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Long-range correlation effects, generalized Brownian motion and anomalous diffusion

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Abstract. We investigate the diffusion motion of a Brownian particle which is acted upon by both a friction force with memory effect and a noise with long-range correlation effects. The noise is expressed as $f(X, t) \sim X^{-\sigma}F(t)$, $\sigma > 0$, where X and t are the displacement and time, respectively, and $F(t)$ has the long-time correlation effect $\langle F(0)F(t)\rangle \sim t^{-\beta}$, $0<\beta<1$, $\beta=1$, $1<\beta<2$. The generalized Langevin equation, corresponding Fokker–Planck equation and its solution at large time are established. A variety of anomalous diffusion patterns are derived. Due to the long-range correlation effects, the effective diffusion coefficient is dependent on both the displacement and time, and the probability density for finding the Brownian particle at displacement X and time t is non-Gaussian distribution. When this model is applied to diffusion on fractals, O'Shaughnessy and Procaccia's results can be naturally derived.

The anomalous diffusion in disordered media or fractal media has recently been receiving much attention [1–6]. Although several approaches [1–6] have been developed to treat the anomalous diffusion, the dynamical mechanisms of anomalous diffusion are not understood throughout. Muralidhar *et al* [3] applied the generalized Langevin equation (GLE) to study the dynamics of anomalous diffusion from the viewpoint of the velocity autocorrelation function of a Brownian particle in disordered media.

Wang [1, 2] has investigated the dynamical mechanisms from the starting point of the GLE and Fokker–Planck equation (FPE), and established the bridge between the long-time correlation effects, fractal Brownian motion [7] and anomalous diffusion. It has been shown that a kind of dynamical mechanism for anomalous diffusion is the long-time correlation effects [1, 2]. Furthermore, Wang [2] has studied biased diffusion and found the probability density function (PDF) for finding the Brownian particle at displacement X and time t. The PDF has Gaussian distribution for displacement X.

However, for single particle diffusion in some disordered media such as fractal media, the PDF is generally not a Gaussian distribution [5, 8, 9] for displacement. Why is the PDF in some disordered media non-Gaussian rather than Gaussian? What is the origin of the non-Gaussian PDF? In this paper, we will focus on these questions.

It is well known that when a Brownian particle moves in a fluid medium, it experiences two forces: one is the determinative dynamical friction force, the other the random fluctuation force originating from random collision between the Brownian particle and the particles of the surrounding medium. In the case where the average value of the randomly fluctuating force equals zero and its correlation function is a Dirac δ function [10], the Langevin equation, the associating Fokker–Planck equation and its solution have been established [10].

When a Brownian particle moves through dense fluids or fluids with internal degree of freedom [11], and on the percolation clusters [6, 12], the randomly fluctuating force correlation function behaves with the so-called long-range correlation. Wang [1, 2] has studied the dynamics of the Brownian particle when it is acted upon by a friction force *with memory and a random fluctuation force with long-time correlation.*

However, in this paper, the dynamics of a Brownian particle moving in a disordered medium is modelled by a friction force with memory and a noise with temporal and spatial correlations rather than white noise. This is different from ordinary Brownian motion, and may be called the generalized Brownian motion. Without loss of generality, we restrict ourselves to the one-dimensional case. If a Brownian particle of mass M starts to move from the origin at time $t=0$, the equation of motion or GLE can be given by

$$\dot{X}=V(t);\ M\ddot{X}+M\int_0^t \alpha(t-\tau)V(\tau)\,\mathrm{d}\tau=f(X,t) \tag{1}$$

where $\alpha(t)$ is friction memory kernel and the noise $f(X, t)$ is assumed to decouple as

$$f(X,t)=BX^{-\sigma}F(t) \tag{2}$$

where σ is an exponent larger than or equal to zero. In the following it will be proved *that σ is related to the fractal dimension if the medium is fractal, and determined by* the structure of the medium. B is a proportionality coefficient independent of time and displacement but dependent on the exponent σ. $F(t)$ has the following properties

$$\langle F(t)\rangle=0 \tag{3}$$

$$\langle F(0)F(t)\rangle=C_f(t)=F_0t^{-\beta}. \tag{4}$$

The values of exponent β can be taken as $0<\beta<1$, or $1<\beta<2$, which is determined by the dynamical mechanisms of the physical processes considered [1, 2]. The proportional coefficient F_0 is independent of time but dependent on the exponent β, which means that the proportionality coefficient depends on the concrete physical processes. In the following B is contracted in F_0. We believe that the particle diffusion in a turbulent medium [8] and a fractal medium, such as percolation clusters [6, 8], encounters this noise, which originates from both the static disorder (fractal structures) and dynamic disorder (random walker).

Now, we take the following variable transformation

$$Y=X^{\sigma+1} \tag{5}$$

in (1). Taking (5) and (2) into (1), we obtain that when only the diffusion motion of Brownian motion is considered, the asymptotic equivalent GLE is

$$\frac{\mathrm{d}Y}{\mathrm{d}t}=u(t);\ M\frac{\mathrm{d}^2Y}{\mathrm{d}t^2}+M\int_0^t \alpha(t-\tau)u(\tau)\,\mathrm{d}\tau=F(t). \tag{6}$$

The memory kernel $\alpha(t)$ can be obtained by the generalized fluctuation-dissipation theorem [2, 10, 13]:

$$C_f(t) = MK_B T\alpha(t) \tag{7}$$

where T is the absolute temperature of the surrounding and K_B is Boltzmann's constant. Immediately, one has

$$\alpha(t) = \alpha_0(\beta)t^{-\beta} \tag{8}$$

where

$$\alpha_0(\beta) = \frac{F_0}{MK_B T}. \tag{9}$$

In addition to the characteristic function and Laplace transformation, and after tedious computation, we can derive the Fokker–Planck equation associated with (1) together with (2) [2].

(i) When $0<\beta<1$ or $1<\beta<2$, the asymptotic form of FPE at large time associated with (1) is [2]

$$\frac{\partial P(X,t)}{\partial t} = \frac{K_B T b_1(\beta)}{M(\sigma+1)^2} X^{-\sigma} \frac{\partial}{\partial X}\left(t^{\beta-1} X^{-\sigma} \frac{\partial P(X,t)}{\partial X}\right) \tag{10}$$

where

$$b_1(\beta) = \frac{b_0}{\Gamma(1-\beta)\Gamma(2-\beta)} > 0 \tag{11}$$

and b_0 is a proportionality coefficient. In fact, we are more concerned with the diffusion motion of the Brownian particle. In the derivation of (10) the terms with $t^{\beta-2}$ have been neglected since they approach zero when t is large. Equation (10) is one of our main results, which is derived in detail in the appendix.

The normalization solution of (10) with the initial condition $P(X,0) = \delta(X)$ can readily be shown to be

$$P(X,t) = (4\pi D t^{\beta})^{-1/2} \exp\left(-\frac{X^{2\sigma+2}}{4Dt^{\beta}}\right) \tag{12}$$

where

$$D = \frac{K_B T b_1(\beta)}{M\beta} > 0. \tag{13}$$

From (12), it is easily shown that the mean-square displacement is

$$\begin{aligned}\langle X^2(t)\rangle &= (2D)^{1/(\sigma+1)} t^{\beta/(\sigma+1)} \\ &\sim t^{\beta/(\sigma+1)} (0<\beta<1 \text{ or } 1<\beta<2, \text{ and } \sigma \geqslant 0).\end{aligned} \tag{14}$$

Equation (14) demonstrates that the Brownian particle obeys anomalously slow ($\beta/(\sigma+1)<1$) and fast ($\beta/(\sigma+1)>1$) diffusions and also is called subdiffusion and superdiffusion [4]. Anomalously slow diffusion like (14) has been reported by other authors [14]. Anomalously fast diffusion(superdiffusion) has been reported by Heinrichs and Kumar [15]. Their superdiffusion is ballistic motion ($\langle X(t)^2\rangle \sim t^2$).

After taking the following scaling transformation in (12)

$$t' = bt \qquad X' = b^{2\sigma+2-\beta}X \tag{15}$$

we have

$$P(X', t') = b^{-\beta/2}P(X, t) \tag{16}$$

which means that the PDF has self-affinity [17].

When $\sigma = 0, 0 < \beta < 1$ or $1 < \beta < 2$, i.e. there is only a long-time correlation, from (14) we have

$$\langle X^2(t)\rangle \sim t^{\beta} \tag{17}$$

which is consistent with our previous results [1, 2]. When $\sigma = 0$, equations (10) and (12) reduce to the FPE and its solution of [2] at large time, respectively. It has been explained that our previous work is a special case of this result.

(ii) In the case $\beta = 1$, the asymptotic FPE when $t \to \infty$ is [2]

$$\frac{\partial P(X,t)}{\partial t} = \frac{K_B T b_2}{(\sigma+1)^2 M} X^{-\sigma} \ln t \frac{\partial}{\partial X}\left(X^{-\sigma} \ln t \frac{\partial P(X,t)}{\partial X}\right) \tag{18}$$

where b_2 is constant. The terms with t^{-1} have been neglected since they approach zero when $t \to \infty$.

The normalization solution of (18) with the initial condition $P(X, 0) = \delta(X)$ is

$$P(X,t) = (4\pi D_2 t(\ln t - 1))^{-1/2} \exp\left(-\frac{X^{2\sigma+2}}{4D_2 t(\ln t - 1)}\right) \tag{19}$$

where $D_2 = K_B T b_2/M$. In addition to (19), the second moment of the displacement is given by

$$\langle X^2(t)\rangle \sim (t \ln t)^{1/(\sigma+1)}. \tag{20}$$

When $\sigma = 0$, this reduces to the result of [2, 3]. However, results similar to (20) have been reported [15, 16]. The case $\sigma \neq 0$, to our knowledge, is a new anomalous diffusion behaviour.

Now, our theory can be applied to the diffusion on fractals. In fact, the major predictions of diffusion on fractals presented in [9] can be derived from our model if $P(X, t)$ is regarded as $\hat{P}(r, t)$ of [9], and X as r of [9]. A random walker on the fractal, which has a fractal dimension d_f, obeys [9, 15]

$$\langle r^2(t)\rangle \sim t^{2/(2+\theta)} \tag{21}$$

where θ is defined in [9, 15]. It is easy to see that (14) is equivalent to (21) for

$$\frac{\beta}{\sigma+1} = \frac{2}{2+\theta}. \tag{22}$$

Therefore (14) is reduced to

$$\langle X^2(t)\rangle \sim t^{2/(2+\theta)}. \tag{23}$$

From (22) and (23), we can obtain

$$t^{\beta-1} \sim X^{2\sigma-\theta}. \tag{24}$$

From (12), we obtain that the probability to return to the origin is

$$P(0, t) \sim t^{-\beta/2}. \tag{25}$$

From (22), we have

$$P(0, t) \sim t^{-d_f/(2+\theta)} \tag{26}$$

for

$$\sigma = d_f - 1. \tag{27}$$

We can see that (26) is the same as (1.3) of [9].

Inserting (24) and (27) into (10), we have

$$\frac{\partial P(X, t)}{\partial t} = D(\theta, d_f) \frac{1}{X^{d_f - 1}} \frac{\partial}{\partial X} X^{d_f - 1 - \theta} \frac{\partial P(X, t)}{\partial X} \tag{28}$$

where $D(\theta, d_f)$ is a constant related to d_f and θ [9]. It is found that (28) is the same as (1.4) in [9]. In analogy with above operations, $\hat{P}(r, t)$ in [9] can be derived according to (12). All predictions of random walker on fractals [9] have been derived in our model.

From the above analysis, it has been found that the diffusion on fractals can be explained in our theoretical framework. That is to say, a random walker on fractals can be approximately viewed as a Brownian particle moving in a disordered medium which provides a noise with decoupled temporal and spatial correlations and a frictional force with memory. Furthermore, we know that the exponent σ is related to the fractal dimension, and smaller than 1 in two-dimensional assembling space, and β is related *to the exponent θ, which describes the decay of the diffusion coefficient with distance* [9]. Therefore, the exponent σ is characteristic of the structure of the disordered medium, and β is characteristic of the dynamics of the Brownian particle.

This paper is a continuation of our efforts [1, 2] to establish the statistical mechanics of damped diffusing particle driven by the noise with long-range correlations. We have established the GLE and corresponding FPE, in which correlation effects are involved. From the FPE, it is easy to see how the correlation affects the law of diffusion. The PDFs corresponding to case (i) and (ii) have the self-affinity property. It is worth noting that when $\beta = 1$, and σ is not equal to zero, the anomalous diffusion behaviour is expressed as $\langle X(t)^2 \rangle \sim (t \ln t)^{1/(1+\sigma)}$, which is a new anomalous diffusion behaviour. Our previous work [1, 2] can be recovered as a special case.

From (10), we may infer that noise with temporal and spatial correlations results in an effective diffusion coefficient depending on both displacement and time. From (2) and (12), we find that a non-Gaussian PDF results from temporal and spatial correlations.

Although our model for the generalized Brownian motion is confined to the one-dimensional case, our model can be extended to higher dimension. In fact, (14) and (10) which are derived for one dimension can be used to derive the results of a particle diffusion on two-dimensional percolation clusters [9]. Our model can be applied to explain the results of diffusion in fractals with higher dimension as long as, in our model, X is regarded as the distance r that the random walker travels from the origin and $P(X, t)$ as the envelope of the probability per site $P(r, t)\,\mathrm{d}r$ that at time t the walker is in the shell between r and $r + \mathrm{d}r$ around the origin, $\hat{P}(r, t)$. It is evident [6] that since the ensemble-averaged diffusion on two-dimensional percolation clusters is approximately isotropic, we can consider the friction kernel and force to be a scalar and the motion along any direction is then described by a scalar GLE. This is reasonable since, on average, one expects a homogeneously disordered system to be rotationally invariant in its properties.

In our theoretical framework, we have derived the all asymptotic expressions characteristic of diffusion on fractals [9], including the diffusion equation and its solution, anomalous diffusion behaviour, as well as the probability of returning to the origin. It should be noted that O'Shaughnessy and Procaccia's results are from the starting point of phenomenological consideration and on the basis of scaling arguments. However, our theory is developed in the framework of strictly statistical mechanics and starts from Brownian motion, which is related to microscopic fluctuations. So, our theoretical framework has a more reliable foundation than that of O'Shaughnessy and Procaccia. It has been shown that a random walker on fractals possibly encounters noise with long-range correlation, which has been little recognized by researchers [3]. According to (27), if the exponent σ in the noise has been determined by experiment, the fractal dimension can be derived from the analysis of the noise. On the other hand, the correlation of noise becomes an effective constitutive property of the fractal medium. Therefore, the fractal dimension of a fractal medium is possibly determined by analysing or 'listening' to the noise of a random walk on the fractal.

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Appendix

The derivation of (10) is as follows. According to the approach developed in [2], we use (6)–(9), and can obtain the asymptotic form of the FPE associated with (6):

$$\frac{\partial P(Y,t)}{\partial t}=b_1(\beta)\frac{K_B T t^{\beta-1}}{M}\frac{\partial^2 P(Y,t)}{\partial Y^2}. \tag{A.1}$$

Our interest is focused on the asymptotic behaviour. Since when $t\to\infty$ $(0<\beta<1$ or $1<\beta<2)$, $t^{\beta-2}\ll 1$ i.e. $t^{\beta-2}\to 0$, we have neglected two terms including $t^{\beta-2}$ in the derivation of (A.1). From (5), we have

$$\frac{\mathrm{d}X}{\mathrm{d}Y}=\frac{X^{-\sigma}}{\sigma+1}. \tag{A.2}$$

According to the derivation of a function of a function and (A.2), we have

$$\begin{aligned}\frac{\partial P(Y,t)}{\partial Y}&=\frac{\partial P(X,t)}{\partial X}\frac{\mathrm{d}X}{\mathrm{d}Y}\\&=\left(\frac{X^{-\sigma}}{\sigma+1}\right)\frac{\partial P(X,t)}{\partial X}.\end{aligned} \tag{A.3}$$

From (A.2) and (A.3), one can obtain

$$\frac{\partial^2 P}{\partial Y^2}=\frac{X^{-\sigma}}{(\sigma+1)^2}\frac{\partial}{\partial X}\left(X^{-\sigma}\frac{\partial P(X,t)}{\partial X}\right). \tag{A.4}$$

By virtue of (A.4) and (A.1), it is straightforward to derive equation (10).

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