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Probability density for diffusion on fractals

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We propose an asymptotic formula for the probabilty density $P_F(x,t)$ that a random walker starts at an arbitrary origin on a fractal at time 0 and arrives at site x at time t. We have numerically verified the proposed form for P_F by testing a composition rule for probabilities which requires that the walker must have been on some site of the fractal at any intermediate time. We further write a Wiener integral representation of P_F.

Let $P_F(x,t)$ denote the probability density that a random walker on a fractal starts at an (arbitrary) origin on the fractal at time 0 and arrives at site x on the fractal at time t. Recently, powerful scaling hypotheses have been advanced for the Laplace transform of this quantity,[1] and in special cases the hypotheses have been verified by explicit calculations.[1,2] In this Rapid Comunication we propose an approximate functional form for $P_F(x,t)$ which realizes these scaling hypotheses directly in space-time, and which should be accurate for large times.[3]

At first sight it might appear that our exercise is a simple application of dimensional analysis. However, in order to arrive at an explicit formula for P_F, we make use of a composition rule for probabilities which requires that at intermediate times, the walker must have visited an arbitrary site on the fractal. As a by-product of this analysis we arrive at a Wiener integral representation of $P_F(x,t)$, which can be applied to compute quantities of interest which depend functionally on the actual path traversed by the walker.

The density $P_F(x,t)$ is constrained to satisfy several requirements. For one, it must be normalizable:

$$\int dx\,\rho(x)P_F(x,t)=1 \quad . \tag{1}$$

Notice that while the integral is defined over all d-dimensional space, restriction to the fractal is implemented by inclusion of a density $\rho(x)$ which (in the sense of a distribution) has support only at points x on the fractal. The density $\rho(x)$ must be specified in detail for a given fractal. However, any fractal must satisfy the scaling condition $\rho(\lambda x)=\lambda^{(d_F-d)}\rho(x)$, where d_F denotes a fractal dimension defined by the mass-volume relation.

A second requirement on the probability density is that the fluctuation of the walk from the origin be governed by the walk exponent d_w,

$$\int dx\,\rho(x)x^2P_F(x,t)\approx t^{2/d_w} \quad . \tag{2}$$

On the basis of dimensional analysis, being careful to include the scaling behavior of $\rho(x)$, one arrives at the hypothesis $P_F(x,t)=g(t)F(x^2/t^{2/d_w})$. But then the normalization condition implies that $g(t)=P_0t^{-d_F/d_w}$, with the normalization constant P_0 given by the expression

$$P_0^{-1}=\int dx\,\rho(x)F(x^2) \quad . \tag{3}$$

[We have set $F(0)=1$ to isolate the above normalization constant.] Thus, in consequence of Eqs. (1) and (2), the return to the origin depends on $t^{-d_s/2}$ with $d_s=2d_f/d_w$, the spectral dimension. As is well known, the density of harmonic excitations at low frequencies scales with this dimensions, hence the name.

We now turn to the composition rule for probabilities which we mentioned earlier. Split the time interval t into two subintervals, λt and $(1-\lambda)t$. At the intermediate time λt the walker could have been at any site y on the fractal. We demand that the walker arrives at $(y,\lambda t)$ with the correct probability density, and that it continues from this intermediate point to (x,t) with the probability density correct for that move as well:

$$P_F(x,t)\equiv\int dy\,\rho(y)P_F(y,\lambda t)P_F(x-y,(1-\lambda)t) \quad . \tag{4}$$

Surely an exact P_F must satisfy this composition rule. An approximate probability density which is appropriate for long times should also satisfy the condition if the intermediate times are also "long," e.g., long enough that the rms distance walked $R(t)\approx t^{1/d_w}$ is large compared to a lattice spacing for a fractal realized on a lattice.

In order to exploit the composition rule Eq. (4) we specialize to the probability of return to the origin. Making use of the restrictions discussed earlier, we again apply dimensional analysis (change of variables) and obtain the condition

$$\int dz\,\rho(z)F(z^2)=[\lambda(1-\lambda)]^{-d_s/2}\int dz\,\rho(z)F(z^2/\lambda^{2/d_w})F(z^2/(1-\lambda)^{2/d_w}) \quad . \tag{5}$$

Equation (5) constitutes a *functional constraint* on the function F. We shall solve the constraint in two steps. First, multiply both sides of Eq. (5) by the factor $[\lambda(1-\lambda)]^{d_s/2}$ and again scale the integration variable to obtain

$$\int dz\,\rho(z)F\{[\lambda(1-\lambda)]^{-2/d_w}z^2\}=\int dz\,\rho(z)F(z^2/\lambda^{2/d_w})F(z^2/(1-\lambda)^{2/d_w}) \quad . \tag{6}$$

Then, denoting $\lambda^{-1}=\alpha_1$, $(1-\lambda)^{-1}=\alpha_2$ we require

$$F[(\alpha_1+\alpha_2)^{2/d_w}z^2]=F(\alpha_1^{2/d_w}z^2)F(\alpha_2^{2/d_w}z^2) \quad . \tag{7}$$

The form of the arguments of F, together with the additive composition property suggested by the above, leads us to the solution

$$F(x^2/\lambda^{2/d_w})=\exp[-(x^2)^{d_w/2}/\lambda] \quad . \tag{8}$$

We can easily illustrate this solution of employing the fractal generated by a self-avoiding walk (SAW), which has $d_s=1, d_f=1/\nu$ (by convention). The rms Euclidean end-to-end distance R for this fractal scales as N^ν, where N is the number of steps of the SAW. A random walker on this fractal experiences a one-dimensional (1D) topology. Thus the probability density to transverse N steps in time t is proportional to $e^{-N^2/t}/t^{1/2}$. Substituting $R^{1/\nu}$ for N, our result follows exactly.

To further verify our continuum approximation, especially regarding the scaling property of the density $\rho(x)$, we have performed numerical simulations on realizations of specific fractals. Equation (4) has been integrated numerically for several choices of (x,t), using Eq. (8) on both the RHS (right-hand side) and LHS, and selecting several values of the intermediate time λt.

Specifically, we have constructed a two-dimensional Sierpinski gasket containing 28 526 sites, and integrated the RHS numerically, using[4] $d_F=\ln 3/\ln 2$, and $d_w=\ln 5/\ln 2$. For the special cases of return to the origin, we have selected the origin to be a symmetry point of the gasket, while for the general case of moving from the origin to a different point the sites are displaced about the symmetry point. We have found that for times ranging from 8000 to 72 000, and for values of λ of 0.4 and 0.5, the ratio of the RHS to the LHS of Eq. (4) is consistently 1.0 ± 0.01. (We shall say more about the time ranges momentarily.)

In addition, as an example of a random fractal we have constructed 30 percolation clusters at threshold on a two-dimensional square lattice of 148×148 sites. Using $d_F=1.89$, and $d_w=2.84$ (as given by the Alexander-Orbach results[5]) we again compute the RHS and LHS of Eq. (4) and form the ratio. The origin and the endpoints for these calculations are chosen randomly to lie within a square window (verified to contain at least one cluster site) of edge 10 lattice spacings centered in the lattice, in order to minimize finite-size effects. The ratios for return to the origin and for the more general case were found to be 0.96 ± 0.08 and 0.95 ± 0.08, respectively, using times ranging between 8000 and 18 000, and factors λ of 0.4, 0.5, 0.6.

Not unexpectedly, the RHS of Eq. (4) is consistently small if short times are used. For example, at $t=8000$, $R(t)\approx24$ for percolation. At length scales much below this the walker is extremely sensitive to the local environment. Thus, intermediate times must also be relatively large. On the other hand, if t becomes too large, $R(t)$ will be larger than the lattice and the integral will be missing support from important regions. It is for these reasons that we have performed our calculations with the times and λ values cited earlier.

In principle, the Wiener representation of $P_F(x,t)$ follows immediately through recursion of the demonstrated subdivision of times. Performing the subdivision so that there are N equally spaced intermediate times, we have

$$P_F(x,t)\equiv\prod_{i=1}^{i=N}P_0\int dx_i\rho(x_i)\frac{\exp\{-[(x_i-x_{i-1})^2]^{(d_w/2)}/\tau\}}{\tau^{d_s/2}} \quad . \tag{9}$$

In this formula, $\tau=t/(N+2)$, x_0 corresponds to the origin, and x_{N+1} corresponds to the final point x.

As is well known for the case of ordinary diffusion the integrand of the Wiener representation provides a mathematically well-defined measure over paths. Thus the integrand is a suitable weight for computing averages over paths of path-dependent functionals. We will not attempt to demonstrate that our integrand satisfies the mathematical requirements on a measure. Nonetheless, we believe it plausible that path-averaged functionals on fractals can be approximated correctly using the same formalism as applies in the case of ordinary diffusion,

$$\langle\Phi[x(t)]\rangle=\prod_{i=1}^{i=N}P_0\int dx_i\rho(x_i)\frac{\exp\{-[(x_i-x_{i-1})^2]^{(d_w/2)}/\tau\}}{\tau^{d_s/2}}[\Phi(x_1,x_2,\ldots,x_N)] \quad . \tag{10}$$

In principle this formula should enable one to compute path-averaged functionals for very long times, longer than what one would care to simulate explicitly on a computer. But in practice, our discussion of accuracy as a function of intermediate time steps implies one must trade off time for using very large lattices. One will have to tailor an explicit calculation carefully in order to extract numerically valid answers. We shall discuss this in greater detail in a lengthier publication.

Note added. After this work was submitted we received a report by B. O'Shaugnessy and I. Procaccia which arrived at the same conclusion, but by different methods. In addition, R. Guyer reports that he has carried out detailed simulations on a Sierpinski gasket in an (x,t) regime complementary to the one in which our results hold. He identifies the distinct regimes of interest in detail in his paper.

[1]S. Alexander and R. Orbach, J. Phys. (Paris) Lett. **43**, L625 (1982); R. Rammal and G. Toulouse, *ibid.* **44**, L13 (1983).

[2]See, e.g., D. Ben-Avraham and S. Havlin, J. Phys. A **15**, L691 (1982).

[3]Inasmuch as fractals are typically neither rotationally nor translationally invariant, one should, in principle, write $P_F=P_F(x,x_0,t)$, exhibiting the origin x_0. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, San Francisco, 1982), quantifies the origin-dependence of the "mass-volume" relation for fractals in terms of "lacunarity": the scaling exponent of the mass-volume relation defines the fractal dimension, but the coefficient exhibits fluctuations which depend upon the choice of origin. We assume that origin-dependent fluctuations are unimportant for the scaling behavior of P_F in this note.

[4]See, e.g., J. R. Banavar and M. Cieplak, Phys. Rev. B **28**, 3813 (1983).

[5]It is our understanding that $d_s=\frac{4}{3}$ is an excellent approximation for percolation.