Critical behavior at the theta point of self-avoiding walks on a Manhattan lattice

1991 J. Phys. A: Math. Gen. 24 L933

(http://iopscience.iop.org/0305-4470/24/16/009)

J. Phys. A: Math. Gen. 24 (1991) L933–L939. Printed in the UK

LETTER TO THE EDITOR

Critical behaviour at the θ point 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 17 May 1991

Abstract. We study the collapse of self-attracting self-avoiding walks on a Manhattan lattice, by means of phenomenological renormalization group techniques. Our results support a recent prediction of non-universality for the entropic exponent γ. The surface exponents are in the same universality class as the θ transition on undirected lattices, thus differing from those of the θ' point. We use a two-parameter renormalization group to obtain estimates of the crossover exponent.

This letter describes a transfer matrix study of the collapse transition 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, such that there is no overall directional bias [1, 2]. In recent work [3, 4], the following exact results have been proposed for the collapse transition (tricritical point) of a self-avoiding walk with nearest-neighbour attractive interactions on a Manhattan lattice. Firstly the critical fugacities are predicted to be $\frac{1}{2}$ and $\sqrt{2}$ for steps of the walk and nearest-neighbour interactions respectively. Secondly the entropic exponent γ is shown to be $\frac{6}{7}$, thus differing from the corresponding value $\frac{8}{7}$ for non-directed, two-dimensional lattices [5, 6]. The correlation-length exponent ν, on the other hand, is expected to be $\frac{4}{7}$ as in the non-directed case.

An argument is given, that γ differs on the Manhattan and non-directed lattices because on the latter the partition function includes contributions from self-trapping configurations excluded in the former. It seems surprising that this, being a purely geometric feature, should affect the value of γ only at the collapse transition: it is known that in the high-temperature phase γ does not differ from the corresponding value for undirected lattices [7, 8].

All the results described above were derived from a correspondence between walks on the Manhattan lattice and the hull of a percolation cluster at criticality, with the help of exact results for the latter.

We present here a direct numerical check of such claims. Our results are consistent with those described above, although some discrepancies are present. We also study the surface and crossover exponents, which do not seem to be accessible by the methods of [3, 4].

† On sabbatical leave from Departamento de Física, PUC/RJ, Cx.P. 38071, 22453 Rio de Janeiro RJ, Brazil, from 1 August 1990 to 31 July 1991.

Indirect support for the location of the tricritical point and for a value of $\gamma = \frac{6}{7}$ can be found by recalling a mapping, proposed in references [3, 4], between tricritical self-avoiding walks on the Manhattan lattice and a restricted model of trails on the square lattice. The latter model is equivalent to the zero-component limit of an $O(n)$ model on a square lattice with a particular set of couplings [9], which has been solved exactly at criticality [10]. Again, surface and crossover exponents have not been discussed.

We consider a self-avoiding walk on a strip of width L. Attractive interactions, $-J$, are introduced as usual between nearest-neighbour sites visited by the walk. An example is shown in figure 2. This model is described by the generating function

$$\mathscr{Z} = \sum_{\text{walks}} \omega^N \tau^{\tilde{N}} \tag{1}$$

where ω is the step fugacity, $\tau = \exp j/kT$ and N and $\tilde{N}$ count the number of steps in the walk and number of interactions respectively. For fixed τ, the partition function becomes singular at a critical fugacity $\omega_c(\tau)$. At high temperatures this corresponds to a second order phase transition, at which the average walk length diverges. The collapse (or θ) transition, to a phase with finite density, occurs at a tricritical point (ω_t, τ_t).

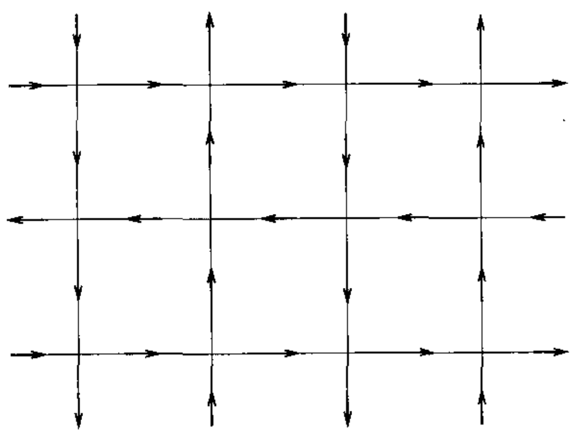

Figure 1. The Manhattan lattice.

The generating function can be written in terms of transfer matrices, $\mathbf{T}^{\uparrow}$, $\mathbf{T}^{\downarrow}$, where the basis states of the transfer matrix are labelled by the configuration of bonds within a vertical column, together with the bonds entering or leaving that column. As bond directionalities alternate, different matrices (labelled $\uparrow$, $\downarrow$) are needed to add successive layers to the strip. The correlation length on a strip of width L is related to the largest eigenvalues $\lambda_L^{\uparrow}$, $\lambda_L^{\downarrow}$ through

$$\xi_L = -2(\ln \lambda_L^{\uparrow} \lambda_L^{\downarrow})^{-1}. \tag{2}$$

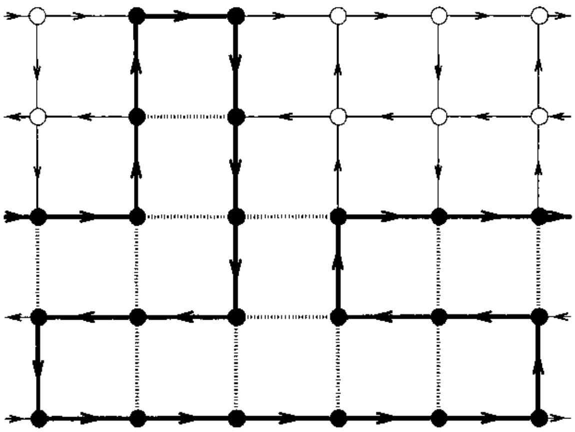

Figure 2. A self-avoiding walk with nearest-neighbour attractive interactions (denoted by hatched lines) on a strip of the Manhattan lattice, of width $L=5$.

Results will be presented for both free and periodic boundary conditions. For the former, in contrast to the case for self-avoiding walks on non-directed lattices [11], only strips of odd widths can be used. This is because a final row of bonds directed on 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. We were able to reach a maximum strip width $L=12$ for the Manhattan lattices with periodic boundary conditions and $L=11$ with free boundary conditions.

We implement the phenomenological renormalization group in three ways.

(i) *One-parameter renormalization group with τ fixed.* The collapse transition is predicted [3, 4] to take place at $(\omega_t, \tau_t)=(\frac{1}{2}, \sqrt{2})$. Therefore, our first approach was to set $\tau=\tau_t=\sqrt{2}$ and to use a one-parameter phenomenological renormalization group to obtain finite-size approximations to the critical fugacity, $\omega_L^*(\tau_t)$, defined by comparing the correlation lengths on strips of two successive widths

$$\frac{\xi_L(\omega_L^*)}{L}-\frac{(\xi_{L-2}(\omega_L^*)}{L-2}. \tag{3}$$

Linearizing around the fixed point of (3) gives a series of approximations for the correlation-length exponent

$$\nu_L^{-1}=\frac{\ln\{(\mathrm{d}\xi_L/\mathrm{d}\omega)_{\omega_L^*}/(\mathrm{d}\xi_{L-2}/\mathrm{d}\omega)_{\omega_L^*}\}}{\ln(L/L-2)}-1. \tag{4}$$

Results for free and periodic boundary conditions are shown in tables 1(a) and (b) respectively. Whenever the sequences of finite-size estimates behave smoothly and converge sufficiently rapidly, extrapolated values can sensibly be obtained by fitting

Table 1. θ point of self-avoiding walks on the Manhattan lattice: results from the one-parameter renormalization group with $\tau=\sqrt{2}$.

L	ω_L^*	ν_L^{-1}	$\eta'_L(\omega_t=\frac{1}{2})$	$\eta'_L(\omega_L^*)$
(*a*) Free foundary conditions				
3	—	—	0.945 38	—
5	0.533 20	1.704 90	1.214 37	0.736 27
7	0.515 90	1.711 51	1.378 23	0.992 44
9	0.508 90	1.715 21	1.487 40	1.167 15
11	0.505 50	1.717 73	1.564 89	1.292 70
Expected	$\frac{1}{2}$	$\frac{7}{4}$	2	2
(*b*) Periodic boundary conditions				
4	—	—	0.485 41	—
6	0.502 16	0.780 79	0.495 61	0.475 74
8	0.502 08	1.732 94	0.507 89	0.476 49
10	0.502 89	1.691 69	0.527 68	0.464 19
12	0.503 64	1.653 98	0.555 34	0.447 46
Expected	$\frac{1}{2}$	$\frac{7}{4}$	$\frac{1}{2}$	$\frac{1}{2}$

the results for the three largest L values to the formula

$$\omega_L^* = \omega_\infty^* + \frac{A}{L^\psi} \tag{5}$$

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

For free boundary conditions, the extrapolations obtained using (5) are $\omega_\infty^*=0.4993$, $\nu_\infty^{-1}=1.734$, in good agreement with the predicted values $\frac{1}{2}$ and $\frac{7}{4}$ respectively. For periodic boundary conditions the results are still moving away from the expected values with increasing L, presumably showing that these strip widths are still far from the asymptotic scaling regime.

Next we examine the exponent γ, with the help of the scaling relation $\eta=2-\gamma/\nu$, where η describes the decay of correlations. Finite-size approximations to η can be obtained from

$$\eta_L = \frac{L}{\pi\xi_L^p} \tag{6}$$

where the correlation length is evaluated for a strip with periodic boundary conditions. Results were obtained by calculating the correlation lengths both at the presumed exact critical fugacity $\omega_t=\frac{1}{2}$ of the infinite lattice [12] and at ω_L^* defined by (3). The latter procedure is especially useful when the location of the critical point is itself under investigation. Here, it provides a convenient estimate of the amount of uncertainty induced by calculating critical quantities at approximate values of the critical parameters. As we shall see below, this can be very large in the present case.

The arguments of [3, 4] give $\gamma=\frac{6}{7}$ and $\nu=\frac{4}{7}$, implying $\eta=\frac{1}{2}$. For two-dimensional, undirected lattices, one has [5, 6] $\gamma=\frac{8}{7}$, $\nu=\frac{4}{7}$, giving $\eta=0$. Results for η from the present calculations are presented in table 1(*b*). There is a very strong dependence of our estimates on fugacity, because the correlation length changes rather quickly as ω is varied. Hence it is difficult to obtain precise results. Nevertheless, it is safe to state that $\eta=0$ is definitely outside our error estimates, no matter how generous these are.

Rough extrapolations of the data in table 1(b) against $1/L$ would give $\eta_\infty(\omega_t=\frac{1}{2})\simeq 0.7$, $\eta_\infty(\omega_L^*)\simeq 0.3$, so a final estimate of $\eta=0.5\pm 0.2$ gives an approximate idea of the uncertainties involved. Thus, our results are a clear sign that the collapse transition of self-avoiding walks on a Manhattan lattice lies in a different universality class to that on non-directed two-dimensional lattices. It must be noted, however, that for each individual sequence of finite-size estimates, the values of η diverge from the expected value of $\frac{1}{2}$ with increasing L. Presumably this is because the asymptotic scaling regime has not yet been reached, with the difficulty being compounded by the large error in η which results from any inaccuracy in the estimates for the critical fugacities.

It is also possible to obtain finite-size approximations to the exponent, η^s, which describes the decay of correlations along the surface

$$\eta_L^s=\frac{2L}{\pi\xi_L^f} \tag{7}$$

where the correlation length is evaluated for strips with free boundary conditions. Again, we have calculated the correlation length both at $\omega=\omega_t=\frac{1}{2}$ and at ω_L^* given by (3). Results are presented in table 1(a). They strongly suggest convergence towards the value 2 conjectured by Seno and Stella [6] for the θ point of self-avoiding walks on non-directed lattices, rather than to $\eta^s=0$ as proposed by Duplantier and Saleur [5] for the so-called θ' point (at which a subset of next-nearest neighbour interactions is present in addition to first-neighbour couplings).

Note that, in using (6) and (7), we have assumed 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 [8].

(ii) *One-parameter renormalization group with ω fixed.* As a complement to the results just described, we fixed $\omega=\omega_t=\frac{1}{2}$ and allowed τ to vary. Fixed points are then located as before through (3), but with ω replaced by τ. Note that at the fixed point the estimate of ν is still given by (4), as the step fugacity is the relevant field for the correlation length in a one-parameter formulation. Results are given in tables 2(a) and

Table 2. θ point of self-avoiding walks on the Manhattan lattice: results from the one-parameter renormalization group with $\omega=\frac{1}{2}$.

L	τ_L^*	ν_L^{-1}	$\eta_L^s(\tau_L^*)$
(a) Free boundary conditions			
5	1.576 03	1.832 94	0.833 99
7	1.490 61	1.792 28	1.064 35
9	1.456 40	1.769 24	1.220 01
11	1.439 98	1.755 95	1.332 51
Expected	$\sqrt{2}$	$\frac{7}{4}$	2
(b) Periodic boundary conditions			
6	1.427 10	1.790 27	0.480 44
8	1.425 45	1.742 98	0.482 41
10	1.429 12	1.707 00	0.473 86
12	1.432 53	1.674 93	0.460 98
Expected	$\sqrt{2}$	$\frac{7}{4}$	$\frac{1}{2}$

(*b*) for free and periodic boundary conditions respectively. A very similar pattern is seen to the case with fixed τ.

For free boundary conditions the results for τ_L^* and ν_L^{-1} extrapolate, using (5), to 1.411 and 1.716 respectively, in reasonable agreement with the predicted values $\sqrt{2}$ and $\frac{7}{4}$. Again, the results obtained for η^s are consistent with a value of 2 rather than zero [5, 6].

For periodic boundary conditions, the finite-size estimates of τ_L^*, ν_L^{-1} and η (the latter calculated at the fixed point of (3)) are again close to the expected values, $\sqrt{2}$, $\frac{7}{4}$ and $\frac{1}{2}$ respectively. However, as was the case for fixed τ, they do move slightly away from these values as L increases.

(iii) *Two-parameter renormalization group.* In an attempt to obtain estimates of the crossover exponent, we performed a two-parameter renormalization group in which the system was allowed the freedom to find a fixed point (ω_L^*, τ_L^*) by comparing the correlation lengths on three strips

$$\frac{\xi_{L-2}(\omega_L^*, \tau_L^*)}{L-2} = \frac{\xi_L(\omega_L^*, \tau_L^*)}{L} = \frac{\xi_{L+2}(\omega_L^*, \tau_L^*)}{L+2}. \tag{8}$$

Linearizing around the fixed points the exponents $y = \nu^{-1}$ and $y_2 = \phi/\nu$, where ϕ is the usual crossover exponent, are solutions of an equation

$$\frac{\dfrac{\partial\xi_{L-2}}{\partial\omega} - \left(\dfrac{L-2}{L}\right)^{1+y^i} \dfrac{\partial\xi_L}{\partial\omega}}{\dfrac{\partial\xi_{L-2}}{\partial\omega} - \left(\dfrac{L-2}{L+2}\right)^{1+y^i} \dfrac{\partial\xi_{L+2}}{\partial\omega}} = \frac{\dfrac{\partial\xi_{L-2}}{\partial\tau} - \left(\dfrac{L-2}{L}\right)^{1+y^i} \dfrac{\partial\xi_L}{\partial\tau}}{\dfrac{\partial\xi_{L-2}}{\partial\tau} - \left(\dfrac{L-2}{L+2}\right)^{1+y^i} \dfrac{\partial\xi_{L+2}}{\partial\tau}} \tag{9}$$

where all the derivatives are evaluated at the fixed point and $y^i = y, y_2$ [13].

For strips with free boundary conditions there was no solution of (8) for physically acceptable values of the fugacities. For periodic boundary conditions the results are displayed in table 3. We have also obtained estimates for η as defined by (6), where the correlation length is evaluated at (ω_L^*, τ_L^*).

Table 3. θ point of self-avoiding walks on the Manhattan lattice: results of the two-parameter renormalization groups on strips of width $L-2$, L, $L+2$, with periodic boundary conditions.

L	ω_L^*	τ_L^*	ν_L^{-1}	$(y_2)_L$	η_L
6	0.502 96	1.409 49	1.505 90	1.188 08	0.474 03
8	0.485 80	1.501 82	1.657 91	1.050 45	0.524 69
10	0.477 23	1.545 50	1.736 40	1.036 46	0.558 05
Expected	$\frac{1}{2}$	$\sqrt{2}$	$\frac{7}{4}$	$\frac{3}{4}$	$\frac{1}{2}$

Extrapolating the results for (ω_L^*, τ_L^*) using (5) gives (0.462, 1.615). These values are not inconsistent with the exact proposal, $(\frac{1}{2}, \sqrt{2})$, given the known difficulty of using the transfer matrix approach to study the collapse transition of self-avoiding walks [14, 15]. However, as already noticed for the one-parameter calculations, the numerical results tend to move away from the values presumed to be exact with increasing L.

Results for ν^{-1} do move towards $\frac{7}{4}$ with increasing L, although an extrapolation using (5) gives 1.89, which has an error of $\simeq 10\%$. The estimates for η again exclude 0 and are close to $\frac{1}{2}$, but there is wide variation with L.

Using the prediction $\phi = \frac{3}{7}$ for the θ' point [5], and with $\nu^{-1} = \frac{7}{4}$, one would expect y_2 to approach $\frac{3}{4}$. Our results tend to a somewhat larger value; however, bearing in mind the uncertainties obtained for ν^{-1}, it is not safe to regard this as indicating a discrepancy.

In conclusion, we have presented a transfer matrix study of a self-avoiding walk with nearest-neighbour attractive interactions on a Manhattan lattice. It has been claimed [3, 4] that this model has a collapse transition at $(\omega_t, \tau_t) = (\frac{1}{2}, \sqrt{2})$, with a non-universal exponent $\eta = \frac{1}{2}$. For the collapse transition on a non-directed two-dimensional lattice η is expected to be zero.

The results from the one-parameter phenomenological renormalization group, assuming either $\tau = \tau_t = \sqrt{2}$ or $\omega = \omega_t = \frac{1}{2}$, are consistent with this. However, for strips with periodic boundary conditions, the estimates for η diverge from $\frac{1}{2}$ for increasing strip width L. Using a two-parameter renormalization group, we also obtain results consistent with those predicted, although our estimates (ω_L^*, τ_L^*) again move away from $(\frac{1}{2}, \sqrt{2})$ as L increases.

The discrepancies are most probably due to the failure to reach the scaling regime. Numerical studies of the collapse transition are known to be extremely difficult, due to strong finite size effects in the collapsed phase [14, 15]. It is therefore hardly surprising that our results are not more precise. However, they do provide support for the claim that η differs at the collapse transition of the Manhattan and non-directed lattices. We have also shown that the surface exponents are in the universality class of the θ, rather than the θ', point. Our results for the crossover exponent are not inconsistent with the value obtained for the θ' point [5], but are very imprecise. Further numerical investigation, by Monte Carlo or exact enumeration methods, would be desirable.

We should like to thank C Vanderzande and A L Stella for interesting conversations. 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] Duplantier B and Saleur H 1987 *Phys. Rev. Lett.* **59** 539
[6] Seno F and Stella A L 1988 *J. Physique* **49** 739
[7] Guttmann A J 1983 *J. Phys. A: Math. Gen.* **16** 3885
[8] de Queiroz S L A and Yeomans J M 1991 *J. Phys. A: Math. Gen.* **24** 1867
[9] Vanderzande C private communication
[10] Blöte H W J and Nienhuis B 1989 *J. Phys. A: Math. Gen.* **22** 1415
[11] Derrida B 1981 *J. Phys. A: Math. Gen.* **14** L5
[12] Cardy J L 1987 *Phase Transitions and Critical Phenomena* vol 11, ed C Domb and J L Lebowitz (New York: Academic) p 55
[13] Derrida B and Herrmann H J 1983 *J. Physique* **44** 1365
[14] Saleur H 1986 *J. Stat. Phys.* **45** 419
[15] Veal A R, Yeomans J M and Jug G 1991 *J. Phys. A: Math. Gen.* **24** 827