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Long-time-correlation effects and biased anomalous diffusion

K. G. Wang

Chinese Center of Advanced Science and Technology (World Laboratory), P. O. Box 8730, Beijing 100 080, China;
Institute of Metal Research, Academia Sinica, Shenyang 100 015, China;*
and International Centre for Materials Physics, Academia Sinica, Shenyang 110 015, China

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This paper investigates the motion of a Brownian particle experiencing both a friction (biased) force and a randomly fluctuating force with a long-time-correlation function $C_f(t) \sim t^{-\beta}$, $0<\beta<1$, $1<\beta<2$, and $\beta=1$, instead of a Dirac δ function. The generalized Langevin equation and Fokker-Planck equation and corresponding solution are presented. It is shown that when $0<\beta<1$ or $1<\beta<2$, the diffusion motion of the Brownian particle is the anomalous diffusion that is related to fractal Brownian motion (FBM). But when $\beta=1$ the diffusion motion is anomalous diffusion with no connection to FBM. The effects of friction retardation result in a probability density function for finding the particle at displacement X at time t that depends on the initial value of velocity of the particle. The approach in this paper may provide a systematic method for the study of particles diffusing in fractal media.

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I. INTRODUCTION

Considerable recent interest has been focused on the attempt to understand anomalous faster and slower than normal diffusion (superdiffusion and subdiffusion). Several approaches have been developed to treat these problems [1–3]. However, the dynamical mechanism of the anomalous diffusion is poorly understood. Recently, Wang and Lung [3] investigated the dynamical mechanism from the starting point of the generalized Langevin equation (GLE) and the Fokker-Planck equation (FPE), and established the bridge between the long-time correlation and fractional (or fractal) Brownian motion (FBM) [4] and anomalous diffusion. Muralidhar *et al.* [5] applied the GLE to study the dynamics of anomalous diffusion from the facet of the velocity autocorrelation function (VACF) of the Brownian particle.

From the starting point of a power law and an oscillating-power-law VACF rather than an exponential VACF, Muralidhar *et al.* [5] have shown the conditions under which anomalous diffusion arises. Although the frictional force (or biased force) acting on the Brownian particle appears in the GLE of their paper, the effects of biased force on the drift motion of the Brownian particle were not studied, an omission also apparent in Ref. [3]. In addition, the very important quantity, the probability density function (PDF) for finding the Brownian particle at displacement X at time t cannot be derived in Muralidhar *et al.*'s paper [5]. However, Wang and Lung [3] have provided an effective FPE which does not include a drift term, and the corresponding solution. From the fact mentioned above, there arise two urgent questions. First, how does one overcome the disadvantages appearing in Refs. [3] and [5]? That is say, how does one deal with the general case of anomalous diffusion with biased effects? Second, how does one not only treat the biased motion and anomalous diffusion of the Brownian particle, but also find the PDF in the unified theoretical framework? The purpose of this paper is to answer these questions.

The outline of this paper is as follows. The long-time correlation and the GLE appear in Sec. II. The associated FPE and PDF are given in Sec. III. The relationship between the long-time-correlation effects and biased anomalous diffusion is discussed in Sec. V. Concluding remarks and the possible applications of this model are presented in the last section. Details of the mathematical derivation appear in the Appendix.

II. LONG-TIME CORRELATION AND THE GENERALIZED LANGEVIN EQUATION

When a Brownian particle moves in a fluid medium, it experiences two forces: one is the determinative dynamical frictional force, the other the random fluctuation force originating from the random collisions between the Brownian particle and the particles of the surrounding medium. If the density of the medium is much smaller than that of the Brownian particle, it is generally thought that the average value of the randomly fluctuating force equals zero and its correlation function is a Dirac δ function [6]. The classical Langevin equation can be written as

$$M\ddot{X}(t)+M\alpha\dot{X}(t)=F(t). \tag{2.1a}$$

The fluctuating force has the following properties:

$$\langle F(t)\rangle=0\ ,$$
$$\langle F(0)F(t)\rangle=D_0\delta(t-0)\ , \tag{2.1b}$$

where M is the mass of the Brownian particle, α is the frictional coefficient per unit mass, $X(t)$ is the displacement of the Brownian particle at time t in one-dimensional space, and D_0 is the diffusion constant. The FPE associated with Eq. (2.1) and its solution can be found in some books on nonequilibrium statistical mechanics [7].

However, when the Brownian particle moves through dense fluids or fluids with internal degrees of freedom [8], and on the percolating cluster [9], the randomly fluctuating force correlation function behaves with a power-law time dependence, the so-called long-time correlation, instead of the Dirac δ function. Recently, long-time-correlation effects have also been found in the dynamics of a growing interface [10].

Now, consider that a Brownian particle is acted upon by a friction force and a fluctuating force with a long-time correlation. The dynamics of the Brownian particle in one-dimensional space is described by the following GLE [3]:

$$\dot{X}(t)=V(t)\ ,$$
$$M\ddot{X}+M\int_0^t \alpha(t-\tau)V(\tau)d\tau=F(t)\ , \tag{2.2}$$

where $\alpha(t)$ represents the friction retardation (or friction memory kernel). The long-time-correlation property of the random fluctuating force is expressed as [3]

$$\langle F(t)\rangle=0\ ,$$
$$\langle F(0)F(t)\rangle=C_f(t)=F_0(\beta)t^{-\beta}. \tag{2.3}$$

The exponent β can be taken as $0<\beta<1$ or $1<\beta<2$, which is determined by the dynamical mechanism of the physical process considered [3]. The proportionality coefficient $F_0(\beta)$ is independent of time but dependent on the exponent β, which means that the proportionality coefficient depends on the physical process.

Due to the long-time correlation, the frictional coefficient is dependent on time instead of constant. The function $\alpha(t)$ can be determined by the generalized second fluctuation-dissipation theorem [7].

$$C_f(t)=Mk_BT\alpha(t)\ , \tag{2.4}$$

where T is the absolute temperature of the surrounding and k_B is Boltzmann's constant. It is straightforward to obtain

$$\alpha(t)=F_0(\beta)/(Mk_BT)t^{-\beta}$$
$$=\alpha_0(\beta)t^{-\beta}\ , \tag{2.5}$$

where

$$\alpha_0(\beta)=F_0(\beta)/(Mk_BT)\ . \tag{2.6}$$

III. FOKKER-PLANCK EQUATION AND ITS SOLUTION

In general, the functional-calculus approach can be used to obtain the FPE associated with the GLE (2.1) with Eq. (2.3). But functional calculus is in general not familiar to physicists. For the purpose of easy acceptability and simplicity, we apply the characteristic function to derive the FPE. The characteristic function associated with the probability density of finding the Brownian particle at displacement X at time t starting at the origin can be defined as

$$\Phi(Y,t)\equiv \exp(iXY)\rangle\equiv\int dX\,P(X,t)\exp(iXY)\ . \tag{3.1}$$

From the Laplace transform of Eq. (2.2), it is easy to obtain the Laplace transform of the VACF $k(t)$

$$k_L(p)=[p+\alpha_L(p)]^{-1}, \tag{3.2}$$

where the subscript L denotes the Laplace transform. The Laplace transform of the integral of $k(t)$ can be written as

$$K_L(p)=\{p[p+\alpha_L(p)]\}^{-1}\ , \tag{3.3}$$

where $K(t)$ describes the influence of the initial velocity of the particle on displacement [7]. From Eq. (2.2), it can be shown that the displacement increment ΔX and velocity increment ΔV are linear functionals of the fluctuating force $F(t)$, given the initial values of displacement and velocity. Therefore we have

$$\Delta X=X(t)-X(0)-V(0)K(t)$$
$$=(1/M)\int_0^t K(t-\tau)f(\tau)d\tau\ , \tag{3.4a}$$

$$\Delta V=V(t)-V(0)k(t)$$
$$=(1/M)\int_0^t k(t-\tau)f(\tau)d\tau\ . \tag{3.4b}$$

Since only the second-order correlation effect of the fluctuating force is considered in Eq. (2.3), the characteristic function can be expressed in term of the corresponding first and second moments. Equation (3.1) can further be changed into the form

$$\Phi(Y,t)=\exp(i\{[X(0)+V(0)K(t)]Y-\tfrac{1}{2}\sigma_{XX}Y^2\})\ , \tag{3.5}$$

where

$$\sigma_{XX}=\langle[X-X(0)-V(0)K(t)]^2\rangle\ . \tag{3.6}$$

By virtue of Eq. (3.4a) and after some computations, Eq. (3.6) can explicitly be rewritten as

$$\sigma_{XX}=(k_BT/M)\left[2\int_0^t K(\tau)d\tau-K(t)^2\right]\ . \tag{3.7}$$

From Eqs. (3.2)–(3.7), one can derive the FPE associated with Eqs. (2.2) and (2.3)

$$\frac{\partial P(X,t)}{\partial t}=-k(t)V(0)\frac{\partial P(X,t)}{\partial X}$$
$$+(k_BT/M)K(t)[1-k(t)]\frac{\partial^2P(X,t)}{\partial X^2}\ . \tag{3.8}$$

The derivation of Eq. (3.8) in detail appears in the Appendix. It should be noted that the PDF depends on the initial value of the velocity of the particle. This feature stems from the non-Markovian process.

In order to solve Eq. (3.8), we must know the explicit expressions for $k(t)$ and $K(t)$. In our previous paper [3], it has been shown that when $1<\beta<2$, the diffusion motion of the Brownian particle is anomalous faster than normal diffusion; when $0<\beta<1$, it is anomalous slower than normal diffusion. Firstly, I consider the cases when $0<\beta<1$ and $1<\beta<2$. Secondly, I consider the case when $\beta=1$, which is different from the first case.

When $0<\beta<1$ and $1<\beta<2$, using the theorems on the asymptotic expansion of Laplace transforms near the origin of Ref. [11], and taking the Laplace transform of Eq.

(2.5), one can easily obtain the asymptotic form when $p \to 0$

$$\alpha_L(p) \sim d_0 \Gamma(1-\beta) p^{\beta-1} , \quad (3.9)$$

where d_0 is a positive proportional constant related to the absolute values of $\alpha_0(\beta)$, and $\Gamma(x)$ is the gamma function. Inserting Eq. (3.9) into (3.2), it is straightforward to yield to leading order

$$k_L(p) \sim p^{1-\beta}/[d_0 \Gamma(1-\beta)] \quad (p \to 0) . \quad (3.10)$$

An unimportant proportionality coefficient is not explicitly expressed. Taking the inverse Laplace transform of Eq. (3.10) and employing the theorems of Ref. [11], we have the following:

(i) When $1<\beta<2$, the asymptotic form of $k(t)$ is

$$k(t) \sim t^{\beta-2}/[d_0 |\Gamma(1-\beta)| \Gamma(\beta-1)] = (\beta-1) t^{\beta-2}/[d_0 \Gamma(\beta-1)\Gamma(2-\beta)] . \quad (3.11)$$

From Eq. (3.11), the VACF $k(t)$ decays with a long positive tail, which means that if the Brownian particle at this instant has a positive velocity value, it has to "remember" to have positive velocity in future time.

(ii) When $0<\beta<1$, the asymptotic form $(t\to\infty)$ $k(t)$ can be written

$$k(t) \sim (\beta-1) t^{\beta-2} [d_0 \Gamma(1-\beta)\Gamma(2-\beta)] = (\beta-1) t^{\beta-2}/[d_0 \Gamma(|\beta-1|)\Gamma(2-\beta)] . \quad (3.12)$$

It is easy to see that when $0<\beta<1$, the VACF $k(t)$ decays with a long negative tail. That implies that, if the particle moves in the positive X direction at this instant, it is more likely to move in the negative direction in the next instant. The negative correlation implies a "whip-back" effect [5]. Combining Eqs. (3.11) and (3.12), the asymptotic behavior of $k(t)$ can be expressed in a unified manner as

$$k(t) \sim (\beta-1) t^{\beta-2}/[d_0 \Gamma(|1-\beta|)\Gamma(2-\beta)] \quad (0<\beta<1 \text{ or } 1<\beta<2) . \quad (3.13)$$

According to the relationship between $k(t)$ and $K(t)$ [Eq. (3.3)], one can obtain the asymptotic form $(t\to\infty)$ of $K(t)$ when $\int_0^\infty k(t)dt \neq E$ $(0<E<\infty)$

$$K(t) = \int_0^t k(t)dt \sim t^{\beta-1}/[d_0 \Gamma(|1-\beta|)\Gamma(2-\beta)] \quad (0<\beta<1 \text{ or } 1<\beta<2) , \quad (3.14a)$$

where the use of Eq. (3.13a) is made.

When $\int_0^\infty k(t)dt = E$ $(0<E<\infty)$, it means that

$$K(t) = \text{const} = E . \quad (3.14b)$$

Combining Eqs. (3.13) and (3.14a) with Eq. (3.8), the Fokker-Planck equation (3.8) can be rewritten as

$$\frac{\partial P(X,t)}{\partial t} = -a_1 V(0) t^{\beta-2} \frac{\partial P(X,t)}{\partial X} + b_1 \frac{k_B T}{M} t^{\beta-1}(1-t^{\beta-2}) \frac{\partial^2 P(X,T)}{\partial X^2} , \quad (3.15)$$

where

$$a_1 = (\beta-1) a_0/[d_0 \Gamma(|1-\beta|)\Gamma(2-\beta)] , \quad b_1 = b_0/[d_0 \Gamma(|1-\beta|)\Gamma(2-\beta)] . \quad (3.16)$$

The symbols a_0 and b_0 are the positive proportional coefficients of Eqs. (3.12) and (3.14), respectively. Our interest is focused on the asymptotic behavior, when $t\to\infty$. When $t\to\infty$, $0<\beta<1$ or $1<\beta<2$, and $t^{\beta-2} \ll 1$, Eq. (3.15) can further be written as

$$\frac{\partial P(X,t)}{\partial t} \approx -a_1 V(0) t^{\beta-2} \frac{\partial P(X,t)}{\partial X} + b_1 \frac{k_B T}{M} t^{\beta-1} \frac{\partial^2 P(X,t)}{\partial X^2} . \quad (3.17)$$

The PDF depends not only on the displacement and time, but also on the initial value of velocity of the particle. It is the essential feature of a non-Markovian process. We now turn to the solution for the Fokker-Planck equation with the initial condition, $P(X,0)=\delta(X)$. Using Fourier's transform of the integral, it is easy to obtain the normalization solution.

$$P(X,t) = (4\pi D t^\beta)^{-1/2} \exp[-(X + a t^{\beta-1})^2/(4Dt^\beta)] , \quad (3.18a)$$

where

$$D = b_1 k_B T/(M\beta) > 0 , \quad a = a_1 V(0)/(\beta-1) . \quad (3.18b)$$

Now, consider the case when $\int_0^\infty k(t)dt = E$ $(0<E<\infty)$. Combining Eqs. (3.14a) and (3.13) with Eq. (3.8), Eq. (3.8) is changed into the following form:

$$\frac{\partial P(X,t)}{\partial t} = -a_1 V(0) t^{\beta-2} \frac{\partial P(X,t)}{\partial X} + \frac{k_B T E}{M} \frac{\partial^2 P(X,t)}{\partial X^2} . \quad (3.19)$$

Its normalization solution with $P(X,0)=\delta(X)$ can easily be obtained,

$$P(X,t)(= (4\pi D' t)^{-1/2} \exp[-(X + a t^{\beta-1})^2/(4D't)] , \quad (3.20a)$$

$$D' = k_B T E/M > 0 , \quad a = a_1 V(0)/(\beta-1) . \quad (3.20b)$$

In the case $\beta=1$, if the VACF can be assumed to be [4]

$$k(t) \sim t^{-1} , \quad (3.21)$$

then

$$K(t) = \int_0^t k(t)dt \sim \ln t . \quad (3.22)$$

Combining Eqs. (3.22) and (3.23) with Eq. (3.8), we have

$$\frac{\partial P(X,t)}{\partial t} = -\left[\frac{a_2 V(0)}{t}\right] \frac{\partial P(X,t)}{\partial x} + \frac{k_B T b_2}{M} \ln t \frac{\partial^2 P(X,t)}{\partial X^2} , \quad (3.23)$$

where a_2 and b_2 are the proportionality coefficients of Eqs. (3.21) and (3.22), respectively.

By virtue of Fourier's integral transform, we can obtain the normalization solution of Eq. (3.23) with the initial condition $P(X,0)=\delta(X)$ as

$$P(X,t)=[4\pi D_2 t(\ln t-1)]^{-1/2} \times\exp\left\{\frac{-[X+a_2V(0)\ln t]^2}{[4D_2t(\ln t-1)]}\right\}, \tag{3.24a}$$

where

$$D_2=k_BTb_2/M>0 . \tag{3.24b}$$

IV. RELATIONSHIP BETWEEN LONG-TIME-CORRELATION EFFECTS AND BIASED ANOMALOUS DIFFUSION

When $0<\beta<1$ or $1<\beta<2$, from Eq. (3.18) it is easily shown that the mean displacement and mean-square displacement of a particle starting at the origin are, respectively,

$$\langle X\rangle=-at^{\beta-1} , \tag{4.1a}$$

$$\langle(X-\langle X\rangle)^2\rangle=2Dt^{\beta} . \tag{4.1b}$$

Equation (4.1a) has demonstrated that the mean displacement of the Brownian particle is proportional to $t^{\beta-1}$. From Eqs. (4.1a), (4.1b), and (3.18b), it can be seen that the initial value of the velocity only influences the drift motion, but does not influence the diffusion motion. Equation (4.1b) implies that the particle experiences an anomalous faster $(1<\beta<2)$ and slower $(0<\beta<1)$ diffusion than regular diffusion. Therefore the Brownian particle "experiences" not only the drift motion but also the anomalous-diffusion motion.

In order to exploit the self-affinity of the PDF, one can take the following scaling transformation in Eq. (3.18):

$$X-\langle X\rangle=b^{\beta/2}(X-\langle X\rangle) , \quad t=bt . \tag{4.2}$$

After simple computation, we have

$$P[X'-\langle X\rangle=b^{\beta/2}(X-\langle X\rangle),t'=bt] =b^{-\beta/2}P(X-\langle X\rangle,t) . \tag{4.3}$$

Equation (4.3) demonstrates that the PDF $P(X-\langle X\rangle,t)$ has the self-affinity [12]. According to the definition of FBM [4], and Ref. [3], we know the diffusion motion above the mean displacement is FBM.

However, when $0<\beta<1$, there is an exception. When $\int_0^\infty k(t)dt=E$ $(0<E<\infty)$, the diffusion motion is normal diffusion, which can be derived from Eq. (3.20a). But the drift motion is the same as that of the corresponding anomalous diffusion.

When $\beta=1$, by virtue of Eq. (3.24), the first and second moments of the displacement can be expressed as

$$\langle X\rangle=-a_2V(0)\ln t , \tag{4.4a}$$

$$\langle(X-\langle X\rangle)^2\rangle=2D_2t(\ln t-1) . \tag{4.4b}$$

When $t\to\infty$, $\ln t\gg1$, Eq. (4.4b) can be rewritten as

$$\langle(X-\langle X\rangle)^2\rangle\approx2D_2t\ln t\sim t\ln t . \tag{4.4c}$$

It is a good agreement with the proposition $2d$ of Ref. [5]. In Ref. [5], the mean displacement was not given.

From Eq. (3.24), it is easy to find the PDF in the case $\beta=1$ does not have self-affinity. In this case, the diffusion motion of the Brownian particle is not FBM, but is an anomalous diffusion. It further demonstrates that FBM corresponds to anomalous diffusion only when $0<\beta<1$ or $1<\beta<2$.

V. CONCLUDING REMARKS

The detailed understanding of transport of particles in disordered systems has been a problem of prime interest recently [1–3,5]. It has been visualized from different points of view and with many approaches [1–3,5]. The method in this paper, which includes both GLE and FPE, has advantages over that of Ref. [5], and over scaling theory [1,2], which cannot give the PDF analytically. However, the approach in this paper can analytically solve the FPE and naturally obtain the PDF and statistical average values. This approach is very suitable to treat dynamics of anomalous diffusion.

It is worth mentioning that in Refs. [3] and [5], the frictional (biased) term had appeared in the GLE, but neither paper gives the influence of bias on the Brownian motion. This paper gives a natural way to treat the bias effects. Our previous result in Ref. [3] can be thought of as a special result of this paper when $k(t)V(0)\to0$, $t\gg t_c$, where t_c is a characteristic time.

It is shown that the long-time correlation of fluctuating force is the physical origin of the anomalous diffusion. The frictional (biased) effect contributes only to drift motion of the Brownian particle, but results in a PDF that depends on the initial velocity of the particle. This is nothing other than the signature of a non-Markovian process.

It is proved that when $0<\beta<1$ or $1<\beta<2$, the PDF for finding the particle at displacement X at time t has self-affinity. It implies that the anomalous diffusion is associated with FBM [3]. However, when $\beta=1$, the probability of displacement is not self-affinite. Also the mean displacement and mean square of displacement is related to logarithmic time rather than a power law of time. That means that this type of anomalous diffusion is not directly related to FBM. To our knowledge, this is the initial recognition of this point.

It must be noted that when $0<\beta<1$, $\int_0^\infty k(t)dt=E$ $(0<E<\infty)$. The diffusion is normal rather than anomalous diffusion. A well-known example has been reported by Alder and Wainright [13] from molecular-dynamics studies.

I strongly believe that the method described in this paper has potential application to diffusion on fractal media [14]. This approach can serve as a general formalism for the study of long-time-correlation effects.

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APPENDIX

The Fokker-Planck equation (3.8) is derived as follows. Through use of Eq. (3.1), we have

$$\frac{\partial \Phi(Y,t)}{\partial t}=\left[iYV(0)k(t)-\frac{1}{2}Y^2\frac{d\sigma_{XX}}{dt}\right]\Phi(Y,t)\ . \quad \text{(A1)}$$

By virtue of Eq. (3.7), one obtains

$$\frac{d\sigma_{XX}}{dt}=\frac{2k_BT}{M}K(t)\left[1-\frac{dK(t)}{dt}\right]=\frac{2k_BT}{M}K(t)[1-k(t)]\ . \quad \text{(A2)}$$

Combining Eq. (A2) with Eq. (A1), we have

$$\frac{\partial \Phi(Y,t)}{\partial t}=\left[iYV(0)k(t)-Y^2\frac{k_BT}{M}\mathbf{K}(t)[1-k(t)]\right]\Phi(Y,t)\ . \quad \text{(A3)}$$

Taking the inverse Fourier transform of Eq. (A3), one can easily obtain the Fokker-Planck equation (3.8).

*Address for correspondence.

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