Conduction and connection properties of self-avoiding walks with bridges

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(Received 24 February 1989; revised manuscript received 1 May 1989)

The voltage drop distribution in the random-resistor networks constituted by all nearest-neighbor bonds connecting points visited by a lattice self-avoiding walk (SAW) is studied by accurate numerical techniques in $d=2$. An analysis of the moments of the distribution allows one to establish the value $\zeta=1.333\pm0.007$ for the resistance exponent and to exclude the possibility of multifractal behavior. These results are also consistent with a topological investigation of the connection properties of SAW, which independently yields $\zeta=1.33\pm0.01$. This clearly supports $\zeta=\frac{4}{3}$ and a spectral dimension $\tilde{d}=1$ for these walks, solving an old controversy. A possible extension of such an analysis to SAW at the Θ point is also discussed.

The simplest and most natural way to associate a nontrivial dynamics to lattice self-avoiding walk (SAW) is that of considering all links between nearest-neighbor (NN) sites visited by the walks as dynamically active, whether they correspond to actual steps or not. So, e.g., one can consider for each SAW configuration a resistor network, in which to every pair of NN lattice sites visited (within one step or more) by the walk, a finite resistance Ω_0 is associated. The same kind of network allows one to define related linear dynamical problems, e.g., diffusion.

The dynamics of structures like those described above, to which we will refer as SAW with bridges, is of potential interest in connection with several physical issues such as electric conduction in linear polymers or anomalous temperature dependences of spin-lattice relaxation times in proteins.[1]

In spite of the fact that SAW are among the most extensively studied fractal structures, the issue of dynamics on SAW with bridges has been addressed relatively recently and does not seem to have been definitely settled. Different numerical and theoretical predictions have been produced so far for both spectral dimension and resistance exponent of such structures. Moreover, these results were never obtained in the context of a systematic investigation of possible multiscaling aspects associated with the random network dynamics.

Ball and Cates first addressed the resistance problem within an ϵ expansion in $d=4-\epsilon$ dimensions.[2] First-order results obtained for SAW with bridges led them to suggest that their end-to-end resistance could be asymptotically proportional to the number of walk steps in all dimensions. Numerical results compatible with this possibility were obtained in $d=2$ for the problem of diffusion on lattice SAW with bridges in Refs. 3 and 4. The SAW is known to have a fractal dimension $\bar{d}=\frac{4}{3}$ in $d=2$ (Ref. 5). Diffusion on SAW with bridges is described by an exponent d_W which yields the spectral dimension $\tilde{d}=2\bar{d}/d_W$ (Ref. 6). This dimension is relevant to the description of low-frequency harmonic vibrational modes of the structure. On the other hand, a scaling relation,[7] $\zeta=d_W-\bar{d}$ links d_W to ζ, the exponent describing how the average resistance $\Omega(R)$ between two points at distance R on the network grows with R:

$$\Omega(R)\propto R^{\zeta},\quad R\to\infty\ . \tag{1}$$

In Ref. 4 $d_W=2.60\pm0.17$ was estimated, and thus $\tilde{d}=1.02\pm0.07$, or $\zeta=1.27\pm0.17$. The values $\zeta=\bar{d}=\frac{4}{3}$ and $\tilde{d}=1$ should be expected if indeed the resistance between two points turns out to be proportional to the number of walk steps separating them.

More recently a number of theoretical and numerical predictions were produced at variance with $\zeta=\bar{d}$ and $\tilde{d}=1$. Both real space renormalization[8,9] and Monte Carlo (MC) results[10] were interpreted as supporting $\tilde{d}\neq1$ for $d=2$ SAW. Moreover, a Levy flight approach to diffusion on SAW with bridges, again predicting $\tilde{d}\neq1$, was recently proposed.[11]

In the present paper we address the issue of electrical conduction across SAW with bridges in $d=2$ (Ref. 12). We study the problem with different numerical techniques. The consistency and accuracy of our estimates should leave little doubt about the correct dynamical properties of these structures. In a broader sense some methods and results presented in this paper could open, in our opinion, new perspectives in the investigation of SAW properties and related problems.

A systematic approach to the conduction properties of a random-resistor network is the study of the voltage distribution across its bonds. SAW with bridges are structures having the same properties as the backbones defined for percolation clusters. Given two points of a SAW, if we consider the union of all self-avoiding paths joining them in the network with bridges, we get a backbone. If, in particular, the two points are the starting and end ones, the backbone coincides with the full network.

Our study in this case follows the main lines of similar investigations of the backbone of the infinite incipient cluster of percolation.[13,14] We generated by standard procedures,[15] a very large number of SAW on a square lattice of lengths ranging from 5 up to a maximum of 95 steps. For each walk the resistor problem with a given voltage difference $V=1$ applied between the ends was solved by rapidly convergent relaxation methods,[16] which also exploit the peculiar topology of SAW with bridges. If we indicate by $n(V)$ the number of links in the network with voltage drop equal to V, the distribution is characterized by its moments:

$$\langle M(q)\rangle \left\langle \sum_V n(V)V^q \right\rangle , \tag{2}$$

in which the average $\langle\ \rangle$ is over the whole sample of walks. We expected, for each q, $\langle M(q)\rangle \propto N^{y_q}$, $N \to \infty$, the scaling exponents y_q giving information about several properties of the resistor network. For example, the zeroth moment is nothing but the average number of links in the network. Since this number is always bounded by a minimum, which is the number of steps N, and a maximum, again proportional to N, we must have $y_0 = 1$. More interesting is the second moment, which can be shown to scale as the inverse of the end-to-end resistance Ω of the SAW with bridges.[13,14] The fourth moment can be seen to be related to $1/f$ noise in the network,[13] while in the limit $q \to \infty$, the moments give information on the number of NN network bonds having the maximum voltage drop V_{max} and thus carrying the total current. These are called links or cutting bonds, because conduction in the network is suppressed when one cuts one of them.

For $d=2$ SAW with bridges the voltage drop distribution and its moments are radically different from those of the percolation backbone. While in the latter case y_q is not linearly varying with q (multiscaling or multifractality) and the voltage distribution is well approximated by a log-normal law,[13,14] for SAW with bridges the moments appear to scale with an exponent which, in the investigated range of q, is linear in q, and the distribution has a very sharp maximum for $V \approx V_{max}$, with secondary peaks at lower V (see Fig. 1).

In Table I we report estimates of some y_q, for both negative and positive q extrapolated from the moments determined as above.

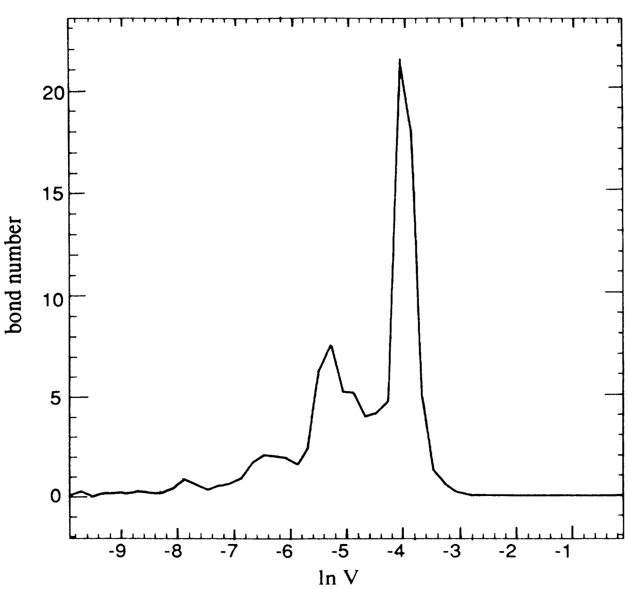

FIG. 1. Voltage drop distribution for walks of 90 steps.

TABLE I. y_q exponents for different q values. In the case $q \geq 0$ the samples for the determination of $\langle M \rangle$ were up to 260 000 walks and the accuracy in the voltage drops determination was 10^{-8}. For $q<0$ the samples contained up to 10^5 walks and accuracy was fixed to 10^{-15}. Extrapolations of y_q were based both on Padè approximants and on standard fitting procedures.

q	y_q
-1	2.00 ± 0.02
-0.6	1.60 ± 0.01
-0.4	1.40 ± 0.01
-0.2	1.200 ± 0.005
0	1.000 ± 0.005
0.5	0.49 ± 0.01
1	0.00 ± 0.01
1.5	-0.51 ± 0.02
2	-1.01 ± 0.02
2.5	-1.45 ± 0.05
3	-1.90 ± 0.08
3.5	-2.35 ± 0.15
4	-2.70 ± 0.20

We already see that within the accuracy, $y_q = 1-q$ seems to be satisfied. In particular we have $y_2 = -1.01\pm0.02$. Since, for an N-step SAW, $N \sim R^{\bar{d}}$, with $\bar{d} = \frac{4}{3}$, we also get $\zeta = -y_2\bar{d} = -4y_2/3 = -1.35 \pm 0.03$. In the last estimate, the inclusion of walk lengths up to $N=95$ appears crucial. Indeed, estimates based on data up to $N \simeq 50-60$ are rather different ($y_2 \simeq -0.92$), due to a clear lack of asymptoticity. A slow onset of the asymptotic regime is the main explanation of the discrepancy of the resistance exponent previously reported in Ref. 10. Statistical fluctuations determine oscillations in the moments which, for $q>0$, are growing with q for a given N. These fluctuations are largely responsible for the uncertainty of the asymptotic estimates. The relatively slow convergence to the asymptotic regime of moments like the second one is due to strong finite size effects: in other words, the conformation of SAW near the ends have a statistics which deviates substantially from that of walk segments deeply inside a long SAW.

In order to test this and to improve the quality of our resistance exponent determinations, we also considered walks of $N+60$ steps, with $N=5,10,\ldots,75,80$. The voltage difference was applied between the sites reached by the 30th and $(N+30)$th steps, respectively, so that the 30 steps initial and final tails of the walk could possibly contribute to the network backbone between these sites. In this way we could simulate the effect of nearby portions of the walk on the conduction properties of any interior segment. As expected, convergence was much more rapid in this case, and even fluctuations were sensibly smaller, at least in the range $q \gtrsim 1$. Results for a few y_q with $q>0$, are reported in Table II, while logarithmic

TABLE II. y_q exponents computed with samples of up to 175 000 walks and accuracy of 10^{-8}.

q	y_q
1	0.000 ± 0.001
1.5	-0.500 ± 0.005
2	-1.000 ± 0.005
2.5	-1.49 ± 0.01
3	-1.99 ± 0.03
3.5	-2.48 ± 0.06
4	-2.9 ± 0.1

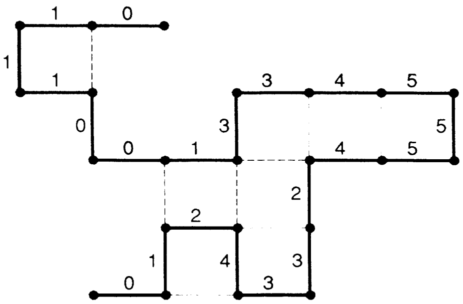

FIG. 3. Example of colors for SAW with bridges.

plots of the moments are given in Fig. 2. For $\langle M(2) \rangle$ we got in this case $y_2 = -1.000 \pm 0.005$, while the general relation $y_q = 1-q$ is very clearly supported by the global trend of the data.

Strong fluctuations hinder the possibility of estimating high-q moments with the above simulations. So, even if the law $y_q = 1-q$ is strongly suggested for $q > 0$, we decided to get an independent test of the scaling properties of the links, or cutting bonds. For SAW with bridges this test can be made without reference to the random-resistor problem, by only taking into account topological properties of the walks.

Let us consider a SAW configuration on the lattice, and attribute to each step a "color" which is equal to the number of NN bridges between nonconsecutive sites, respectively preceding and succeeding the step itself along the walk (see Fig. 3). More precisely, one can say that the color of a given step is the number of distinct connections between its extrema, each exploiting one and only one of the network bridges. Steps with color equal to zero are clearly the links of the SAW with bridges. For steps with color greater than zero it seems more difficult to find a physically relevant meaning in addition to the topological one. The statistics of the above colors can be easily studied, e.g., within a MC approach. To our knowledge such a study was never performed before.

Indicating by c ($=0,1,2,\ldots$) the color, and by N_c the average number of steps with color c, we could extrapolate behaviors of the form $N_c \propto N^{x_c}$, $N \to \infty$, with $x_0 = 1.00 \pm 0.01$, $x_1 = 1.00 \pm 0.01$, and $x_2 = 0.99 \pm 0.02$. The samples considered were of up to 7×10^6 walks of up to 100 steps. The x_c estimates were based on Padè approximant methods. We also extrapolated the ratios N_c / N for $N \to \infty$, obtaining $N_0 / N \to 0.52 \pm 0.05$, $N_1 / N \to 0.27 \pm 0.03$, and $N_2 / N \to 0.16 \pm 0.03$.

Of direct relevance for the resistance of SAW with bridges is the result for x_0. The fact that N_0 is proportional to N, within the numerical error, implies by necessity that the resistance must also be proportional to N, as we were finding independently by analysis of the second moment of the voltage drop distribution. So, from the above determination of x_0, we get an independent estimate of $\zeta = \bar{d} x_0 = 1.33 \pm 0.01$.

Coming back to our voltage drop distribution, of which a typical realization is shown in Fig. 1, we notice that the linear growth of N_0 with N is fully consistent with the fact that $y_q = 1-q$, for positive q. Indeed, in a distribution like this, positive moments are always expected to be dominated by the peak at $V = V_{\max}$, which is extremely sharp, and $n(V_{\max}) \sim N_0 \sim N$, while $V_{\max}$ is inversely proportional to N.

The fact that $y_q = 1-q$ also for (at least moderately) negative q tells something about the role of the rest of the network bonds. The secondary peaks are not strong enough to usurp the role of the links in controlling the moments, also for negative q. This circumstances is not *a priori* obvious. In analogy with work done previously for percolation backbones,[14] one can easily formulate deterministic hierarchical models of the SAW network, in which still $N_0 \propto N$, but while, for $q > 0$, $y_q = 1-q$ is satisfied, for $q < 0$ there is onset of multiscaling, with a sort of first-order transition in the spectrum. The occurrence of transitions of any kind seems to be excluded by our results here.

The results of this work, in our opinion, should give a final clear-cut solution to the doubts and controversies

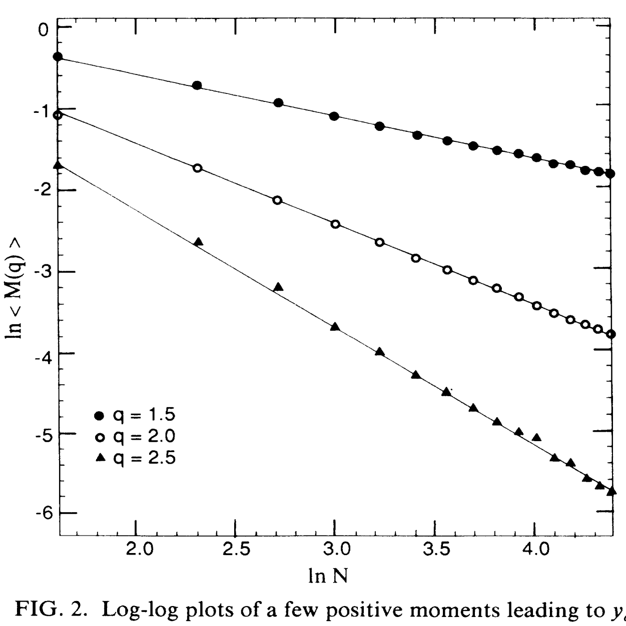

FIG. 2. Log-log plots of a few positive moments leading to y_q exponents reported in Table II.

raised in the recent literature on SAW with bridges. The ζ exponent for these walks is just equal to their fractal dimension in $d=2$. In particular the Levy flight picture of Ref. 11 clearly does not apply to our walks. Based on the Einstein relation,[7] our results also obviously imply $\bar{d}=1$ for SAW with bridges, as appropriate to essentially linear structures. Apart from the possible implications for physical problems like those mentioned above, it is worthwhile to remark that our results firmly establish an important topological property of SAW, which, somewhat surprisingly, was never investigated carefully enough before.

We finally call attention on the fact that the approach developed here can also be applied to other problems of considerable interest.

A possible extension of this work is, e.g., the study of conduction, or colors for SAW with bridges, when these SAW obey the statistics of the Θ point. One considers SAW configurations which are not all equally probable, but are weighted by a Boltzmann factor $\exp(\omega N_b)$, N_b being the number of bridges and $\omega>0$ some dimensionless attractive energy between NN visited points. Very recently a systematic investigation of this problem in $d=2$ was performed by the present authors.[17] In particular this study allowed to locate with reasonable precision the value of the energy ω_Θ, marking the separation between the SAW $(0=\omega<\omega_\Theta)$ and collapsed-chain $(\omega>\omega_\Theta)$ regimes. Clearly the conformations at the Θ point or in the collapsed regime are expected to be very different from those in the SAW regime studied above. In particular, in the collapsed phase we definitely expect the links to become a vanishing fraction of the total number of steps for $N\to\infty$. For $\omega=\omega_\Theta$ the situation is not *a priori* clear, even if one can expect of course N_0 to be definitely less than in the corresponding $\omega=0$ case. Using our previous determinations of ω_Θ in $d=2$, we obtained the following preliminary estimates of x_c exponents at the Θ point: $x_0=0.42\pm0.05$, $x_1=0.55\pm0.10$, and $x_2=0.7\pm0.2$. The trend of these data shows that at the Θ point links of SAW have a fractal dimension which is much less than that of the walk itself ($\bar{d}_0=x_0\bar{d}$, while $\bar{d}=\frac{7}{4}$).[17]

Steps with increasing color c seem to have increasing fractal dimensions. These results indicate that at the Θ-point SAW with bridges are qualitatively more similar to percolation backbones. A study of the voltage drop distribution in the case of the Θ point would most probably reveal multifractal properties. Investigations based on the conduction properties or on the colors of SAW with bridges thus seem to be a promising new way of characterizing the Θ point itself.

Financial support from the Gruppo Nazionale di Struttura della Materia and the Centro Interuniversitario di Struttura della Materia is gratefully acknowledged.

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