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J. Phys. A: Math. Gen. 17 (1984) L457–L461. Printed in Great Britain

LETTER TO THE EDITOR

A generalised self-avoiding walk

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Received 28 March 1984

Abstract. We study a generalised self-avoiding walk on a lattice in which each vertex may be visited less than k times. Turban has argued that, for this model, the critical exponents should change continuously with k from the standard self-avoiding walk exponents ($k=2$) to mean-field exponents. By generating series expansions for both two- and three-dimensional lattices, we find strong support for the conventional, and opposing, view that the critical exponents remain unchanged for finite k, only taking on their mean-field values in the limit $k \to \infty$.

Recently Turban (1983) suggested a generalised self-avoiding lattice walk in which the usual self-avoiding constraint does not apply until a particular vertex has been visited $k-1$ times. A kth visit is forbidden. For $k=2$ the usual self-avoiding walk (SAW) is recovered, while in the limit $k \to \infty$ it is clear that the pure random walk is obtained. Intermediate values of k therefore interpolate between these two limits.

During 1983 we investigated this problem, by series analysis, but did not publish our results as they were indicative of the behaviour we expected, which was that the critical exponents do not change with k (for finite k), and so the generalised problem remains in the same universality class as the SAW problem, a result we considered unsurprising.

Turban (1983), however, has given arguments to suggest totally different behaviour. His arguments, based both on a Flory theory argument and on the properties of fractals, suggest that the critical exponent characterising the mean square end-to-end distance through the relation $\langle R_N^2 \rangle \sim aN^{2\nu}$, should vary with k like

$$\nu_k = (k+1)/[(k-1)d+2] \tag{1}$$

whenever the spatial dimension $d \leqslant d_c(k) = 2k/(k-1)$.

This surprising result has prompted us to extend our series data and analyse it more carefully. Our re-analysis confirms our earlier results, which are therefore totally different from those obtained by Turban.

The problem appears to have been first suggested by Malakis (1975), who defined the model in passing and suggested the results found in this paper, that is, that there is no change in the critical exponents from the SAW values. In a subsequent paper, Malakis (1976) called these walks 'k-tolerant walks', where 'k' in Malakis's notation is '$k-1$' in the notation of Turban, and this paper. Malakis suggested that the problem is essentially different to the SAW problem in three dimensions (but not one and two) by invoking an argument based on the properties of pure random walks, and hence

0305-4470/84/090457+05$02.25 © 1984 The Institute of Physics

raised the possibility that the exponents may differ in the three-dimensional case. We shall show that this does not appear to be the case.

Firstly, let us look in more detail at the predictions of Turban's results. For $d=2$, $d<d_c(k)$ for all finite k, and $\nu_k=(k+1)/2k$, so that $\nu_2=\frac{3}{4}$, $\nu_3=\frac{2}{3}$, $\nu_4=\frac{5}{8}$, $\nu_5=\frac{3}{5}$, etc. Thus ν decreases monotonically with increasing k from the SAW value ($\nu=\frac{3}{4}$) to the mean-field value ($\nu=\frac{1}{2}$). Consider now the 'susceptibility' exponent γ characterising the growth in the number of chains C_n of length n through $C_n \sim A\mu^n n^{\gamma-1}$, where μ is a lattice-dependent growth constant. Clearly γ must also decrease from its value at $k=2$ ($\gamma=1.34375$) to the mean-field value of $\gamma=1$ as $k\to\infty$. Analogy with Turban's results for ν suggest that this decrease should be monotonic in k. Our findings are that γ remains constant for finite k at the $k=2$ (SAW) value, as might be expected from the following heuristic argument due to C J Thompson (private communication). Drawing on the analogy between the $n>0$ and the $n=0$ realisation of the n-vector model, we would expect that setting $k>2$ in the generalised SAW model corresponds to increasing the range of the interaction in an n-vector model, while still keeping the range finite. Under such circumstances one expects the exponents to remain unchanged.

For the two-dimensional triangular lattice we have generated series expansions for the number of n-step chains and for a range of values of k. The triangular lattice was chosen in order that the characteristic alternation of loose-packed lattice series would be absent. In table 1 we display the series coefficients for $k=2$ (the SAW problem) to $k=6$. Note that, in each case, for $0\leq n<2k-2$, the coefficients are given by 6^n, which is the pure random walks result. Therefore only for $n\geq 2k-2$ do the series coefficients reflect the self-avoiding constraint, and for that reason, as k increases, an increasing number of series coefficients are needed for the series to be analysed with confidence. Accordingly, we concentrate our analysis on those series with low values of k.

For $k=2$ we have the SAW series, for which 18 terms are known, and for which we find (Guttmann 1984) $\mu=4.1508$ and $\gamma=1.34375$ (Nienhuis 1982). A simple dlog Padé analysis of the series for $k>2$ (not shown) gives $\mu\approx 5.306$, $\gamma\approx 1.39$ for $k=3$, $\mu\approx 5.68$ and $\gamma\approx 1.4$ for $k=4$. These results immediately cast doubt on Turban's results, as they superficially suggest that γ *increases* with k, rather than decreasing as

Table 1. Chain generating function coefficients for generalised SAW on the triangular lattice.

$n \backslash k$	2	3	4	5	∞
0	1	1	1	1	1
1	6	6	6	6	6
2	30	36	36	36	36
3	138	216	216	216	216
4	618	1 260	1 296	1 296	1 296
5	2 730	7 206	7 776	7 776	7 776
6	11 946	40 650	46 440	46 656	46 656
7	51 882	227 256	276 054	279 936	279 936
8	224 130	1 262 832	1 633 848	1 678 320	1 679 616
9	964 134	6 983 730	9 633 366	10 051 782	10 077 696
10	4 133 166	38 470 220	56 616 140	60 132 100	60 466 176
11	17 668 938	211 220 800	331 847 200	359 296 300	362 797 056
12	75 355 206	1 156 490 000	1 940 717 000	2 144 325 000	2 176 782 336
13	320 734 686	6 317 095 284	11 327 957 196		
14	1 362 791 250	34 435 495 872	66 010 769 382		

Turban's theory would suggest. The reason for this apparent increase seems likely to be due to the presence of confluent singularities, and we investigate this in the following manner. We assume that the general coefficient C_n behaves in the following manner for sufficiently large n:

$$C_n \sim A\mu^n n^g(1 + B/n^\Delta + C/n + D/n^{\Delta+1} + \ldots) \tag{2}$$

where $g = \gamma - 1$, and Δ is the exponent corresponding to the confluent singularity. Then the ratio of successive terms is

$$r_n = C_n/C_{n-1} \sim \mu[1 + g/n - B\Delta/n^{1+\Delta} + \mathrm{O}(n^{-2}) + \mathrm{O}(n^{-3\Delta}) + \mathrm{O}(n^{-2-\Delta}) + \mathrm{O}(n^{-1-2\Delta})]. \tag{3}$$

To eliminate μ, we form ratios of ratios, and find

$$s_n = r_n/r_{n-1} - 1 \sim -g/n^2 + h/n^{2+\Delta} + \mathrm{O}(n^{-3}) + \mathrm{O}(n^{-2-2\Delta}) \tag{4}$$

where h can be expressed in terms of Δ, g and B. If γ (and hence g) is known, the quantity

$$t_n = s_n + g/n^2 \sim h/n^{2+\Delta} + \mathrm{O}(n^{-3}). \tag{5}$$

A plot of $\ln|t_n|$ against $\ln n$ should then produce a straight line with gradient $\Delta + 2$. If the value of g used is inaccurate, say $g^* \neq g$, the straight line should then have gradient 2, with intercept giving $g - g^*$. In figure 1 we show the log–log plot for $k = 2$ and 3, with g chosen to be 0.34375, in agreement with the $k = 2$ (SAW) result of Nienhuis (1982). The plots display decreasing curvature with increasing n, and from the obvious trend we obtain, from the last two points, that $\Delta_3 > 0.11$ ($k = 3$) and $\Delta_2 > 0.26$ ($k = 2$). Further, for $k = 3$ we have repeated the analysis using $g^* = 0.23$, and find that the last three points lie on a straight line of gradient 2.0, the intercept of which suggests $g - g^* \approx 0.16$, in agreement with the Padé approximant analysis cited earlier.

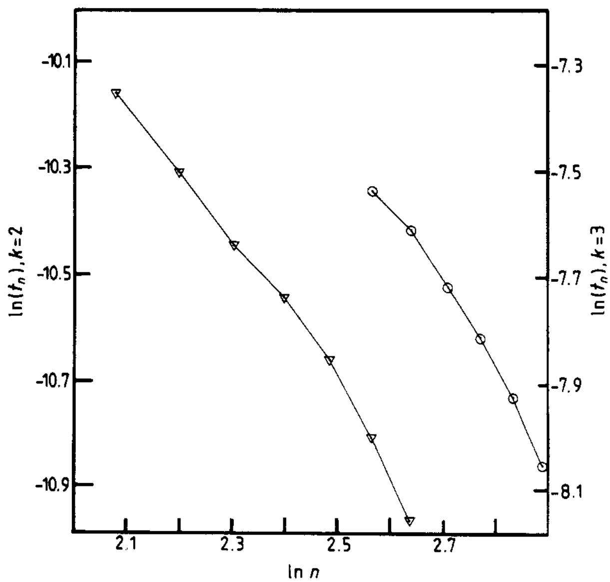

Figure 1. Log–log plot of t_n(equation (5)) against n for $k = 2$ ($\odot$) and $k = 3$ (∇) generalised SAWs on the triangular lattice. Gradient is a measure of $-(2 + \Delta)$.

For $k=4$ our series are too short to be successfully analysed by this technique, though the log–log plot of t_n against n does have gradient greater than 2, implying $\Delta_4 > 0$.

While this analysis is by no means conclusive, we believe that the fact that elementary methods of series analysis suggest $\gamma(k=3,4) > \gamma(k=2)$, in addition to the analysis given here, which gives a consistent interpretation that $\gamma(k<\infty) = \gamma(k=2)$, would seem to rule out $\gamma(k>2) < \gamma(k=2)$, as suggested by Turban's results.

Our results based on three-dimensional data lend stronger support to this view. In three dimensions, Turban predicts that only for $k=2$ is $d < d_c$, while for $k=3$, $d=3$ is the critical dimension. At the critical dimension we would expect mean-field exponents, modified by confluent logarithmic singularities. That is, for $d=3$, $k=3$ Turban predicts $\nu=\frac{1}{2}$, while for $d=3$, $k=2$ we expect $\nu \approx 0.59$ from RG results and series analysis. To check this result, we have generated series on the simple cubic

Table 2. Chain generating function coefficients and mean square end-to-end distances for simple cubic lattice $k=3$ SAWs.

n	C_n	$\langle R_n^2 \rangle$
0	1	1.000 000 00
2	36	2.000 000 00
3	216	3.000 000 00
4	1 260	4.114 285 71
5	7 350	5.231 836 73
6	42 462	6.412 886 82
7	245 664	7.589 097 30
8	1 412 568	8.820 938 89
9	8 131 062	10.046 906 79
10	46 617 096	11.319 872 69
11	267 490 638	12.586 548 61
12	1 530 512 418	13.894 446 64
13	8 763 095 548	15.195 887 58

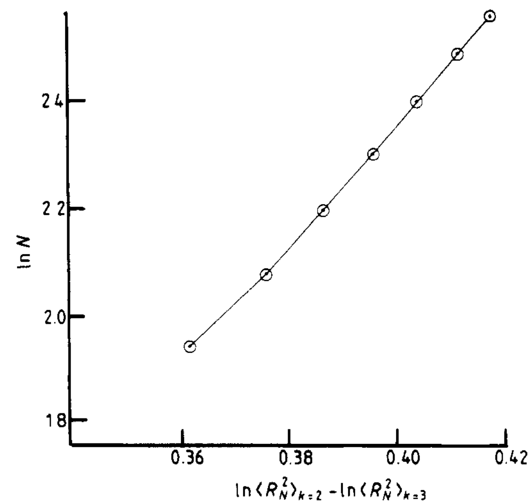

Figure 2. Log–log plot of $\langle R_N^2\rangle_{k=2}/\langle R_N^2\rangle_{k=3}$ against N for $k=3$ generalised SAWs on the simple cubic lattice. Gradient is a measure of $2(\nu_2-\nu_3)$.

lattice for $k=3$. We have obtained both the number of chains and their mean square end-to-end distance. If Turban is correct, the ratio $\langle R_N^2\rangle_{k=2}/\langle R_N^2\rangle_{k=3} \sim CN^{2(\nu_2-\nu_3)} \approx CN^{0.18}$. A log–log plot of this ratio should be linear with slope given by $2(\nu_2-\nu_3)$. The raw data are shown in table 2, and the log–log plot is shown in figure 2. It can be seen from figure 2 that the gradient is *decreasing* with increasing N, and the last two points already yield a straight line with gradient 0.074.

Assuming this trend continues then yields $\nu_2-\nu_3<0.37$, compared with Turban's prediction of 0.09. The behaviour we observe is entirely consistent with the expected behaviour $\nu_2=\nu_3$, and the previously expressed view that, for $k=3$, the model has the same critical exponents as for $k=2$. Thus in conclusion we find that the generalised SAW belongs to the same universality class as the usual SAW, contrary to Turban's arguments.

We have benefited from discussions and correspondence with Professors Colin J Thompson and Stuart G Whittington.

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