

Random Walks on a Fractal Solid

John J. Kozak¹

Received January 10, 2000; final March 10, 2000

It is established that the trapping of a random walker undergoing unbiased, nearest-neighbor displacements on a triangular lattice of Euclidean dimension $d=2$ is more efficient (i.e., the mean walklength $\langle n \rangle$ before trapping of the random walker is shorter) than on a fractal set, the Sierpinski tower, which has a Hausdorff dimension D exactly equal to the Euclidean dimension of the regular lattice. We also explore whether the self similarity in the geometrical structure of the Sierpinski lattice translates into a "self similarity" in diffusional flows, and find that expressions for $\langle n \rangle$ having a common analytic form can be obtained for sites that are the first- and second-nearest-neighbors to a vertex trap.

KEY WORDS: Random walks; fractals; fractal dimension; lattices.

1. INTRODUCTION

In the last decade much work have been done examining problems of diffusion on percolation networks.⁽¹⁻⁵⁾ For example, Gefen, Ahrony and Alexander⁽¹⁾ proved that diffusion on percolation networks is slower than on Euclidean ones, and, in particular, the mean-square displacement of a random walker is given in their work by

$$\langle r^2(t) \rangle \sim t^{2/(2+\theta)}$$

with $\theta=0.8$ in dimension $d=2$ for percolating networks versus $\theta=0$ for the corresponding Euclidean one.

Complementary to the above work has been studies of random walks on lattices of fractal dimension⁽⁶⁻¹¹⁾ with traps. A random walk on a lattice

¹ Department of Chemistry, Iowa State University, Ames, Iowa 50011-3111.

with N sites can be characterized by an $N \times N$ Markov transition matrix, denoted here by P . The (i, j) th element of this matrix, $p(i, j)$, is the probability, conditional on being in state i at any time, such that the next step of the random walk takes the walker to state j . The sites corresponding to state i on a lattice are traps if the sum of the elements $p(i, j)$, $j = 1, \dots, N$ of row i if P is less than 1. There is then a nonzero probability that the walk will end if it reaches state i . The case studied here is that of a deep trap; all the elements $p(i, j)$ are zero, so that the walk ends with certainty whenever it reaches state i .

The mean walklength $\langle n \rangle$ before trapping on the Sierpinski gasket, a two-dimensional uncountable set with zero measure and Hausdorff dimension

$$D = \log 3 / \log 2 = 1.584962$$

was found to be distinctly longer than $\langle n \rangle$ calculated for the corresponding $d=2$ triangular lattice.⁽⁶⁻⁸⁾ And, values of $\langle n \rangle$ calculated for random walks on the Menger sponge, a symmetric fractal set in three dimensions of Hausdorff dimension

$$D = \log 20 / \log 3 = 2.7268\dots$$

were found to be longer than on the corresponding $d=3$ simple cubic lattice (but shorter than on the corresponding $d=2$ square-planar lattice).⁽⁹⁻¹¹⁾

Evolution profiles generated from solutions to the stochastic master equation for the trapping problem were also presented in refs. 6-8. The mean walklength $\langle n \rangle$ is related (via the lattice valency) to the reciprocal of the smallest eigenvalue of the time-dependent solution to the stochastic master equation, but the full profiles showed that the conclusion was valid in the initial stages of evolution where more than one eigenvalue contributed significantly to the temporal behavior of the system.

The question posed in the present contribution can now be stated. In the studies referenced above, fractal sets were studied which were characterized by a Hausdorff dimension intermediate between the dimensionality of two, regular Euclidean lattices. It is therefore of interest to calculate (numerically-exact) values of the mean walklength $\langle n \rangle$ of a random walker on a fractal set whose Hausdorff dimension D happens to be the same as the Euclidean dimension d of a companion lattice, and to determine quantitatively whether (or not) the $\langle n \rangle$ values on the fractal set are larger (and the corresponding decay times longer) than on the comparison, Euclidian lattice.

2. RESULTS

Figure 1 illustrates a three-dimensional generalization of the Sierpinski gasket. To construct this lattice, sometimes called the Sierpinski tower, one proceeds in the same way that one constructs the planar Sierpinski gasket, only here one starts with a regular tetrahedron and then removes a half-size, upside-down regular tetrahedron. On each of the resulting tetrahedra, one repeats this procedure, and generates, eventually, the structure displayed in Fig. 1.

The Hausdorff dimension of this self-similar construction can be determined by noting that one has $N=4$ pieces in the first step of the iteration, each of size $r=1/2$, so that

$$D = \log N / \log(1/r) = \log 4 / \log 2 = 2$$

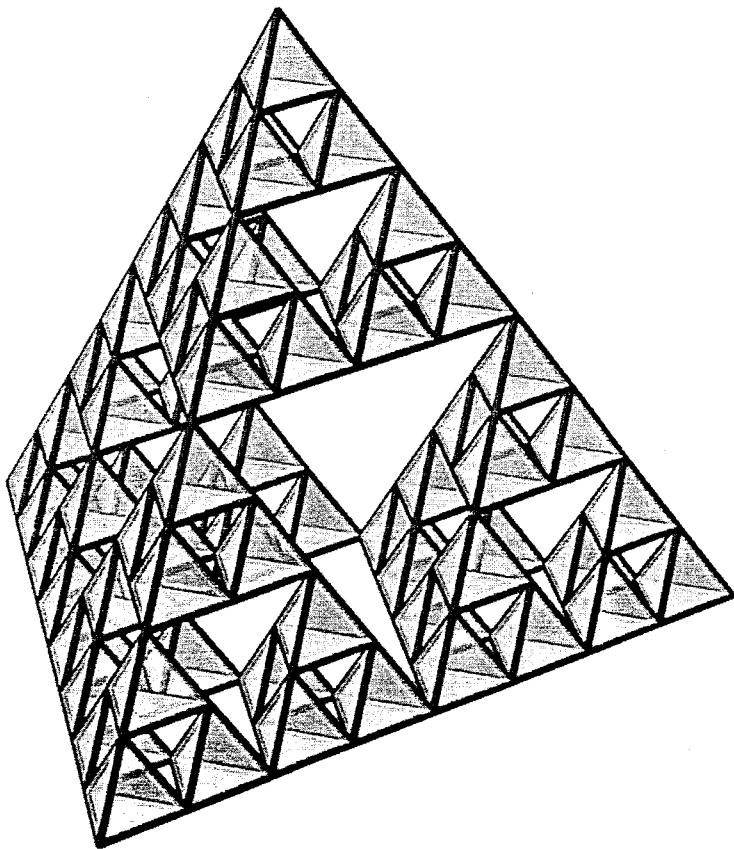


Fig. 1. The Sierpinski tower (see text).

a fractal dimension that happens to be an integer, one less than the embedding Euclidean dimension, $d = 3$.

Each node of the structure displayed in Fig. 1 is of coordination $v = 6$, except the vertex points which are of coordination $v = 3$. To make a direct comparison with the companion Euclidean lattice, a triangular lattice, all nodes of which are of uniform coordination $v = 6$, one imposes the condition that if the random walker happens to land on a vertex site in Fig. 1, it can either move away from that site (in one of three directions) or take three "virtual" steps, simply remaining at that site.

Displayed in Table 1 are numerically-exact values of $\langle n \rangle$ for the $D = 2$ Sierpinski lattice. N denotes, for each generation g , the total number of sites for which calculations were performed. The ratio of prime numbers reported in each case is the exact result, with the decimal value given to the nearest 1/1000th to facilitate comparison with the values of $\langle n \rangle$ calculated for a companion $d = 2$, $v = 6$ triangular lattice and a $d = 3$, $v = 6$ simple cubic lattice. The latter values were computed from asymptotic expressions which give the "best-fit" to the numerically-exact values of $\langle n \rangle$ reported in the literature⁽¹²⁻¹³⁾ (see later text).

The direct comparisons are for the N values, $N = 10, 34, 130$, and 514 . Placing the trap at the midpoint base site at each stage in the self-similar generation of Fig. 1 yields the smallest value of $\langle n \rangle$; placing the trap at the vertex site yields the largest values of $\langle n \rangle$. One finds that $\langle n \rangle$ for the

Table 1. Comparison of $\langle n \rangle$ Values for $d \geq 2$ Lattices

N	Sierpinski Lattice $D = 2; v = 6$		Triangular Lattice	Simple Cubic Lattice
	Vertex Trap	Midpoint Base Trap	$d = 2; v = 6$	$d = 3; v = 6$
10	$\frac{83}{2^2} = 20.75$	$\frac{(7)(17)}{(2^2)(3)} = 9.916$	9.382	5.846
34	$\frac{(3)(3049)}{(2^3)(11)} = 103.943$	$\frac{(3^3)(461)}{(2^3)(11)} = 47.147$	42.032	37.393
130	$\frac{(3)(23)(61)(97)}{(2^4)(43)} = 593.420$	$\frac{(3)(60821)}{(2^4)(43)} = 265.208$	206.348	159.566
517	$\frac{(11)(13)(127)(353)}{(2^5)(3)(19)} = 3514.711$	$\frac{(179)(839)}{(2^5)(3)} = 1564.386$	1007.078	693.933

Sierpinski “tower” is always greater than the $\langle n \rangle$ value calculated on the companion $d = 2$ triangular lattice and, certainly, for the $d = 3$ simple cubic lattice. This answers the question posed earlier and is the principal result of this study.

Whereas the comparisons in Table 1 for fixed N were based on asymptotic expressions for $\langle n \rangle$ for the companion Euclidean lattices, numerically-exact values of the mean walklength were reported in earlier work for symmetric $d = 2$, $v = 6$ triangular lattices subject to a variety of boundary conditions.⁽¹²⁾ Listed in Table 2 are the values of $\langle n \rangle$ for a triangular lattice subject to confining boundary conditions. The latter boundary condition permits the generation of the full triangular lattice from the “unit cells” displayed in Fig. 2, and is realized by imposing the constraint that when a walker attempts to step outside the unit cell from a boundary site, it simply returns to the site from whence it came. Note that the result calculated for the $N = 19$, $d = 2$, $v = 6$ triangular lattice coincides exactly with the value calculated for the (smaller) $N = 10$, $D = 2$, $v = 6$ Sierpinski lattice with a trap located at the vertex. This result complements the asymptotic results reported in Table 1. The further (numerically-exact results reported in Table 2 document further the conclusion that values of $\langle n \rangle$ calculated for the $D = 2$ lattices are systematically larger than values calculated for the companion $d = 2$ lattice.

Table 2. $\langle n \rangle$ Values for $d = 2$, $v = 6$ Triangular Lattices

N	Centrosymmetric Trap
19	$\frac{83}{2^2} = 20.75$
37	$\frac{(5)(149)}{2^4} = 46.563$
61	$\frac{(2^2)(3^3)(19)(53)}{(5)(257)} = 84.635$
91	$\frac{(3^3)(863)(3833)}{(2^2)(5)(13)(281)} = 135.829$
127	$\frac{(3^3)(11)(23)(43)(38971)}{(2^2)(7)(2035757)} = 200.822$
169	$\frac{(3^2)(23)(47)(2713)(91009)}{(2^5)(7)(647)(59159)} = 280.175$

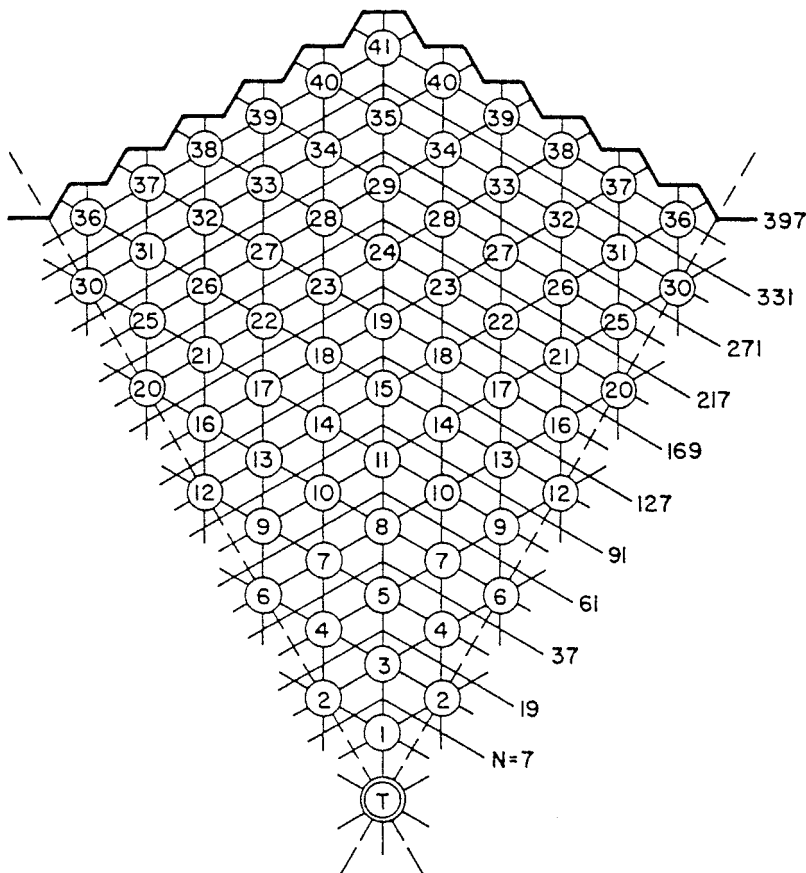


Fig. 2. Unit cells of the $d=2, v=6$ triangular lattice; the symmetry-distinct sites are denoted by integers.

3. SELF SIMILARITY

The figure displayed in Fig. 1 is self similar. A natural question is whether this self similarity translates into a "self similarity" in the diffusional flows, as monitored by values of the $\langle n \rangle$. A first response to this question can be given by placing a trap at the top vertex site, and calculating changes in the values of $\langle n \rangle$ at the sites which are the first- and second-nearest neighbor sites to this vertex site as one considers sequentially the first ($N=10$), second ($N=34$), third ($N=130$), fourth ($N=517$), ..., g th generation lattice.

Table 3. Comparison of $\langle n \rangle_i$ Values for First- and Second-Nearest Neighbors for the Sierpinski vs. Triangular Lattice

N	1st	2nd	
		corner site	midpoint base site
<i>D</i> = 2 Sierpinski Lattice			
10	(2)(3 ²)	$\frac{(3^2)(5)}{2} = 22.5$	$\frac{(3)(29)}{(2^2)} = 21.75$
34	(2)(3)(11)	$\frac{(3^2)(21)}{2} = 94.5$	$\frac{(3)(109)}{(2^2)} = 81.75$
130	(2)(3)(43)	$\frac{(3^2)(5)(17)}{2} = 382.5$	$\frac{(3)(429)}{(2^2)} = 321.75$
514	(2)(3)(171)	$\frac{(3^2)(341)}{2} = 1534.5$	$\frac{(3)(1709)}{(2^2)} = 1281.5$
<i>d</i> = 2 Triangular Lattice			
19	18	$\frac{(3^2)(5)}{2} = 22.5$	$\frac{(3)(29)}{(2^2)} = 21.75$
37	36	$\frac{(3^3)(7)}{2^2} = 47.25$	$\frac{(3)(11^2)}{(2^3)} = 45.375$
61	60	$\frac{(3^2)(2297)}{257} = 80.437$	$\frac{(3^2)(5)(877)}{(2)(257)} = 76.780$
91	90	$\frac{(3^2)(17)(19)(613)}{(2^2)(13)(281)} = 121.954$	$\frac{(3)(103)(10973)}{(2^3)(13)(281)} = 116.023$
127	126	$\frac{(3)(5)(13)(29)(123677)}{(2)(2035757)} = 171.777$	$\frac{(3)(7)(23)(479)(5741)}{(2^2)(2035757)} = 163.111$
169	168	$\frac{(3)(11733154931)}{(2^2)(647)(59159)} = 229.906$	$\frac{(3)(7)(61)(239)(218081)}{(2^3)(647)(59159)} = 218.046$

Let us denote the first nearest-neighbor site by *n*, and the two, second nearest-neighbor sites, the corner site and the midpoint base site, by *c* and *m*, respectively. Displayed in Table 3 are the numerically-exact values of $\langle n \rangle$ for the first-nearest neighbor site *n*, and the two second-nearest sites, viz., *c* and *m*, for the first four generations of the Sierpinski tower.

The values reported in Table 3 for the three cases (*n*, *c*, *m*) can be generated from the following expressions:

n site:

$$\langle n \rangle = (2 \cdot 3) \left\{ 4^{g-1} f(n) - \frac{1}{3} (4^{g-1} - 1) \right\}$$

with $f(n) = 3$;

c site:

$$\langle n \rangle = \frac{3^2}{2} \left\{ 4^{g-1} f(c) + \frac{1}{3} (4^{g-1} - 1) \right\}$$

with $f(c) = 5$;

m site:

$$\langle n \rangle = \frac{3}{2^2} \left\{ 4^{g-1} f(m) - \frac{7}{3} (4^{g-1} - 1) \right\}$$

with $f(m) = 29$.

As is evident, the three expressions for $\langle n \rangle$ have a common analytic form, and it is reasonable to suppose that this commonality is a consequence of the underlying self-similarity in the Sierpinski fractal.

Similar calculations for the first six generations of the $d=2, v=6$ triangular lattice were performed; the results are also displayed in Table 3. Several points are worth noting. First, analytic expressions similar to those reported above could not be found for the triangular lattice. Second, as expected from the results presented in Table 1, values of $\langle n \rangle$ for the sites n, c and m for the $g=1$ generation are identical for the $N=10$ fractal lattice and the $N=19$ Euclidean lattice; however, on comparing results for the $g=2$ generation, one finds already that the value of $\langle n \rangle$ for the corner site on the $N=37$ triangular is half the value of $\langle n \rangle$ for the corner site on the $N=34$ Sierpinski lattice, demonstrating again the consequences of modifying the regular Euclidean lattice structure, even in a self-similar way. Third, from these results, and those reported earlier, it is clear that the values of $\langle n \rangle$ for the Sierpinski lattice have a stronger N -dependence than the $(N \ln N)$ -dependence one expects for $d=2$ Euclidean lattices (see following section).

4. CONCLUSIONS

The role of lattice dimensionality and coordination in influencing the efficiency of trapping of a random walker on regular, Euclidean lattices was addressed in a classic series of papers by Montroll and Weiss thirty years ago.⁽¹⁴⁻¹⁶⁾ It was proved that the mean walklength before trapping was given by the expressions

$$\langle n \rangle = N(N+1)/6, \quad d=1$$

$$\langle n \rangle = N/(N-1)[A1N \ln N + A2N + A3 + A4/N], \quad d=2$$

where the coefficients $\{A_1, A_2, A_3, A_4\}$ were determined by the lattice coordination, and

$$\langle n \rangle = 1.516\,386\,0591N + O(N^{1/2}), \quad d = 3$$

for simple cubic lattices. The significant dependence of $\langle n \rangle$ on the Euclidean dimension d is clearly displayed in these analytic results. For given N , the efficiency of trapping increases with increase in d .

Taking together the results presented in the earlier contributions, refs. 6–12, and the result reported here, the conclusion reached by Montroll and Weiss on the role of dimensionality in influencing the trapping efficiency can be extended.

First, if the Hausdorff dimension D is less than or equal to the Euclidean dimension d of the companion lattice, trapping on the fractal lattice will be less efficient. Intuitively, fractal lattices tend to be “more disordered” than Euclidean lattices, and this slows down the trapping process. In fact, as noted in the previous section, values of $\langle n \rangle$ for the Sierpinski tower increase with N faster than $N \ln N$, the asymptotic, dependence which characterizes the companion $d = 2$ lattice.

Second, for the particular fractal sets studied in refs. 6–12, when the Hausdorff dimension D is greater than the Euclidean dimension d , trapping on the fractal set was found to be more efficient. The referee has noted, however, that when D is only slightly larger than d , this ordering may not hold. The two effects, “randomness” versus system dimensionality, may balance or either one may still “win” out in this situation. This phenomenon is well known in models of localization in which a distribution of weak barriers is stronger than a strong one.

Preliminary evidence that self-similarity in the geometrical structure of the Sierpinski lattice can translate into a self similarity in diffusional flows was presented in Section 3. The same procedure can be used to determine whether the overall walklength $\langle n \rangle$ also satisfies expressions similar to those found for the first- and second-nearest neighbor sites, and this will be pursued in further work.

ACKNOWLEDGMENTS

It is a pleasure to contribute to this volume in honor of Professor Gregoire Nicolis, Director of the Centre for Nonlinear Science and Complex Phenomena at the Université libre de Bruxelles. The importance of his contributions to thermodynamics and statistical mechanics sustains the traditions of the Brussels school and contributes significantly to the legacy of Theophile De Donder and Ilya Prigogine.

REFERENCES

1. Y. Gefen, A. Aharony, and S. Alexander, *Phys. Rev. Lett.* **50**:77 (1983).
2. G. Weiss and R. J. Rubin, *Adv. Chem. Phys.* **52**:363 (1983).
3. A. Blumen, J. Klafter, and G. Zumofen, *Optical Spectroscopy of Glasses*, I. Zschokke, ed. (D. Reidel, Dordrecht, 1986).
4. S. Havlin and D. Ben-Avraham, *Adv. Phys.* **36**:695 (1987).
5. J. M. Drake and J. Klafter, *Phys. Today* **43**:46 (1990).
6. G. D. Abowd, R. A. Garza-Lopez, and J. J. Kozak, *Phys. Lett. A* **127**:155 (1988).
7. R. A. Garza-Lopez and J. J. Kozak, *Phys. Rev. A* **40**: 7325 (1989).
8. R. A. Garza-Lopez, J. K. Rudra, R. Davidson, and J. J. Kozak, *J. Phys. Chem.* **94**:8315 (1990).
9. J. J. Kozak, *Chem. Phys. Lett.* **275**:199 (1997).
10. R. A. Garza-Lopez, M. Ngo, E. Delgado, and J. J. Kozak, *Chem. Phys. Lett.* **306**:411 (1999).
11. R. A. Garza-Lopez and J. J. Kozak, *J. Phys. Chem.* **103**:9200 (1999).
12. P. A. Politowicz and J. J. Kozak, *Langmuir* **4**:305 (1988).
- 13.(a) C. A. Walsh and J. J. Kozak, *Phys. Rev. B* **26**:4166 (1983); (b) P. A. Politowicz and J. J. Kozak, *Mol. Phys.* **62**:939 (1987).
14. E. W. Montroll, *Proc. Symp. Appl. Math. Am. Math. Soc.* **16**:193 (1964).
15. E. W. Montroll and G. H. Weiss, *J. Math. Phys.* **6**:167 (1965).
16. E. W. Montroll, *J. Math. Phys.* **10**:753 (1969).