposite wall having  $M$  monomers into the bulk and  $K$  monomers lying on the walls.



a)



b)



c)

Fig. 1. Examples of the polymer configurations modelled as: (a) site lattice animals, (b) site lattice animals without loops and (c) partially directed site lattice animals without loops (only  $+X$  and  $\pm Y$  steps are allowed) on the square lattice of length  $b=6$ . Each occupied site has a fugacity  $z$  if it is situated on any wall of the lattice (black square) and the normal bulk-fugacity  $x$  otherwise (black circle). For the present examples this leads to the renormalization equations: (a)  $z' = x^{13}z^{14}$ ,  $x' = x^{27}$ , (b)  $z' = x^{11}z^{15}$ ,  $x' = x^{26}$  and (c)  $z' = x^{11}z^{12}$ ,  $x' = x^{23}$ .

In the similar way the bulk generating function has the form

$$\Xi^b(x) = \sum \omega(N) x^N \quad (2)$$

where  $N$  is the total number of monomers in one connected cluster defined as above.

The renormalization group recursion relation is defined by requiring that the generating function is invariant on the original and rescaled levels. We now have two recursion relations

$$x' = \Xi^b(x) \quad (3)$$

$$z' = \Xi^s(x, z) \quad (4)$$

where the renormalized fugacities  $x'$  and  $z'$  are the generating functions of a single site on the rescaled lattice. These equations have three relevant fixed points, one of which is the non trivial fixed point

$$(x_c, z_c) = (x_0, x_0) \quad (5)$$

that describes an adsorption transition (parameters  $x_0$  are given in the Table 1).

Linearising the transformation around the non trivial fixed point we have found two eigenvalues,  $\lambda_b$  and  $\lambda_s$  greater than 1, corresponding to the bulk relation (3) and to the surface one (4) respectively. These two eigenvalues give the gyration-radius critical exponent<sup>(1, 2, 10)</sup>  $\nu$  as

$$\nu = \ln b / \ln \lambda_b \quad (6)$$

and the crossover exponent  $\phi$  as

$$\phi = \ln \lambda_s / \ln \lambda_b \quad (7)$$

### 3. RESULTS

The results for  $x_0$ ,  $\nu$  and  $\phi$  of these transformations are given in Table 1 for branched polymers on the square lattice. They are calculated for the lattice lengths up to  $b = 8$  for site lattice animals with and without loops and up to  $b = 9$  for partially directed site lattice animals without loops.

In order to check the method, first we calculate the critical exponent  $\nu$ , characterizing the asymptotic behavior of the gyration-radius, by fitting the data of Table 1 using the well known method<sup>(4, 11)</sup> from previous RG studies. We find  $\nu^{-1} = 1.5359 \pm 0.00074$  and  $\nu^{-1} = 1.535.3 \pm 0.00074$ , i.e.,

Table 1. The Critical Fugacity  $x_0$  and Critical Exponent  $\nu$  and  $\phi$  for the Three Types of Branched Polymers

$b$	Branched polymers with loops			Branched polymers without loops			Partially directed branched polymers without loops		
	$x_0$	$\nu$	$\phi$	$x_0$	$\nu$	$\phi$	$x_0$	$\nu$	$\phi$
2	0.4142136	0.7093612	1	0.4342585	0.7356318	1	0.4342585	0.7356318	1
3	0.3753542	0.6988892	0.9140544	0.400784	0.7223553	0.9212795	0.4071852	0.7306958	0.9198715
4	0.3486432	0.6915812	0.8246388	0.3738285	0.7120518	0.8316720	0.3856786	0.7258583	0.8304434
5	0.3301402	0.6872023	0.7565650	0.3548813	0.7056771	0.7631695	0.3710354	0.7238691	0.7623623
6	0.3167621	0.6842946	0.7043124	0.3408167	0.7011724	0.7102433	0.3602381	0.7229523	0.7098788
7	0.3067325	0.6821372	0.6630225	0.3301334	0.6977803	0.6682530	0.3521470	0.7226918	0.6686098
8	0.2989777	0.6803934	0.6295093	0.3217905	0.6950506	0.6341411	0.3458856	0.7227126	0.6353874
9							0.3409241	0.7228735	0.6080247

$\nu = 0.6511 \pm 0.00034$  and  $\nu = 0.6513 \pm 0.00034$  for branched polymers modeled as site lattice animals with loops and site lattice animals without loops on the simple square lattice. We can see that these two models, within error bars, give the consilient value for the critical exponent  $\nu$ , so these results prove that the hypothesis<sup>(3, 12)</sup> that branched polymers with and without loops, in a good solvent, belong to the same universality class is valid for the case of branched polymers modeled as a site lattice animals. The results we have got for critical exponent  $\nu$  are in good agreement with these already found for site lattice animals.<sup>(4, 13, 14)</sup> It is easy to see from the Table 1 that the partially directed polymers without loops do not belong to the same universality class as the above two models. The same is true for the partially directed polymers with loops. We can conclude that partially directed site lattice animals is a too simplified model and it can not be used for studying branched polymers in a good solvent. However, this model gives the similar behavior for the surface crossover exponent (see Table 1) which is in favor of the hypothesis of universality.

Our analyses show that in order to find the crossover exponent  $\phi$  for the infinite system it is convenient to introduce a new variable  $l = \exp(-\frac{2}{9}b)$ . The data for the crossover exponent  $\phi$  of Table 1, for not too small  $b$ , can be fitted well as a function of  $l$  by the second degree polynomial function

$$\phi(b) = \phi + c_1 l + c_2 l^2 \quad (8)$$

see Fig. 2. Fitting the data of Table 1 to (8), where we have omitted the first two points in order to have a smaller error, we extrapolate the finite- $b$  results to the limit  $b \rightarrow \infty$ . We have found  $\phi = 0.502 \pm 0.003$  for branched polymers and  $\phi = 0.503 \pm 0.003$  for branched polymers without loops modeled as a site lattice animals. For both models the crossover exponent  $\phi$  is consistent with the hyperuniversality conjecture  $\phi = \frac{1}{2}$ .<sup>(5, 6)</sup>

#### 4. CONCLUSION

We have studied branched polymers modeled as site lattice animals situated on the square lattice with adsorbed surfaces using a renormalization group approach. The three cases studied are: (a) randomly branched polymers without loops (tree-like branched polymers) where two elements belonging to it are connected through one and only one path in the animal, (b) randomly branched polymers with loops in which branch endpoints are allowed to be connected to other elements of the polymer, thereby forming loops and (c) partially directed randomly branched polymers without loops where every polymer configuration is represented by one connected cluster starting from the lower left hand corner that may grow only in the positive

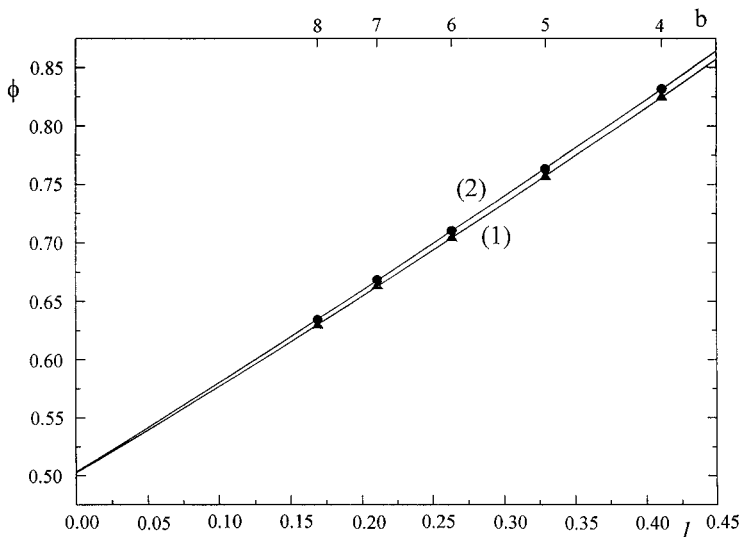


Fig. 2. Dependence of  $\phi$  against  $l = \exp(-\frac{2}{3}b)$  from Table 1. The curves through the points are the best fit to our two sets of data; (1) for branched polymers with loops and (2) for branched polymers without loops.

$X$  direction while walks in the  $Y$  direction are without limitation. But we have found that the third model is too simplified to be used for studying branched polymers.

We have found the gyration radius critical exponent for the branched polymers with loops  $\nu = 0.6511 \pm 0.0003$  and for the branched polymers without loops  $\nu = 0.6513 \pm 0.0003$  which is in good agreement with results already found for site animals<sup>(4, 13, 14)</sup> and supports the hypothesis that branched polymers with and without loops, in a good solvent, belong to the same universality class.<sup>(3, 12)</sup>

The crossover exponent  $\phi$  has the value  $\phi = 0.502 \pm 0.003$  for branched polymers with loops and  $\phi = 0.503 \pm 0.003$  for branched polymers without loops. This is consistent with the exact value of the crossover exponent<sup>(5, 6)</sup> ( $\phi = 1/2$ ) for the adsorption problem and agrees well with transfer-matrix<sup>(7)</sup> and series expansion.<sup>(8)</sup>

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