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Self-interacting self-avoiding walks on the Sierpinski gasket (*)

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Résumé. — Nous donnons les relations de récurrence exactes pour les fonctions génératrices décrivant les marches aléatoires sans recoupement et avec volume exclu sur la famille des tamis de Sierpinski. Leur étude révèle que la moyenne des distances parcourues pour des marches de N pas varie comme N^ν avec $\nu = \ln(2)/\ln\{(7 - \sqrt{5})/2\}$, indépendamment de la force (limitée) d'interaction. Nous donnons également un certain nombre d'autres propriétés asymptotiques dans la limite N grand.

Abstract. — Exact recurrence relations for generating functions for self-interacting self-avoiding random walks on a Sierpinski gasket lattice are given. Their analysis reveals that the mean end-to-end separation of N -step walks varies as N^ν with $\nu = \ln(2)/\ln\{(7 - \sqrt{5})/2\}$, regardless of the (finite) strength of the self-interaction. Some other properties are also determined in the large- N limit.

1. Introduction

B. Mandelbrot [1] has emphasized that many self-similar structures (fractals) occur in nature. Thus it is of interest to investigate simple models of fractals, one such model being the Sierpinski gasket, with a Hausdorff dimension of $\ln(3)/\ln(2)$. Indeed, the Sierpinski gasket has now been much studied [2], particularly with reference to its similarities to percolation clusters (at threshold).

Here we develop exact results for self-avoiding walks on the lattice of the Sierpinski gasket including self-interaction, thereby generalizing Dhar's treatment of non-interacting walks on simplex lattices [3]. This then is to be added to the brief list of exactly solved self-avoiding walk problems, which includes walks on Bethe lattices [4], on finite-width strips [5], and Nienhuis' [6] recent nontrivial results on the honeycomb lattice. The present solution is obtained *via* a real-space renormalization group kind of technique [7], in common both with Dhar's work and with other renormalization group treatments [8] of self-avoiding walks.

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The Sierpinski gasket, as well as the various self-avoiding walks on it, may be built up in a hierarchy of stages. The method of procession from one stage to the next is indicated in figure 1, where three triangular blocks are joined together to form a block of the next larger size. Examples of blocks, with walks on them, are shown in figures 2 and 3. The blocks in figures 2 and 3 are at stages $n = 1$ and $n = 2$ respectively, where the step length along the side of a block is 2^n .

Fig. 1. — The manner of joining three gaskets at one stage to form a gasket at the next higher stage.

Fig. 2. — The various self-avoiding walks between the lower-left and top apices of a stage 1 Sierpinski gasket.

Fig. 3. — Two examples of (type a) self-avoiding walks between two apices of a stage 2 Sierpinski gasket.

We introduce generating functions for various types of self-interacting self-avoiding walks on a Sierpinski gasket at stage n . The walks, between two extreme (apex) vertices of the gasket, are classified into four types :

- (a) those walks visiting neither the third apex nor the two vortices adjacent to this third apex ;
 - (b) those walks visiting exactly one of the two vertices adjacent to the third (unvisited) apex ;
 - (c) those walks visiting both the vertices adjacent to the third apex which is not itself visited ;
- and
- (d) those walks visiting the third apex.

These types of walks, and their associated generating functions, at stage n are denoted as a_n, b_n, c_n and d_n . All the a_1, b_1, c_1, d_1 walks between two given apices are shown in the corresponding rows a, b, c, d of figure 2. The generating functions are defined to be a sum of monomials in variables u, v and z . Each monomial corresponds to a single walk between two fixed apices, such that : first, the power of u is the number of unoccupied gasket bonds which terminate at the walk with one site on the walk and the other off ; second, the power of v is the number of unoccupied gasket bonds connecting vertices of the walk ; and third, the power of z is the number of steps in the walk. Thus at stage 1 the four generating functions, corresponding to the four rows of figure 2 are

$$\begin{aligned} a_1 &= u^4 z^2 \\ b_1 &= 2 u^4 v z^3 \\ c_1 &= 3 u^2 v^3 z^4 + u^6 z^3 \\ d_1 &= u^4 v z^4 + 2 v^4 z^5 . \end{aligned} \quad (1)$$

The variables u and v are positive weights measuring the interaction strengths between each of the walk's vertices and other adjacent vertices.

Recurrence relations for the generating functions may be developed in parallel to the construction of figure 1. That is, the walks on the $(n + 1)$ -stage gasket are composed from (two or three) properly adjoined walks on the component n -stage gaskets. This leads to

$$\begin{aligned} a_{n+1} &= (a_n + b_n + c_n + u^2 d_n)^2 + \Delta_n a_n \\ b_{n+1} &= \Delta_n b_n \\ c_{n+1} &= \Delta_n c_n \\ d_{n+1} &= \Delta_n d_n \end{aligned} \quad (2)$$

where

$$\Delta_n = (a_n + b_n + c_n)^2 + 2 d_n (u^2 a_n + v b_n + [v^2/u^2] c_n) . \quad (3)$$

Here in (2) the term $(a_n + b_n + c_n + u^2 d_n)^2$ arises from all walks visiting just two of the n -stage blocks each factor $(a_n + b_n + c_n + u^2 d_n)$ being associated with one of these two n -stage blocks. An example of a walk counted in the product $u^2 d_1 c_1$ is shown in the first part of figure 3. The weights u (and v) in Δ_n appear explicitly so as to account for new contacts introduced between different n -stage blocks. An example of an a walk counted in the product $d_1 [v^2/u^2] c_1 a_1$ (which arises in $\Delta_1 a_1$) is shown in the second part of figure 3.

2. Analysis of the generating functions.

The coefficient of a particular power of z , say z^N , in the sum $a_n + b_n + c_n$ is a polynomial in u and v ; this polynomial represents a (monodisperse) partition function for all weighted N -step walks between the two fixed apices of the stage- n Sierpinski gasket. The corresponding coefficient in a particular generating function ξ_n represents the particular corresponding type- ξ N -step walks.

The « dominant » partition functions in these generating functions are expected to grow like κ^N for some appropriate u - and v -dependent connective constant. This may be numerically checked and evaluated if one simply determines (for any given u and v) the radius of convergence z_c of the generating functions as polynomials in z . Then $z_c = 1/\kappa$. For $z > 1/\kappa$ all ξ_n should diverge as the stage index n is iterated upward, whereas for $z < 1/\kappa$ all ξ_n should converge to 0.

The general behaviour of the ξ_n at $z = 1/\kappa$ can be elucidated. From the relation (2) it is seen that if $\Delta_m > 1$ at any given m , then a_{m+1} , Δ_{m+1} , and the subsequent ξ_n increase, ultimately diverging. If Δ_m remains less than 1, then the b_n , c_n , d_n converge to 0 and the recurrence relation for type- a walks approaches

$$a_{n+1} \cong a_n^2 + a_n^3, \quad \text{as } n \rightarrow \infty. \quad (4)$$

Here the a_n take (non-negative) values causing the recurrence (4) to give convergence, since otherwise Δ_n would become greater than 1 and all the ξ_n would diverge. As a consequence (4) implies a_n approaches a fixed point a which is a solution to $a^3 + a^2 - a = 0$. Then either $a = 0$ or

$$a = (\sqrt{5} - 1)/2 \cong 0.61803399. \quad (5)$$

Now as $z \rightarrow 1/\kappa$ from below, we expect the maximum a_n value to increase while the n value at which this maximum is achieved also increases. But at such larger values of n the b_n , c_n , d_n should approach very close to zero and the behaviour of a_n be governed by (4). Thus as $z \rightarrow 1/\kappa$ from below the maximum a_n value should increase toward a of (5), regardless of the positive values for u and v .

All this is indeed numerically found for a wide range of weights u and v . Such resulting κ values are given in figure 4, where we have constrained

$$u + v = 1. \quad (6)$$

Rescaling to any other (positive) value for this sum can be readily handled *via* the relation

$$\xi_n(u, v, z) = \xi_n(su, s^2 v, z/s^2). \quad (7)$$

Further it may be noted that the maximum a value we achieved for $v \gtrsim 0.82$ is very close to the value of (5); whereas for $v \lesssim 0.86$ the value we achieved is less than half of (5). Evidently to come closer to the precise value of (5) at these larger values of v one must approach $1/\kappa$ more accurately than the 1 part in 10^{16} which we achieved.

The asymptotic behaviour of the mean end-to-end separation $\langle R \rangle_N$ for walks of a fixed number of steps can be deduced. Indeed

$$\langle R \rangle_N \cong AN^v \quad (8)$$

where, for large n ,

$$N \sim \left(\frac{1}{a_n} \frac{\partial a_n}{\partial \ln z} \right)_{z=1/\kappa} \quad \text{and} \quad \langle R \rangle_N \sim 2^n. \quad (9)$$

Thus the desired exponent is given as

$$v = \lim_{n \rightarrow \infty} n \ln 2 \left(\frac{\partial a_n}{\partial \ln z} \right)_{z=1/\kappa}. \quad (10)$$

These partial derivatives with respect to z are obtained *via* recurrence relations which result from taking derivatives of the equations (2) and (3). The result can be expressed in terms of a column

Fig. 4. — The variation (as a function of contact activity v) of the per-site count κ and of the fraction ρ of possible near-neighbour contacts.

4-vector $\mathbf{Z}_n$ with ξ th component $(\partial \xi_n / \partial \ln z)_{z=1/\kappa}$. Then

$$\mathbf{Z}_{n+1} = T_n \mathbf{Z}_n . \tag{11}$$

Here T_n is a 4 by 4 matrix with (ξ, ζ) th element

$$(T_n)_{\xi\zeta} = \frac{\partial F_{\xi}(a, b, c, d, u, v)}{\partial \zeta} \quad \text{at} \quad a = a_n, b = b_n, c = c_n, d = d_n \tag{12}$$

where the recurrence relations of (2) are summarized as

$$\xi_{n+1} = F_{\xi}(a_n, b_n, c_n, d_n, u, v) \tag{13}$$

The initial $\mathbf{Z}_1$ is obtained on taking derivatives of equations (1). From the asymptotic behaviour of the ξ_n at $z = 1/\kappa$ it is seen that as $n \rightarrow \infty$ the matrices T_n approach an asymptotic n -independent form T . Then

$$\mathbf{Z}_{n+1} \rightarrow T \mathbf{Z}_n \rightarrow B \lambda^n \mathbf{e} \tag{14}$$

where $\mathbf{e}$ is the vector with ξ component $\delta(\xi, a)$ and λ is the maximum eigenvalue to T . Through the use of (12) and the asymptotic behaviour of the ξ discussed near equation (5), we find $\lambda = 3 - a$.

Thus

$$\nu = \ln(2)/\ln\left(\frac{7-\sqrt{5}}{2}\right) \cong 0.79862456 \quad (15)$$

This exponent applies over the full range of positive u and v .

The asymptotic behaviour of the ratio ρ of the average number of near-neighbour contacts between sites of the walk to the maximum achievable number of contacts can also be deduced. This is given by

$$\rho \rightarrow \left(\frac{\partial a_n}{\partial \ln v} \bigg/ \frac{\partial a_n}{\partial \ln z} \right)_{z=1/\kappa} \quad \text{for large } n. \quad (16)$$

The formulae for the derivatives with respect to $\ln(v)$ may be derived much as for those with respect to $\ln(z)$. Letting U and X be the column 4-vectors with components $(\partial \xi_n / \partial \ln v)_{z=1/\kappa}$ and ξ_n respectively, we find

$$U_{n+1} = T_n U_n + 2 d_n \left(v b_n + 2 \frac{v^2}{u^2} c_n \right) X_n \quad (17)$$

where T_n is as in (12). Asymptotically as $n \rightarrow \infty$ at $z = 1/\kappa$ the terms which multiply X_n in (17) vanish, and then

$$U_{n+1} \rightarrow T U_n \rightarrow C \lambda^n \mathbf{e}. \quad (18)$$

Thus $\rho \rightarrow C/B$. Numerically we find the results also shown in figure 4.

In the limits of strongly self-repelling ($u \rightarrow 1, v \rightarrow 0$) or self-attracting ($v \rightarrow 1, u \rightarrow 0$) walks some additional comments can be made. Taking the $u \rightarrow 0$ or $v \rightarrow 0$ limits for the ξ_n in (1) and (2), one finds these relations simplify substantially, and exact values for κ can be found, as indicated in figure 4. Moreover in the $u \rightarrow 0$ and $v \rightarrow 0$ limits we anticipate that the pre-exponential factor A of (8) varies as v^α and u^β , respectively. While the numerical data indicates that $\alpha = 0$, it is insufficient to determine β , for the reasons indicated following (7). Corresponding limiting forms involving the ratio of (16) are also expected, namely $\rho \sim v^{\alpha'}$ and $(1 - \rho) \sim u^{\beta'}$. The numerical data indicates $\alpha' = 1$ and $\beta' = 0$.

Finally we note Dhar's case [3] of unweighted walks has $u = v = 1$. Here κ^N gives an asymptotic count of the number of N -step walks. We find $\kappa \cong 2.288029891153$. Because of the close relation of Dhar's 3-simplex lattice to the Sierpinski gasket, he obtains the same value for ν but a different value for κ .

3. Conclusion.

An exact approach for self-interacting self-avoiding walks on the Sierpinski gasket has been given. The exponent for the mean end-to-end separation of N -step walks is independent of the (finite) interaction strength. This last fact is evidently due to the Sierpinski gasket's low degree of ramification, i.e., the low number of sites far from two given distant sites which if deleted would cut all paths between the two given sites.

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