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Resistance and spectral dimension of self-avoiding walks with local bridges

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Self-avoiding-walk (SAW) configurations are considered by incorporating local bridges, i.e., connecting any two nearest-neighbor sites visited by the SAW by massless cross links. Introducing a new elegant method of estimating the resistance of an arbitrary network, we find the resistance exponent $\delta = 0.920 \pm 0.005$ in $d = 2$ by enumerating the random samples of SAW's using a Monte Carlo method. We also find the shortest-connecting-path-length exponent t to be equal to 0.975 ± 0.005 using a simulation technique in two dimensions. Random walks on SAW networks with local bridges are studied using a scaling formalism in the "grand canonical ensemble" picture of SAW's. We fit the mean end-to-end distance $\langle R_t \rangle$ of random walks of t steps with a scaling form $\langle R_t \rangle \sim t^{1/d_w} F((f - f_c)t^x)$ (f being the fugacity of SAW's) and find $d_w = d_F(1+\delta)$. In two dimensions this predicts the spectral dimension d_S ($= 2d_F/d_w$) of SAW networks with bridges to be equal to 1.042.

I. INTRODUCTION

Self-avoiding walks (SAW's) are random walks with the restriction that no site of a lattice is visited more than once. Recently, interest has been growing in the investigation of the scaling properties of the average end-to-end resistance[1,2] $\langle r_N \rangle$ and also of the shortest connecting path[1,3] length $\langle L_N \rangle$ of N-stepped SAW's. Also the critical behavior of the Ising model[3,4] and diffusion[2,5-7] (random walk) on SAW structures have been studied with great interest. Nontriviality in such problems on SAW fractal structures comes from the random nearest-neighbor connections arising as a result of the random folding of SAW chains. Let us consider, for example, the SAW configuration as shown in Fig. 1. Here, apart from the SAW backbone ("streets," solid lines in Fig. 1), any two nearest-neighbor sites visited by the SAW are connected by massless links ("bridges," broken lines in Fig. 1). In fact, it is to be noted that the fractal dimension (d_F) of SAW chains remains unchanged even by the introduction of bridges.[8]

To find the average end-to-end resistance of each conducting SAW networks one places unit conductors along streets as well as along the bridges. Ball and Cates[1] argued, with the help of a direct renormalization-group method to first order in ε ($= 4 - d$), that $\langle r_N \rangle$ is still proportional to N, i.e., $\delta = 1$ ($\langle r_N \rangle \sim N^{\delta}$, δ being the resistance exponent) even though the SAW network contains a considerable number of loops. Chowdhury and Chakrabarti,[2] on the other hand, studying the problem using a small-cell real-space renormalization-group treatment, concluded that $\delta \sim 0.88$ for $d = 2$. Here, we estimate the resistance exponent δ by enumerating the random SAW samples in two dimensions, both for square and triangular lattices using a Monte Carlo simulation method. We measure the resistance for each of them, introducing a new elegant method of estimating the resistance of an arbitrary network and we find $\delta = 0.920 \pm 0.005$ for $d = 2$. We also find the shortest-connecting-path-length exponent t to be equal to 0.975 ± 0.005 ($\langle L_N \rangle \sim N^t$), using the Monte Carlo simulation technique in two dimensions. These results are in disagreement with those of Ball and Cates,[1] but consistent with the physically obvious bound that $\langle r_N \rangle \leq \langle L_N \rangle$. Again, the simulation result for t is in good agreement with the numerical result of Bhattacharya and Chakrabarti[3] who found $t = 0.977 \pm 0.007$ for $d = 2$, using an exact enumeration technique.

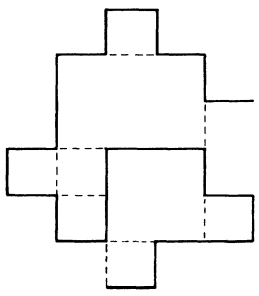

FIG. 1. A typical self-avoiding walk configuration on a square lattice with local bridges. "Streets" are shown by full lines and "bridges" by broken lines.

For random walks or diffusion along such chains, one makes the problem nontrivial in the sense that the random walker can move or hop along the chain backbone or streets and also along the bridges. For simplicity one can take the hopping probability along the street and the bridge to be the same, although in reality these two hopping probabilities may be quite different because of the different character in the corresponding bonds in linear polymers (however, it may be noted that the universality class remains the same for any finite ratio of the two hopping probabilities[9]). Much attention has been paid to the diffusion problem in the context of the experimental measurement[10] of the spectral dimension d_S and the fractal dimension d_F of some proteins. Stapleton *et al.*[10] conjectured that $d_S = d_F$ for these proteins. To reproduce this

experimental fact Helman, Coniglio, and Tsallis[5] modeled proteins as self-avoiding-walk networks with nearest-neighbor (local) bridges (hydrogen bonds acting as "massless bridges") and predicted that as a result of the presence of a sufficiently large number of bridges a random walker might effectively see the embedding Euclidean lattice when moving on the SAW networks with bridges giving thereby $d_w=2$ ($\langle R_t\rangle \sim t^{1/d_w}$, $\langle R_t\rangle$ the mean end-to-end distance of t-stepped random walks). Thus the spectral dimension becomes equal to the fractal dimension because of the Alexander-Orbach conjecture[11] $d_S=2d_F/d_w$. However, subsequent numerical studies by Chowdhury and Chakrabarti[2] and also by Yang, Lin, and Lam[6] in $d=2$ did not support this prediction of $d_w=2$. The numerical simulation of Chowdhury and Chakrabarti[2] gave $d_w\sim 2.78$ and they argued that $d_w > 2d_F$ ($=\frac{8}{3}$ for $d=2$) in this model because of random lavy flights. In a recent letter, Christou and Stinchcombe[7] agree with Chowdhury and Chakrabarti[2] in finding $d_w\sim 2.78$ with the use of a real-space renormalization-group treatment. At this point, we note that $d_w(\sim 2.78) > 2d_F(=\frac{8}{3})$ poses a serious problem in that it requires d_S to be less than 1. We think that this cannot be true; in any case for scalar harmonic excitation. On the other hand, the numerical value of $d_w=\frac{8}{3}$ is also inconsistent with the model defined because this value of d_w leads to a spectral dimension of 1, whereas d_S should be greater than 1, as SAW networks with bridges are not at all linear structures. Here, to clarify the situation, we study random walks on SAW chains in two dimensions (with nearest-neighbor hopping along the chain backbone and also the bridges with same hopping probability), using a scaling formalism in the "grand canonical ensemble" picture of SAW's. We fit the mean end-to-end distance $\langle R_t\rangle$ of random walks of step sizes t with a scaling form $\langle R_t\rangle \sim t^{1/d_w}F((f-f_c)t^x)$ (f being the fugacity of SAW's) and find $d_w=d_F(1+\delta)$, δ being the resistance exponent. With $\delta\sim 0.920$, we find $d_w < 2d_F$, leading to a spectral dimension d_S ($=2d_F/d_w$) of SAW networks with bridges of 1.042. This value of d_S also does not agree with the prediction of Stapleton, Allen, and Flynn[10] for proteins that $d_S=d_F$.

II. COMPUTER SIMULATION FOR δ AND t

We generated SAW's of step sizes (N) from 10 to 65 on a square lattice and from 10 to 40 on a triangular lattice, by the usual Monte Carlo method. We estimate the resistance exponent δ for self-avoiding-walk networks with bridges by measuring the resistance for each of the randomly generated samples of SAW networks and then averaging. We introduce here a simple method of estimating the resistance of an arbitrary network of resistors. This method is general and it can be applied to any complicated random resistor network (e.g., to find the resistance of an infinite percolation cluster). We apply it here to get the resistance of SAW networks with bridges.

Because there can be no accumulation of electric charge in a network of conductors, it follows that Laplace's equation $\nabla^2 V=0$ will hold good for the network where V is the potential at any point in the network. Here, we apply a unit potential difference across the initial and final positions of the self-avoiding walker. Our aim is to find out the potential gradient along the SAW chain with bridges. Values of the potential at all intermediate sites are obtained by discretization of Laplace's equation. In our case the discretized version would be

$$V=\left(\sum_i V_i\right)/n \ , \tag{1}$$

where the summation would run over all the occupied nearest neighbors (n). We assign the potential value of V at the starting point to be 1 and at the finishing point it is 0, whereas all other intermediate points are assigned any arbitrary fixed initial value. In the first iteration potential values at all intermediate sites are replaced by Eq. (1), and this process is repeated. We stop this process until the maximum of the difference between the potentials at any site between two successive iterations converges to a value less than some small number (we take it to be 10^{-5}). We assume this to be the potential distribution and, calculating the current, we find that average resistance of the SAW chain. We measure $\langle r_N\rangle$ of SAW chains with bridges both for a square lattice (step sizes N varying from 10 to 65, 2500 configurations for each length) and for a triangular lattice (N varying from 10 to 40, 2000 configurations for each length). We then have a log-log plot of $\langle r_N\rangle$ vs N (see Fig. 2), and fitting the results of $\langle r_N\rangle$ with the scaling form $\langle r_N\rangle \sim N^{\delta}$, the exponent δ is found to be equal to 0.920 ± 0.005.

Our result of δ is in contradiction with the field-theoretic treatment[1] of δ value which predicted $\delta=1$. Ac-

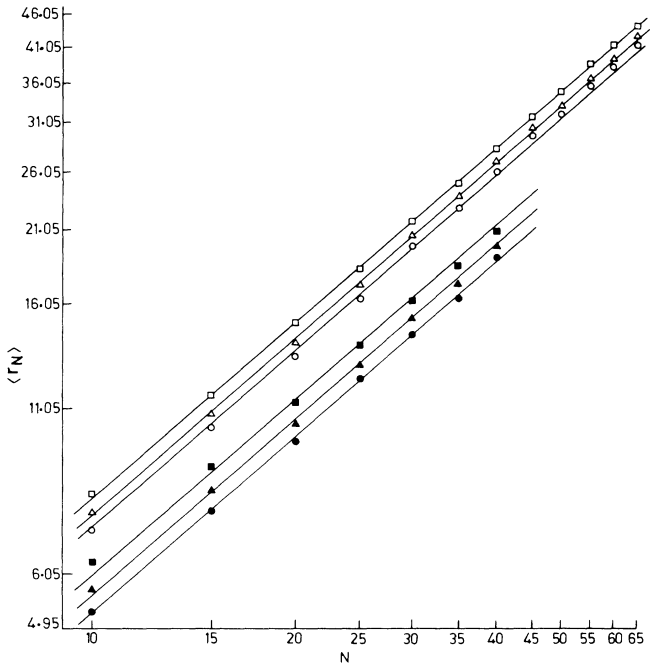

FIG. 2. Log-log plot of the average resistance vs step sizes (N) of SAW's. Points for $\langle r_N\rangle$, $\langle r_N^2\rangle^{1/2}$, and $\langle r_N^4\rangle^{1/4}$ for square lattice are denoted by symbols ○, △, and □, respectively. Filled symbols denote corresponding values for triangular lattice.

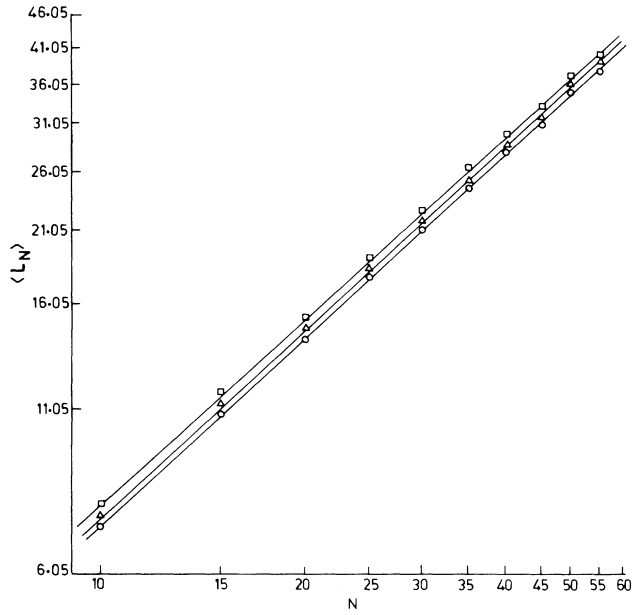

FIG. 3. Log-log plot of the average shortest path length vs step sizes (N) of SAW's on square lattice. Points for $\langle L_N\rangle$, $\langle L_N^2\rangle^{1/2}$, and $\langle L_N^4\rangle^{1/4}$ are denoted by ○, △, and □, respectively.

cording to Ball and Cates[1] the average resistance is proportional to the step sizes of the SAW's because the fraction of chain arc in no loop remains finite (nonvanishing). However, we claim that this is not true; rather the fraction of the number of bridges remains finite and nonvanishing,[8] leading to the nontrivial value of $\delta\sim 0.920$. On the other hand, small-cell renormalization-group results[2] indicated $\delta\sim 0.88$ which compares well with our Monte Carlo result.

Next, we measure the mean shortest connecting path length $\langle L_N\rangle$ for SAW's (with bridges) of step sizes (N) varying from 10 to 60 on a square lattice using a Monte Carlo simulation technique. For this we first connect all the nearest-neighbor sites, starting from the initial position and ending at the final position of the self-avoiding walker. Thus we make a cluster for the SAW configuration with local bridges. Then we measure all the connecting path lengths between the initial and the final positions of the walker and calculate the shortest connecting path length and then average it out for different configurations (~ 2500) of SAW's. We then have a log-log plot of $\langle L_N\rangle$ vs N (see Fig. 3) and fitting the results of $\langle L_N\rangle$ with the scaling form $\langle L_N\rangle\sim N^t$ the exponent t is found to be equal to 0.975 ± 0.005. This is in good agreement with exact enumeration result of Bhattacharya and Chakrabarti[3] who found $t=0.977\pm 0.007$.

III. SCALING THEORY FOR $\langle R_t\rangle$ OF RANDOM WALKS ON SAW NETWORKS WITH BRIDGES

In this section we try to formulate a scaling formalism for the average end-to-end distance $\langle R_t\rangle$ of a t-stepped random walk on SAW networks of N steps with bridges. Here, we adopt a grand canonical ensemble picture[12,13] of SAW's. In fact, it is seen that grand canonical ensemble of SAW's is a very useful picture to know the scaling properties of the statistics of SAW's on randomly diluted lattices.[14] In the canonical ensemble, the end-to-end distance $\langle R_N\rangle$ of N-stepped SAW's is averaged over all SAW's of the same number of steps $[\langle R_N^2\rangle = G_N^{-1}\sum_{r_{ij}} r_{ij}^2 G_N(r_{ij})]$, whereas for the grand canonical ensemble of SAW's all step lengths N are allowed, with a weight f^N for an N-stepped walk in the ensemble. One then defines the mean end-to-end distance of SAW's ($\xi_{\rm SAW}$) as

$$\xi_{\rm SAW}^2(f)=\sum_{r_{ij}} r_{ij}^2 \sum_N G_N(r_{ij}) f^N \times\left[\sum_{r_{ij}}\sum_N G_N(r_{ij}) f^N\right]^{-1}, \tag{2}$$

and one observes (using $\langle R_N\rangle\sim N^{\nu}$ and $G_N\sim\mu^N N^{\gamma-1}$) that at a critical fugacity f_c ($=1/\mu$) $\xi_{\rm SAW}\sim(f-f_c)^{-\nu}$. The fundamental role played by the fugacity f per unit step as the unique scaling field of SAW's leads to the emergence of an ordered and a disordered phase of SAW chains in the thermodynamic description.[13] For $f>f_c$, only a chain of finite length can occur, which corresponds to the disordered or the high-temperature phase. For $f<f_c$, on average an infinite chain with a compact structure of dimensionality d occurs; this corresponds to the ordered or low-temperature phase. At $f=f_c$, an infinite chain with a ramified structure of fractal dimensionality d_F occurs. This description of a single chain is very similar to percolation.[13] One defines here an order parameter (P) in the ordered phase and relates it to the monomer density, and since there is only one chain, the monomer density is just the probability that a given bond (occupied or empty) belongs to an infinite chain. Redner and Reynolds[13] defined $P\sim(f-f_c)^{\beta}$ and found $\beta=d\nu-1$ where $\nu=\frac{3}{4}$ and 0.588 in $d=2$ and 3. Here we make a scaling formulation for the end-to-end distance $\langle R_t\rangle$ of random walks on SAW's with bridges, similar to the study of random walks on percolation clusters.[15]

In the ordered phase ($f>f_c$) of the SAW chain because the infinite SAW chain has a compact structure, there will be normal diffusion on the SAW chains (with only a fugacity dependence on $\langle R_t\rangle$) and we thus write for $\langle R_t\rangle$ of the t-stepped random walk for $f>f_c$,

$$\langle R_t\rangle\sim(f-f_c)^{\sigma} t^{1/2}. \tag{3a}$$

It may be mentioned that 2σ is the diffusivity exponent and is related to the resistance exponent δ. For $f=f_c$, since the SAW chains have fractal structure, there will be anomalous diffusion on the SAW chains. Let us have k as the average end-to-end distance exponent of random on SAW chains at $f=f_c$. Thus at $f=f_c$,

$$\langle R_t\rangle\sim t^{k}. \tag{3b}$$

For f below f_c, obviously there will be no t dependence on $\langle R_t\rangle$, and $\langle R_t\rangle$ will be of the order of the average size of the SAW chain for $t\to\infty$ because in this limit of f only as SAW chain of finite length can occur. So for $f<f_c$,

$$\langle R_t\rangle\sim\xi_{\rm SAW}\sim(f_c-f)^{-\nu}. \tag{3c}$$

We now combine all results for $\langle R_t\rangle$ in three different

limits of f in one scaling form:

$$\langle R_t \rangle \sim t^k F(t^x(f-f_c)) \ . \tag{4}$$

For $f > f_c$ and for $Z \to \infty$ [where $Z = t^x(f-f_c), t \to \infty$] the scaling function $F(Z)$ must be proportional to Z^σ so as to be consistent with Eq. (3a) and thus $\sigma = (\frac{1}{2} - k)/x$. Again, for $f < f_c$, $F(Z)$ should be proportional to $Z^{-\nu}$ so as to be consistent with Eq. (3c) and thus $x = k/\nu$. So we get $k = \nu/2(\nu+\sigma)$. As the grand canonical ensemble picture of SAW's is similar to percolation in the thermodynamic description we can have a relation between the diffusivity exponent 2σ and the conductivity exponent τ of SAW's and thus (see, e.g., Stauffer[16]) $2\sigma = \tau - \beta$, where $\tau = (d-2)\nu + \delta$ and $\beta = d\nu - 1$; δ being the resistance exponent. With this value of 2σ we get

$$k = \nu/(1+\delta) \ . \tag{5}$$

Thus we find that the walk dimensionality $d_w [= 1/k = d_F(1+\delta), \sim 2.56$ in $d = 2]$ is not 2 and therefore is in contradiction and Helman, Coniglio, and Tsallis.[5] This result also does not support the numerical work of Chowdhury and Chakrabarti[2] and Yang *et al.*[6] Subsequently, this is also in disagreement with the real-space renormalization-group result of Christou and Stinchcombe.[7] But our result is consistent with the physical condition $d_w < 2d_F$ $(= \frac{8}{3})$.

Now we can have a knowledge of the scaling behavior of the low-frequency density of states $\rho(\omega) \sim \omega^{d_S - 1}$ (d_S is spectral dimension) through the Alexander-Orbach[11] relation $d_S = 2d_F/d_w$ and we see that $d_S = 2/(1+\delta)$. As $\delta = 0.92$ for SAW's with bridges we find $d_S = 1.042$ for $d = 2$. This value of d_S (> 1) is quite justified because SAW's with bridges is not a linear structure (it may be noted that for SAW's without bridges $\delta = 1$, and from our scaling argument we find that $d_S = 1$ which is obvious because SAW's without bridges are linear in structure).

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