Use of combinatorial algebra for diffusion on fractals

Akhlesh Lakhtakia
The Center for Engineering of Electronic and Acoustic Materials and Laboratory for Electromagnetic and Acoustic Research, Department of Engineering Science and Mechanics, The Pennsylvania State University, University Park, Pennsylvania 16802

Russell Messier
Materials Research Laboratory and Department of Engineering Science and Mechanics, The Pennsylvania State University, University Park, Pennsylvania 16802

Vijay K. Varadan and Vasundara V. Varadan
The Center for Engineering of Electronic and Acoustic Materials and Laboratory for Electromagnetic and Acoustic Research, Department of Engineering Science and Mechanics, The Pennsylvania State University, University Park, Pennsylvania 16802
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The use of combinatorial algebra for understanding diffusive motion on a geometrically ordered fractal lattice is demonstrated. The specific example of the fractal lattices used are the Pascal-Sierpiński gaskets of prime orders of which the well-known Sierpiński gasket is a special case. It is shown that the conclusions obtained from such an analysis can be meaningfully interpreted in physical terms.

Renormalization procedures[1-3] have been widely employed recently for understanding diffusion on the Sierpiński gasket, and with great success. For example, Guyer[1] has pointed out that comparison of calculated and experimentally obtained results will make sense only if the length-scale and the time-scale regimes coincide; and O'Shaughnessy and Procaccia[2] have confirmed the validity of a scaled diffusion equation. The techniques used for obtaining these and other results can hardly be considered simple. It is surprising, therefore, that the use of combinatorial algebra has not been made in investigating diffusion on geometrically self-similar fractal lattices, particularly when this algebra is very well known. By its very nature, combinatorial algebra is particularly suited for analyzing such fractals because these fractals can be thought of as *structures of structures,* not unlike the concept of *arrays of arrays* put forward in 1943 by Schellkunhoff.[4] It is the object of this report to introduce the use of combinatorics for this purpose by considering diffusive motion on the Pascal-Sierpiński gaskets,[5] of which the Sierpiński gasket is a special case. Some results derived by this approach are given with emphasis on physical interpretation.

The Pascal-Sierpiński gaskets (PSG's) are constructed on a symmetric triangular grid, in which the nth row, $n=0,1,2,\ldots$, contains $n+1$ number of sites $\{n,m_n\}$, $m_n=0,1,2,\ldots,n$. Attached with each site is the binomial coefficient $\{n![m_n!(n-m_n)!]^{-1}\}$, so that the resulting map of the binomial coefficients forms the famous Pascal's triangle.[6] Now, all sites whose binomial coefficients are multiples of some prime N, $N\neq 1$, should be made to vanish. The first $N^{(L+1)}$ rows of the surviving sites form a PSG of order N which has evolved to a stage L, $L\geq 1$. The similarity fractal dimension of these PSG's has been shown to be[4]

$$d_N=\ln[(1/2)N(N+1)]/\ln(N)\,, \tag{1}$$

and for $N=2$ the PSG generated is the same as the Sierpiński gasket. The PSG of order 5, thus generated, is shown in Fig. 1.

The diffusion experiment to be performed on a PSG is now described. Let a particle enter the PSG at the site $\{0,0\}$ and move on downwards. Let the (vertical) distance between successive rows be c, and let the (horizontal) intersite distance between adjacent sites on the same row be $2d$. The rules applicable to its motion are as follows: (a) it can move downwards one row at a time, and it can never move either upwards or laterally; (b) there cannot be more than two sites available in the next row, one im-

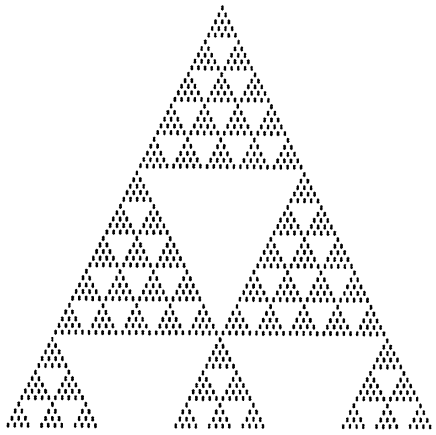

FIG. 1. The first 64 rows of the Pascal-Sierpiński gasket of order $N=5$.

mediately to the right at a horizontal distance of d, and the other immediately to the left at the same horizontal displacement from its present position; (c) if there are two possible paths permitted by rules (a) and (b), it can move leftwards with a probability $p<1$, or to the right with a probability $q=1-p$; (d) if there is only one permitted path, it surely takes it; and (e) if there is no permissible path, then that site is a sink into which the particle falls and is removed from the gasket. In Fig. 2 these various possibilities have also been illustrated. The object of this experiment to determine the chance a particle has of making its way up to some specified site in the PSG.

Parenthetically, we observe here that the prescribed set of rules has some basis in reality. Messier and Yehoda[7] have shown that the morphology of vapor-deposited thin films, in which the condensing atoms aggregate in a random ballistic fashion, form a cauliflowerlike structure. The random ballistic aggregation process leads to clustering, with the variously sized clusters competing for growth. The boundaries between the resulting growth cones, commonly called voids, form a random array of cones, which themselves cluster to form yet larger cones. These void boundaries are known to be related to diffusion. For instance, films with a lower density always etch chemically faster[8,9] and the etching proceeds preferentially along the void networks.[10] Also, hydrogen in an electrochemical cell configuration is known to have high diffusion through tungsten oxide films, and that the diffusion is predominantly along the void boundaries.[11] A mathematical description of the void network, when coupled to a realistic diffusion description, would be a significant contribution to quantitative preparation-morphology-property relations in thin films.

The use of combinatorial algebra is best illustrated by an example, like the one shown in Fig. 3 for the $N=2$ gasket. For this purpose, the basic gasket unit is made up of its first N rows. In Fig. 3 the arrival probabilities on the sites of the second row are, leftmost first $\{p,q\}$. Then, the arrival probabilities on the four sites of the last row of the stage $L=1$ are $(p\{p,q\},q\{p,q\})=(p^2,pq,pq,q^2)$. Next the arrival probabilities on the eight sites of the last row of the stage $L=2$ are

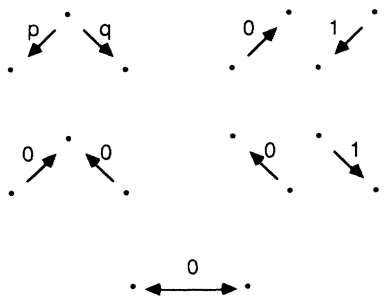

FIG. 2. Probabilities for elementary diffusive motions on a PSG.

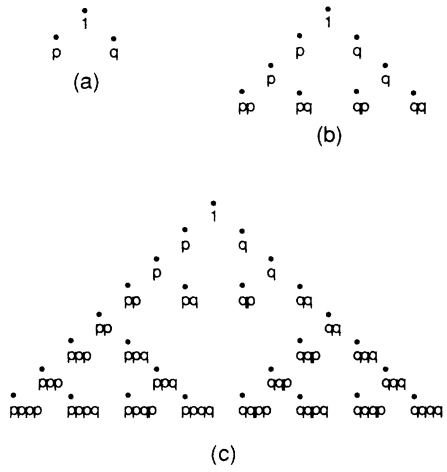

FIG. 3. To illustrate the use of combinatorial algebra on the PSG of order $N=2$. (a) Arrival probabilities for the first N rows of the PSG, to be used for calculating (b) the arrival probabilities for stage $L=1$, which, in turn, are used for computing (c) the arrival probabilities for stage $L=2$.

$$[p^2(p\{p,q\},q\{p,q\}),q^2(p\{p,q\},q\{p,q\})]$$
$$=(p^4,p^3q,p^3q,p^2q^2,p^2q^2,pq^3,pq^3,q^4)\ ,$$

and so on. The chance of arrival at other sites can also be computed in this recursive fashion. Thus, it becomes clear that the arrival probabilities for the sites of stage $L+1$ are simply related to those for the sites of the stage L.

Based on studies done on the PSGs in this manner, some remarks applicable to diffusion on these fractal structures can now be made.

Remark No. 1. The probability of arrival at any site on the last row of the Lth stage is given by

$$PQ(N,L)=\left[(p+q)\prod_{i=1,2,\ldots,L-1}[p^{i(N-1)}+q^{i(N-1)}]\right]^{N-1}$$
$$<1\ . \tag{2a}$$

This remark has been stated without proof here, but it can be easily derived by following the combinatorial procedure given above for a general PSG of order N. In particular, if $p=\frac{1}{2}$, then

$$PQ(N,L)=2^{-N(N^L-L-1)}\ , \tag{2b}$$

and it becomes clear from (2a) that as L increases, the chance of the particle getting lost in sink sites increases.

Remark No. 2. The probability of arrival at the leftmost site of the last row of the Lth stage is given by

$$P(N,L)=p^{(N-1)N^L}=[P(N,L-1)]^N\leq 1\ ; \tag{3a}$$

also the probability of arrival at the rightmost site of the same row is given by

$$Q(N,L)=q^{(N-1)N^L}=[Q(N,L-1)]^N\leq 1\ . \tag{3b}$$

To prove this remark, one needs to extract the highest exponent of either p or q in (2a), which turns out to be

$$(N-1)\left[1+(N-1)\sum_{i=1,2,\ldots,L-1}(N^i)\right]=(N-1)N^L. \tag{3c}$$

The cumulative effect of these two remarks can be discussed qualitatively now. Since it is impossible to find primes N_1 and N_2 and integers L_1 and L_2, such that

$$N_1{}^{L_1}=N_2{}^{L_2}\ , \tag{4}$$

an exact comparative study is not possible. However, a PSG of order 3 and stage 4 contains 243 rows, and a PSG of order 2 and stage 7 contains 256 rows: They may be considered roughly equal in size and compared with each other. It is seen from Eqs. (3a) and (3b) that

$$P(3,4)=p^{34}P(2,7);\quad Q(3,4)=q^{34}Q(2,7)\ , \tag{5}$$

which implies that, because $p,q<1$, the probability of arrival at the leftmost or the rightmost sites on the last rows of comparably sized order N gaskets decreases with increasing N. This is because the number of sink sites is less when N is higher, and that the sink sites are concentrated towards the median of the gasket, away from its sides.

Let us also compute $PQ(N,L)$ with $p=\frac{1}{2}$ for the two PSG's under investigation. Then,

$$PQ(3,4)=2^{19}PQ(2,7)\ , \tag{6}$$

which means that the probability of reaching any one of the sites on the last rows of comparably sized gaskets increases with increasing N. Again, the number of sink sites explains this conclusion easily.

As a result of Eqs. (5) and (6) it becomes apparent that as N increases, the tendency of the particle to travel towards the median of the gasket increases. To examine this contention further, the following remark can be made.

Remark No. 3. The probability of arrival at the central site of the last row of the Lth stage is given by

$$C(N,L)=\{(N-1)![(N/2-\tfrac{1}{2})!]^{-2}\}^{L+1}\times(pq)^{(1/2)(N-1)N^L}\ , \tag{7a}$$

the formula being valid only for the odd primes N. The proof for this remark can be obtained simultaneously with that for Remark No. 1. It can be easily seen that the ratio

$$C(N,L)[P(N,L)Q(N,L)]^{-1/2}=\{(N-1)![(N/2-\tfrac{1}{2})!]^{-2}\}^{L+1} \tag{7b}$$

increases unboundedly as N increases. Consequently, the tendency to diffuse towards the median increases with increasing N. In light of the previous three remarks, it should be noted that the probabilities of arrival on a given site are symmetric about the median axis of the PSG's if $p=\frac{1}{2}$. If $p>\frac{1}{2}$ (respectively, $p<\frac{1}{2}$), the chances of arrival in the left (respectively, right) half of the gaskets increase. Finally, with regard to counting the number of various types of sites, the following remark can be made.

Remark No. 4. There are exactly $B(N,L)$ branching sites in a PSG of order N and evolutionary stage L where the diffusing particle has a choice of two downward paths, and this number bears a direct correspondence with the similarity dimension of the PSG. This number is given by

$$B(N,L)=(\tfrac{1}{4})N^2(N^2-1)[(\tfrac{1}{2})N(N+1)]^{L-1}\ . \tag{8a}$$

To prove this statement, consider that the first N rows of the gaskets contain exactly $(\frac{1}{2})N(N-1)$ such sites. In the first stage this primitive structure comprising the first N rows is contained $(\frac{1}{2})N(N+1)$ times; so

$$B(N,1)=(\tfrac{1}{4})N^2(N^2-1)\ . \tag{8b}$$

But each PSG of stage $L>1$ contains $(\frac{1}{2})N(N+1)$ of PSG's of the previous stage $L-1$. Hence, $B(N,L)=(\frac{1}{2})N(N+1)B(N,L-1)$, and the formula (8a). In addition, the ratio

$$B(N,L)/B(N,L-1)=(\tfrac{1}{2})N(N+1)=N^{d_N}\ , \tag{9}$$

as per Eq. (1). This means that a gasket containing only the branching sites of a PSG of order N is also a geometrically ordered fractal possessing the similarity dimension d_N. This is interesting, since the total number of sites of all kinds can be enumerated as

$$T(N,L)=[(\tfrac{1}{2})N(N+1)]^{L+1}\ , \tag{10a}$$

whence

$$T(N,L)/T(N,L-1)=N^{d_N}\ , \tag{10b}$$

the right-hand side of Eq. (10b) being identical to that of Eq. (9).

In the same vein as of the previous remark, two further statements can be made, one regarding the number $S(N,L)$ of sink sites, and the other for the number $O(N,L)$ of sites from which only one downward path is possible. Without giving any proofs for them (which can be found using procedures similar to that for Remark No. 4), they are as follows.

Remark No. 5. The number of sink sites in stage L, including those in the last row of the stage, can be computed recursively as

$$S(N,L)=S(N,L-1)(N^{d_N})+2(N-1)\ , \tag{11a}$$

with

$$S(N,1)=(N-2)(N^{d_N})+2(N-1)\ . \tag{11b}$$

Remark No. 6. The number of sites in stage L, including those in the last row, from which only one downward path is available can also be computed recursively as

$$O(N,L)=O(N,L-1)(\tfrac{1}{2})(N^2-N-4)-2\ , \tag{12a}$$

with

$$O(N,1)=2(\tfrac{1}{2})(N^2-N-4)-2\ . \tag{12b}$$

In the limit that L is large, the ratio

$$S(N,L)/S(N,L-1)\approx(N^{d_N}) , \tag{13}$$

implying that although a gasket made of the sink sites of a PSG is not exactly self similar, it is still a fractal structure whose fractal dimension is close to d_N. On the other hand, from Eq. (12a), the ratio

$$O(N,L)/O(N,L-1)\approx(N^{d_N})-(N-2) \tag{14}$$

in the same limit. For $N=2$, the gasket made up of the single-path sites of the PSG, though not exactly self-similar, does certainly tend to have a fractal dimension close to d_N. For very high N, say $N>23$, a similar conclusion can also be drawn.

In summary, it has been shown here by the use of combinatorial algebra on the Pascal-Sierpiński gaskets, that this simple algebra can be employed to glean some understanding of diffusive motion on geometrically ordered, self-similar fractals. Fractal lattices different from the ones employed here can be considered, and different rules for diffusive motion can be prescribed, along with the incorporation of stage-dependent and position-dependent probabilities. Since this approach requires effort on only the primitive structure (for a PSG, the first N rows), while the evolution of stages can be analyzed recursively, the use of combinatorial algebra appears to be promising.

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