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Diffusion on self-avoiding walk networks

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Abstract. Two properties of self-avoiding walk networks, constructed by connecting the nearest-neighbour points of self-avoiding walks on the square lattice, are studied numerically. The average end-to-end linear part of such networks is investigated, and is found to be proportional to the length of the walk. Secondly, random walks on this structure are studied and the associated spectral dimension of such networks is estimated to be 1.03 ± 0.03, which implies that the effect of such connections affects the spectral dimension only weakly, if at all.

1. Introduction

Self-avoiding walks (SAW) form a subset of Polya random walks in which no site has been visited more than once. Such walks model linear polymers in dilute solution. The excluded-volume effect is represented by self-avoidance in SAWs [1]. However, distinct points on such a walk can be situated very close to one another. In the lattice version of this walk, steps are denoted by bonds of the lattice and the walk is represented by joining successive bonds. The minimum distance of separation between two sites on the walk is the lattice constant. One can make this simple structure somewhat more complex by connecting any two neighbouring sites on the SAW, and the resulting structure is called the SAW network (see figure 1(*a*)). We call these link bonds 'bridges', and bonds on the walk 'streets' [2]. This network is used to study a number of properties such as electrical conductivity, or the spectral distribution of low-energy phonons in linear polymers [4]. Recently there has been renewed interest in problems of diffusion on random structures [3], because of their application to these and related problems, such as the reptation problem in three dimensions introduced by de Gennes [1].

2. Linear part

Consider an electrical circuit constructed by placing unit resistors both along the streets and the bridges of the SAW network. Now if a current I is introduced at the initial point and emerges from the final point of the network of length N, then within the network there is a distribution of currents. Let i be the current in a particular bond; then a bond can be labelled by a number $\alpha = i/I$ which has a distribution $n(\alpha)$. One can construct the moments $M(k) = \Sigma\, \alpha^k n(\alpha)$ and fit $\langle M(k) \rangle \sim N^{\xi(k)}$ where $\langle \ldots \rangle$ denotes the average over different configurations of the SAW network. Here $M(0)$ is

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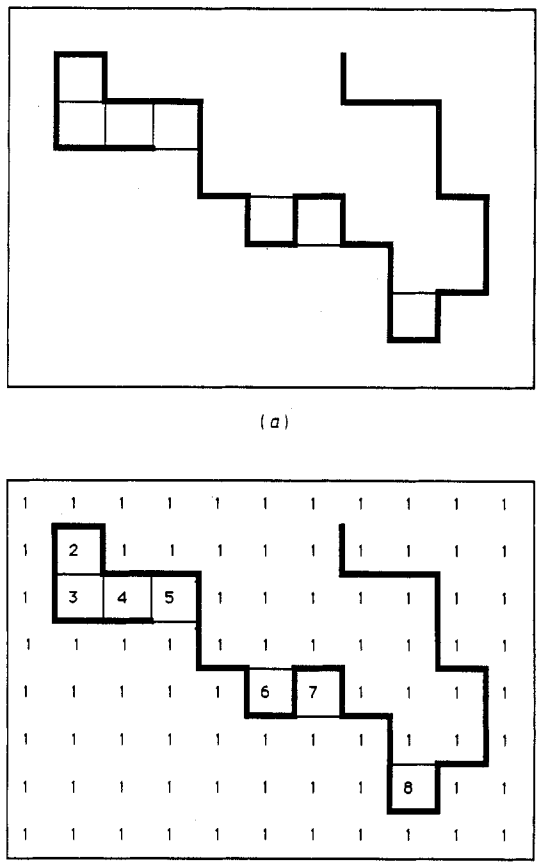

Figure 1. (*a*) A typical SAW network of 30 steps; 'streets' are shown by thick lines and 'bridges' are shown by thin lines. (*b*) The linear part calculation. Both streets and bridges are shown by thick lines; bonds of the network with squares on both sides with the same number constitute the linear part; here it is of length 13 units.

the total number of bonds of the network, and from an estimate of $\xi(0)$ the value of the fractal dimension of the network can be obtained. $M(2)$ is the end-to-end resistance of the network, and $\xi(2)$ is the average end-to-end resistance exponent. $M(\infty)$ is the number of bonds in the network carrying the total current I, and constitutes the linear part of the network, while the corresponding exponent $\xi(\infty)$ is the linear part exponent. As α is less than or equal to 1, one has the inequality $M(0) \geqslant M(2) \geqslant \ldots \geqslant M(\infty)$ and this implies a similar inequality for the exponents $\xi(k)$. For percolation clusters this type of calculation has already been done [5].

The resistance of such networks has been studied by a direct renormalisation method, and the average resistance was predicted to be proportional to the chain length, which implies $\xi(2) = 1$ [6]. However, the same exponent is claimed to be 0.88 by a small-cell real-space renormalisation group (RSRG) method [2] and 0.92 by a computer simulation method [7]. We study here the linear part of this network, and estimate the value of the corresponding exponent $\xi(\infty)$ with the expectation that if the SAW network is a non-trivial one (with exponent $\xi \neq 1$) the non-triviality should

be most prominent for the linear part. Using the method of extensive computer simulations by both exact enumeration and Monte Carlo methods, we estimate the linear part exponent $\xi(\infty) = 0.99 \pm 0.01$ which suggests that the exponent is very likely to be 1. This implies that the result of $\xi(2) = 1$ in [6] is entirely consistent with our result of $\xi(\infty) \simeq 1$. We now believe that the earlier result $\xi(2) = 0.92$ is an effective exponent for small values of N [7].

The linear part between the endpoints of a SAW network consists of those bonds of the network which carry the total current. A second definition is: those bonds of the network which are common to all distinct self-avoiding walks between the endpoints of the SAW network constitutes the linear part.

We use the second definition to estimate the linear part exponent of the SAW network for small values of walk length N (up to 18). Here we exactly enumerate all distinct SAWs on the square lattice for a particular walk length. For each walk configuration we first construct the SAW network by joining the nearest-neighbour sites on the walk. Then on that network we enumerate all distinct SAWs starting from the initial point and ending at the final point. We count (a) total number of bonds in the network $M(0)$, (b) the minimum length s_N of all these SAWs which is the minimum path between the endpoints and (c) the number of bonds of the network which are traversed by all walks contributing to the linear part $M(\infty)$. We sum these quantities over all distinct walks and get $\Sigma M(0)$, Σs_N and $\Sigma M(\infty)$ (see table 1). The average minimum path $\langle s_N \rangle$ has already been calculated (up to $N = 14$ on square lattice) in the literature in the context of the Ising model on a SAW network [8].

We used the method of differential approximants [18, 19] to fit generating functions for the averages of these quantities assuming standard algebraic singularities, which implies the forms $\langle M(0) \rangle \sim N^{\xi(0)}$, $\langle s_N \rangle \sim N^{x}$ and $\langle M(\infty) \rangle \sim N^{\xi(\infty)}$. In this manner we used the protocol described in [18, 19] to form exponent estimates and error estimates, and find $\xi(0) = 0.996 \pm 0.005$, $x = 0.991 \pm 0.010$ and $\xi(\infty) = 0.990 \pm 0.010$.

We know that the average size of SAWs, $\langle R_N \rangle$, varies with walk length N as $\langle R_N \rangle \sim N^{\nu}$ with $\nu = \frac{3}{4}$ in two dimensions [9]. Using this relation we can write $\langle M(0) \rangle \sim \langle R_N \rangle^{\xi(0)/\nu}$ where $\xi(0)/\nu$ gives the fractal dimension of the SAW network. Our estimate of $\xi(0) = 1$ implies that the fractal dimension of a SAW network is the same as that of ordinary SAW. This result is not unexpected since by the inclusion of bridges we only add mass to a particular length scale whereas to change the fractal dimension one should add mass to all length scales. Therefore with the values of $\xi(0)$ and $\xi(\infty)$ both equal to 1 we conclude that all intermediate moment exponents must be equal to 1.

The linear part exponent $\xi(\infty)$ was also estimated by the Monte Carlo simulation method. Here we generate SAWs of large lengths (N up to 640) using the dynamic Monte Carlo method called the 'pivot' algorithm [10]. We connect all neighbouring site pairs on a walk and thus get the SAW network. The linear part of this network is obtained by using the recently introduced algorithm of Roux and Hansen to find the backbone of a percolation cluster [11]. In this method we consider the clusters whose elements are unit squares on the lattice. Two such squares separated by a vacant bond are said to belong to the same cluster. A distinct cluster of such squares is surrounded by streets or bridges. We number these clusters of squares following the cluster counting algorithm [12]. After this numbering we count those bonds of the network which have squares on both sides with the same number. These bonds constitute the linear part of the network (see figure 1(b), which has linear part 13).

Using this method we have calculated the average linear part $\langle M(\infty) \rangle$ and the mean-square end-to-end distance $\langle R_N^2 \rangle$ of SAW networks of lengths $N = 28, 32, 40, 48, \ldots,$

Table 1. Exact enumeration data (a) for the sum over linear part ($\Sigma M(\infty)$), minimum path (Σs_N) and total mass ($\Sigma M(0)$) for SAW networks. For the Monte Carlo data (b), the average linear part $\langle M(\infty)\rangle$, the mean-square end-to-end distance $\langle R_N^2\rangle$ and the number of configurations considered is given.

(a) N	$\Sigma M(\infty)$	Σs_N	$\Sigma M(0)$
1	1	1	1
2	6	6	6
3	21	23	29
4	76	84	108
5	249	283	393
6	814	930	1 298
7	2 521	2 921	4 271
8	7 824	9 096	13 312
9	23 473	27 507	41 469
10	70 590	82 930	125 042
11	207 345	244 819	376 747
12	610 356	722 116	1 111 144
13	1 765 959	2 096 603	3 274 475
14	5 119 006	6 087 290	9 505 054
15	14 643 993	17 458 887	27 573 041
16	41 958 852	50 090 544	79 086 964
17	118 976 633	142 317 089	226 727 667
18	337 823 486	404 543 142	644 301 026

(b) N	Number of configurations	$\langle M(\infty)\rangle$	$\langle R_N^2\rangle$
28	1000 000	16.371	118.06
32	5000 000	18.581	143.94
40	5000 000	22.989	200.20
48	5000 000	27.406	262.11
64	6000 000	36.200	401.62
80	5000 000	45.008	559.77
96	5000 000	53.795	734.22
128	3500 000	71.430	1 127.7
160	2500 000	88.998	1 573.0
192	2500 000	106.62	2 065.6
256	3500 000	141.80	3 174
320	1550 000	176.84	4 429
384	1550 000	211.93	5 825
512	1550 000	282.68	8 973
640	1550 000	352.7	12 518

640. The number of configurations considered for each length varied from 100 000 to 500 000 (see table 1). A log-log plot of $\langle M(\infty)\rangle$ against N gives a value of $\xi(\infty) = 0.99 \pm 0.02$ (see figure 2), while a similar plot of $\langle R_N^2\rangle$ against N gives $\nu = 0.745 \pm 0.01$ (see figure 3).

3. Spectral dimension

Recently diffusion on different fractal structures and the associated spectral dimensions of such processes have been studied with great interest [13]. The spectral dimension

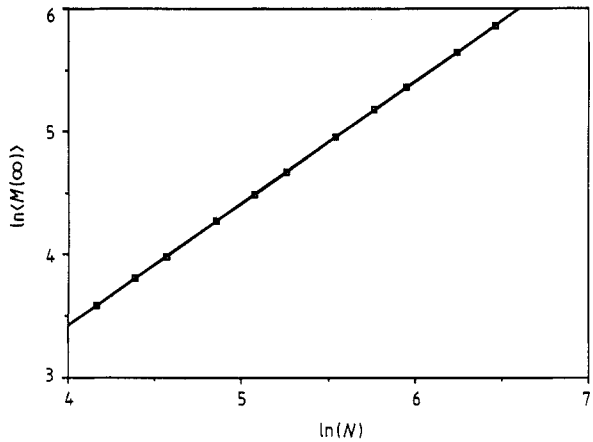

Figure 2. Log-log plot of average linear part $\langle M(\infty)\rangle$ against walk length N with a slope $\xi(\infty) = 0.99 \pm 0.02$.

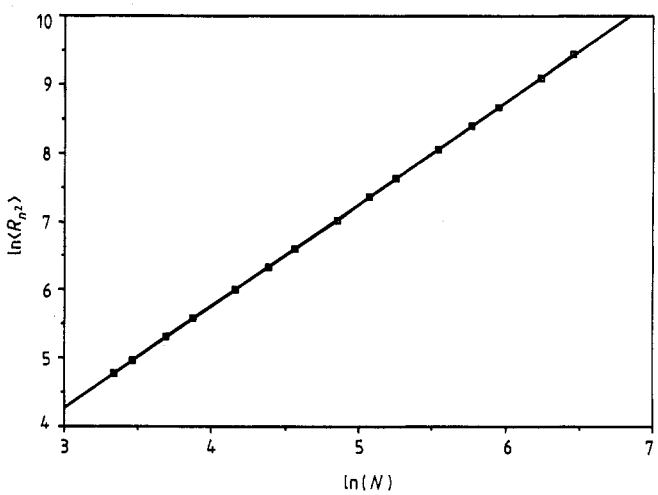

Figure 3. Log-log plot of mean-square end-to-end distance $\langle R_N^2\rangle$ against walk length N which gives $\nu = 0.745 \pm 0.010$.

d_s of some proteins has been measured by electron-spin-lattice relaxation experiments via the temperature dependence of the relaxation rate [14]. The spectral dimension describes the variation of the phonon density of states $\rho(\omega) \sim \omega^{d_s - 1}$ in the limit $\omega \to 0$. A value of $d_s = 1.65 \pm 0.04$ was obtained which is close to the value of the fractal dimension $d_f \simeq \frac{5}{3}$ and the conjecture was made that $d_s = d_f$ [14].

This result was used to explain the role of additional 'massless springs' present in protein molecules (e.g. hydrogen bonds) and thus to suggest modelling this system by a SAW network with bridges [4]. It is known that the phonon problem is equivalent to a diffusion problem of a random walker moving on a fractal lattice with the mean square end-to-end distance $\langle R_t^2\rangle$ varying with time t as $t^{2\nu}$ where $2\nu = d_s/d_f$ [20]. Therefore the dimension seen by a random walker is $d_w = 1/\nu = 2d_f/d_s$. In the absence of the bridges, the SAW structure is linear and its spectral dimension is 1. However, d_s

may be different for an SAW network due to the presence of bridges. It is argued in [4] that the number of bridges in a SAW network is so high that the diffusing particle will see the underlying Euclidean space which implies that d_s should be equal to d_f. This implies in two dimension that d_s should have a value of $\frac{4}{3}$. A Monte Carlo simulation has been done with random walks of 70 steps on SAW networks of 75 steps and $\nu = 0.72$ was obtained which implies $d_s = 0.96$ [2]. Alternatively, from a resistance measurement and subsequent application of scaling arguments it was claimed that $d_s = 1.04$ [7], while $d_s = 1$ was claimed in [15].

Recently this problem was also studied by using a Levy flight argument [16]. A jump of the walker across a bridge is considered as a step of length equal to the length I of the segment cut out by the jump along the walk. The probability distribution of such jumps is considered to be the same as the loop distribution deep inside the SAW chains, and is described by $P(I) \sim I^{-\mu}$, and the spectral dimension was estimated to be $d_s = 2(\mu - 1)/(3\mu - 5)$. With a value of $\mu = 2.95 \pm 0.20$ in $2d$ [17], d_s is estimated to be 1.01.

For this diffusion problem we simulate SAWs up to 10 000 steps using hash coding techniques in conjunction with the pivot algorithm from which we construct our SAW network. We start from an initial rod configuration and consider one configuration every 50th move. We discard the first 240 000 such configurations to get an equilibrium configuration. After that we generate a large number of SAW networks (up to 70 000 for $N = 10\,000$) for diffusion. We start a blind random walker† from the centre point of the walk, and it makes 100 steps through occupied sites (both streets and bridges are allowed). For each SAW network 100 such random walks are simulated. Data for the mean square end-to-end distance is accumulated in an array which is then averaged and analysed. We analysed the data by the ratio method with Neville-Aitken extrapolation [19] after applying a mild Euler transformation to eliminate the effect of the loose-packed lattice structure. We found the following exponents as a function of SAW length: $2\nu(1250) = 0.773 \pm 0.010$, $2\nu(2500) = 0.745 \pm 0.010$, $2\nu(5000) = 0.750 \pm 0.010$ and $2\nu(10\,000) = 0.762 \pm 0.008$. This suggest an increasing sequence of estimates of 2ν with increasing SAW length for walks longer than 1250 steps, though the evidence is not strong enough to rule out the value of $\nu = \frac{3}{8}$. Our preferred value is $2\nu = 0.77 \pm 0.03$. Using the relation $d_s = 2d_f\nu$ we find $d_s = 1.03 \pm 0.03$.

4. Conclusion

In this paper we have made a numerical study of two properties of SAW networks on a square lattice. In the first part, the average linear part and the average total number of bonds of the network are calculated, and the associated exponents are estimated. Both the exponents are found to be equal to 1 which implies that in spite of the presence of bridges the SAW network is basically a linear structure. However, the bridge connections still have some effect in some other phenomena, e.g. diffusion on such networks as those studied in the latter part of the paper. We estimate the spectral dimension of the network to be 1.03 ± 0.03 which shows that the effect of bridges, if any, is quite small.

† A blind random walker attempts steps in all possible lattice directions, whether allowed or not and pauses if a forbidden direction is chosen.

Acknowledgments

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References

[1] Montroll E W 1950 *J. Chem. Phys.* **18** 734
de Gennes P G 1979 *Scaling Concepts in Polymer Physics* (Ithaca, NY: Cornell University Press)
[2] Chowdhury D and Chakrabarti B K 1985 *J. Phys. A: Math. Gen.* **18** L377
[3] Kehr K W and Kutner R 1982 *Physica* A **110** 535
Dekeyser R, Maritan A and Stella A 1987 *Phys. Rev. Lett.* **58** 1758; 1987 *Phys. Rev.* A **36** 2238
Manna S S, Guttmann A J and Hughes B D 1989 *Phys. Rev.* A **39** 4337
[4] Helman J S, Coniglio A and Tsallis C 1984 *Phys. Rev. Lett.* **53** 1195
[5] de Arcangelis L, Redner S and Coniglio A 1985 *Phys. Rev.* B **31** 4725
[6] Ball R C and Cates M E 1984 *J. Phys. A: Math. Gen.* **17** L531
[7] Manna S S and Roy A K 1987 *Phys. Rev.* A **35** 4023
[8] Bhattacharya S and Chakrabarti B K 1984 *Z. Phys.* B **57** 151
[9] Nienhuis B 1982 *Phys. Rev. Lett.* **49** 1063
[10] Lal M 1969 *Mol. Phys.* **17** 57
Madras N and Sokal A D 1988 *J. Stat. Phys.* **50** 109
Kremer K and Binder K 1988 *Comput. Phys. Rep.* **7** 259
[11] Roux S and Hansen A 1987 *J. Phys. A: Math. Gen.* **20** L1281
[12] Hoshen J and Kopelman R 1976 *Phys. Rev.* B **14** 3438
[13] Stauffer D 1985 *Introduction to Percolation Theory* (London: Taylor and Francis)
Havlin S and Ben-Avraham D 1987 *Adv. Phys.* **36** 695
[14] Stapleton H J, Allen J P, Flynn C P, Stinson D G and Kurtz S R 1980 *Phys. Rev. Lett.* **45** 1456
[15] Stella A L, Dekeyser R and Maritan A 1986 *Fractals in Physics* ed L Pietronero and L Tosatti (Amsterdam: Elsevier)
[16] Bouchaud J P and Georges A 1987 *J. Phys. A: Math. Gen.* **20** L1161
[17] Redner S 1980 *J. Phys. A: Math. Gen.* **13** 3525
[18] Guttmann A J 1987 *J. Phys. A: Math. Gen.* **20** 1839
[19] Guttmann A J 1989 *Phase Transitions and Critical Phenomena* vol 13, ed C Domb and J Lebowitz (London: Academic)
[20] Alexander S and Orbach R 1982 *J. Physique Lett.* **43** L625