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Probability distribution of random walks on self-avoiding walks

H Eduardo Roman

Institut für Theoretische Physik III, Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

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Abstract. The probability distribution of random walks on one-dimensional fractal structures generated by random walks (RW chains) and self-avoiding walks (SAW chains) in d -dimensional space, $P_d(r, t)$, is studied analytically in the case $\xi \equiv r/t^{1/d_w} \ll 1$, where d_w is the fractal dimension of the random walk, $\langle r^2(t) \rangle \sim t^{2/d_w}$. It is shown that there exists an infinite hierarchy of critical dimensions, $d = d_c = 4n + 2$, with $n \geq 0$ for RW chains and $n \geq 1$ for SAW chains, for each term in the ξ -expansion of $f_d(\xi)$, the scaling part of $P_d(r, t)$. Each transition is characterized by its own logarithmic correction.

1. Introduction

Random fractals represent useful models for a variety of disordered systems found in nature. In addition to their novel structural properties, fractals have attracted much attention in recent years because of the interesting transport phenomena resulting from the self-similarity of the conduction paths [1–8].

A great deal of interest has been devoted to the question of how the distribution of random walks, $P_d(r, t)$, representing the probability density that a walker is at distance r from its starting point at time $t = 0$, is modified on fractal structures with respect to the standard Gaussian form valid on regular d -dimensional systems, i.e.

$$P_d(r, t) \sim t^{-d/2} \exp(-\text{constant} \times r^2/t).$$

On fractals, the form of $P_d(r, t)$ depends on the value of the scaling variable $\xi = r/t^{1/d_w}$, where d_w denotes the fractal dimension of the random walk characterizing the time evolution of the mean-square displacement of the walks, $\langle r^2(t) \rangle \sim t^{2/d_w}$, $d_w > 2$. So far, much interest has been devoted to the tail of the distribution, corresponding to the limit $\xi \gg 1$ [2–8]. As a result of these works, it is now generally accepted that $P_d(r, t)$ displays a stretched Gaussian shape asymptotically, i.e.

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

where $\rho(r) \sim r^{d_f-d}$ is the density of the fractal structure, d_f the fractal dimension, $d_s = 2d_f/d_w$ the spectral dimension [1], α the power-law correction exponent [5–8], $u = d_w/(d_w - 1)$, and $P_d(r, t)$ is normalized according to $\int dr r^{d-1} P_d(r, t) = 1$.

The behaviour of $P_d(r, t)$ around its maximum value, i.e. when $\xi \rightarrow 0$, is much less well known at present. The study of this ‘small- r ’ regime is interesting from a theoretical point of view, since the form of $P_d(r, t)$ in this case is determined by the exponents describing the structure of the fractal on which diffusion takes place. This gives us a new perspective

for learning about the structure of the fractal itself in those cases where it is not accurately known.

In order to understand this point better, it is convenient to start considering the simplest random fractals available, i.e. paths generated by random walks and self-avoiding random walks (SAWs). The latter are useful models of linear polymers in a good solvent, and the study of diffusion processes on them is also relevant for understanding the transport properties of such linear polymers.

In this paper we consider diffusion processes on linear fractals generated by random walks and self-avoiding random walks. Recently it has been suggested, by means of scaling arguments and numerical simulations, that on linear fractals generated by random walks in d dimensions (RW chains) [9]

$$P_d(r, t) \sim \rho(r) t^{-1/2} (1 - \text{constant} \times \xi^{d-2}) \quad \xi \rightarrow 0$$

for all dimensions d . More recently, it has been shown that this result is valid only for dimensions $2 < d < 5$, and that

$$P_d(r, t) \sim \rho(r) t^{-1/2} (1 - \text{constant} \times \xi^4) \quad \xi \rightarrow 0$$

for $d > 6$ [10]. In addition, it was found that the small- ξ expansion of $P_d(r, t)$ displays logarithmic corrections for the terms of order $\xi^{d_c-2} \log(1/\xi)$, where $d_c = 4n + 2$, with $n \geq 0$, play the role of critical dimensions in the expansion.

In this paper we extend those studies to the case of linear structures generated by self-avoiding walks (SAW chains) and obtain the corresponding small- ξ expansion of $P_d(r, t)$ for arbitrary dimensions. We start in section 2 briefly reviewing the main results for random walks on RW chains, presenting a different approach to that discussed in [10]. The method is generalized and applied to the case of random walks on SAW chains in section 3. Finally, in section 4 we summarize our main results.

2. The short-distance shape of random walks on random-walk chains

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

2.1. Diffusion in ℓ -space

Along the one-dimensional path, the probability distribution of walkers, at topological ('chemical') distance ℓ 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

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

normalized according to $\int_0^\infty d\ell P(\ell, t) = 1$. Thus, diffusion along the chain (i.e. in ℓ -space) is normal and $\langle \ell^2(t) \rangle = t$.

2.2. Diffusion in r -space

The time behaviour of the random walkers in r -space can easily be obtained from their time behaviour in ℓ -space and the spatial behaviour of the fractal substrate. First note that for a RW-chain, the mean square displacement of the chain, averaged over all chain configurations, $\langle r^2(\ell) \rangle$, behaves linearly with its length ℓ , i.e. $\langle r^2(\ell) \rangle \sim \ell$. Since the mass M of the chain is proportional to its length ℓ , one has that $M \sim r^{d_f}$, where the fractal dimension $d_f = 2$, independently of d . Now, along the chain the mean chemical distance explored by the walker, $\langle \ell \rangle$, scales with time t as $\langle \ell \rangle \sim t^{1/2}$, from which we obtain the scaling relation between r and t as

$$\langle r^2(\ell) \rangle \sim t^{2/d_w}$$

where $d_w = 2d_f = 4$ is the fractal dimension of the random walk in r -space.

To obtain the behaviour of the probability distribution in r -space, averaged over all RW chain configurations, $P_d(r, t)$, we note that it is related to $P(\ell, t)$ by [3]

$$P_d(r, t) = \int_0^\infty d\ell \Phi(r, \ell) P(\ell, t) \tag{2}$$

where $\Phi(r, \ell)$ is the probability that two sites on the chain at distance r in space are at distance ℓ along the chain[†].

The probability density $P_d(r, t)$ is normalized in the Euclidean space according to

$$\int dr r^{d-1} P_d(r, t) = 1. \tag{3}$$

Another possibility is the normalization on the fractal set, i.e.

$$\int_0^\infty dr r^{d_f-1} P(r, t) = 1. \tag{4}$$

Both distributions are simply related to each other by

$$P_d(r, t) = \rho(r) P(r, t) \tag{5}$$

where $\rho(r) \sim r^{d_f-d}$ is the density of the fractal structure in r -space.

The structural function $\Phi(r, \ell)$ for RW chains which has been introduced in (2), can be obtained straightforwardly by noting that the chemical distance ℓ plays the role of the time variable in (1), and one can immediately write

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

and $\Phi(r, \ell) = 0$ for $\ell < r$, where A_d is a normalization factor such that $\int_0^\infty dr r^{d-1} \Phi(r, \ell) = 1$. Therefore, by inserting equations (1) and (6) in (2) we obtain

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

Now, by performing the transformation $x = \ell/t^{1/2}$, equation (7) becomes

$$P_d(r, t) \sim t^{-d/4} \int_{r/t^{1/4}}^\infty dx x^{-d/2} \exp\left(\frac{-\xi^2}{2x}\right) \exp\left(\frac{-x^2}{2}\right) \tag{8}$$

[†] Actually, the function $\Phi(r, \ell) = 0$ when $\ell < \ell_{\min}$, and $\ell_{\min} = r$ when all RW-chain configurations are considered (see [11]).

where the scaling variable $\xi = r/t^{1/d_w}$ with $d_w = 4$. Since the lower integration limit $\xi/t^{1/4}$ vanishes for fixed ξ and $t \rightarrow \infty$, which is the limit we are interested in here, we set it equal to zero in what follows. After some minor manipulations we obtain

$$P_d(r, t) \sim \rho(r) t^{-1/2} \xi^{d-2} \int_0^\infty dx x^{-d/2} \exp\left(\frac{-\xi^2}{2x}\right) \exp\left(\frac{-x^2}{2}\right) \quad (9)$$

from which we can identify the probability $P(r, t)$ according to (5) as,

$$P(r, t) \sim t^{-1/2} f_d(\xi) \quad (10)$$

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

$$f_d(\xi) = \xi^{d-2} \int_0^\infty dx x^{-d/2} \exp\left(\frac{-\xi^2}{2x}\right) \exp\left(\frac{-x^2}{2}\right). \quad (11)$$

Equation (11) can be solved exactly [10]. However, since we are interested in the asymptotic limit $\xi \rightarrow 0$, we proceed differently than in [10] by performing suitable expansions in the integrand of (11). The present approach yields essentially the same results as those of [10], but are obtained in a more intuitive fashion, also allowing us to study other linear structures for which the structural function $\Phi(r, \ell)$ is not known exactly (see section 3).

We start by splitting the integrand in (11) into two parts as

$$f_d(\xi) = \xi^{d-2} [I_1(\xi) + I_2(\xi)] \quad (12)$$

where

$$I_1(\xi) = \int_0^{\xi^2/2} dx x^{-d/2} \exp\left(\frac{-\xi^2}{2x}\right) \exp\left(\frac{-x^2}{2}\right) \quad (13)$$

and

$$I_2(\xi) = \int_{\xi^2/2}^\infty dx x^{-d/2} \exp\left(\frac{-\xi^2}{2x}\right) \exp\left(\frac{-x^2}{2}\right). \quad (14)$$

The idea is to calculate I_1 and I_2 in an approximate way in the case $\xi \rightarrow 0$.

Consider I_1 first. Since in this case $x < \xi^2/2$, we make the approximation $\exp(-x^2/2) \cong 1$, and by setting $y = x/(\xi^2/2)$ we obtain

$$I_1(\xi) \cong \xi^{2-d} A(d) \quad (15)$$

where $A(d) = 2^{(d/2)-1} \int_0^1 dy y^{-d/2} \exp(-1/y)$ can be related to the incomplete gamma function [12].

Now consider I_2 . Since in this case $x > \xi^2/2$, we make the approximation $\exp(-\xi^2/2x) \cong 1$ and set the upper integration limit to 1, so that

$$I_2 \approx \int_{\xi^2/2}^1 dx x^{-d/2} \exp\left(\frac{-x^2}{2}\right). \quad (16)$$

Now, by expanding the exponential in its power series we finally obtain

$$I_2 \approx \sum_{n=0}^{\infty} \frac{(-)^n}{2^n n!} \frac{1}{(2n+1-d/2)} \left[1 - \left(\frac{\xi^2}{2}\right)^{2n+1-d/2} \right] \quad 2n+1 - \frac{d}{2} \neq 0. \quad (17)$$

Logarithmic corrections, contained in the terms denoted by $L_{d_c}(\xi)$, occur for dimensions $d = d_c$ such that

$$d = d_c = 4n_c + 2 \quad n_c \geq 0 \quad (18)$$

i.e. $d_c = 2, 6, 10, 14, 18, \dots$, and the corresponding terms behave as

$$L_{d_c}(\xi) = \frac{2(-)^{n_c}}{2^{n_c} n_c!} \xi^{d_c-2} \log\left(\frac{1}{\xi}\right) \tag{19}$$

in agreement with the exact results [10]. In what follows we consider the case $d = 1$ separately, and summarize the results for higher d afterwards.

2.2.1. *Dimension $d = 1$.* The one-dimensional case is interesting, since $f_1(\xi) \rightarrow \infty$ when $\xi \rightarrow 0$. According to (12) and our approximate results (15) and (17), we immediately find

$$f_1(\xi) \approx 2 \xi^{-1} \quad \xi \rightarrow 0$$

which can be compared with the exact result obtained by direct integration of (14) (setting $\xi = 0$ in the integral) as

$$f_1(\xi) = 2^{-3/4} \Gamma(\frac{1}{4}) \xi^{-1} \cong 2.1558 \xi^{-1}.$$

Thus, in one dimension the probability of random walks $P(r, t)$ behaves, when $r \rightarrow 0$ and $t \rightarrow \infty$, as

$$P(r, t) \sim \frac{1}{t^{1/4}} \frac{1}{r} \quad r \rightarrow 0 \quad \text{and} \quad t \rightarrow \infty$$

reflecting the persistence of the walks in returning close to the origin. In other words, for small but otherwise fixed r , i.e. $r = \epsilon$, $P(\epsilon, t) \sim t^{-1/4}$ for $t \rightarrow \infty$, different to the behaviour in ℓ -space, i.e. $P(\ell = 0, t) \sim t^{-1/2}$.

2.2.2. *Dimension $d \geq 2$.* From equations (12), (15) and (17) it can be shown that when $\xi \rightarrow 0$:

$$2 < d < 6: \quad f_d(\xi) \cong a_d + b_d \xi^{d-2} + O(\xi^4)$$

$$6 < d < 10: \quad f_d(\xi) \cong a_d + b_d \xi^4 + c_d \xi^{d-2} + O(\xi^8)$$

$$10 < d < 14: \quad f_d(\xi) \cong a_d + b_d \xi^4 + c_d \xi^8 + e_d \xi^{d-2} + O(\xi^{12})$$

$$14 < d < 18: \quad f_d(\xi) \cong a_d + b_d \xi^4 + c_d \xi^8 + e_d \xi^{12} + f_d \xi^{d-2} + O(\xi^{16})$$

etc. For the corresponding critical dimensions we find

$$d = 2: \quad f_2(\xi) \cong \text{constant}_2 + 2 \ln(1/\xi) + O(\xi^4)$$

$$d = 6: \quad f_6(\xi) \cong \text{constant}_6 - \xi^4 \ln(1/\xi) + O(\xi^4)$$

$$d = 10: \quad f_{10}(\xi) \cong \text{constant}_{10} + \text{constant}'_{10} \xi^4 + \frac{1}{4} \xi^8 \ln(1/\xi) + O(\xi^8)$$

etc.

In summary, for $d > 6$ the scaling function $f_d(\xi)$ behaves asymptotically as

$$f_d(\xi) \sim a_d + b_d \xi^4 \sim \exp(-\text{constant} \times \xi^{d_w}) \quad \xi \rightarrow 0 \tag{20}$$

where $d_w = 4$, independently of d .

3. The short-distance shape of random walks on SAW chains

We now consider one-dimensional structures generated by self-avoiding random walks (SAW) in d -dimensional space [13, 14]. Such structures, denoted here as SAW chains, are fractal with a mass fractal dimension $d_f = 1/\nu = (d+2)/3$ when $d < 4$, and $d_f = 2$, when $d \geq 4$ (see, e.g., [2]).

Since SAW chains are topologically one-dimensional, diffusion is normal in ℓ -space and equation (1) still holds here, while in r -space, the diffusion exponent $d_w = 2d_f = 2/\nu$, which becomes anomalous when $d > 4$ †. The probability distribution $P_d(r, t)$ can be obtained from (2), where $\Phi(r, \ell)$ is now not known exactly but is expected to obey the scaling form [13, 14]

$$\Phi(r, \ell) = \frac{1}{\ell^{\nu d}} \phi(r/\ell^\nu) \quad (21)$$

when $d \geq 2$. The scaling function $\phi(x)$ is expected to behave asymptotically as

$$\phi(x) \sim x^{g_1} \quad \text{for } x \ll 1 \quad (22)$$

and

$$\phi(x) \sim x^{g_2} \exp(-c x^\delta) \quad \text{for } x \gg 1. \quad (23)$$

Here $g_1 = (\gamma - 1)/\nu$, $\delta = (1 - \nu)^{-1}$, $g_2 = \delta[d(\nu - \frac{1}{2}) - (\gamma - 1)]$ [13, 14], γ is the enhancement exponent and is given approximately by [8] $\gamma - 1 \cong (4 - d)/6$, and c is a constant. For spatial dimensions $d \geq 4$, one has $\nu = \frac{1}{2}$ and $\gamma = 1$, thus $g_1 = g_2 = 0$, and $\Phi(r, \ell)$ scales as in (6).

From equations (1) and (2), together with (21), (22) and (23), and by making the substitution $x = \ell/t^{1/2}$, we can write

$$P_d(r, t) \sim t^{-\nu d/2} \int_{\xi/t^{(1-\nu)/2}}^{\infty} dx x^{-\nu d} \phi[(\xi^{1/\nu}/x)^\nu] \exp\left(\frac{-x^2}{2}\right) \quad (24)$$

where we have taken $\ell_{\min} = r$, and $\xi \equiv r/t^{1/d_w}$. Since we are interested in the asymptotic behaviour $t \rightarrow \infty$, for vanishing ξ , the lower integration limit in (24) can be set equal to zero (cf equation (9)). By making use in (24) of the asymptotic forms for $\phi(x)$ (cf equations (22) and (23)), and employing (5), for $P(r, t)$ we obtain

$$P(r, t) \sim \frac{1}{t^{1/2}} \xi^{d-d_f} [\xi^{g_1} I_2(\xi) + \xi^{g_2} I_1(\xi)] \quad (25)$$

where

$$I_1(\xi) \sim \int_0^{\xi^{1/\nu}} dx x^{-\nu(d+g_2)} \exp\left[-c \left(\frac{\xi^{1/\nu}}{x}\right)^{\nu\delta}\right] \exp\left(\frac{-x^2}{2}\right)$$

and

$$I_2(\xi) \sim \int_{\xi^{1/\nu}}^{\infty} dx x^{-\nu(d+g_1)} \exp\left(\frac{-x^2}{2}\right)$$

which generalize our previous results (10)–(14). Note that the exponent g_1 occurs in I_2 and g_2 in I_1 .

To obtain the leading behaviours of I_1 and I_2 when $\xi \rightarrow 0$, we proceed similarly as in section 2. Let us start by I_1 , where we take $\exp(-x^2/2) \cong 1$. By performing a simple transformation we find

$$I_1(\xi) \cong \xi^{d_f-d-g_2} A_d(g_2) \quad (26)$$

† In one dimension, both ℓ - and r -spaces are equivalent for SAWs, and $d_w = 2$.

where $A_d(g_2) = \int_0^1 dy y^{-v(d+g_2)} \exp(-cy^{-v\delta})$. To estimate I_2 , we expand the exponential in power series, and set the upper integration limit to one, i.e.

$$I_2(\xi) \cong \int_{\xi^{1/\nu}}^1 dx x^{-v(d+g_1)} \left(1 - \frac{x^2}{2} + \frac{1}{3!} \left(\frac{x^2}{2} \right)^2 - \dots \right) \tag{27}$$

which can be integrated immediately. Thus, altogether $P(r, t)$ behaves, when $\xi \rightarrow 0$ and $1 < d < 4$, as

$$P(r, t) \sim \frac{1}{t^{1/2}} [a_d - b_d \xi^\beta + c_d \xi^{d_w} + O(\xi^{2d_w})] \tag{28}$$

where

$$\beta = d - d_f + g_1$$

and

$$a_d \cong A_d(g_2) + \frac{1}{[v(d + g_1) - 1]} \quad b_d \cong \frac{1}{[v(d + g_1) - 1]} + c_d$$

and

$$c_d = \frac{1}{2[3 - v(d + g_1)]}$$

We see that, in contrast to diffusion on RW chains, $P(r, t)$ behaves regularly when $d = 2$, i.e. $d = 2$ is no longer a critical dimension. Employing the above quoted expressions for ν and γ , we estimate

$$\beta \cong \frac{10}{9} = 1.11 \quad \text{when } d = 2$$

where $d_w = \frac{8}{3} = 2.67$ and

$$\beta \cong \frac{29}{18} = 1.61 \quad \text{when } d = 3$$

where $d_w = \frac{10}{3} = 3.33$.

When $d \geq 4$, SAWs reduce to simple random walks, i.e. $g_1 = 0$, $d_f = 2$, and the critical dimensions $d_c = 4n + 2$, with $n \geq 1$, i.e. $d_c = 6, 10, 14, \dots$, are recovered. We further note that when $d > 6$, $\beta = d - 2 > d_w = 4$, the coefficient $c_d < 0$ and $P(r, t)$ behaves asymptotically as

$$P(r, t) \sim \frac{1}{t^{1/2}} \left[a_d - \frac{1}{d-6} \xi^4 + \dots \right] \quad d > 6 \tag{29}$$

when $\xi \rightarrow 0$.

4. Summary

In summary, we have studied the asymptotic form of random walks on random fractals, such as paths generated by random walks (RW chains) and self-avoiding random walks (SAW chains) in d -dimensional space. We have shown that the mean probability density of random walks in r -space, $P(r, t)$, normalized on the fractal, i.e. $\int_0^\infty dr r^{d_f-1} P(r, t) = 1$, behaves asymptotically when $\xi = r/t^{d_w} \rightarrow 0$, as

$$P(r, t) \sim \frac{1}{t^{1/2}} [1 + \text{constant}_1 \xi^\beta + \text{constant}_2 \xi^{d_w} + O(\xi^{2d_w})] \quad \beta \neq d_w$$

where d_w is the anomalous diffusion exponent, $\beta = d - d_f + g_1$ and d_f is the fractal dimension. Here, g_1 characterizes the asymptotic shape of the fractal structure when $r \ll \ell^v$, where

$\nu = 1/d_f$. For RW chains, $g_1 = 0$ for all dimensions, and for SAW chains, $g_1 = 0$ for $d \geq 4$.

The actual dependence of $P(r, t)$ on ξ , when $\xi \rightarrow 0$, is determined by $\min(\beta, d_w)$. There exists a critical dimension $d_c = 6$ below which $\beta < d_w$, and

$$P(r, t) \sim t^{-1/2} (1 - \text{constant} \times \xi^\beta) \quad \beta < d_w$$

where β depends on d , while when $d > 6$, $d_w = 4 < \beta = d - 2$, and

$$P(r, t) \sim t^{-1/2} (1 - \text{constant} \times \xi^{d_w}) \quad d_w < \beta$$

where $d_w = 4$ independently of d . Logarithmic corrections occur when $d = d_c = 4n + 2$, with $n \geq 0$ for RW chains and $n \geq 1$ for SAW chains.

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