Generalized diffusion equation for anisotropic anomalous diffusion

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Motivated by studies of comblike structures, we present a generalization of the classical diffusion equation to model anisotropic, anomalous diffusion. We assume that the diffusive flux is given by a diffusion tensor acting on the gradient of the probability density, where each component of the diffusion tensor can have its own scaling law. We also assume scaling laws that have an explicit power-law dependence on space and time. Solutions of the proposed generalized diffusion equation are consistent with previously derived asymptotic results for the probability density on comblike structures.

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I. INTRODUCTION

Anomalous diffusion and its applications to fractal and disordered systems have been intensively studied for over two decades [1,2]. One object of particular interest in these studies is the probability density of random walkers. Due to the presence of obstacles and dangling ends at all scales, the probability density can exhibit non-Gaussian behavior so that it no longer satisfies the classical diffusion equation. The exact nature of the probability density for anomalous diffusion and the differential equation, if any, that it satisfies are still open questions.

O'Shaughnessy and Procaccia [3,4] first proposed an equation for isotropic diffusion on fractals based on a probability balance supplemented with the usual gradient law for diffusive flux, but where the diffusion coefficient scales with distance to a power. This scaling gave rise to anomalous diffusion with a non-Gaussian probability density. Using a different method, Guyer [5] directly obtained a different stretched Gaussian for the asymptotic form of the probability density of random walkers on the Sierpinski gasket. Guyer attributed the two different results to different regimes of validity. Various other authors also obtained similar stretched Gaussians for diffusion on a wide range of structures, including percolation clusters and combs [6–8]. In fact, Havlin and ben-Avraham [1] noted the similarity of these results with those for anomalous continuous-time random walks and self-avoiding walks obtained by a variety of different techniques. In addition to being supported by numerical simulations [1], these stretched Gaussians are also consistent with rigorous derivations of bounds on the probability density for diffusion in several fractals [9–11].

Alternatively, Metzler *et al.* [12] and Giona and Roman [13,14] proposed differential equations involving fractional time derivatives. Furthermore Compte and Jou [15] proposed a nonlinear constitutive relation for the diffusive flux to account for the anomalous diffusion. All these proposed equations do give rise to anomalous diffusion. In order to determine which, if any, was appropriate for diffusion on a specific fractal, Schulzky *et al.* [16] compared the solutions of the proposed equations with extensive random walk simulations on the Sierpinski gasket and showed that, while there may be some partial agreement, *none* agreed with the simulation results over a wide range of time scales.

Recently Campos *et al.* [17] proposed a generalized diffusion equation for isotropic diffusion based on a probability balance and a gradient law for the diffusive flux. In contrast to previous work, they allowed the diffusion coefficient to depend on *space and time*, which yielded the desired stretched Gaussian for the probability density.

Here we extend this work to present a generalization of the classical diffusion equation that models anisotropic anomalous diffusion. We are motivated by results for comblike structures that show that diffusion along the backbone can be significantly different from that along the teeth. In fact, a steepest descent approximation for the asymptotic probability density on a comb yields an *anisotropic stretched Gaussian* [2,7]. To account for the anisotropy we introduce a diffusion tensor where each component can have its own scaling law. As in Campos *et al.* [17], we allow for an explicit space and time dependence in the scaling of the diffusion coefficients and thereby obtain solutions that are consistent with the previously obtained anisotropic stretched Gaussians for comblike structures. The explicit time dependence of the diffusion tensor is critical to this consistency and can be attributed to the tendency for random walkers to spend more time wandering in the teeth as time increases so that the effective diffusion along the comb backbone decreases in time.

This work indicates that a unified description of anomalous diffusion can describe a wide range of objects where the response can be anisotropic or isotropic. There are limitations however to using differential equations to model transport on fractals and other complex structures. Arkhincheev and Baskin [18–20] have shown how nonlocal effects such as a dependence on history arise. Our work is restricted to the asymptotic regime where such effects take a simpler form. Furthermore, detailed random walk simulations for the Sierpinski gasket indicate that the probability density can be nonanalytic as well as multiple valued [4,21]. Thus the probability density cannot always satisfy a differential equation in the classical sense. However, its asymptotic or leading order behavior may be smooth and effectively described by a differential equation. We therefore interpret here the probability density as a smooth approximation to the actual probability density. Another approach suggested by Davison *et al.* [21] introduces equivalence classes among the points of a fractal. They showed then that the probability distribution is smooth for each such equivalence class. The probability density can also exhibit periodic oscillations in space and time [22]. Such oscillations are not captured by our proposed generalized diffusion equation. There are also indications of multifractal response not accounted for in the stretched Gaussians [23,24]. We ignore such complications in the following.

II. ISOTROPIC DIFFUSION

We first consider the special case of isotropic diffusion, which is commonly assumed for many fractals. This case has been treated by Campos *et al.* [17]. Let the fractal dimension be denoted by d_f. We assume that at time $t=0$ simple independent random walkers are placed at the origin. Due to the isotropy, the diffusive growth will be radially symmetric. The mean-squared displacement of the walkers is [25]

$$\langle r^2(t)\rangle \sim t^{2/d_w}, \tag{1}$$

where r is the Euclidean distance from the origin and d_w the random walk dimension. For this case, Mosco [8] proposed the long-time asymptotic probability density,

$$P(r,t) \sim \frac{1}{t^{d_s/2}} \exp\left[-c\left(\frac{r^{d_w}}{t}\right)^{d_{\min}/(d_w-d_{\min})}\right], \tag{2}$$

with $d_{\min}$ the exponent for the chemical distance [2] and d_s the spectral dimension given by

$$d_s = \frac{2d_f}{d_w}. \tag{3}$$

The expression (2) is consistent with other asymptotic results for a variety of structures [6,7]. The probability density (2) indicates that three scaling exponents are important for isotropic diffusion: d_w, d_s, and $d_{\min}$. Given the relation (3), these three exponents are also equivalent to d_w, d_f, and $d_{\min}$. Henceforth, we assume that (2) is valid and construct a generalized diffusion equation that yields (2) as the solution. The procedure is to use a probability balance supplemented with a constitutive relation for the diffusive flux. The probability balance in this radially symmetric case was given by O'Shaughnessy and Procaccia [3,4],

$$\frac{\partial P(r,t)}{\partial t} = \frac{1}{r^{d_f-1}}\frac{\partial}{\partial r}[r^{d_f-1}J_r(r,t)]. \tag{4}$$

For the radial flux $J_r(r,t)$, we assume the gradient law

$$J_r(r,t) = D_r(r,t)\frac{\partial P(r,t)}{\partial r}, \tag{5}$$

where the radial diffusion coefficient D_r is allowed to be a function of space and time. Campos *et al.* [17] first showed that the time dependence is important. Consistency of (4) and (5) with the desired solution (2) now requires that the diffusion coefficient D_r have the following form:

$$\begin{aligned} D_r(r,t) &= \frac{(d_w-d_{\min})}{cd_w^2 d_{\min}}\left(\frac{r}{t}\right)^{(d_w-2d_{\min})/(d_w-d_{\min})} \\ &= \frac{(d_w-d_{\min})}{cd_w^2 d_{\min}}\left(\frac{r^2}{t}\right)\left(\frac{t}{r^{d_w}}\right)^{d_{\min}/(d_w-d_{\min})}. \end{aligned} \tag{6}$$

This diffusion coefficient is defined by the gradient law (5) and generally differs from the coefficient D defined by

$$D \propto \frac{\langle r^2(t)\rangle}{t} \sim t^{(2/d_w)-1}. \tag{7}$$

In the special case of regular diffusion with $d_w=2$, the two definitions coincide.

In conjunction with the probability balance (4) and gradient law (5), (6) leads to the generalized diffusion equation,

$$\begin{aligned} &\frac{cd_w^2 d_{\min}}{(d_w-d_{\min})} r^{d_f-1}\frac{\partial P(r,t)}{\partial t} \\ &\quad = \frac{\partial}{\partial r}\left[\left(\frac{r}{t}\right)^{(d_w-2d_{\min})/(d_w-d_{\min})} r^{d_f-1}\frac{\partial P(r,t)}{\partial r}\right] \\ &\quad = \frac{\partial}{\partial r}\left[\left(\frac{r^{d_w}}{t}\right)^{(d_w-2d_{\min})/(d_w-d_{\min})} r^{d_f-d_w+1}\frac{\partial P(r,t)}{\partial r}\right]. \end{aligned} \tag{8}$$

This equation is equivalent to within a constant to that obtained by Campos *et al.* [17]. Direct substitution verifies that (2) is the solution to (8).

Note that (2) is consistent with the rigorous bounds obtained by Barlow and Perkins [9] for the Sierpinski gasket (for which $d_{\min}=1$),

$$\begin{aligned} &\frac{c_1}{t^{d_s/2}} \exp\left[-c_2\left(\frac{r^{d_w}}{t}\right)^{1/(d_w-1)}\right] \\ &\quad \leqslant P(r,t) \leqslant \frac{c_3}{t^{d_s/2}} \exp\left[-c_4\left(\frac{r^{d_w}}{t}\right)^{1/(d_w-1)}\right], \end{aligned} \tag{9}$$

where the c_i are constants. It is an inequality because the actual solution oscillates in space and time due to the presence of obstacles at all scales. These oscillations are not captured by the differential equation (8).

III. ANISOTROPIC DIFFUSION ON COMBS

We now extend these ideas to allow for anisotropic diffusion. For concreteness we consider a n-dimensional comb with teeth orthogonal to the backbone. The teeth and backbone are taken parallel to Cartesian coordinate axes x_i. Again simple random walkers are placed at the origin on the backbone. In this case, the response can be anisotropic so that the mean-squared displacements of the walkers scale with the time t as [1]

$$\langle x_i^2(t)\rangle \sim t^{2/d_{w_i}}. \tag{10}$$

Here d_{w_i} is the random walk dimension in the x_i direction. For example, for the case of the two-dimensional (2D) comb with the backbone along the x axis and teeth with infinite length parallel to the y axis, we have [26]

$$d_{w_x} = 4, \quad d_{w_y} = 2, \tag{11}$$

so the random walkers will undergo anomalous diffusion along the backbone but regular diffusion along the teeth. For the hierarchical three-dimensional (3D) comb with backbone along the x axis and teeth with infinite length parallel to the y and z axes [26],

$$d_{w_x} = 8, \quad d_{w_y} = 4, \quad d_{w_z} = 2. \tag{12}$$

The anisotropic behavior is also evident in the form of the probability density $P(\mathbf{r},t)$. The long-time asymptotic response has been estimated to be the anisotropic stretched Gaussian [7]

$$P(\mathbf{r},t) \sim \frac{1}{t^{d_s/2}} \exp\left[\sum_{i=1}^{n} -a_i\left(\frac{|x_i|^{d_{w_i}}}{t}\right)^{1/(d_{w_i}-1)}\right], \tag{13}$$

where the spectral dimension d_s in this case satisfies

$$\frac{d_s}{2} = \sum_{i=1}^{n} \frac{d_{f_i}}{d_{w_i}} = \sum_{i=1}^{n} \frac{1}{d_{w_i}}, \tag{14}$$

since the fractal dimensions $d_{f_i}=1$ for each i. Note that for linear structures, such as the combs considered here, we also have $d_{\min}=1$. Thus the scaling exponents important for diffusion on combs are the spectral dimension d_s and the n random walk dimensions d_{w_i}.

In particular, for the 2D case of infinite tooth length, substitution of (11) into (13) yields

$$P(x,y,t) \sim \frac{1}{t^{3/4}} \exp\left(-\frac{a_x|x|^{4/3}}{t^{1/3}} - \frac{a_y y^2}{t}\right). \tag{15}$$

In the anisotropic case considered here, the conservation of probability in local form is given by

$$\frac{\partial}{\partial t}P(\mathbf{r},t) = \operatorname{div}\mathbf{J}(\mathbf{r},t) = \sum_{i=1}^{n} \frac{\partial}{\partial x_i}J_i(\mathbf{r},t), \tag{16}$$

where $\mathbf{J}(\mathbf{r},t)$ is the flux vector. We now need a constitutive relation for $\mathbf{J}$. We assume a relation linear in the gradient of probability

$$\mathbf{J}(\mathbf{r},t) = \mathbf{D}(\mathbf{r},t)\operatorname{grad} P(\mathbf{r},t), \tag{17}$$

where $\mathbf{D}(\mathbf{r},t)$ is the effective diffusion tensor which is a function of position $\mathbf{r}$ and time t. Substitution of (17) into the probability balance (16) leads to

$$\frac{\partial}{\partial t}P(\mathbf{r},t) = \sum_{i,j}^{n} \frac{\partial}{\partial x_i}\left(D_{ij}(\mathbf{r},t)\frac{\partial P(\mathbf{r},t)}{\partial x_j}\right). \tag{18}$$

An explicit relation for the diffusion tensor $\mathbf{D}$ is still needed. The classical diffusion equation is obtained when the diffusion coefficients D_{ij} are constants. Consistency with the anisotropic stretched Gaussian (13) requires the following form:

$$\begin{aligned} D_{ij} &= \frac{(d_{w_i}-1)}{a_i d_{w_i}^2}\left(\frac{|x_i|}{t}\right)^{(d_{w_i}-2)/(d_{w_i}-1)} \delta_{ij} \\ &= \frac{(d_{w_i}-1)}{a_i d_{w_i}^2}\left(\frac{x_i^2}{t}\right)\left(\frac{t}{|x_i|^{d_{w_i}}}\right)^{1/(d_{w_i}-1)} \delta_{ij}, \end{aligned} \tag{19}$$

which yields the generalized diffusion equation

$$\frac{\partial P}{\partial t} = \sum_{i=1}^{n} \frac{(d_{w_i}-1)}{a_i d_{w_i}^2} \frac{\partial}{\partial x_i}\left[\left(\frac{|x_i|}{t}\right)^{(d_{w_i}-2)/(d_{w_i}-1)} \frac{\partial P}{\partial x_i}\right]. \tag{20}$$

Direct substitution of (13) verifies this result.

Equation (20) is our main result. It describes anisotropic anomalous diffusion on n-dimensional combs. The only scaling properties involved are those that arise in the expression (19) for the diffusion tensor. In the case of regular diffusion with constant diffusion coefficients D_{ij} and random walk dimensions $d_{w_i}=2$, the differential equation (20) reduces to the classical anisotropic diffusion equation

$$\frac{\partial P}{\partial t} = \sum_{i=1}^{n} \frac{1}{4a_i}\frac{\partial^2 P}{\partial x_i^2}. \tag{21}$$

In the case of 2D combs with infinite tooth-length, (19) becomes

$$D_{xx} = \frac{3}{16a_x}\left(\frac{|x|}{t}\right)^{2/3}, \quad D_{yy} = \frac{1}{4a_y}, \quad D_{xy} = 0, \tag{22}$$

and the generalized diffusion equation (20) becomes

$$\frac{\partial P}{\partial t} = \frac{3}{16a_x}\frac{\partial}{\partial x}\left[\left(\frac{|x|}{t}\right)^{2/3}\frac{\partial P}{\partial x}\right] + \frac{1}{4a_y}\frac{\partial^2 P}{\partial y^2}. \tag{23}$$

As in the radially symmetric case (6), the diffusion coefficients (19) depend explicitly on time. As time increases, the diffusion coefficients at a fixed point decrease. If we accept the probability balance (16), the gradient law for the flux (17) and the asymptotic solution (13), then this time dependence is necessary for consistency, in agreement with Campos *et al.* [17] for isotropic situations. For 2D combs, we can intuitively interpret it as the tendency for more and more random walkers to wander off and get stuck in the teeth as time increases, so the effective diffusion along the backbone appears to slow down with time.

IV. DISCUSSION

We have presented a unified description of the long-time asymptotic regime of anomalous diffusion that allows for anisotropic response, which is observed in comblike structures. The result is a generalized diffusion equation in which the diffusion coefficients are functions of space and time.

In an alternative approach, Arkhincheev and Baskin [18–20] developed an explicit model for diffusion on 2D combs based on a linear diffusion equation,

$$\left(\frac{\partial}{\partial t} - D_{xx}\delta(y)\frac{\partial^2}{\partial x^2} - D_{yy}\frac{\partial^2}{\partial y^2}\right)P(x,y,t) = 0, \tag{24}$$

where δ is the Dirac delta function. The solution along the axis $y=0$ can be expressed as [20]

$$P(x,0,t) = D_{xx}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{t} \frac{P(x,0,\tau)}{\sqrt{\pi D_{yy}(t-\tau)}}d\tau. \tag{25}$$

This expression involves a history term similar in form to the Basset history term for drag on an unsteady sphere in a fluid [27,28]. Differentiation of (25) by fractional degree $\frac{1}{2}$ yields

$$\frac{\partial^{1/2}P(x,0,t)}{\partial t^{1/2}} = D_{xx}\frac{\partial^2 P(x,0,t)}{\partial x^2}. \tag{26}$$

Thus the probability density along the backbone satisfies an integro-differential equation involving a fractional time derivative of order $\frac{1}{2}$. The asymptotic response is given by [18]

$$P(x,0,t) \sim \frac{1}{t^{3/4}} \exp\left(-\frac{c|x|^{4/3}}{t^{1/3}}\right), \tag{27}$$

which corresponds to (15).

In order to make a comparison with our derived equation (23), we can differentiate (25) with respect to time to obtain

$$\frac{\partial P(x,0,t)}{\partial t} = D_{xx}\frac{\partial^2}{\partial x^2}\frac{\partial}{\partial t}\int_{-\infty}^{t} \frac{P(x,0,\tau)}{\sqrt{\pi D_{yy}(t-\tau)}}d\tau. \tag{28}$$

In this context, we can view (23) as an asymptotic form of (28). It shows that asymptotic response is governed by a simpler equation where the diffusion coefficient can be viewed as a function of space and time rather than a functional of the total history. Note however that (23) is not restricted to the axis $y=0$.

Furthermore Campos *et al.* [17,29] found that (8) can reproduce the best-known asymptotic results for isotropic diffusion on fractals. We would also expect (20) to be useful in reproducing asymptotic results for anisotropic diffusion.

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