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LETTER TO THE EDITOR

Analytical enumeration of Hamiltonian walks on a fractal

R M Bradley
Department of Physics, Colorado State University, Fort Collins, CO 80523, USA

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Abstract. The connectivity constant ω for Hamiltonian walks on Dhar's 4-simplex is found using an exact set of recursion relations. The result $\omega = 1.399\,710\ldots$ differs from the value of ω for Hamiltonian walks on the square lattice. As a consequence, ω must depend on other lattice characteristics besides the coordination number and the fractal dimension. The first correction to the leading-order asymptotic behaviour is also obtained.

Hamiltonian walks are self-avoiding walks (SAW) which visit every site in a lattice, and are often used as a model of collapsed polymer chains in the zero-temperature limit (see, for example, [1]). The enumeration of these walks is also important in the theory of the glass transition of polymer melts [2]. The number of Hamiltonian walks on a finite subset of the lattice with N points, C_N, grows as ω^N for large N. More precisely,

$$\lim_{N\to\infty} \frac{\ln C_N}{N}$$

exists and is defined to be $\ln \omega$. The constant $\ln \omega$ is the configurational entropy per monomer of a collapsed single chain at $T = 0$. The value ω is called the connectivity constant.

The connectivity constant is known exactly for a small number of lattices. Some time ago, Kasteleyn [3] found ω for the Manhattan lattice, while Malakis [4] used this result to compute the connectivity constant for Hamiltonian walks on coverings of the Manhattan lattice. More recently, Suzuki [5] determined the value of ω for the hexagonal and 3–12 lattices. Finally, Bradley [6] found that $\omega = 12^{1/9}$ for Hamiltonian walks on the Sierpinski gasket. Since the Sierpinski gasket is frequently employed as a simple model of the infinite cluster at the percolation threshold in two dimensions [7], this result is relevant to the theory of collapsed polymer chains in random media.

Dhar's 4-simplex [8] is a regular fractal with Hausdorff dimension $D = 2$. The critical exponents of the self-avoiding walk on this lattice have been computed analytically [9]. In addition, Dhar and Vannimenus [10] recently established that a self-attracting linear polymer on the 4-simplex has a collapse transition at finite temperature and determined the critical exponents at the theta point exactly. In this letter, I show that the zero-temperature entropy in the collapsed phase can be computed for polymer chains on the 4-simplex using a set of exact recursion relations. The result $\omega = 1.399\,710\ldots$ which I obtain extends the short list of lattices where the connectivity constant for Hamiltonian walks has been computed analytically†. I also show that

† Parenthetically, it is trivial to see that $\omega = 1$ for the 3-simplex.

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the leading-order correction to the asymptotic behaviour of C_N has the same form as was recently obtained for Hamiltonian walks on the even–even Manhattan lattice with free boundaries [11]†.

Let C_l be the number of closed Hamiltonian walks on the 4-simplex of order l (see figure 1). Each of these walks visits each site once and ultimately returns to its starting point. To compute C_l, we let $C_{1,l}$ be the number of Hamiltonian walks which start at one corner of the lth 4-simplex and end at another. A Hamiltonian walk of this kind will be represented schematically as shown in figure 2. Figure 3 illustrates how each closed Hamiltonian walk on the $(l+1)$th 4-simplex can be decomposed into Hamiltonian walks which enter and exit 4-simplices of order l. As a result

$$C_{l+1} = 3C_{1,l}^4 \qquad \text{for } l \geq 1. \tag{1}$$

To obtain a closed set of recursion relations, walks of a different type must also be considered. The corners of the lth 4-simplex are all equivalent by symmetry, and we arbitrarily label them by the numbers 1 to 4. Consider a SAW which enters at corner 1, exits at corner 2, re-enters at corner 3 and exits once more at corner 4. The total

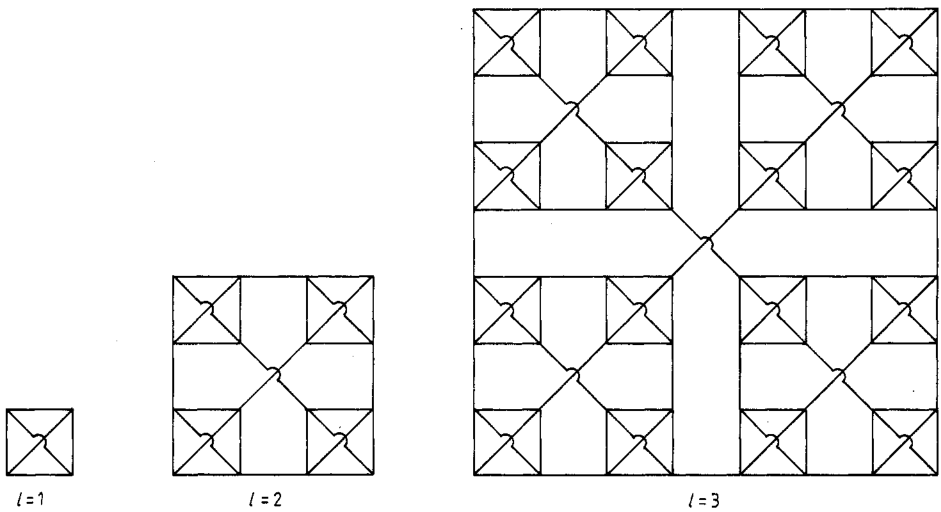

Figure 1. Dhar's 4-simplices of order $l = 1$, 2 and 3.

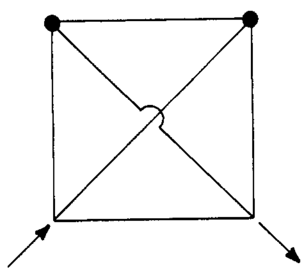

Figure 2. Schematic representation of a Hamiltonian walk which enters and exits the lth 4-simplex at different corners.

† This was conjectured earlier in [4].

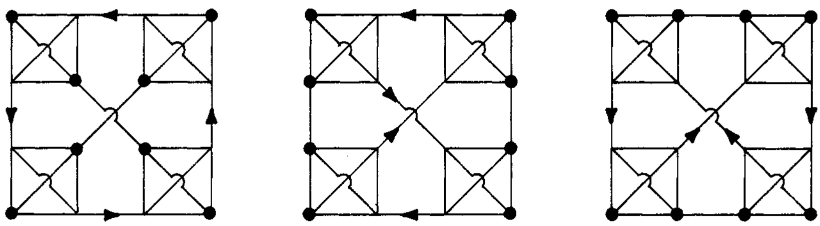

Figure 3. Decomposition of a closed Hamiltonian walk on the $(l+1)$th 4-simplex into Hamiltonian walks which enter and exit 4-simplices of order l. The three possible decompositions are shown in (a), (b) and (c).

number of such walks which visit each site on the lth 4-simplex once will be denoted by $C_{2,l}$. It is straightforward but tedious to show that

$$C_{1,l+1}=2C_{1,l}^4+4C_{1,l}^3C_{2,l}+6C_{1,l}^2C_{2,l}^2 \tag{2}$$

$$C_{2,l+1}=C_{1,l}^4+4C_{1,l}^3C_{2,l}+22C_{2,l}^4 \tag{3}$$

for all $l \geqslant 1$. Equations (2) and (3) are the exact recursion relations for the problem. They are similar in form to the recursion relations for the generating functions for SAW on the 4-simplex [9, 10], but do not contain terms involving non-Hamiltonian walks. The initial values are

$$C_{1,1}=2 \qquad C_{2,1}=1. \tag{4}$$

To obtain the connectivity constant, we first let

$$x_l \equiv \frac{C_{1,l}}{C_{2,l}}$$

and

$$y_l \equiv \frac{\ln C_{2,l}}{4^l} - \frac{\ln 22}{3}\left(\frac{1}{4}-\frac{1}{4^l}\right)$$

for all $l \geqslant 1$. We also define $\tilde{\omega}$ by

$$\ln \tilde{\omega} \equiv \lim_{l\to\infty} \frac{\ln C_{2,l}}{N_l} \tag{5}$$

where $N_l = 4^l$ is the number of sites in the lth 4-simplex. Clearly,

$$\lim_{l\to\infty} y_l = \ln \tilde{\omega} - \frac{\ln 22}{12}. \tag{6}$$

Equations (2) and (3) yield recursion relations for x and y valid for all $l \geqslant 1$:

$$x_{l+1} = \frac{2x_l^4+4x_l^3+6x_l^2}{x_l^4+4x_l^3+22} \tag{7}$$

$$y_{l+1} = y_l + \frac{1}{4^{l+1}} \ln(1+\tfrac{2}{11}x_l^3+\tfrac{1}{22}x_l^4). \tag{8}$$

The initial values are $x_1 = 2$ and $y_1 = 0$. Numerically iterating x and y, we find that x_l tends to zero as $l \to \infty$, while y_l quickly asymptotes to 0.078 678 .... (The second term was included in the definition of y_l to speed convergence.) Equation (6) now gives

$$\tilde{\omega} = 1.399\,710\ldots. \tag{9}$$

It remains to demonstrate that $\tilde{\omega}$ is equal to the connectivity constant ω. Equation (1) shows that C_l and $C_{1,l}$ have the same leading-order asymptotic behaviour, so

$$\lim_{l\to\infty} \frac{\ln C_{1,l}}{N_l} = \ln \omega. \tag{10}$$

Using (2), we obtain

$$\frac{\ln C_{1,l+1}}{4^{l+1}} = \frac{1}{2}\left(\frac{\ln C_{1,l}}{4^l} + \frac{\ln C_{2,l}}{4^l}\right) + \frac{\ln 6}{4^{l+1}} + \frac{1}{4^{l+1}} \ln(1 + \tfrac{2}{3}x_l + \tfrac{1}{3}x_l^2).$$

Taking the $l \to \infty$ limit of this expression and employing (5) and (10), we have the desired result $\omega = \tilde{\omega}$. We conclude that

$$\omega = 1.399\,710\ldots. \tag{11}$$

It may at first glance seem surprising that $\omega = \tilde{\omega}$, even though the ratio $x_l \equiv C_{1,l}/C_{2,l}$ tends to zero. The reason x_l goes to zero is that $C_{1,l}$ and $C_{2,l}$ have the same leading-order asymptotic behaviour but have different correction terms. Indeed, as l grows large, x_l tends to zero and (7) may be replaced by

$$x_{l+1} \simeq \tfrac{3}{11} x_l^2. \tag{12}$$

Equation (12) shows that

$$C_{1,l}/C_{2,l} = x_l \sim \lambda^{2^l} \qquad \text{as } l \to \infty \tag{13}$$

where λ is a positive constant smaller than 1. The constant λ can be computed by letting

$$z_l = \frac{\ln x_l}{2^l} - \ln(\tfrac{3}{11})\left(\frac{1}{2} - \frac{1}{2^l}\right) \tag{14}$$

so

$$\lim_{l\to\infty} z_l = \ln \lambda - \tfrac{1}{2}\ln(\tfrac{3}{11}). \tag{15}$$

As before, the second term in (14) has been added to $\ln x_l/2^l$ to increase the rate of convergence. From (7) we have

$$z_{l+1} = z_l + \frac{1}{2^{l+1}} \ln\left(\frac{1 + \tfrac{2}{3}x_l + \tfrac{1}{3}x_l^2}{1 + \tfrac{2}{11}x_l^3 + \tfrac{1}{22}x_l^4}\right) \tag{16}$$

for $l \geq 1$. The initial value of z is $z_1 = (\ln 2)/2$. Iterating x and z using (7) and (16), we find that z_l converges to 0.471 256 ... as $l \to \infty$. Equation (15) then gives

$$\lambda = 0.836\,620\ldots.$$

Having determined λ, we are in a position to find the leading-order correction to the asymptotic behaviour of C_l. First note that, from (8), we have

$$y_l = \sum_{k=1}^{l-1} (y_{k+1} - y_k) + y_1 = \sum_{k=1}^{l-1} \frac{1}{4^{k+1}} \ln(1 + \tfrac{2}{11}x_k^3 + \tfrac{1}{22}x_k^4). \tag{17}$$

Taking the $l \to \infty$ limit in (17) and using (6), we obtain

$$\ln \omega - \frac{\ln 22}{12} = \sum_{k=1}^{\infty} \frac{1}{4^{k+1}} \ln(1 + \tfrac{2}{11}x_k^3 + \tfrac{1}{22}x_k^4).$$

We now apply this and the definition of y_l to (17) to get

$$\frac{\ln C_{2,l}}{4^l} = \ln \omega - \frac{\ln 22}{3}\frac{1}{4^l} - \sum_{k=l}^{\infty} \frac{1}{4^{k+1}} \ln(1 + \tfrac{2}{11}x_k^3 + \tfrac{1}{22}x_k^4). \qquad (18)$$

A simple inductive argument shows that $x_l \leq 2$ for all l, so

$$\sum_{k=l}^{\infty} \frac{1}{4^{k+1}} \ln(1 + \tfrac{2}{11}x_k^3 + \tfrac{1}{22}x_k^4) \leq \ln(\tfrac{35}{11}) \sum_{k=l}^{\infty} \frac{1}{4^{k+1}} = \tfrac{1}{3}\ln(\tfrac{35}{11})\frac{1}{4^l}.$$

Equation (18) then gives

$$\ln C_{2,l} = (\ln \omega) N_l + O(1) \qquad (19)$$

for large l. Combining (13) and (19), we have

$$\ln C_{1,l} \sim (\ln \omega) N_l + (\ln \lambda) N_l^{1/2}.$$

We now have the desired result:

$$\ln C_l \sim (\ln \omega) N_l + (2 \ln \lambda) N_l^{1/2} \qquad \text{for } l \gg 1$$

which shows that the leading-order correction to the asymptotic behaviour of $\ln C_l$ is proportional to the simplex perimeter. Recently, the leading-order correction term in $\ln C_N$ for Hamiltonian walks on the even–even Manhattan lattice with free boundaries has also been shown to be proportional to the perimeter [11].

It is interesting to compare our result (11) to the predictions of the various mean-field theories of Hamiltonian circuits which have been proposed [2–4]. These theories give estimates of ω that depend only on the coordination number of the lattice, z. For a lattice with $z=4$, a Flory–Huggins type of theory [13] yields $\omega_{FH} = 3/e \simeq 1.1036$, Huggins [14] predicts that $\omega_H = 1.5$, and Orland *et al* [12] give the value $\omega_0 = 4/e \simeq 1.4715$. None of these values is a good approximation to the value of ω for the 4-simplex.

The 4-simplex, square lattice and Sierpinski gasket all have coordination number $z=4$, but each has a different connectivity constant [6]†. Thus, ω cannot depend on z alone, contrary to the prediction of the mean-field theories. In fact, since the square lattice and 4-simplex both have coordination number $z=4$ and fractal dimension $D=2$, the connectivity constant must depend on other lattice characteristics besides z and D. Clearly, the universality of ω is quite low.

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† Schmalz *et al* [15] obtained $\omega \sim 1.472$ for the square lattice. B Derrida (unpublished) found that ω lies between 1.4725 and 1.4730.

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