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Spectral dimension and the shortest path of SAWs with multi-neighbour interactions

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Abstract. The spectral dimension and the shortest path of self-avoiding walks (SAWs) with bridge length (interaction range) $b = 1, \sqrt{2}, \sqrt{3}, 2$ are studied numerically. The spectral dimension is calculated by performing exact multi-neighbour random walks on the Monte Carlo generated SAW configurations. It is found that the spectral dimension is not affected by the finite range of interactions (finite bridge length), and approach to $d_s = 1$ both in dimensions $d = 2$ and 3. The shortest path length S_N of the N-step SAW with local bridges is also investigated. It is shown that $S_N/N = A + N^{-\Delta}(B + C/N)$. Our numerical simulation results indicate that the exponent Δ is independent of the dimensionality, and is about 3/16 in dimensions $d = 2$-5.

1. Introduction

In the last fifteen years, many experiments [1] have been performed to study the spin-lattice relaxation in some proteins (large linear polymer molecules). It is found that, by fitting the experimentally observed spin-lattice relaxation time to the theoretical formula [2], the spectral dimension d_s [3] of ferredoxin comes to about 4/3 and that of the haemoproteins to about 5/3. In fact, it was found that for these polymer molecules, d_s equals to the respective fractal dimension d_f. If we consider that the protein (polymer) backbones to be self-avoiding walk (SAW) configurations and that the ferredoxin form the planner structures and haemoproteins form ball-like structures, one gets the observed values for the fractal dimensions of the proteins. But, as the SAWs are chain-structured objects, assuming the isotropic interactions between monomers, the spectral dimension d_s should be unity. This is in conflict with the experimental observations ($d_s = d_f > 1$).

In 1984, Helman *et al* [4] proposed a 'SAW with bridges' model, and they argued for a conjecture that the inclusion of the cross chain bridging interactions would eventually allow the diffusive modes to 'see' the embedding Euclidean space rather than the linear structure, so that normal diffusion would take place and d_s would be equal to d_f. Since then, many authors did extensive numerical simulations and theoretical analysis [5-9] essentially in the two-dimensional lattice with the nearest-neighbour bridges, and the conjecture was clearly disproved. People are also seeking other solutions to the problem [10]. It seems that the above theoretical efforts to deal with the problem went in the wrong direction: the experiments are done in the solvent

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(water), but the above theoretical models do not incorporate the solvent effect. In fact, in a different approach, proposed by one of the authors [11], it was argued that the solvent effect could make $d_s = d_f$.

Although the 'SAW with bridges' model is inappropriate for explaining the above-mentioned experimental observations regarding d_s, it remains a problem whether the inclusion of the local bridges into the SAW configurations could significantly change the predominant linear structure of the SAW chains and thereby change their spectral dimension or not. Actually, different authors give different results and conjectures [5-8]. Recently, Bouchaud *et al* [9] presented a Levy flight approach to the problem, and by using the known results for the statistics of finite loops in a SAW, they estimated that the spectral dimension for the three-dimensional 'SAW with bridges' model would be about 1.69. However, as the SAWs should be less compact than the random walks due to the excluded volume effect, it is hard to accept the result that the SAWs could have a larger spectral dimension than that of the random walks in a three-dimensional lattice. The spectral dimension of the random walks is approximated by the formula $d_s = 8/(4+d)$ [12]. In three dimensions, it is much smaller than the above-estimated spectral dimension of the SAWs. We tend to argue that in higher-dimensional spaces, the walker has more choice of directions to go; therefore it has a smaller probability of meeting the previously visited sites, and the structure would be more ramified and the spectral dimension should be smaller. In fact, above four dimensions, the cross chain interaction dies out and the scaling properties of the SAWs converge to that of the random walks [13], and the spectral dimension is exactly 1. It was already conjectured [5] that the inclusion of the finite length bridges would not change the spectral dimension of the system. This paper presents an extensive Monte Carlo simulation of the problem on the square lattice and on the cubic lattice with different bridge length b. Our numerical results indicate that the dynamical properties of SAWs with (finite length) bridges are essentially one dimensional: $d_s = 1$ in all d.

Also, the multifractal property of the 'SAW with bridges' network is of current interest. For example, the resistance $R_N \sim N^{\delta}$ of a SAW chain of length N (bridge bonds having identical resistance to the chain bonds), with δ as the resistance exponent [14, 6, 8], and the shortest path length $S_N \sim N^{\varepsilon}$, where ε is the shortest path exponent [15, 8] have recently been investigated in great detail and exponents δ and ε have been estimated (see also [16] for a recent study of the multifractal properties of the SAW networks in $d = 2$). All these results (mostly numerical, and in $d = 2$) indicate that the 'SAW with bridges' network is dominantly linear in structure ($\delta = \varepsilon = 1$). In fact, since the diffusion on the network is related to its conductivity, δ is related to d_s by a scaling relation [8] $d_s = 2/(1+\delta)$. Our results $d_s = 1$ for all d thus also implies $\delta = \varepsilon = 1$ for all d. However, there are expected to be significant finite-size scaling corrections to the leading linear scaling behaviour. On average, SAWs with finite range bridging interactions are expected to have significant corrections to scaling due to the local blobs (coming from the multiply connected structure due to local bridges), over the finite fraction of the linear region (not connected to other parts of the SAW by any finite range bridges or interactions). Quantities of interest therefore, say the average shortest path length S_N, are expected to be proportional to N in the large-N limit, i.e.

$$S_N/N = A + N^{-\Delta} f(1/N, d, b) \qquad \varepsilon = 1. \tag{1}$$

The finite-size correction to this major linear scaling behaviour is determined by the exponent Δ, which is contributed by the non-trivial blob structures of the network. The function f is an analytic function of its argument, and approaches a constant

when $1/N \to 0$. The simplest possible form for f is expected to be $B + C/N$. Therefore, we could approximate (1) by the following:

$$S_N/N = A + N^{-\Delta}(B + C/N). \tag{2}$$

We numerically evaluated S_N by Monte Carlo simulation in $d = 2$–5 hypercubic lattices with different bridge lengths. A least-squares fit to (2) gives $\Delta \simeq 0.19 \pm 0.01$ in $d = 2$–5. It seems that Δ is a superuniversal constant, and we conjecture it to be $3/16$ for all $d \geqslant 2$.

2. Computer simulations

2.1. The spectral dimension

The models are similar to the one described in an earlier publication [5], except that here we allow multi-neighbour random walks. The multi-neighbour random walk is equivalent to the vibrational motion with multi-neighbour interactions. Taking the lattice constant to be unity, on the square lattice, the nearest-neighbour distance is 1, the next-nearest-neighbour distance is $\sqrt{2}$, and the third-neighbour distance is 2. Two lattice sites are connected by the bridging interaction if the distance between them is less than or equal to the bridge length b.

In performing the random walk on the SAW configurations, we use the same random walk jump probabilities to all the accessible sites (within the interaction range). A SAW configuration on the square lattice with bridge length $b = 2$ is shown in figure 1, and models with other interaction lengths and in different dimensions could be constructed in a similar fashion.

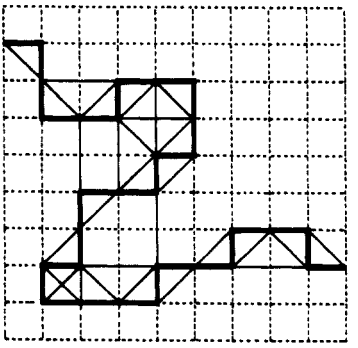

Figure 1. A SAW configuration with third-neighbour bridges on the square lattice. The thick lines represent the SAW backbone; the thin lines represent the 'bridges'.

If R_n denotes the average end-to-end distance of the n-step random walks on the SAW configurations, the random walk dimension d_w is defined through the equation

$$R_n \sim n^{1/d_w} \qquad n \to \infty. \tag{3}$$

We use the computer-simulated R_n to calculate $d_w(n)$ through the formula:

$$d_w(n) = \ln[(n+1)/(n-1)]/\ln[R_{n+1}/R_{n-1}]. \tag{4}$$

We also calculated $P_n(0)$, the probability of returning to origin after an n-step random walk. It has the following asymptotic form [3]:

$$P_n(0) \sim n^{-d_s/2}. \tag{5}$$

$d_s(n)$ is calculated via the equation:

$$d_s(n) = -2 \ln[P_{n+1}(0)/P_{n-1}(0)]/\ln[(n+1)/(n-1)]. \tag{6}$$

If C_N denotes the total number of N-step SAW configurations, then asymptotically

$$C_N \sim N^{\gamma-1} K_c^{-N} \qquad N \to \infty \tag{7}$$

We could, therefore, calculate K_c using the formula:

$$K_c(N) = [C_{N-1}/C_{N+1}]^{1/2}. \tag{8}$$

The error in neglecting the $N^{\gamma-1}$ term indeed disappears as N becomes large.

Using a very efficient constant fugacity Monte Carlo enumeration method [17], we generated the 65-step SAW configurations on a 70×70 site square lattice with an IBM-PC/XT personal computer. On each of the generated SAW configurations, we performed the exact multi-neighbour random walks [18] up to 50 steps. By the same method, we generated the 100-step SAW configurations on a $70 \times 70 \times 70$ cubic lattice with a Motorola 68020 based minicomputer, and performed the same 100-step exact multi-neighbour random walks on each of the SAW configurations. In figure 2, we plotted the calculated $d_s(n)$, $d_w(n)$, $(d_w(n)^{-1})$ against $1/\ln(n)$, and $K_c(N)$ against $1/N$ (calculated from equations (6), (4) and (8) respectively). It is clear that for different bridge lengths on the square lattice and for the nearest-neighbour bridge on the cubic lattice, d_s converges to 1. For next-nearest-neighbour bridges on the cubic lattice, d_s becomes less than 1. This is caused by the finite SAW chain length and the comparatively large random walk length. In fact, d_s in such cases is never expected to be less than unity and the inclusion of the bridge interactions can only increase the spectral dimension. We thus take the results as indicative of $d_s = 1$. The large n value of the d_w are unreliable when the random walk step size n is comparable to the SAW chain length N. When the step length of the random walk is large, the random walker has a non-negligible probability of reaching the edge of the SAW configuration, and the random walk end-to-end distance becomes incorrect. However, as the probability of returning to origin after an n-step random walk is affected only when the random walkers are reflected from the edge of the SAW configuration, it is less sensitive to the SAW chain length. Neglecting therefore, the very large n (compared with N) results, $d_w/2$ converges to d_f. Knowing that d_s could also be expressed as $d_s = 2d_f/d_w$, here d_f being the fractal dimension of the SAWs, we also arrive at the same result $d_s \to 1$. For checking the convergence to the asymptotic limit of SAW step sizes, we also calculated the critical fugacity K_c, and it converges to the known value [19].

2.2. The shortest path

The SAW configurations are again generated by the constant fugacity Monte Carlo method [17]. For an N-step SAW configuration, the middle site, i.e. the $(N/2)$th site counted from one end of the SAW configuration, is labelled the 0-site, all the sites which belong to the SAW configuration and can be connected to the middle site are labelled as 1-site and all the unlabelled sites which belong to the SAW configuration and can be connected to the 1-sites are labelled as 2-sites, etc. Thus, the labelling of each site is equal to the shortest path from that site to the middle one. On the $d = 2$–5-dimensional hypercubic lattices, for each bridge length, with a Motorola 68020-based minicomputer, we generated typically 20 000–80 000 SAW configurations and calculated the shortest path. Our algorithm can calculate the shortest path for

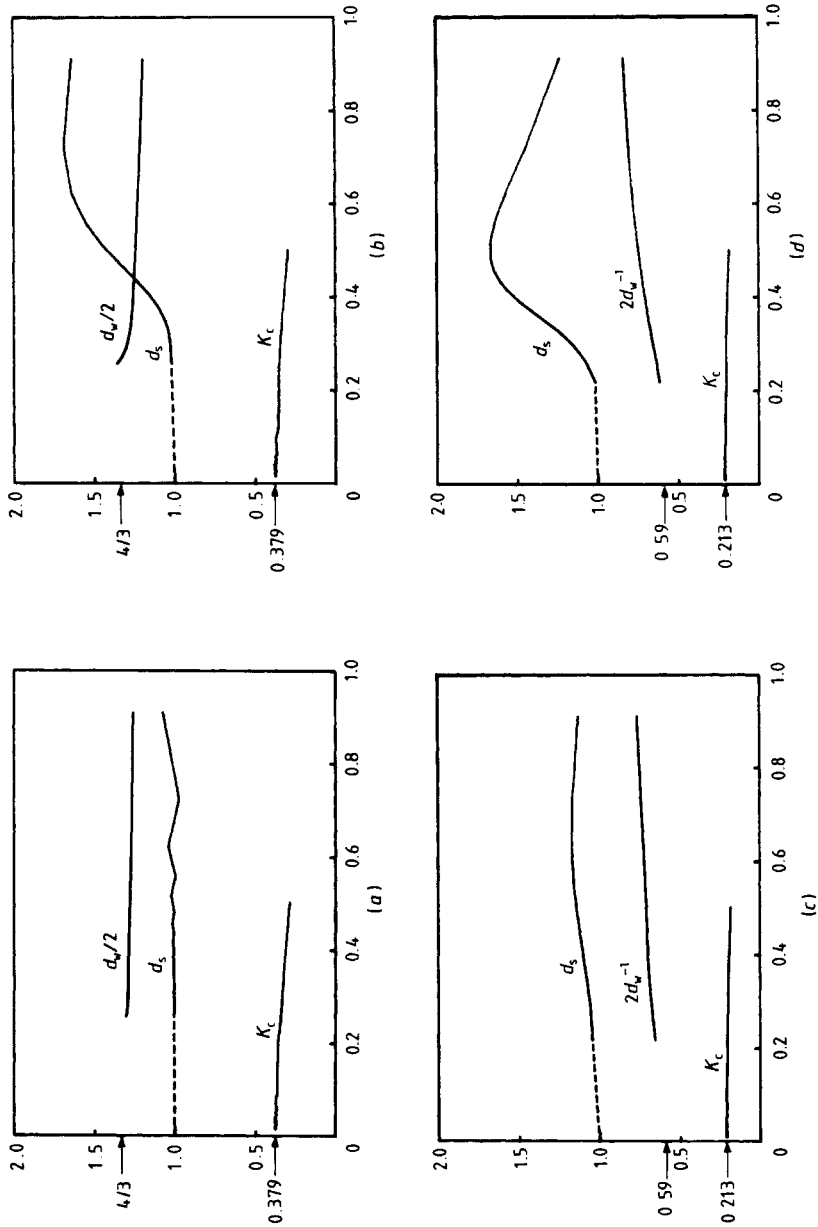

Figure 2. Monte Carlo simulation of the 'SAW with bridges' model. The broken lines represent the expected extrapolation to the n, $N \to \infty$ limit. d_s and $d_w/2(2d_w^{-1})$ are plotted against $1/\ln(n)$, and K_c is plotted against $1/N$. (*a*) The nearest-neighbour bridge model on the square lattice. The number of SAW configurations (taken) is 13 498. (*b*) The third-neighbour bridge model on the square lattice. The number of SAW configurations is 5361. (*c*) The nearest-neighbour bridge model on the simple cubic lattice. The number of SAW configurations is 5358. (*d*) The third-neighbour bridge model on the cubic lattice. The number of SAW configurations is 8214.

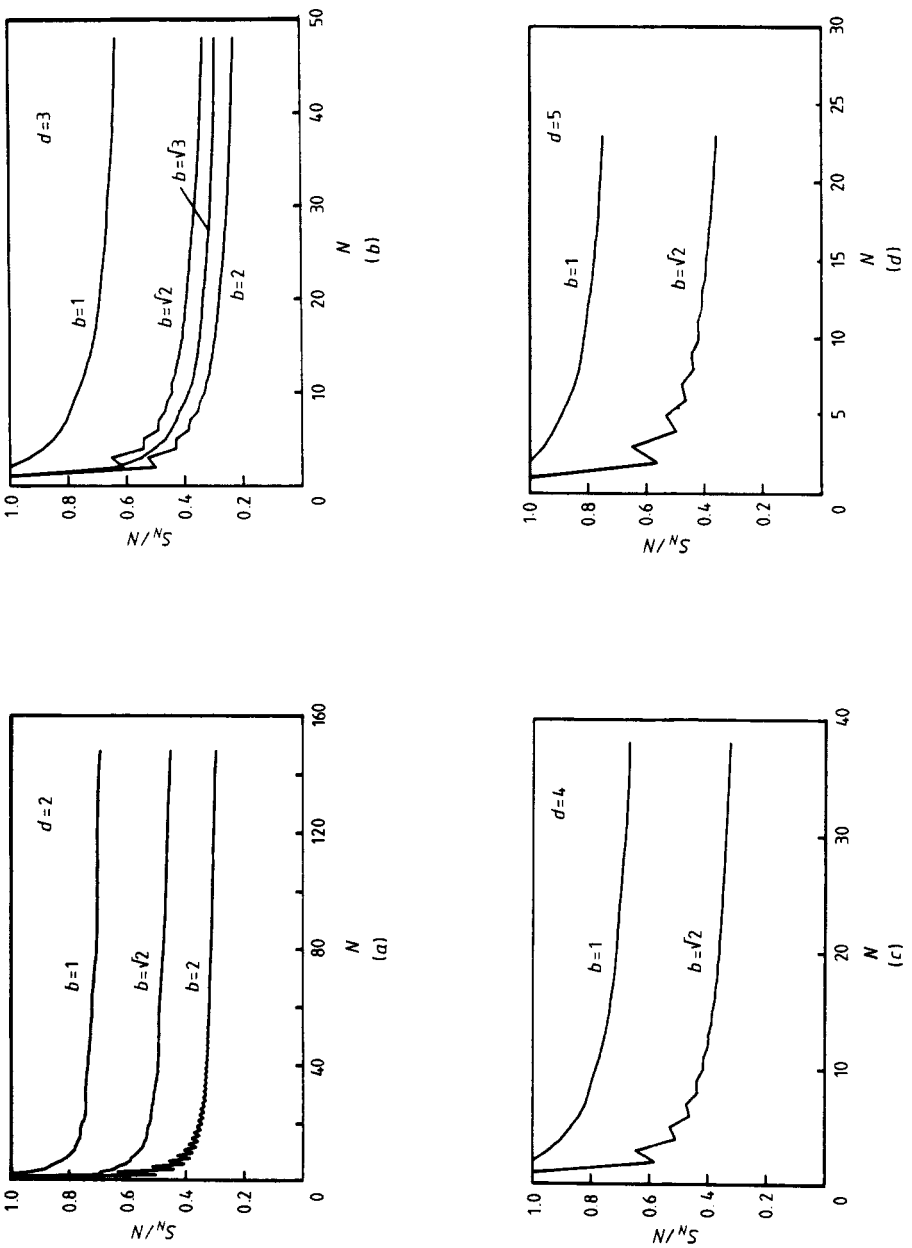

Figure 3. The renormalised shortest path length S_N/N against the SAW chain length N. (*a*) Square lattice. (*b*) Simple cubic lattice. (*c*) 4D hypercubic lattice. (*d*) 5D hypercubic lattice.

1000–2000 SAW configuration in one minute of CPU time. Figure 3 is the configuration-averaged S_N/N plotted against the path length N along the SAW chain, and the least-squares fit of the computed data to (2) is shown in table 1. As (2) is supposed to be correct only in the large-N limit, in our least-squares fit, we only use the large-N values for S_N/N. For the M-site SAW configurations, we use the data for $N>(2/5)M$, $N>(1/2)M$, and $N>(2/3)M$ respectively in three independent fittings. The error bars in the table are the largest deviations from the mean value. It is concluded by inspecting table 1 that Δ is a superuniversal exponent and its value is 0.19 ± 0.01 for $d=2$–5. It is related to the non-trivial blob structure of the SAWs with finite range bridging interactions. It should be mentioned that, for $d=6$, our simulation indicated a lower value of Δ ($\simeq 0.14$). However, we believe that this is due to the insufficient lattice size (11^6) and the SAW chain length ($N=40$) which we could simulate in such a high dimension.

Figure 4 is our simulated critical fugacity K_c calculated via (8) for $d=4$, 5 and 6. It is found from our computer simulation that $K_c=0.148\pm0.002, 0.113\pm0.001, 0.0916\pm0.0004$ in four-, five- and six-dimensional hypercubic lattices respectively. Defining the effective connective constant $z_{\text{eff}}=2+z-1-1/K_c$ [15], where z is the lattice

Table 1. Exponent Δ and the parameters A, B, C from the least-squares fit to (2).

b	d	A	B	C	Δ
	2	0.502 ± 0.004	0.496 ± 0.005	-0.1 ± 0.8	0.191 ± 0.008
	3	0.390 ± 0.000	0.501 ± 0.000	0.96 ± 0.21	0.200 ± 0.002
1	4	0.416 ± 0.000	0.500 ± 0.001	0.91 ± 0.09	0.197 ± 0.003
	5	0.455 ± 0.000	0.495 ± 0.001	0.61 ± 0.04	0.182 ± 0.001
	2	0.263 ± 0.003	0.498 ± 0.003	0.2 ± 0.8	0.194 ± 0.006
$\sqrt{2}$	3	0.0924 ± 0.0004	0.500 ± 0.000	1.00 ± 0.06	0.200 ± 0.001
	4	0.0648 ± 0.0000	0.494 ± 0.000	0.57 ± 0.08	0.185 ± 0.002
	5	0.0680 ± 0.0000	0.498 ± 0.000	0.740 ± 0.002	0.188 ± 0.000
$\sqrt{3}$	3	0.044 ± 0.006	0.500 ± 0.005	-0.3 ± 0.7	0.182 ± 0.006
	2	0.103 ± 0.006	0.494 ± 0.006	-1.0 ± 1.0	0.186 ± 0.012
2	3	-0.015 ± 0.002	0.500 ± 0.000	0.7 ± 0.3	0.196 ± 0.004

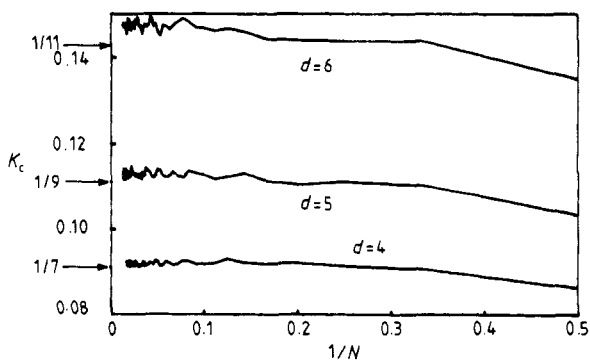

Figure 4. The computer-simulated K_c on $d=4$, 5, 6 hypercubic lattices. The values of $1/(z-1)$ for the corresponding lattices are indicated.

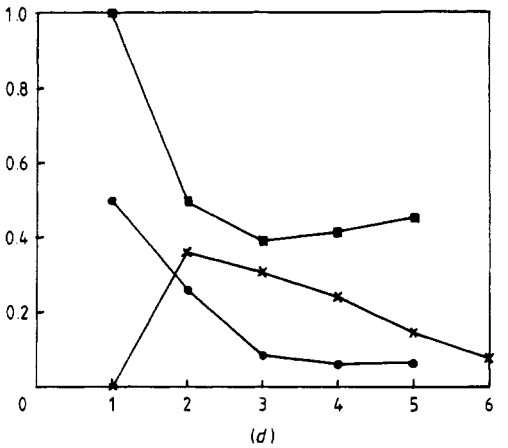

Figure 5. d-dependence of $z_{\text{eff}}-2$ and of parameter A. ■, A for $b=1$; ●, A for $b=\sqrt{2}$; ×, $Z_{\text{eff}}-2$.

coordination number, the d dependence of $z_{\text{eff}}-2$ and of the parameter A in (1) is depicted in figure 5.

3. Discussion

From our computer simulation, it is seen clearly that the inclusion of the massless bridges into the SAWs will not change their spectral dimension. If we think that the 'SAW with bridges' model still forms a fractal structure, i.e. if it were self-similar in a large length scale, then upon a change of the length scale, the interaction length would shrink, and finally arrive at the nearest-neighbour model. The above argument indicates that any finite length bridge models belong to the same universality class, and have the same scaling behaviour. As the 'SAW with bridges' model has a finite fraction (finite A in (2)) of steps which form the linear structure, the dynamic properties of the model can only be one dimensional, i.e. $d_s=\delta=\varepsilon=1$. The existence of the finite fraction of the linear portion in the SAW with bridges model also explains the disagreement of our results with that of Bouchaud *et al* [9]. But the inclusion of the bridges will have an effect on the short length scale behaviour. The effect can be seen in figure 2. It seems that the inclusion of the bridges tend to increase the spectral dimension when the random walk is short (finite-size crossover effect). Therefore, the data from the smaller SAW chain lengths and shorter random walks tend to be misleading.

For bridge length $b=1$, let $\mathscr{L}$ denote the fraction of sites in a SAW configuration which form the linear structure, and b_{eff} the effective (chemical) length of a bridge. We then have $A=\mathscr{L}/b_{\text{eff}}$. This can be readily seen for $d=1$, where $b_{\text{eff}}=b$. In a one-dimensional SAW, no blob can be formed by the bridges and all the sites in the SAW configuration belong to the linear part, $\mathscr{L}=1$. The shortest path S_N in this case is equal to $(1/b)\,N$, i.e. $A=1/b$. In higher dimensions, as the fraction of sites which form loops by the nearest-neighbour bridges is related to $(z_{\text{eff}}-2)$, we would expect [15] $\mathscr{L}\sim 1-[(z-1)-1/K_c]$ for the linear fraction. Its minimum value occurs at $d=2$. However, b_{eff} is larger than b for $d>1$, and decreases to b again for $d\to\infty$. As a consequence, the minimum value of A is expected to be found at a higher d $(d>2)$.

This can be observed from table 1 and figure 5. The argument is also true for $b > 1$, with a smaller $\mathcal{L}$ and a larger b_{eff}. The observed negative value of A for $b = 2$ on cubic lattice is due to the finite SAW chain length.

One of the interesting observations of our simulation is that the exponent Δ in (2) is superuniversal. The shortest path is closely connected to the dynamic aspect of the problem, and the dynamic properties are more likely to be superuniversal, like the spectral dimension of the percolation. Since the second term in (2) is coming from the blob structure of the model, we conclude that the dynamic properties of the blobs might be superuniversal. It may be noted that the value of the exponent Δ (contributed by the blob structures) is not observed to have any significant change at $d = 4$, the upper critical dimension for SAWs. This shows that although the random (long distance: greater than the bridge or interaction range) folding of the linear part (given by fraction A), determines the SAW size exponent and the excluded volume effect (size exponent more than that of random walk) disappears above $d = 4$, the short-range blob structural singularities do not feel any such disappearance of fluctuations at and above $d = 4$.

In conclusion, our numerical results suggest that the 'SAW with bridges' models in two and three dimensions all give $d_s \simeq 1$, and the spectral dimension is not affected by the bridge length. As it is known exactly that $d_s = 1$ for $d = 1$ and for $d \geq 4$, it is conjectured that the 'SAW with bridges' model belongs to the same universality class as the ordinary SAW, i.e. $d_s = 1$ for all d. Our numerical simulation also indicates that the same structural properties of the blobs, related to the exponent Δ in (2) in the 'SAW with bridges' model, might be superuniversal.

Acknowledgment

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Note added in proof. Apart from [16], the multifractal property of the SAW with bridges network has again been investigated numerically in two dimensions in a recent publication [20], where the authors also obtain $d_s = 1$, in agreement with ours (for $d = 2, 3$). The finite-size correction exponent Δ for S_N has recently been studied [21] using small-N series enumeration (up to $N = 18$, 11 and 12 only for square, triangular and simple cubic lattices respectively) and the extracted values of Δ are $\Delta \simeq 0.15$ and 0.33 for $d = 2$ and 3 respectively. However, larger series results for S_N are being tried [22].

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