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LETTER TO THE EDITOR

Self-avoiding walks with nearest- and next-nearest-neighbour steps

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Abstract. Self-avoiding walks of 12 steps and fewer have been enumerated for the square lattice, for the case in which steps can occur between both nearest-neighbour and next-nearest-neighbour lattice sites. The appropriate two-variable generating function diverges along a critical line with a constant exponent $\gamma \sim \frac{4}{3}$, in agreement with general universality expectations.

The properties of self-avoiding walks (chains) on a regular lattice are of theoretical interest, as a general problem in lattice statistics. Their interest in physics stems mainly from their use in polymer physics, as models of polymer chains which incorporate excluded-volume effects. Self-avoiding walks also provide the largest contribution to the high-temperature susceptibility of the Ising model and are consequently of interest in the field of critical phenomena. A review by Domb (1969) gives an extensive discussion of the field.

Exact enumerations of short chains (up to ~10–20 steps) have been carried out for all of the regular two- and three-dimensional lattices, primarily at King's College, London (Martin *et al* 1967, Sykes *et al* 1972). From this work it has been well established that the chain generating function $C(x)$ has a power-law singularity at a 'critical point' x_c with asymptotic behaviour $C(x) \sim A(1-x/x_c)^{-\gamma}$. The critical exponent γ appears to be universal and has values close to, and possibly exactly equal to, $\frac{4}{3}$ and $\frac{7}{6}$ in two and three dimensions respectively. The amplitude A and the critical point x_c vary from lattice to lattice.

All of the previous studies have considered self-avoiding walks with only nearest-neighbour steps, or chains with only nearest-neighbour links. It is possible to consider a more general problem, in which next-nearest-neighbour steps are also permitted. As part of a study of the Ising model with nearest- and next-nearest-neighbour interactions, we have enumerated such chains with up to and including 12 links on the square lattice. This Letter presents the data and a numerical analysis of the appropriate two-variable generating function. The enumeration was carried out directly, using the University of Alberta Amdahl 470 computer, and took about $3\frac{1}{2}$ hours of CPU time.

We denote by $c_{m,n}$ the number of chains consisting of m nearest-neighbour links and n next-nearest-neighbour links. Table 1 gives the values of these coefficients for the

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Table 1. Values of $c_{m,n}$—the number of chains with m nearest-neighbour and n next-nearest-neighbour steps, for the square lattice.

1	0	0·400 000 000 0E+01	0	1	0·400 000 000 0E+01	2	0	0·120 000 000 0E+02
1	1	0·320 000 000 0E+02	0	2	0·120 000 000 0E+02	3	0	0·360 000 000 0E+02
2	1	0·136 000 000 0E+03	1	2	0·160 000 000 0E+03	0	3	0·360 000 000 0E+02
4	0	0·100 000 000 0E+03	3	1	0·528 000 000 0E+03	2	2	0·936 000 000 0E+03
1	3	0·672 000 000 0E+03	0	4	0·100 000 000 0E+03	5	0	0·284 000 000 0E+03
4	1	0·182 400 000 0E+04	3	2	0·456 800 000 0E+04	2	3	0·508 800 000 0E+04
1	4	0·252 800 000 0E+04	0	5	0·284 000 000 0E+03	6	0	0·780 000 000 0E+03
5	1	0·614 400 000 0E+04	4	2	0·190 080 000 0E+05	3	3	0·302 400 000 0E+05
2	4	0·240 480 000 0E+05	1	5	0·892 800 000 0E+04	0	6	0·780 000 000 0E+03
7	0	0·217 200 000 0E+04	6	1	0·195 840 000 0E+05	5	2	0·745 360 000 0E+05
4	3	0·148 600 000 0E+06	3	4	0·170 056 000 0E+06	2	5	0·103 272 000 0E+06
1	6	0·301 120 000 0E+05	0	7	0·217 200 000 0E+04	8	0	0·591 600 000 0E+04
7	1	0·617 920 000 0E+05	6	2	0·271 864 000 0E+06	5	3	0·669 040 000 0E+06
4	4	0·968 960 000 0E+06	3	5	0·853 872 000 0E+06	2	6	0·414 104 000 0E+06
1	7	0·984 000 000 0E+05	0	8	0·591 600 000 0E+04	9	0	0·162 680 000 0E+05
8	1	0·188 800 000 0E+06	7	2	0·962 896 000 0E+06	6	3	0·275 779 200 0E+07
5	4	0·494 871 200 0E+07	4	5	0·556 484 000 0E+07	3	6	0·394 500 000 0E+07
2	7	0·157 628 000 0E+07	1	8	0·313 504 000 0E+06	0	9	0·162 680 000 0E+05
10	0	0·441 000 000 0E+05	9	1	0·573 696 000 0E+06	8	2	0·326 860 800 0E+07
7	3	0·108 707 680 0E+08	6	4	0·228 242 400 0E+08	5	5	0·319 150 240 0E+08
4	6	0·290 704 240 0E+08	3	7	0·170 920 960 0E+08	2	8	0·576 264 000 0E+07
1	9	0·979 808 000 0E+06	0	10	0·441 000 000 0E+05	11	0	0·120 292 000 0E+06
10	1	0·170 673 600 0E+07	9	2	0·109 055 840 0E+08	8	3	0·406 804 640 0E+08
7	4	0·993 782 720 0E+08	6	5	0·163 309 072 0E+09	5	6	0·185 617 480 0E+09
4	7	0·141 067 904 0E+09	3	8	0·703 711 360 0E+08	2	9	0·203 943 040 0E+08
1	10	0·301 347 200 0E+07	0	11	0·120 292 000 0E+06	12	0	0·324 932 000 0E+06
11	1	0·506 022 400 0E+07	10	2	0·353 781 760 0E+08	9	3	0·148 160 432 0E+09
8	4	0·407 264 240 0E+09	7	5	0·780 257 600 0E+09	6	6	0·104 626 505 6E+10
5	7	0·995 441 568 0E+09	4	8	0·645 195 808 0E+09	3	9	0·277 937 792 0E+09
2	10	0·702 884 240 0E+08	1	11	0·914 883 200 0E+07	0	12	0·324 932 000 0E+06

square lattice (for $m+n \leqslant 12$). A generating function can be defined by

$$C(x, y) = \sum_{m,n=0}^{\infty} c_{m,n} x^m y^n \tag{1}$$

with $c_{0,0} = 1$. For $y = 0$ (or equivalently for $x = 0$) the problem reduces to the usual one of chains with only nearest-neighbour links. We expect that the function $C(x, y)$ will diverge along a critical line in the (x, y) plane with a characteristic exponent γ which, according to general ideas of universality, should remain constant along this line.

Techniques for numerical analysis of such power series have been used with considerable success in the field of critical phenomena (see e.g. Gaunt and Guttmann 1974), and we have used these methods to determine the position of the critical line and to estimate the value of the exponent γ. We introduce polar coordinates (z, θ) and analyse single-variable series in z for fixed values of θ. For fixed θ the generating function is expected to have the asymptotic behaviour

$$C(z) \sim A(\theta)(1 - z/z_c(\theta))^{-\gamma}. \tag{2}$$

The series are most amenable to analysis by Padé approximants, and in table 2 we give some details for the case $\theta = 45°$. Results of similar consistency are obtained for

Table 2. Series analysis for $\theta = 45°$.

(a) Estimates of z_c from poles of $[N, D]$ Pade approximants to the series for $(d/dz) \log C(z)$.

[7, 4]	[6, 5]	[5, 6]	[4, 7]	[6, 4]	[5, 5]	[4, 6]
0·242 284	0·242 285	0·242 273	0·242 287	0·242 287	0·242 265	0·242 266

(b) Estimates of γ from Pade approximants to the series for $(z_c - z)(d/dz) \log C(z)$, evaluated at $z_c =$ 0·24228.

[7, 4]	[6, 5]	[5, 6]	[4, 7]	[6, 4]	[5, 5]	[4, 6]
1·333 35	1·333 43	1·333 43	1·333 49	1·333 45	1·333 35	1·333 46

(c) Estimates for z_c from poles of $[N, D]$ Pade approximants to the series for $[C(z)]^{1/\gamma}$, with $\gamma = \frac{4}{3}$.

[8, 4]	[7, 5]	[6, 6]	[5, 7]	[4, 8]	[6, 5]	[5, 6]
0·242 280	0·242 280	0·242 278	0·242 278	0·242 280	0·242 278	0·242 278

other values of θ, and yield the locus of the critical line in the (x, y) plane as shown in figure 1. Ratio analysis is complicated by the presence of odd–even oscillations, characteristic of bipartite lattices. These oscillations are due to interfering negative singularities and are most pronounced near $\theta = 0°$ and $\theta = 90°$. The ratio results are consistent with but less precise than the Padé results. Estimates of the exponent γ are marked by a high degree of consistency, and provide strong evidence for the hypothesis that γ is constant along the entire critical line, and takes the value $\gamma = 1·333$ $(=\frac{4}{3})$.

It is hoped that these results may be of some interest to workers in the field of lattice statistics. They are certainly of relevance in the study of the Ising model with nearest- and next-nearest-neighbour interactions on the square lattice, and this topic will be discussed in a future publication. It is not clear whether chains of this type have any useful application in polymer problems.

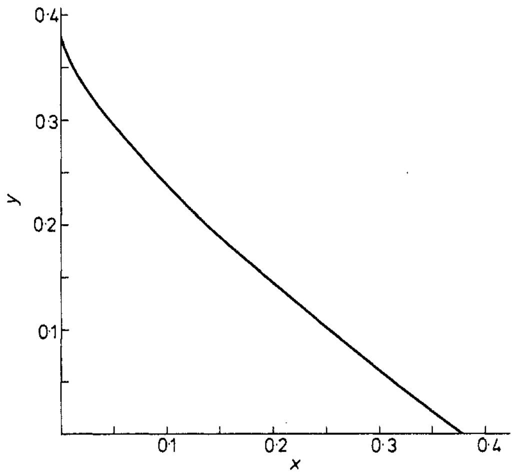

Figure 1. The locus of the line of singularities of the generating function $C(x, y)$ in the (x, y) plane. The uncertainty is estimated to be considerably less than the drawn width of the line.

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