Transition density of diffusion on the Sierpínski gasket and extension of Flory's formula

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Some problems related to the transition density $u(t,x)$ of the diffusion on the Sierpínski gasket are considered, based on recent rigorous results and detailed numerical calculations. The main contents are an extension of Flory's formula for the end-to-end distance exponent of self-avoiding walks on the fractal spaces and evidence of the oscillatory behavior of $u(t,x)$ on the Sierpínski gasket.

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In this paper we report our study on the transition density $u(t,x)$ of the diffusion and the random walk on the Sierpínski gasket, based on recent rigorous results and detailed numerical calculations. The main contents are an extension of Flory's formula for the end-to-end distance exponent of self-avoiding walks on the fractal spaces and evidence of the oscillatory behavior of $u(t,x)$ on the Sierpínski gasket.

Recently, rigorous justification of the (symmetric and isotropic) diffusion on the Sierpínski gasket and analysis of its behavior have appeared in mathematics literature [1,2]. Among the results in these studies, we focus on the transition density $u(t,x)$, the density at point x at time $t>0$, for the diffusion starting at $t=0$ from the origin of the Sierpínski gasket. In [2] $u(t,x)$ is rigorously shown to exist, and the following form of bound is proved to hold for all $t>0$ and at any point x on the Sierpínski gasket:

$$f(t,x;C_1,C_2) \le u(t,x) \le f(t,x;C_3,C_4)\,, \qquad (1)$$

where C_i's are some positive constants independent of t and x, and the function f is given by

$$f(t,x;C_1,C_2) = C_1 t^{-d_s/2} \exp\{-C_2(|x|t^{-1/d_w})^{2\eta}\}$$
$$\eta = d_w/(2d_w-2)\,. \qquad (2)$$

The exponents d_w and d_s in (2) are the walk dimension and the spectral dimension, respectively, whose values for the Sierpinski gasket are $d_w = \log 5/\log 2$, and $d_s = 2d_f/d_w = 2\log 3/\log 5$, where $d_f = \log 3/\log 2$ is the fractal dimension [3–5]. The specific form $|x|t^{-1/d_w}$ in (2) implies anomalous diffusion $\langle |x(t)|^2\rangle \sim t^{2/d_w}$ (or rather, this relation defines d_w). Note that the value of η in (2) cannot be determined from this relation alone. Bounds of the form (1) with η as in (2) are mathematically proven to hold also for a wide class of finitely ramified fractals [6] (with some generalizations, which we will not deal with here), and even on some infinitely ramified fractals such as the Sierpínski carpet [7]. The wide applicability of (2) suggests that we may take this formula as one of the bases in the studies of $u(t,x)$. We consider two problems related to $u(t,x)$. One is the extension of Flory's formula for self-avoiding walks (SAW's) to fractal spaces, and the other is the oscillatory behavior of $u(t,x)$ on the Sierpínski gasket.

It is to be noted here that there is a rigorous analogy between diffusion and harmonic vibration [4], and the behavior of $u(t,x)$ carries information on the density of eigenstates of the "Laplacian" and so forth. We ask readers to see [8] for a recent overview of the dynamical properties of fractal networks, and references therein for numerous results on fractal vibrations.

Consider a SAW on a fractal with fractal dimension d_f and spectral dimension d_s. The end-to-end distance exponent ν is defined by $R(N) \sim N^{\nu}$ $(N \gg 1)$, where N is the number of steps of a SAW and $R(N) = \langle |x(N)|\rangle$ is the average end-to-end distance of the N-step SAW. According to the mean-field-type arguments for SAW's, Flory's value ν_F [9,10] for the exponent ν is obtained by finding the solution $R = R_F(N)$, which attains the minimum of the "free energy" $-\log u(N,R) + V(N,R)$ for each N, where we wrote $u(N,R)$ for an average of the transition density $u(N,x)$ of the simple random walk over x with $|x| \approx R$, and $V(N,R) = N^2/R^{d_f}$ represents the volume exclusion effects. ν_F is then determined by $R_F(N) \sim N^{\nu_F}$. The studies that derived (2) for finitely ramified fractals start with an analysis of simple random walks and then reach the diffusions by taking continuum limits. Therefore the long time behavior $(N \gg 1)$ of the transition density $u(N,x)$ for a random walk also satisfies (1) with (2). We use the form (2) for $u(N,R)$ to obtain

$$\nu_F = \nu_F(\eta) = 2\frac{1+\eta/d_w}{d_f+2\eta}\,, \quad \eta = d_w/(2d_w-2)\,. \qquad (3)$$

The argument holds for any network with definite fractal dimension d_f and walk dimension d_w. The value $\eta = d_f/d_s = d_w/2$ was proposed at times when the form of (2) was not settled, resulting in a simpler formula $\nu_F(d_w/2) = 3/(d_f+d_w)$ [10,11]. In [10] it was pointed out that there was no justification in this choice other than simplicity, and that the problem of the choice of η remained open. A heuristic explanation of the rigorous proof [2] for the value $\eta = d_w/(2d_w-2)$ is as follows.

Fix the step N and the distance R such that $R = |x| \gg N^{1/d_w}$ and consider walks of N steps that reach

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a point at distance R; i.e., look at walks going outwards quickly. Classify the random walk sample paths by the scale r_0, such that for scale r larger (smaller) than r_0 the random walker walks straight (walks randomly; $\Delta N \sim \Delta r^{d_w}$). A walk specified by the scale r_0 passes straight through R/r_0 blocks of scale r_0, by definition. Since it takes steps of order $r_0^{d_w}$ to pass through each block, we have $N \sim (R/r_0) r_0^{d_w}$, which implies that the dominant contribution to the quick diffusion specified by (N, R) comes from the walks with $r_0 \sim (N/R)^{1/(d_w-1)}$. Each time the walker passes the block straight through it loses probability by 1/4, because, at each node, there are four possible directions (i.e., the four outmost vertices of the two blocks connected to the node) in which to go. The total decay of probability, which gives an estimate of the transition density is $u(N, R) \sim 4^{-(R/r_0)}$, because the walker passes R/r_0 blocks straight through. Using the estimate for r_0 given above, we have $-\log p_N(R) \sim (R N^{-1/d_w})^{d_w/(d_w-1)} \log 4$, which implies $\eta = d_w/(2d_w - 2)$.

The reason that (2) is to be used for Flory's formula can be seen from the above argument; compared to random walks, the SAW is "pushed outwards" owing to self-repulsion or volume exclusion effects. Therefore, the dominant contribution to the SAW comes from those walks that move quickly away. The argument given above explains that the value $\eta = d_w/(2d_w - 2)$ is the consequence of the contribution from walks that quickly move away; hence, it is reasonable to use this form in deriving Flory's formula.

The explicit values of d_f and d_w are known for the Sierpínski gasket and its natural d-dimensional generalizations (dSG's), constructed by a $(d+1)$ simplex instead of by a triangle. The values are $d_f = \log(d+1)/\log 2$ and $d_w = \log(d+3)/\log 2$ for dSG's [3–5], with which $\nu_F = \nu_F(d_w/(2d_w - 2))$ can be calculated from (3). For 2SG (= Sierpínski gasket) and 3SG, the values of ν_F (0.8249... and 0.724588..., respectively) are to be compared with the exact values of ν, which are

$$\begin{aligned} \nu(\mathrm{2SG}) &= \log 2/\log(7-\sqrt{5})/2 = 0.79862\ldots, \\ \nu(\mathrm{3SG}) &= 0.67402\ldots. \end{aligned} \tag{4}$$

The value of ν(3SG) has an exact expression similar to that for ν(2SG), but in place of integers 7 and 5 appear roots of a 14th order algebraic equation [12]. The values in (4) have been known for some time [13] (see also [10,14]), and have recently been proved rigorously in [15,12]. Flory's formula (3) is within a 3% and 8% precision from the exact values for 2SG and 3SG, respectively. Flory's formula is known to be numerically very good for SAW's on Euclidean lattices (for a recent review of SAW's on Euclidean lattices, see [16]). The extended Flory's formula (3) that we have is not bad, but it is not very close to the exact values compared to Euclidean cases. If we put $\eta = 1$, the values become closer (in fact, they are close to the best choice) to the exact results (0.06% and 3% deviation for 2SG and 3SG, respectively). The choice $\eta = d_w/(2d_w - 2)$ has the soundest basis (1) and (2), but the value is better for 2SG and 3SG with $\eta = 1$. Deviation of (3) from the rigorous and exact results (4) leads our interest to detailed numerical studies of $u(t, x)$.

Two open problems are found in the literature concerning the detailed structure of $u(t, x)$. One problem is the value of η; the results given in [17] agree with (2), while those in [18] claim the value $\eta = d_w/2$. The other problem is the observation in [2,19] that there are "oscillations" in $u(t, x)$.

To perform numerical calculations, we regard $u(t, x)$ as the electric charge density of a point x at time t, and reformulate the problem in terms of the impedance circuits. We consider a d-dimensional Sierpínski gasket dSG. The corresponding electrical circuit has an impedance distribution on the gasket, and also impedance between the gasket and the ground. By symmetry and star-triangle (Y-Δ) type relations, a unit block of the gasket (a subcircuit of d-dimensional simplex with side length 1) can effectively be represented by a device with $d+1$ terminals, each connected by an impedance $a(s)$ to the center point of the simplex, to which the ground is connected by an impedance $b(s)$. s is the dual variable to t in the Laplace transform. The self-similarity of the diffusion implies the scaling behavior $B\,u(Lt, 2x) = u(t, x)$ [1–5], where we put $L = d+3 = 2^{d_w}$ and $B = d+1 = 2^{d_f}$. Using the scaling behavior, the self-similarity of the gasket, and the similarity among $d+1$ terminals of a block simplex, together with star-triangle-type relations, we find

$$(a(Ls)\,L/B,\ g(Ls)) = W(a(s),\ g(s))\,, \tag{5}$$

where $g(s) = 2a(s)/b(s)$, and $W(x, y) = (x(y+L)/(y+B), y(y+L))$. We also find $g(0) = 0$. $g'(0)$ and $a(0)$ determine the normalization of u and t. We focus on the normalization independent quantities such as exponents and oscillations. By fixing $g'(0)$ and $a(0)$, the solution of the functional equation (5) is determined uniquely. The equation for $g(s)$ is known as Schröder's functional equation. The existence of the solution has been studied [20], but its detailed behavior seems to be unknown.

We define two asymptotic functions $C(s) = s^{1-d_s/2} \lim_{n\to\infty} (L/B)^n a(L^n s)$ and $k(s) = s^{-1/d_w} \lim_{n\to\infty} 2^{-n} \ln g(L^n s)$, for $s > 0$. These functions are periodic in $\log s$ with period $\log L$, and hence can be expanded in Fourier series:

$$\begin{aligned} C(s) &= c_0 + \sum_{n=1}^{\infty} c_n \sin(2\pi n \log_L s + \phi_n)\,, \\ k(s) &= k_0 + \sum_{n=1}^{\infty} k_n \sin(2\pi n \log_L s + \phi_n')\,. \end{aligned} \tag{6}$$

We numerically obtained by double precision FORTRAN calculations for $d = 2$, the Sierpínski gasket; $c_1/c_0 = 1.219\,294\,38 \times 10^{-5}$ and $c_2/c_1 = 3.68 \times 10^{-6}$, for $C(s)$; and $k_1/k_0 = 1.526\,419\,1 \times 10^{-6}$ and $k_2/k_1 = 5.6 \times 10^{-7}$, for $k(s)$. The results show a strong hierarchy of coefficients, such that the higher frequency components have exponentially small values [$c_n = O(10^{-5n})$, $k_n = O(10^{-6n})$]. Note that we have small but nonzero numbers of $O(10^{-6})$ out of Eq. (5) with $O(1)$ coefficients, which is potentially an interesting phenomenon. We performed the numerical calculations up to $d = 10$, and obtained qualitatively similar behavior, with somewhat larger amplitudes of oscillations for larger d. For a precision check, we performed

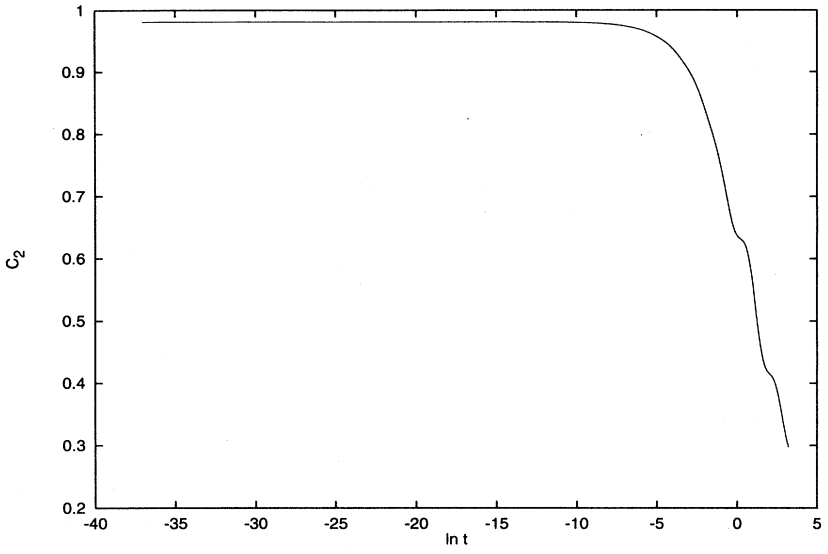

FIG. 1. $C_2(t) = t^{2\eta/d_w} \ln[u(t,0)/u(t,1)]$.

the calculations for $d = 1$, corresponding to the diffusion on a line, and obtained the correct constant values $C(s) = 2^{1/2}$ and $k(s) = 2^{1/2}$, within an error of 10^{-14}. The peak values of $k(s)$ are consistent with the numerically obtained values in [2].

We can calculate the Laplace transform $\tilde{u}(s,x)$ of the density using the impedances. For the transition density at the origin, we have $\tilde{u}(s,0) = a_\infty(s)/2$, where $a_\infty(s) = C(s)\, s^{d_s/2-1}$ is the impedance corresponding to a simplex of "infinite" size. Using (6), we can evaluate the inverse Laplace transformation of $\tilde{u}(s,0)$, term by term in the Fourier series, using a change of contours. We have

$$u(t,0) = N\, t^{-d_s/2}\left[c_0 p_0 + \sum_{n=1}^{\infty} c_n p_n \cos(2\pi n \log_L t - \psi_n)\right],$$

with c_n as in (6) and $p_n = |\Gamma(2^{-1}d_s + \pi^{-1}\Omega n i)|2^{-1/2}[\cosh(2\Omega n) - \cos(\pi d_s)]^{1/2}$ for $n \geq 0$, where $\Omega = 2\pi^2/\ln L$. N is a normalization constant. Thus the oscillation in $C(s)$ explains that in $u(t,0)$.

We parametrize $u(t,x) = f(t,x;C_1(t),C_2(t,x))$ with f as in (2), and consider the oscillations in C_i's. Using the values given below (6) for c_n's, we have, for $d = 2$, $C_1(t) = t^{d_s/2}u(t,0) = C_{10} + C_{11}\cos(2\pi \log_L t - \psi_1) + \cdots$, with $C_{11}/C_{10} = 8.096\,478 \times 10^{-3}$. We performed a numerical Laplace inverse transformation of $\tilde{u}(s,0)$ and obtained a consistent value. The Laplace transform of the density $u(t,1)$ at a vertex of a unit simplex is given by $\tilde{u}(s,1)/\tilde{u}(s,0) = [1 + g(s)/(2d)][1 - a(s)/a_\infty(s)] - a(s)/[da_\infty(s)]$. $C_2(t) = C_2(t,1)$ is then given by $C_2(t) = t^{2\eta/d_w}\log[u(t,0)/u(t,1)]$. To calculate the inverse Laplace transforms for small t ($t \leq 10^{-2}$), we find $s = s_0 > 0$, which gives a minimum of $\tilde{u}(s,1)\exp(st)$ (as we do in the steepest descent method of complex contour integration), and numerically evaluate the contour integration with the contour $\mathrm{Re}(s) = s_0$. For larger t we use the contour $\mathrm{Re}(s) = 1/t$. (The details of the numer-

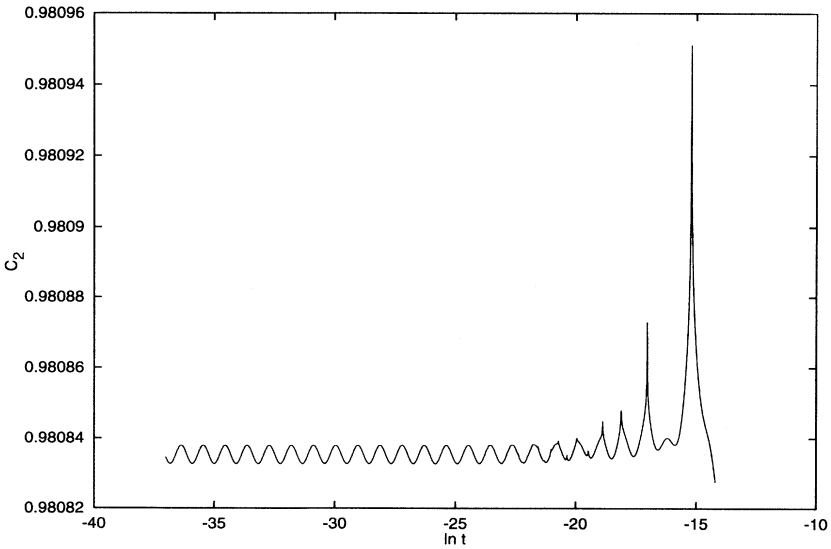

FIG. 2. Oscillation of $C_2(t)$ for small t.

ical calculations will be reported elsewhere.) Figures 1 and 2 show $C_2(t)$ for $d = 2$ as a function of $\ln t$. Figure 2 shows the small oscillation [$O(10^{-6})$ in amplitude] in $C_2(t)$ for very small t. We performed similar calculations for the exactly solvable $d = 1$ case, and checked that the error in the range of Fig. 2 is $O(10^{-11})$. Small t corresponds to large s in the Laplace transform, where we have an asymptotic formula $\tilde{u}(s,1)/\tilde{u}(s,0) \sim \exp[-s^{1/d_w}k(s)]$. Thus the oscillation in $k(s)$ explains that in $C_2(t)$ for very small t.

From Fig. 1 we see that (besides the tiny oscillation) $C_2(t)$ is flat for small t. This is consistent with the fact [2] that the value $\eta = d_w/(2d_w - 2)$ explains the asymptotic behavior of $u(t,x)$ as $t \to 0$. For larger t, $C_2(t)$ is decreasing with a significant size of oscillation. If we try to explain this decrease in terms of "effective (dynamical)" changes in the value of η, i.e., keep C_2 constant and let η change as $\eta = \eta_{eff}(t)$, we see that the effective value $\eta_{eff}(t)$ increases as t is increased. Our data are in favor of the argument in [17] that $\eta_{eff}(t) = d_w/2$ [18] may be effectively good for $t = O(1)$, while $\eta = d_w/(2d_w - 2)$ is good for $t \ll 1$. Note also that $d_w/(2d_w - 2) < 1 < d_w/2$, where $\eta = 1$ gives good $\nu_F(\eta)$. The oscillatory behavior of the data prevents us from obtaining precise results on the value of η_{eff}. In contrast to the clarity in the meaning of the value $\eta = d_w/(2d_w - 2)$, the theoretical basis for η_{eff} is still unclear, which has to be settled before we can be conclusive about its value and implications.

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