Analytical Solutions for Diffusion on Fractal Objects

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A generalization of the Euclidean diffusion equation is proposed for diffusion on fractals on the basis of a scaling argument, a renormalization-group theory for the Green's function, and numerical tests. Conjectures on the applicability to natural fractals (such as porous media) are presented.

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The wide interest in the rich variety of natural objects which are best modeled as fractals[1,2] has increased further since the discovery of their unusual dynamical properties.[3-6] The unusual forms of the density of states on fractals,[4,5] their anomalous diffusion properties,[6] and the scaling laws for conductivity[3,6] have all attracted intensive research.

In this Letter we address the issue of diffusion on fractal structures. We go one step beyond previous research by proposing a generalization of the diffusion equation for Euclidean lattices to the case of lattices of noninteger dimension (section 1). When we assume a scaling form for the conductivity the equation can be solved exactly; all the well-known scaling properties follow[4,6] while the information contained in the full probability distribution is far greater. The equation should provide a theoretical framework for transport processes in, e.g., porous media in natural environments (section 4).

To help judge the arguments of section 1 we present a renormalization-group theory for the Green's function on simple fractals and numerical tests in sections 2 and 3, respectively. Throughout we emphasize the shortcomings of the smooth scaling form assumed for the conductivity and the solution of section 1 which results.

(1) *Scaling argument.*—Consider diffusion on a fractal object of fractal dimension D, embedded in space of dimension d. Let $M(r,t)$ be the probability at time t to be within the hyperspherical shell between r and $r+dr$ centered on some origin chosen to lie on the fractal. Conservation of probability requires that

$$\partial M(r,t)/\partial t = \partial J(r,t)/\partial r \tag{1}$$

where $J(r,t)$ is the total radial current. Define $p(r,t)$ as the average probability per site, i.e., $M(r,t) \sim r^{D-1} p(r,t)$. Assume now that there exists a constitutive relationship of the form

$$J(r,t) = K(r) r^{D-1} \partial p(r,t)/\partial r \tag{2}$$

where $K(r) r^{D-1}$ is defined as the total conductivity of a shell of r^{D-1} sites. Generally speaking Eq. (2) is an approximation; it involves a product of spherically averaged quantities rather than an average of a product. Equation (2) in Eq. (1) yields the diffusion equation

$$\frac{\partial p(r,t)}{\partial t} = \frac{1}{r^{D-1}} \frac{\partial}{\partial r}\left[K(r) r^{D-1} \frac{\partial p(r,t)}{\partial r}\right]. \tag{3}$$

Equation (3) is a natural generalization of the spherically symmetric diffusion equation in Euclidean spaces. For the latter D is integer and $K(r)=K$ is the constant diffusion coefficient. To calculate $K(r)$ we exploit the equivalence of the electrical conductivity problem and the stationary diffusion problem and consider a fixed potential ϕ at the origin and a zero (ground) potential at the shell at r. The total *integral* resistance $R(r) = \phi/J$. Let us assume $R(r)$ scales like $R(r) \sim r^{\alpha}$; then the conductivity at the shell r is $\sigma(r) \sim [\partial R/\partial r]^{-1} \sim r^{1-\alpha}$. From this we get $K(r) \sim r^{1-D}\sigma(r) \sim r^{2-\alpha-D}$. We thus have

$$K(r) = K r^{-\theta}, \quad \theta = D + \alpha - 2. \tag{4}$$

With use of Eq. (4) in Eq. (3) we get a diffusion equation whose exact solution is[7]

$$p(r,t) = \frac{(2+\theta)}{D\Gamma(D/(2+\theta))}\left[\frac{1}{K(2+\theta)^2 t}\right]^{D/(2+\theta)} \exp\left[-\frac{r^{2+\theta}}{K(2+\theta)^2 t}\right] \tag{5}$$

where the normalization $\int_0^\infty D r^{D-1} p(r,t)\, dr = 1$ has been used.

From (5) we obtain the exact result

$$\langle r^2(t) \rangle = [K(2+\theta)^2 t]^{2/(2+\theta)} \Gamma((D+2)/(2+\theta))/\Gamma(D/(2+\theta)) \tag{6}$$

and therefore we identify θ as the exponent of anomalous diffusion[6] and Eq. (4) (hitherto only a definition of θ) as a scaling law. Wilke *et al.*[8] have argued differently for the same law (they related the resistance to the effective number of one-dimensional links between shells) and Guyer[9] has argued for a similar law involving the couplingconstant exponent instead of the resistance exponent α. From (5), $p(0,t) \sim t^{-D/(2+\theta)}$ from which we find the usual relation for the spectral (fracton) dimension[4] $\tilde{d} = 2D/(2+\theta)$. Equation (5) appears to agree with the form suggested by Banavar and Willemsen[10] based on a different argument.

It must be emphasized that the factors $Kr^{-\theta}$ and r^{D-1} in (3) which yield (5) are the *smooth envelopes* of the conductivity and number of sites in a shell which can be highly singular functions of r in all lacunar[1] fractals. Indeed, these singularities *occur on all length scales.* In turn the solution (5) is anticipated to be the envelope of an equally singular distribution $p(r,t)$.

To illustrate the determination of K and θ and to analyze the Green's function in section 2, we need a simple fractal on which calculations can be done exactly. The obvious choice is the Sierpinski gasket which has been the testing ground for so many ideas on fractals.[3,5,9–13] For this fractal we have calculated the equilibrium current J exactly as a function of lattice size using a decimation method[14] for the case of the origin at the top triangle [Fig. 1(a)]. Now in steady state, Eq. (3) yields a current as a function of K and θ; by requiring this to equal J, both K and θ are determined. For the gasket in d dimensions we find in this way[14]

$$K = \frac{2dW}{D(2+\theta-D)(d+1)} \tag{7}$$

where W is the conductance of a bond.

(2) *Renormalization-group theory for the Green's function.*—In contrast with previous studies of the Green's function for the diffusion equation on the Sierpinski gasket[9,11,15] we deal with explicit spatial coordinates, in terms of which theory is developed. For the purpose of analysis, it is essential to choose a coordinate system which reflects the dilatational invariance. For the triangular gasket the appropriate coordinate system was suggested in Ref. 13. In a gasket with 3^n triangles, *the triangles* are labeled (see Fig. 1)

$$i = \sum_{k=0}^{n-1} a_k 3^k, \quad a_k = 0, 1 \text{ or } 2.$$

Given an inner length scale, the diffusion occurs by hopping from *site to site* with a diffusion equation $W^{-1}\dot{Q}_p = -4Q_p + \sum_q Q_q$ where q runs over four nearest-neighbor *sites.* By summing over the three vertices that belong to a given triangle we have derived the equivalent equation for triangles

$$\dot{P}_i = W\left(\sum\nolimits_j P_j - 3P_i\right) \tag{8}$$

where P_i is the probability to belong to the ith *triangle* at time t. The factor of 3 reflects the fact that triangles have three neighbors rather than four.

Consider now the Green's function $G_{i,j}^{(n)}(t)$, which is the probability to be at triangle i at time t with initial conditions $P_i(0) = \delta_{ij}$, on a gasket of 3^n triangles. $G_{ij}^{(n)}(t)$ is the Laplace transform of the Green's function $G_{i,j}^{(n)}(E)$ for the diffusion or Schrödinger equation. We wish to develop a fixed-point equation by relating it to $G_{\alpha i,\alpha j}^{(n-1)}(\beta t)$. To do so we pick four neighboring triangles on the $(n-1)$ lattice, denoted by i, k, l, m [see Fig. 1(b)]. On the (n) lattice each of these consists of three triangles, $i_\alpha = 3i + \alpha$, etc., with $\alpha = 0$, 1, 2 [Fig. 1(b)]. From Eq. (8)

$$[3 - (E/W)]G_{i,j}^{(n)}(E) = \sum\nolimits_k G_{k,j}^{(n)}(E) + \delta_{ij}. \tag{9}$$

We pick now an initial condition on a triangle j [which on the (n) lattice is composed of j_0, j_1, j_2], and derive the equations for $G_{i_\alpha,j_s}^{(n)} = \sum_\beta G_{i_\alpha,j_\beta}$, subject to $P_{i_\beta}(0) = \delta_{i_\beta j_\alpha}$. With the notation $\lambda = 1-\epsilon$, $\epsilon = E/W$, and $\delta_{i_\alpha j_s} = \sum_\beta \delta_{i_\alpha j_\beta}$ these read

$$\lambda G_{i_2,j_s}^{(n)}(\epsilon) = G_{i_1,j_s}^{(n)}(\epsilon) + G_{i_0,j_s}^{(n)}(\epsilon) + G_{l_0,j_s}^{(n)}(\epsilon) + \delta_{i_2 j_s}, \tag{10a}$$

$$\lambda G_{l_0,j_s}^{(n)}(\epsilon) = G_{i_2,j_s}^{(n)}(\epsilon) + G_{l_1,j_s}^{(n)}(\epsilon) + G_{l_2,j_s}^{(n)}(\epsilon) + \delta_{l_0 j_s}, \tag{10b}$$

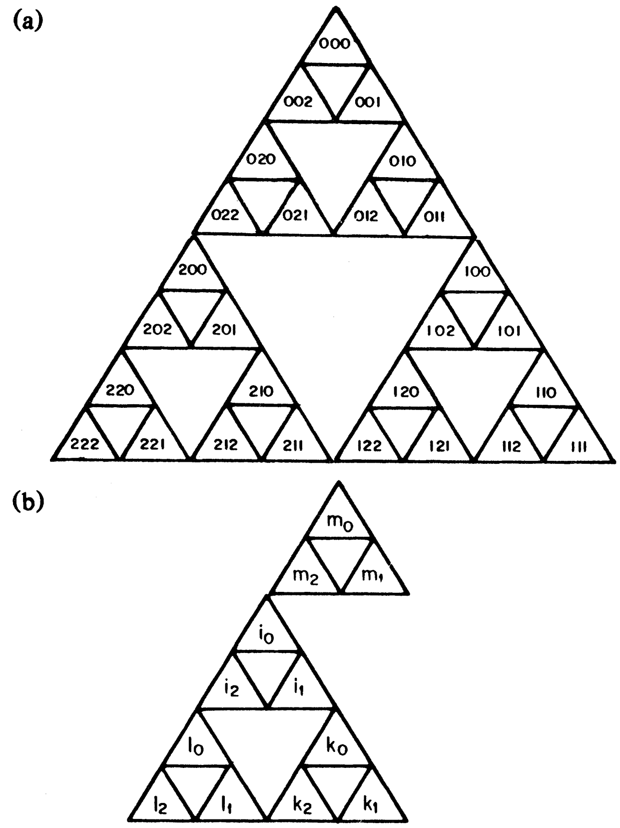

FIG. 1. (a) The Sierpinski gasket and the coordinate system used here. (b) The four triangles that are explicitly considered in the renormalization-group theory.

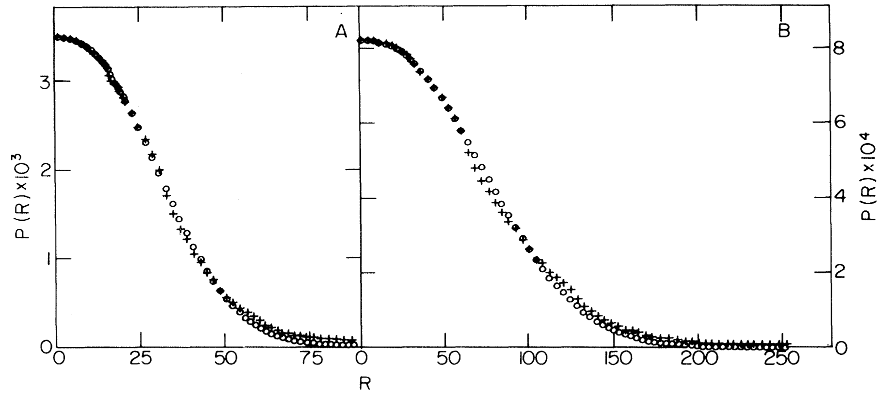

FIG. 2. Typical plots of $p(r,t)$ vs r along the edge of the gasket with δ-function initial conditions at the top, and $W=0.25$. (a) $t=3000$, r in dimensionless units, numerical experiments plotted with crosses, analytical predictions with open circles. (b) $t=25\,000$, otherwise identical to (a). Notice that the analytical predictions have no free parameters.

with similar equations for $G^{(n)}_{i_0,j_s}(\epsilon)$ $G^{(n)}_{i_1,j_s}(\epsilon)$, $G^{(n)}_{k_0,j_s}(\epsilon)$, and $G^{(n)}_{m_2,j_s}(\epsilon)$. Multiplying Eq. (10a) by $(1+\lambda)$ and adding to Eq. (10b) we find

$$(\lambda^2+\lambda-1)G^{(n)}_{i_2,j_s}(\epsilon)=(1+\lambda)[G^{(n)}_{i_0,j_s}(\epsilon)+G^{(n)}_{i_1,j_s}(\epsilon)]+G^{(n)}_{l_s,j_s}(\epsilon)+(1+\lambda)\delta_{i_2 j_s}+\delta_{l_0 j_s}, \tag{11}$$

where $G_{l_s,j_s}\equiv\sum_\alpha G_{l_\alpha,j_s}$. Analogous equations are easily found for $G^{(n)}_{i_0,j_s}(\epsilon)$ and $G^{(n)}_{i_1,j_s}(\epsilon)$. When these three equations are all summed we find

$$(\lambda^2-\lambda-3)G^{(n)}_{i_s,j_s}(\epsilon)=G^{(n)}_{l_s,j_s}(\epsilon)+G^{(n)}_{m_s,j_s}(\epsilon)+G^{(n)}_{k_s,j_s}(\epsilon)+(1+\lambda)\delta_{i_s j_s}+\delta_{l_0 j_s}+\delta_{k_0 j_s}+\delta_{m_0 j_s}. \tag{12}$$

We note that $\delta_{i_s}\delta_{j_s}=3\delta_{ij}$; the key point is that the system (12) has the same structure as a sum of systems (9). By denoting $(\lambda^2-\lambda-3)$ by $(3-\epsilon')$, we have

$$G^{(n)}_{i_s,j_s}(\epsilon)=3(1+\lambda)G^{(n-1)}_{i,j}(\epsilon')+\sum\nolimits_q G^{(n-1)}_{qj}(\epsilon') \tag{13}$$

where q are nearest neighbors to i.

To compare with the diffusion equation approach, we consider now Eq. (13) for i and j which are far apart. We then have $G^{(n-1)}_{q,j}\simeq G^{(n-1)}_{i,j}$ and also $G^{(n)}_{i_\alpha,j_\beta}\simeq G^{(n)}_{i_0,j_0}=G^{(n)}_{3i,3j}$. Accordingly we finally find

$$G^{(n)}_{3i,3j}(\epsilon)\simeq\tfrac{1}{3}(5-\epsilon)G^{(n-1)}_{i,j}(5\epsilon-\epsilon^2). \tag{14}$$

On the infinite lattice, since boundary effects are immaterial, we expect the Green's function to be the fixed-point function $G^*_{i,j}(\epsilon)$ of the rescaling procedure (14). By considering the limit $\epsilon\to 0$ we find that[14] for large times Eq. (14) predicts that

$$G^*_{3i,3j}(t)=\tfrac{1}{3}G^*_{i,j}(\tfrac{1}{5}t). \tag{15}$$

Although this equation is derived for the gasket embedded in $d=2$, its generalizations to higher d are available and will be reported elsewhere.[14]

The crucial point now is that Eq. (15) can be used on the one hand to support the validity of Eq. (3) and on the other hand to expose its shortcomings. Firstly, it is apparent that the solution of Eq. (3), i.e., Eq. (5), is a solution of the fixed-point equation (15). To see this pick, for example, $j=0$ (the uppermost triangle) for which Eq. (15) reads $G_{3i}(t)=\frac{1}{3}G_i(\frac{1}{5}t)$. A solution of this equation [together with $G_i(t=0)=\delta_i$] when expressed in terms of the distance r in the embedding space which satisfies $r\propto j^{\ln 2/\ln 3}$ is

$$G(r,t)=C_1\exp(-r^{\ln 5/\ln 2}/C_2 t)/t^{\ln 3/\ln 5}. \tag{16}$$

Remember that for the example at hand[3] $D=\ln 3/\ln 2$ and $\theta=\ln 5/\ln 2-2$; thus we see that Eq. (16) agrees exactly with Eq. (5). On the other hand we realize that Eq. (15) has information on triangles i, j and $3^n i$, $3^n j$ *only*. Therefore an analytic solution like (16) for any k, $l\neq 3^n i, 3^n j$ should be interpreted as an *envelope*. To appreciate these points further we turn now to some numerical simulations.

(3) *Numerical simulations.*.—We have solved numerically the random-walk problem [Eq. (8)] on the Sierpinski gasket with three[9] sites with delta-function initial conditions at the top triangle. We have tested the predictions of Eq. (5) by (i) plotting (see Fig. 2) the numerical values of $p(r,t)$ *along the edge* of the gasket together with the right-hand side of Eq. (5), using the theoretical value of K, Eq. (7). Notice that Eq. (5) contains no free parameters. As anticipated theoretically, Eq. (5) appears to be an envelope to the numeri-

cal results which display the expected nonanalyticities; these have interesting self-similar properties which will be discussed elsewhere.[14] (ii) We plotted $\ln[p(r,t)/p(r,0)]$ vs $[r^{2+\theta}/t]$, for many values of r and t. Satisfactory straight lines are found.[14] (iii) Lastly, we tested the scaling Eq. (15) at many general (i,j) sites at various times. The scaling prediction is confirmed.[14]

(4) *Conjectures.*—Given a fractal of dimension D, be it random or not, we conjecture that when the resistance envelope scales like r^α the diffusion problem should be describable by Eqs. (3) and (5). Similarly we suggest that in natural materials, such as porous media, a link between the scaling of conductivity and the existence of a diffusion equation like (3) should be sought experimentally.

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