Critical dimensions for random walks on random-walk chains

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The probability distribution of random walks on linear structures generated by random walks in d-dimensional space, $P_d(r,t)$, is analytically studied for the case $\xi \equiv r/t^{1/4} \ll 1$. It is shown to obey the scaling form $P_d(r,t)=\rho(r)t^{-1/2}\xi^{-2}f_d(\xi)$, where $\rho(r)\sim r^{2-d}$ is the density of the chain. Expanding $f_d(\xi)$ in powers of ξ, we find that there exists an infinite hierarchy of critical dimensions, $d_c=2,6,10,\ldots$, each one characterized by a logarithmic correction in $f_d(\xi)$. Namely, for $d=2$, $f_2(\xi)\simeq a_2\xi^2\ln\xi+b_2\xi^2$; for $3\leqslant d\leqslant 5$, $f_d(\xi)\simeq a_d\xi^2+b_d\xi^d$; for $d=6$, $f_6(\xi)\simeq a_6\xi^2+b_6\xi^6\ln\xi$; for $7\leqslant d\leqslant 9$, $f_d(\xi)\simeq a_d\xi^2+b_d\xi^6+c_d\xi^d$; for $d=10$, $f_{10}(\xi)\simeq a_{10}\xi^2+b_{10}\xi^6+c_{10}\xi^{10}\ln\xi$, etc. In particular, for $d=2$, this implies that the temporal dependence of the probability density of being close to the origin $Q_2(r,t)\equiv P_2(r,t)/\rho(r)\simeq t^{-1/2}\ln t$. [S1063-651X(96)13410-3]

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I. INTRODUCTION

Random fractals represent useful models for a variety of disordered systems found in nature. In addition to their structural properties, fractals have attracted much attention in recent years because of their interesting transport properties [1–4].

Of particular interest is the question of how the probability density of random walks, $P_d(r,t)$, is changed on fractal structures with respect to its Gaussian form valid on regular d-dimensional systems, $P_d(r,t)\sim t^{-d/2}\exp(-\text{const}\times\eta^2)$, where $\eta=r/t^{1/2}$. The form of $P_d(r,t)$ on fractals has been extensively studied in the asymptotic limit $\xi=r/t^{1/d_w}\gg 1$ [2,5–12], where d_w is the anomalous diffusion exponent characterizing the time behavior of the random walks, $\langle r^2(t)\rangle\sim t^{2/d_w}$. As a result of these investigations, it is now generally accepted that $P_d(r,t)$ displays a stretched Gaussian form

$$P_d(r,t)\sim\rho(r)t^{-d_s/2}\exp(-\text{const}\times\xi^u),\quad \xi\gg 1, \tag{1}$$

where $\rho(r)\sim r^{d_f-d}$ is the density of the fractal structure, d_f is the fractal dimension, $d_s=2d_f/d_w$ is the spectral dimension [1], $u=d_w/(d_w-1)$, and is normalized according to $\int dr r^{d-1}P_d(r,t)=1$. However, much less is known about the behavior of $P_d(r,t)$ in the opposite limit when ξ approaches zero.

In this paper we concentrate on diffusion in linear random fractal structures generated by random walks [random-walk chains (RWC)] in d-dimensional systems, where $P_d(r,t)$ can be obtained exactly. Recently, using numerical simulations, it has been suggested that for such linear fractals [13],

$$Q_d(r,t)/Q_d(0,t)\sim(1-\text{const}\times\xi^{d-2}),\quad \xi\to 0, \tag{2}$$

for all dimensions d, where $Q_d(r,t)=\rho(r)^{-1}P_d(r,t)$ is normalized on the fractal chain, i.e., $\int dr r^{d_f-1}Q_d(r,t)=1$, with $d_f=2$, $d_w=4$ for RWC, $\xi=r/t^{1/4}$ and $Q_d(0,t)$ is the probability density to return to the origin.

In the following, we derive an exact expansion for $P_d(r,t)$ in the limit of $\xi\to 0$. Surprisingly, $P_d(r,t)$ displays an extremely rich behavior as a function of both ξ and dimensionality d. We show, among other results, that Eq. (2) can only be valid for $3\leqslant d\leqslant 5$, and

$$P_d(r,t)\sim\rho(r)t^{-1/2}(1-\text{const}\times\xi^4)\quad\text{for}\quad d\geqslant 7. \tag{3}$$

Moreover, we find that the small-ξ expansion of $P_d(r,t)$ is characterized by a hierarchy of critical dimensions, $d_c=2,6,10,14,\ldots$, where logarithmic corrections of the form $\xi^{d_c-2}\ln(1/\xi)$ occur. In particular, for $d=2$ we obtain $P_2(r,t)\simeq 2\rho(r)t^{-1/2}\ln(t^{1/4}/r)$.

II. RANDOM WALKS ON RANDOM-WALK CHAINS

We consider linear structures generated by random walks in d-dimensional systems. Such structures are fractals with fractal dimension $d_f=2$, independently of d. To study diffusion of particles along such linear chains, we assume that the diffusing particles (random walkers) can move only along the structure (path) which has been created sequentially by the generating walks. Thus, although the structure can intersect itself in space, the walkers see just a linear path. We denote such paths as random-walk chains.

Along the linear path, the probability density of random walkers, at chemical distance ℓ along the RWC from their starting point after time t, $p(\ell,t)$, subject to the initial condition $p(\ell,0)=\delta(\ell)$, approaches the well-known Gaussian distribution

$$p(\ell,t)=\frac{2}{(2\pi t)^{1/2}}\exp\left(-\frac{\ell^2}{2t}\right), \tag{4}$$

normalized according to $\int_0^\infty d\ell\, p(\ell,t)=1$. Thus, diffusion along the chain (i.e., ℓ space) is normal and $\langle\ell^2\rangle=t$. On the contrary, in Euclidean r space diffusion is anomalous with $d_w=2d_f=4$ (see, e.g., [2]).

To obtain the behavior of the probability density in r space, averaged over all RWC configurations, $P_d(r,t)$, we note that it is related to $p(\ell,t)$ by

$$P_d(r,t)=\int_0^\infty d\ell\,\Phi_d(r,\ell)p(\ell,t) \tag{5}$$

and is normalized according to $\int d^d r P_d(r,t)=1$. Another possibility is a normalization on the RWC fractal, i.e., $\int_0^\infty dr r^{d_f-1}Q_d(r,t)=1$. Both distributions are simply related to each other by $P_d(r,t)=\rho(r)Q_d(r,t)$.

In Eq. (5), $\Phi_d(r,\ell)$ represents the probability for a site r to belong to a RWC at distance ℓ from the origin along the chain. The chemical distance ℓ plays the role of the time variable in Eq. (4), and one can immediately write

$$\Phi_d(r,\ell)=A_d\left(\frac{1}{2\pi\ell}\right)^{d/2}\exp\left(-\frac{r^2}{2\ell}\right), \tag{6}$$

where A_d is a normalization factor such that $\int d^d r\Phi_d(r,\ell)=1$. Therefore, by inserting (4) and (6) in (5) we infer [4,14]

$$P_d(r,t)=\left(\frac{1}{2\pi}\right)^{d/2}\frac{2A_d}{(2\pi t)^{1/2}}\int_0^\infty d\ell\,\ell^{-d/2}\exp\left(-\frac{r^2}{2\ell}\right)\times\exp\left(-\frac{\ell^2}{2t}\right). \tag{7}$$

Now, the elementary transformation $x=\ell/r^2$ brings (7) to the form

$$P_d(r,t)=2A_d(2\pi)^{-(d+1)/2}r^{-d}f_d(\xi), \tag{8}$$

where the scaling function $f_d(\xi)$ is defined by

$$f_d(\xi)=\xi^2\int_0^\infty dx x^{-d/2}\exp\left[-\frac{1}{2}\left(\xi^4x^2+\frac{1}{x}\right)\right] \tag{9}$$

for the scaling variable $\xi\equiv r/t^{1/4}$. If the RWC normalization is chosen, the distribution $Q_d(r,t)=\rho^{-1}(r)P_d(r,t)\cong t^{-1/2}\tilde{f}_d(\xi)$, where $\tilde{f}_d(\xi)=\xi^{-2}f_d(\xi)$.

To deal now with the evaluation of $f_d(\xi)$ when $\xi\to 0$, it is convenient to rewrite the integrand exponent as

$$\exp\left[-\frac{1}{2}\left(\xi^4x^2+\frac{1}{x}\right)\right]=\exp\left[-\frac{1}{2}\left(\xi^4x^2+\frac{1}{x^2}\right)\right]\times\exp\left[-\frac{1}{2x}\left(1-\frac{1}{x}\right)\right]$$

and expand the second exponential factor in Taylor series. The remaining integrals can be solved exactly (see, e.g., [15]), and one arrives at the following expression for (9):

$$f_d(\xi)=\xi^2\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{1}{2}\right)^n\sum_{k=0}^{n}(-1)^k\binom{n}{k}\xi^{d/2-1+n+k}\times K_{1/2(d/2-1+n+k)}(\xi^2), \tag{10}$$

where K_ν is the modified Bessel function of order ν.

Let us consider Eq. (10) in some particular cases of interest. The results for spatial dimensions $d\leqslant 7$ are summarized in Table I. All the coefficients were calculated numerically by computing the double sums explicitly. In some cases they are available in analytic form, but we include their numerical values to make the table uniform.

TABLE I. The leading and correction terms for the series expansion of $f_d(\xi)$, with $\xi\equiv r/t^{1/4}$, when $\xi\to 0$, Eq. (10), as a function of dimension d.

d	Leading term	First correction	Second correction
1	2.1558ξ	$-2.5066\xi^2$	$O(\xi^5)$
2	$2\xi^2\ln(1/\xi)$	$0.1738\xi^2$	$O(\xi^6)$
3	$2.5066\xi^2$	$-0.0609\xi^3$	$O(\xi^6)$
4	$2\xi^2$	$-1.2533\xi^4$	$O(\xi^6)$
5	$2.5066\xi^2$	$-1.4372\xi^5$	$O(\xi^6)$
6	$4\xi^2$	$-\xi^6\ln(1/\xi)$	$-0.3369\xi^6$
7	$7.5199\xi^2$	$-1.2533\xi^6$	$0.8244\xi^7$

However, besides the coefficients, the main properties of these expansions can be obtained readily as follows. The key parameter is $s=1/2\,(d/2-1)$. The corresponding values of $d=2(2s+1)$ for integer s should be referred to as *critical dimensions*, $d_c=2,6,10,\ldots$. Each order in the expansion has its own critical dimension. The leading term has $d_c=2$, the first correction term has $d_c=6$, the second correction term has $d_c=10$, etc. This has to do with the functional form of $f_d(\xi)$ in the corresponding order which for $d<d_c$ depends on d, at $d=d_c$ it has a logarithmic correction and for $d>d_c$ becomes independent of d. In particular, the leading term of $f_d(\xi)$ behaves as ξ for $d=1$ and $\xi^2\ln(1/\xi)$ for $d=d_c=2$ and as ξ^2 for all $d>d_c=2$, the first correction term behaves as ξ^d for $2\leqslant d<6$, and for $d=d_c=6$ as $\xi^6\ln(1/\xi)$ and as ξ^6, for all $d>d_c=6$, and so on.

Mathematically, this behavior can be explained by the intrinsic properties of the Bessel function $K_s(\xi^2)$. By its definition, $K_s(\xi^2)=(\pi/2)\csc(\pi s)[I_s(\xi^2)-I_{-s}(\xi^2)]$ for noninteger s and, in turn, $I_s(\xi^2)=\xi^{2s}\Sigma_{k=0}{}^{\infty}b_k(s)\xi^{4k}$ and $\xi^{2s}I_{-s}(\xi^2)=\Sigma_{k=0}{}^{\infty}b_k(-s)\xi^{4k}$. As one can see this expansion has *s-independent* powers of ξ that form the *invariant* part of $f_d(\xi)$. The first terms of $\xi^{2s}K_s(\xi^2)$ expansion are

$$\xi^{2s}K_s(\xi^2)\approx b_0(s)\xi^{4s}+b_1(s)\xi^{4s+4}+\cdots-b_0(-s)-b_1(-s)\xi^4-\cdots.$$

Thus, for $0<s<1$ (i.e., $2<d<6$) $f_d(\xi)$ has the form $f_d(\xi)\approx\xi^2[a_0(-d)-a_0(d)\xi^{d-2}]$. We see that the first term of this expansion is the invariant part (up to numerical coefficients) of $f_d(\xi)$, which remains unchanged when varying d. The same argument shows that for $1<s<2$ $(6<d<10)$ $f_d(\xi)$ takes the form $f_d(\xi)\approx\xi^2[a_0(-d)-a_1(-d)\xi^4+a_0(d)\xi^{d-2}]$ and now *two* first terms of this expansion are the invariant part of $f_d(\xi)$. A special case in our problem is $d=1$, i.e., $s=-1/4<0$. Then the leading term of $f_d(\xi)$ is $\xi^2\xi^{-4|s|}=\xi$, which is easily seen by noting that $K_{-s}(\xi^2)=K_s(\xi^2)$.

For integer values of s, the small-ξ expansion of $\xi^{2s}K_s(\xi^2)$ has a logarithmic term of form $\xi^{4s}\ln(1/\xi)=\xi^{d-2}\ln(1/\xi)$ [15].

In general, there are $[s]+1$ ($[s]$ is the integer part of s) terms in the invariant part of $f_d(\xi)$.

III. CONCLUSIONS

We have studied analytically the small-ξ expansion of the mean probability density, $P_d(r,t)$, of random walks on random-walk chains in d-dimensional space. We have shown that the leading terms of the expansion of, $P_d(r,t)$, behaves, in the limit $\xi = r/t^{1/4} \rightarrow 0$, as

$$P_d(r,t) \propto \rho(r) t^{-1/2}(1 - a_d \xi^{d-2}) \quad \text{when} \quad 3 \leqslant d \leqslant 5,$$

and as

$$P_d(r,t) \propto \rho(r) t^{-1/2}(1 - c_d \xi^4) \quad \text{when} \quad d \geqslant 7,$$

where $\rho(r) \sim r^{d_f - d}$ and $d_f = 2$. This implies that the probability density $Q_d(r,t) = P_d(r,t)/\rho(r)$ on the fractal chain behaves for $d \geqslant 7$ as $Q_d(r,t) \sim t^{-1/2}(1 - c_d r^4/t)$, consistent with the behavior of diffusion in ℓ space, i.e., $p(\ell,t) \sim t^{-1/2}(1 - \ell^2/2t)$, for $\ell^2 \ll t$, and the fact that $Q_d(r=1,t) \sim p(\ell=1,t)$ when $d \rightarrow \infty$. We see that this already occurs when $d \geqslant 7$.

We have shown that logarithmic corrections occur at critical dimensions $d = d_c = 4n + 2$, with $n = 0,1,2, \ldots$, i.e., $d_c = 2,6,10, \ldots$, for the terms $\xi^{d_c - 2}\ln(1/\xi)$. In particular for $d = 2$, $Q_2(r,t) \simeq t^{-1/2}\ln(t^{1/4}/r)$, for $r \ll t^{1/4}$, and the probability density for the random walker to be close to the origin, $Q_2(r,t)$ behaves as $t^{-1/2}\ln t$. This logarithmic correction is due to the fact that in two dimensions the RWC returns to its starting point with probability 1. In one dimension, $Q_1(r,t) \simeq t^{-1/4}/r$, and in $d = 3$, $Q_3(0,t) \simeq t^{-1/2}$. One can say that $d = 2$ plays the role of a marginal dimensionality for the probability density of being at the origin of random walks on RWC, while for larger r each order in the expansion has its own critical dimension.

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