Universality of surface exponents of self-avoiding walks on a Manhattan lattice

1991 J. Phys. A: Math. Gen. 24 1867

(http://iopscience.iop.org/0305-4470/24/8/026)

J. Phys. A: Math. Gen. 24 (1991) 1867–1874. Printed in the UK

Universality of surface exponents of self-avoiding walks on a Manhattan lattice

S L A de Queiroz† and J M Yeomans

Department of Theoretical Physics, University of Oxford, 1 Keble Road, Oxford OX1 3NP, UK

Received 1 February 1991

Abstract. We use phenomenological renormalization group techniques to study the bulk and surface properties of self-avoiding walks on a Manhattan lattice. We find that, as is the case for the bulk exponents, the underlying bond directionality does not change the universality class of the surface exponents relative to undirected lattices. We also obtain an estimate for the position of the binding transition.

We present a transfer matrix study of a self-avoiding walk on a Manhattan lattice. The Manhattan lattice is a two-dimensional square lattice on which bonds are directed, as shown in figure 1(*a*), so there is no overall directional bias [1,2]. Recent work [3,4] has suggested that the collapse transition (tricritical point) of a self-avoiding walk on Manhattan lattices lies in a different universality class from that on non-directed, two-dimensional lattices. Our aim in this paper is to discuss whether a similar division occurs for the surface critical exponents. This seems a possibility given that surface phenomena along, for example, the (1,0) direction would take place in a locally directed environment. To this end we study the adsorption transition: in addition to exponents, we also obtain estimates for the critical fugacity and the value of the surface interaction at which the walk becomes bound.

We consider a self-avoiding walk on a strip of width L. To implement the phenomenological renormalization group [5], a transfer matrix is constructed for the strip. The critical fugacities and exponents can be calculated from the largest eigenvalue. Extrapolation to $L \to \infty$ then gives estimates for the behaviour of the two-dimensional system [6].

Both free and periodic boundary conditions will be used, the latter in order to provide estimates of bulk quantities for comparison. In the case of free boundary conditions an energy $-\epsilon^s$ is assigned to each bond that lies along either side of the strip. If ω is the monomer fugacity the generating function of the model can be written

$$\mathcal{Z} = \sum_{\text{walks}} \omega^N \kappa^{N^s} \tag{1}$$

† On sabbatical leave from Departamento de Física, PUC/RJ, CxP 38071, 22453 Rio de Janeiro RJ, Brazil.

0305-4470/91/081867+08$03.50

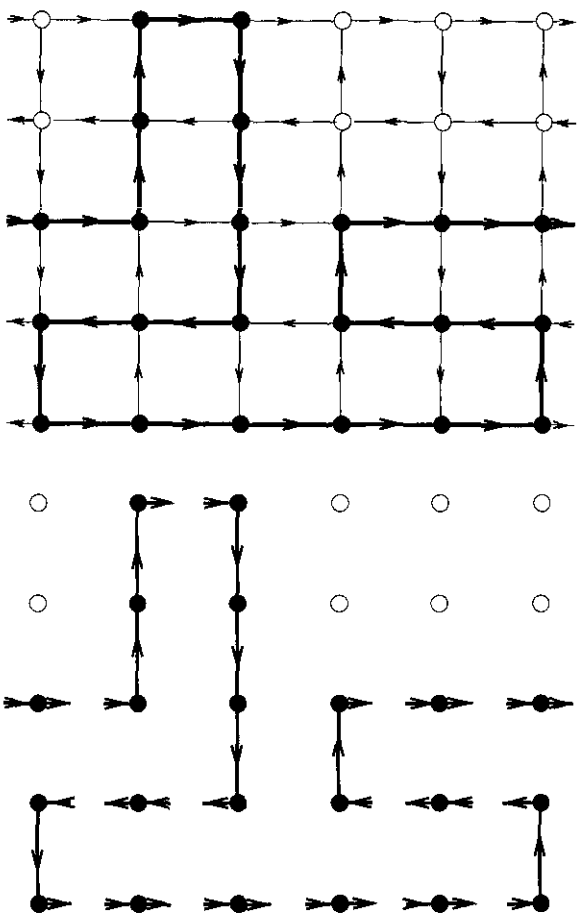

Figure 1. (*a*) A self-avoiding walk on a strip of the Manhattan lattice, of width $L = 5$. Note the underlying bond directionality of the lattice itself. (*b*) The self-avoiding walk decomposed into a sequence of column states.

where $\kappa = \exp \epsilon^s/kT$ and N and N^s count the total number of steps in the walk and at the surface respectively.

The generating function can be written in terms of transfer matrices, $\mathbf{T}^{\uparrow}$, $\mathbf{T}^{\downarrow}$. The first step is to divide all the self-avoiding walk configurations on a strip into a sequence of columns. Figure 1(*b*) shows the decomposition of the walk in figure 1(*a*). The set of allowed column states forms the basis for the transfer matrices. Transfer matrix elements, $\mathbf{T}_{jk}$, are labelled by the states of consecutive columns, j and k, and are defined as

$$\mathbf{T}_{jk}^{\uparrow,\downarrow} = \omega^{N_{jk}} \kappa^{N_{jk}^s} \tag{2}$$

if the states can be connected to form a self-avoiding walk and zero otherwise. Different transfer matrices (which we label $\uparrow$ and $\downarrow$) are needed to add states preceded by columns of bonds pointing upwards and downwards, as the connectivity is different in the two cases. N_{jk} and N_{jk}^s are respectively the total number of steps and of surface steps between the centres of the columns j and k.

For free boundary conditions, in contrast to the case for self-avoiding walks on non-directed lattices, only strips of odd widths can be used. This is because a final row of bonds directed to the left, say, forms a trap for a walk progressing from the left. As a result the transfer matrices for strips of width L and $L+1$ are identical for odd L. For periodic boundary conditions only even L must be used, to avoid two adjacent rows of bonds pointing in the same direction. It is possible to reach a maximum strip width $L = 12$ for the Manhattan lattice with periodic boundary conditions and $L = 13$ with free boundary conditions. In table 1 we compare the sizes of the transfer matrices for self-avoiding walks on the Manhattan and the non-directed square lattice [7], both with free boundary conditions.

Table 1. A comparison of the sizes of the transfer matrices for self-avoiding walks on the non-directed square and Manhattan lattices, for free boundary conditions.

	No of basis states		No of non-zero matrix elements	
L	Square	Manhattan	Square	Manhattan
3	5	4	15	7
4	12		60	
5	30	16	247	48
6	76		1040	
7	196	68	4453	353
8	512		19328	
9	1353	304	84848	2745
10	3610		376064	
12				
13		6752		185534

The partition function for a walk with ends respectively in the 0th and Rth columns can be written in terms of the transfer matrix

$$\mathcal{Z}_{L,R} = \boldsymbol{v}^{t}(\mathbf{T}^{\alpha}\mathbf{T}^{\beta})^{R/2}\boldsymbol{u} \qquad (R \text{ even})$$
$$\mathcal{Z}_{L,R} = \boldsymbol{v}^{t}(\mathbf{T}^{\alpha}\mathbf{T}^{\beta})^{(R-1)/2}\mathbf{T}^{\alpha}\boldsymbol{u} \qquad (R \text{ odd}) \tag{3}$$

where $\boldsymbol{u}$ and $\boldsymbol{v}$ are vectors which depend on the initial and final positions of the walk and R is the end-to-end distance measured along the strip. Summing over all R gives the generating function.

As $R \to \infty$ the expression for $\mathcal{Z}_{L,R}$ is dominated by the largest eigenvalue of the transfer matrix, λ_L, and the partition function is given by

$$\mathcal{Z} \sim (\lambda_L)^R \qquad R \to \infty. \tag{4}$$

Hence the generating function diverges as $\lambda_L \to 1$. The singularity in $\mathcal{Z}_L$ is due to the divergence of the average length of the self-avoiding walk and defines the critical fugacity ω_L^* for a strip of width L

$$\lambda_L(\omega_L^*(\kappa)) = 1. \tag{5}$$

The correlation length on a strip of width L is related to the largest eigenvalue through

$$\xi_L = -(\ln \lambda_L)^{-1}. \tag{6}$$

We shall be concerned with the critical behaviour at two fixed points.

1. The ordinary fixed point, $(\omega^*, \kappa^*)_{\text{ord}}$, which governs the critical behaviour of the unbound phase. Here the surface interactions are irrelevant.
2. The special fixed point, $(\omega^*, \kappa^*)_{\text{sp}}$, which describes the binding transition.

For large enough L the correlation length on a strip of width L is expected to scale as

$$L^{-1}\xi = F(L^{y}(\omega - \omega^*); L^{y^s}(\kappa - \kappa^*)) \tag{7}$$

where $\nu = 1/y$ is the usual bulk correlation length exponent

$$\xi \sim (\omega - \omega^*)^{-\nu} \tag{8}$$

and the crossover exponent

$$\phi = y^s/y. \tag{9}$$

The leading relevant exponent y is expected to be the same at the ordinary and special fixed points. y^s describes an irrelevant variable at the ordinary fixed point and a relevant variable at the special fixed point; hence it is negative at the former and positive at the latter. We shall use the notation $(y^s)_{\text{ord}}$ and $(y^s)_{\text{sp}}$ to distinguish the two cases where necessary. At the binding transition $\nu^s = 1/y^s$ describes the divergence of the thickness of the adsorbed layer

$$\xi^{\perp} \sim (\kappa - \kappa^*)^{-(\nu^s)_{\text{sp}}}. \tag{10}$$

We shall also calculate the decay-of-correlation exponents η and η^s given through:

$$\Gamma_b(r) \sim 1/r^{\eta} \tag{11}$$

and

$$\Gamma_s(r) \sim 1/r^{\eta^s} \tag{12}$$

where $\Gamma_b(r)$, $\Gamma_s(r)$ are correlation functions at criticality between points separated by r, in the bulk and along the surface respectively.

We implement the phenomenological renormalization group in two ways.

(i) *One-parameter renormalization group*

We first consider no surface binding ($\kappa = 1$). A series of approximations to the critical fugacity, ω_L^*, are obtained by comparing the correlation lengths on strips of two successive widths

$$\frac{\xi_L(\omega_L^*)}{L} = \frac{\xi_{L-2}(\omega_L^*)}{L-2}. \tag{13}$$

By linearising about the (ordinary) fixed point a series of approximations to the exponent y, defined in equations (7) and (8), can be obtained

$$y_L = \frac{\ln\{(\mathrm{d}\xi_L/\mathrm{d}\omega)_{\omega_L^*} / (\mathrm{d}\xi_{L-2}/\mathrm{d}\omega)_{\omega_L^*}\}}{\ln(L/L-2)} - 1. \tag{14}$$

We assume that the system is conformally invariant, even though the bonds are directed. Directionality is expected to be irrelevant here, since it has only a local (as opposed to global) character for the Manhattan lattice. We may then calculate a series of finite-size estimates to η

$$\eta_L^{\$} = \frac{2L}{\pi \xi_L(\omega_\infty^*)} \tag{15}$$

for free boundary conditions and

$$\eta_L = \frac{L}{\pi \xi_L(\omega_\infty^*)} \tag{16}$$

for periodic boundary conditions. Here, ω_∞^* stands for the critical fugacity of the infinite lattice [8]. We have used the series estimate $\omega_\infty^*=0.5771 \pm 0.0002$ [9].

Results for free and periodic boundary conditions are shown in tables 2 and 3 respectively. The extrapolated values were obtained by fitting the results for the three largest L values to the formula

$$\omega_L^* = \omega_\infty^* + \frac{A}{L^\psi} \tag{17}$$

where A and ψ are constants, and similarly for the other quantities.

(ii) *Two-parameter renormalization group*

We next consider a strip with free boundary conditions and allow the surface interaction to vary [10, 11]. Fixed points (ω_L^*, κ_L^*) are obtained by comparing the correlation length on three strips

$$\frac{\xi_{L-2}(\omega_L^*, \kappa_L^*)}{L-2} = \frac{\xi_L(\omega_L^*, \kappa_L^*)}{L} = \frac{\xi_{L+2}(\omega_L^*, \kappa_L^*)}{L+2}. \tag{18}$$

These equations give two fixed points: the ordinary fixed point, which describes the behaviour of the unbound walk and the special fixed point which describes the walk's behaviour at the binding transition.

Table 2. Critical properties of the Manhattan lattice: results from one-parameter renormalization group with free boundary conditions.

L	ω_L^*	y_L	$\eta_L^{\$}$
3	—	—	0.7070 ± 0.0009
5	0.61246	1.4231	0.8752 ● 0.0018
7	0.59405	1.4018	0.968 ± 0.003
9	0.58660	1.3856	1.026 ± 0.004
11	0.58296	1.3739	1.064 ± 0.005
13	0.58096	1.3654	1.090 ● 0.006
Extrapolated	0.5766	1.303	1.25 ± 0.02
Best estimates	0.5771 ± 0.0002	4/3	5/4

Table 3. Critical properties of the Manhattan lattice: results from the one-parameter renormalization group with periodic boundary conditions.

L	ω_L^*	y_L	η_L
4	—	—	0.3136 ± 0.0007
6	0.56590	1.5172	0.2801 ± 0.0013
8	0.57150	1.4524	0.2611 ± 0.0020
10	0.57429	1.4141	0.2507 ± 0.0027
12	0.57568	1.3892	0.2503 ± 0.0035
Extrapolated	0.5780	1.307	0.23 ± 0.02
Best estimates	0.5771 ± 0.0002	4/3	5/24

Linearizing around the fixed points the exponents y and y^s are found to be solutions of an equation

$$\frac{\frac{\partial \xi_{L-2}}{\partial \omega} - \left(\frac{L-2}{L}\right)^{1+y^i} \frac{\partial \xi_L}{\partial \omega}}{\frac{\partial \xi_{L-2}}{\partial \omega} - \left(\frac{L-2}{L+2}\right)^{1+y^i} \frac{\partial \xi_{L+2}}{\partial \omega}} = \frac{\frac{\partial \xi_{L-2}}{\partial \kappa} - \left(\frac{L-2}{L}\right)^{1+y^i} \frac{\partial \xi_L}{\partial \kappa}}{\frac{\partial \xi_{L-2}}{\partial \kappa} - \left(\frac{L-2}{L+2}\right)^{1+y^i} \frac{\partial \xi_{L+2}}{\partial \kappa}} \tag{19}$$

where all the derivatives are evaluated at the fixed point in question, and $y^i = y$, y^s [12]. $(\eta_L^s)_{\mathrm{ord}}$ and $(\eta_L^s)_{\mathrm{sp}}$ are then calculated from (15) where ξ_L is estimated at the finite-size estimates to the critical point. This is because, in contrast to the one-parameter case, estimates of $(\omega_\infty^*, \kappa_\infty^*)$ more accurate than our own are not available. Of course ω_∞^*, as a bulk property, is independent of κ for $\kappa \leq (\kappa^*)_{\mathrm{sp}}$; however, it would be inconsistent to use, for example, the series estimate of [9] while the corresponding κ_L^* suffers from unknown finite-size inaccuracies.

The results are shown in tables 4 and 5 for the ordinary and special fixed points respectively. Where possible, the data were extrapolated using (17); where this did not give a sensible result because of non-monotonic convergence, data for the largest two strip widths were extrapolated against L^{-1}. This was the case for all quantities evaluated at the ordinary fixed point except y_L.

Table 4. Critical properties of the Manhattan lattice at the ordinary fixed point results of the two-parameter renormalization group.

L	ω_L^*	κ_L^*	y_L	$(y_L^s)_{\mathrm{ord}}$	$(\eta_L^s)_{\mathrm{ord}}$
7	0.57981	0.7507	1.4956	−1.5598	1.2542
9	0.57560	0.6863	1.4298	−0.9697	1.3662
11	0.57576	0.6913	1.3987	−0.9420	1.3601
13	0.57612	0.7101	1.3801	−0.9518	1.3412
Extrapolated	0.5781	0.814	1.327	−1.006	1.238
Best estimates	0.5771 ± 0.0002	—	4/3	−1	5/4

It is always difficult to assess the accuracy of a phenomenological renormalization group calculation, as corrections to scaling introduce unknown systematic errors for finite values of L. One way is to compare results from several different implementations of the technique where such alternatives exist. Comparing the results for ω_∞^* from tables 2–5 we would conclude $\omega_\infty^* = 0.577 \pm 0.001$. This agrees well with, but is less precise than, the best series estimate available, 0.5771 ± 0.0002 [9].

Table 5. Critical properties of the Manhattan lattice at the special fixed point: results of two-parameter renormalization group.

L	ω_L^*	κ_L^*	y_L	$(y_L^s)_{sp}$	$(\eta_L^s)_{sp}$
7	0.57871	1.4448	1.3730	0.7844	−0.0353
9	0.57777	1.4556	1.3582	0.7437	−0.0478
11	0.57738	1.4611	1.3518	0.7232	−0.0555
13	0.57719	1.4643	1.3482	0.7112	−0.0606
Extrapolated	0.5769	1.472	1.339	0.679	−0.084
Best estimates	0.5771 ± 0.0002	—	4/3	2/3	−1/12

For the value of κ at which the walk binds to the surface, we have only one estimate, namely $(\kappa^*)_{sp} = 1.472$ (table 5). Using the extrapolation (17) on $L = 7, 9, 11$ rather than $L = 9, 11, 13$ gives an identical result, suggesting that corrections to scaling may be unimportant. Thus, this may be a good estimate; however, it is not possible to give realistic error bars.

Our results for critical exponents are less precise. Averaging over results from the different approaches gives $y = 1.32 \pm 0.02$, in good agreement with the exact value for isotropic two-dimensional lattices, 4/3 [13]. Our value for the exponent which describes the decay of correlations in the bulk is $\eta = 0.23 \pm 0.02$, where the error bars arise from the uncertainty in the series estimate of ω_∞^*. This value is very close to the exact one for non-directed lattices, 5/24 (see for example [14] and references therein). This corroborates series results [9, 15, 16] which, taken together, indicate that all bulk exponents are the same for the Manhattan and non-directed lattices.

If the same is true for surface critical exponents, $(\eta^s)_{ord}$ is expected to take the value 5/4 [17]. Taking into account the extrapolated results from the one- and two-parameter renormalization groups (tables 2 and 4 respectively), one obtains $\eta_L^s = 1.25 \pm 0.02$. Furthermore, at the ordinary fixed point (table 4), the extrapolation for the irrelevant eigenvalue $(y^s)_{ord} = -1.006$ is in good agreement with the corresponding exact value of -1 for isotropic lattices [10, 11, 17]. A similar picture holds at the special fixed point (table 5); the extrapolated exponent estimates $(y^s)_{sp} = 0.679$ and $(\eta^s)_{sp} = -0.084$ agree very well with the exact values for undirected lattices, 2/3 and $-1/12$ respectively [10, 11, 17]. Thus there is no evidence that the surface critical behaviour of self-avoiding walks on the Manhattan lattice lies in a new universality class.

Our work is tantamount to a check of the universality of the high-temperature phase of self-attracting self-avoiding walks on the Manhattan lattice. It is interesting to note that the universality of all bulk and surface exponents with those for undirected lattices has already been obtained for Hamiltonian walks (which correspond to the low-temperature phase) on the Manhattan lattice [18]. With all exponents equal to their undirected-lattice counterparts at both ends of the temperature range, the non-universality found at the collapse point [3, 4] becomes an even more interesting effect. We hope to explore this in the future.

Acknowledgments

We should like to thank Andrew Veal for access to the transfer-matrix programmes for isotropic self-avoiding walks, and Rob Hutchings of OUCS for computational advice.

SLAdQ thanks R M Bradley for sending his results prior to publication, and Brazilian Government agencies CNPq, CAPES and FINEP for financial support.

References

[1] Kasteleyn P W 1963 *Physica* **29** 1329
[2] Barber M N 1970 *Physica* **48** 237
[3] Bradley R M 1989 *Phys. Rev.* A **39** 3738
[4] Bradley R M 1990 *Phys. Rev.* A **41** 914
[5] Derrida B 1981 *J. Phys. A: Math. Gen.* **14** L5
[6] Barber M N 1983 *Phase Transitions and Critical Phenomena* vol 8, ed C Domb and J L Lebowitz (New York: Academic) p 145
[7] Veal A R 1990 *DPhil Thesis* University of Oxford unpublished
[8] Cardy J L 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55
[9] Enting I G and Guttmann A J 1985 *J. Phys. A: Math. Gen.* **18** 1007
[10] Guim I and Burkhardt T W 1989 *J. Phys. A: Math. Gen.* **22** 1131
[11] Veal A R, Yeomans J M and Jug G 1991 *J. Phys. A: Math. Gen.* **24** 827
[12] Derrida B and Herrmann H J 1983 *J. Physique* **44** 1365
[13] Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1062
[14] Saleur H and Derrida B 1986 *J. Stat. Phys.* **44** 225
[15] Malakis A 1975 *J. Phys. A: Math. Gen.* **8** 1885
[16] Guttmann A J 1983 *J. Phys. A: Math. Gen.* **16** 3885
[17] Duplantier B and Saleur H 1986 *Phys. Rev. Lett.* **57** 3179
[18] Duplantier B 1987 *J. Stat. Phys.* **49** 411