Fractional Langevin Equation to Describe Anomalous Diffusion

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A Langevin equation with a special type of additive random source is considered. This random force presents a fractional order derivative of white noise, and leads to a power-law time behavior of the mean square displacement of a particle, with the power exponent being noninteger. More general equation containing fractional time differential operators instead of usual ones is also proposed to describe anomalous diffusion processes. Such equation can be regarded as corresponding to systems with incomplete Hamiltonian chaos, and, depending on the type of the relationship between the speed and coordinate of a particle, yields either usual or fractional long-time behavior of diffusion.

§1. Introduction

In recent years, growing attention has been focused on the processes that take place in random disordered media, and in dynamic systems demonstrating chaotic behavior. A special place here is taken by the systems with incomplete Hamiltonian chaos, of which trajectories in the phase space can be portrayed as a set of "islands around islands" with self-similar (fractal) structure. In such systems the lifetime of any state of regular motion is also random. Incomplete chaos results in a few interesting phenomena that, among others, include anomalous properties of transport processes. That is associated with the fact that the islands of stability in this case act as a system of traps with a certain given distribution of the trapping time. For example, well known is the phenomenon of anomalous diffusion that is characterized by the time dependence of the mean squared displacement of a diffusing particle, which is described not by the Einstein's law but by a power function with noninteger exponent: [1),2)]

$$\langle (\Delta x)^2 \rangle \propto t^\alpha, \quad \alpha \neq 1.$$

In most cases, such behavior is considered to be connected with self-similar properties of the diffusion medium. Then it becomes possible to describe it by introducing fractional integrals I^α and derivatives $D^\alpha, (0 \leq \alpha < 1)$ [3)]

$$I^\alpha f(t) =_\circ I_t^\alpha f(t) \equiv \frac{1}{\Gamma(\alpha)} \int_0^t \frac{f(t')}{(t-t')^{1-\alpha}} dt',$$

$$D^\alpha f(t) =_\circ D_t^\alpha f(t) \equiv \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t \frac{f(t')}{(t-t')^{\alpha}} dt' \qquad (1)$$

into the equations of motion, either into the macroscopic Fokker-Planck equation (that leads to the fractional Fokker-Planck equation, [4)-8)]) or into the stochastic process defining microscopic motion of the particle. In the latter case a generalization of Wiener process called fractional Brownian motion was invented and gave way to the fractional noise which is obtained by fractional integration or differentiation of the Gaussian white noise.[9),10)] Possible interpretation of the physical meaning of fractional integrals and derivatives was offered in Refs. 4) and 11), and assumes that a system described by equations with fractional derivatives or integrals possesses a "selective" memory that acts only in the points within a fractal Cantor-type set and is in accordance with the ideas about a certain self-similar (say, Levy-type or fractal) distribution of traps and waiting times.[4)]

Fractal Brownian motion is of great interest not only from mathematics and theory of stochastic processes points of view but also in terms of physical applications. It can be used in describing polymer chains, electric transport in disordered semiconductors, diffusion on comb-like structures, and so on. However, it is well known that in many cases the most convenient way of describing the Brownian diffusion of particles is not the Wiener process but rather the Ornstein-Uhlenbeck process (or Langevin method[2),13)]) that is based on the solution of stochastic differential equation

$$\frac{d}{dt}v = -\gamma v + F(t), \tag{2}$$

where v is the velocity of a Brownian particle, γ is the liquid friction coefficient, and $F(t)$ is the random source characterizing the properties of medium where diffusion occurs. Apart from the problem of Brownian motion itself, this method is widely applied to describe various systems subjected to external noise. This brings up the question of whether the Langevin equation can be written for anomalous diffusion as well, and if so, what will be the structure of the corresponding random source in it.

§2. Fractional Langevin equation

a. As it has been mentioned above, introducing the fractional differential operators into the Fokker-Planck equation or Wiener process makes it possible to describe the anomalous transport process quite correctly. Therefore, let us consider the following equation that differs from the usual Langevin equation by replacing the first derivative with respect to time by the fractional derivative of order ν

$$\frac{d^\nu}{dt^\nu}v = -\gamma v + F(t). \tag{3}$$

Applying the fractional integral operator to both left-hand and right-hand sides of this equation in order to incorporate the initial condition $v_{t=0} = v_0$, we have

$$v - v_0 = {}_0I_t^\nu(-\gamma v + F(t)). \tag{4}$$

Expressing the fractional integral in the explicit form as in Eq. (1), this equation can be easily solved by standard techniques, and its solution has the form

$$v = v_0 E_{1,\nu}(-\gamma t^\nu) + \int_0^t F(t')(t-t')^{\nu-1} E_{\nu,\nu}[-\gamma(t-t')^\nu]dt', \tag{5}$$

where $E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} z^k/\Gamma(\alpha+\beta k)$ is so called Mittag-Leffleur function. If $\nu = 1$ then Eq. (5) the solution of the usual Langevin equation recovers. Provided that $F(t)$ is taken, as usual, to be a Gaussian δ-correlated source with zero mean, the velocity correlation function has the form

$$\langle v(t_1)v(t_2)\rangle = v_0^2 E_{1,\nu}(-\gamma t_1^\nu)E_{1,\nu}(-\gamma t_2^\nu) + q\int_0^{\min(t_1,t_2)} dt' \frac{E_{\nu,\nu}\left[-\gamma(t_1-t')^\nu\right]}{(t_1-t')^{1-\nu}} \frac{E_{\nu,\nu}\left[-\gamma(t_2-t')^\nu\right]}{(t_2-t')^{1-\nu}}. \quad (6)$$

One can then calculate the mean squared displacement of a particle of which motion is described by Eq. (3) as

$$\langle(\Delta x)^2\rangle = \int_0^t \int_0^t \langle v(t_1)v(t_2)\rangle dt_1 dt_2 \quad (7)$$

that can be reduced to

$$\langle(\Delta x)^2\rangle = v_0^2\left[tE_{2,\nu}(-\gamma t^\nu)\right]^2 + \frac{q}{\gamma^2}\left(t - 2tE_{2,\nu}(-\gamma t^\nu) + \int_0^t \left[E_{1,\nu}(-\gamma t^\nu)\right]^2 dt\right). \quad (8)$$

At large values of the argument $E_{1,\nu}(-\gamma t^\nu) \propto E_{2,\nu}(-\gamma t^\nu) \propto 1/\gamma t^\nu$. Therefore, the integral in Eq. (8) necessarily converges at $t \to \infty$ for $1/2 < \nu < 1$, and the leading term in the asymptotics is

$$\langle(\Delta x)^2\rangle = \frac{q}{\gamma^2} t \quad (9)$$

just as it is the case for the usual Langevin equation with the first derivative with respect to time.

b. However, it must be noted that in Eq. (8) we assumed that, as usually, the velocity v was defined as the first derivative of the coordinate with respect to time and, therefore, $x = \int_0^t v(t)dt$. Actually, it makes sense to consider a more general relationship

$$x = \frac{1}{\Gamma(\nu)} \int_0^t \frac{v(t')}{(t-t')^{1-\nu}} dt', \quad (10)$$

that corresponds to the most complete possible description of the system memory by means of the fractional integrals — the particle's displacement is defined by velocity only in the points within a time interval of dimension ν. In order to clear this point, let us recollect that microscopic motion of a diffusing particle represents a twisted and everywhere nondifferentiable curve. For such curve, however, one can often find a derivative of fractional order [14] that, in fact, is a derivative of the trajectory, averaged with a power weight, and the observed motion of the particle is the thus averaged motion. In terms of memory, it means that for fractal paths (which are even the paths of classical Brownian particle) some of the instant velocities and displacements do not contribute into the resulting macroscopic motion. As this occurs, the behavior of the solution changes, and diffusion becomes anomalous. In this case instead of Eq. (8) we obtain

$$\langle(\Delta x)^2\rangle = {}_0I^{\nu}_{t_1}\,{}_0I^{\nu}_{t_2}\langle v(t_1)v(t_2)\rangle = v_0^2\frac{\Big[E_{1,\nu}(-\gamma t^{\nu})-1\Big]^2}{\gamma^2}$$
$$+\frac{2qt^{2\nu-1}}{\gamma^2}\sum_{k,l=1}^{\infty}\frac{(-\gamma)^{k+l}}{\Gamma(\nu+\nu k)\Gamma(\nu l)}\frac{\Gamma(\nu k+\nu l+\nu-1)}{\Gamma(\nu k+\nu l+2\nu)}t^{\nu k+\nu l}. \quad (11)$$

At large times the first term tends to v_0^2/γ^2, and the sum in the second term converges. Therefore we finally have (assuming $1/2<\nu<1$)

$$\langle(\Delta x)^2\rangle \propto N\frac{q}{\gamma^2}t^{2\nu-1}, \quad 1<N<\frac{2}{\Gamma(\nu)} \quad (12)$$

that coincides with the asymptotics of fractional Brownian motion. [9)-12)]

c. Let us now investigate separately the influence of memory and fractal behavior on the regular and random components of the force acting on a particle. It turns out that the same fractal asymptotic behavior can be demonstrated by taking into account only the memory for the random force component in the initial Langevin equation, which has a more clear physical meaning (cf. Eq. (4)):

$$v = v_0 - \gamma\int_0^t v(t')dt' + \frac{1}{\Gamma(\nu)}\int_0^t \frac{F(t')}{(t-t')^{\nu}}dt'. \quad (13)$$

In fact, it means that in Eq. (2) the random source is not δ-correlated but represents a fractional derivative of white noise

$$F(t) = {}_0D_t^{1-\nu}g(t), \qquad \langle g(t_1)g(t_2)\rangle = q\delta(t_1-t_2). \quad (14)$$

Equation of this type was actually considered in Ref. 15). It was shown numerically there that when in the Langevin equation Gaussian white noise is replaced by the fractional noise it can yield the spectrum for homogeneous Eulerian and Lagrangian turbulence. However, Eq. (13) can be easily solved analytically. Its solution reads

$$v = v_0e^{-\gamma t} + \int_0^t F(t')(t-t')^{\nu-1}E_{\nu,1}\Big[-\gamma(t-t')\Big]dt' \quad (15)$$

and calculation of the mean squared displacement results in the following asymptotic behavior

$$\langle(\Delta x)^2\rangle \propto \frac{1}{(2\nu-1)\Big[\Gamma(\nu)\Big]^2}\frac{q}{\gamma^2}t^{2\nu-1}, \qquad t\to\infty, \quad (16)$$

which agrees with Eq. (12) up to the constant factor and coincides exactly with the results of Ref. 12).

d. Finally, let us consider the third case, that is when the memory is taken into account only for the friction force

$$v = v_0 - \gamma\frac{1}{\Gamma(\nu)}\int_0^t\frac{v(t')}{(t-t')^{\nu}}dt' + \int_0^t v(t')dt', \quad (17)$$

where $F(t)$ is again the Gaussian white noise (cf. Eqs. (4) and (13)). It means that now it is the dissipative force that is proportional to the fractional derivative of velocity $f_{\rm diss} = {}_0D_t^{1-\nu}v(t)$. Its solution is

$$v = v_0 E_{1,\nu}(-\gamma t^\nu) + \int_0^t F(t')E_{\nu,\nu}\Big[-\gamma(t-t')^\nu\Big]dt'. \tag{18}$$

The contribution from the second term in the mean squared displacement results in the power function of time in the following form

$$\langle(\Delta x)^2\rangle \propto M\frac{q}{\gamma^2}t^{3-2\nu}, \quad 1 < M < \frac{1}{\Gamma(1+\nu)}. \tag{19}$$

§3. Probability distributions

The probability distributions that arise from the stochastic processes described above can easily be obtained by calculating the moments

$$M_n = |x-y|^n = \int_t^{t+\Delta t}\cdots\int_t^{t+\Delta t}\langle v(t_1)\cdots v(t_n)\rangle dt_1\cdots dt_n. \tag{20}$$

Our equations are linear both with respect to the external additive noise and the stochastic variable. Hence, the distribution for the particle coordinate $W(x,t)$ must be Gaussian. Moreover, taking into account Eq. (6) — like expressions for velocity correlations, it can be shown that dispersion of this Gaussian distribution is proportional to the mean squared displacement during time t. In particular, considering the Ornstein-Uhlenbeck process with the fractional noise Eq. (13) it the transition probability $P(x,t+\Delta t;y,t)$ has the form

$$P(x,t+\Delta t;y,t) = \frac{1}{\sqrt{2\pi B\Delta t^{2\nu-1}}}\exp\left(-\frac{|x-y|^2}{2B\Delta t^{2\nu-1}}\right), \tag{21}$$
$$B = \frac{1}{(2\nu-1)\Big[\Gamma(\nu)\Big]^2}\frac{q}{\gamma^2}$$

provided $\Delta t \ll t$ and the result for the coordinate distribution $W(x,t)$ of the wandering particle agrees with [2), 12)]

$$W(x,t) = \frac{1}{\sqrt{2\pi Bt^{2\nu-1}}}\exp\left(-\frac{x^2}{2Bt^{2\nu-1}}\right). \tag{22}$$

It should also be noted that such process on any time scales is not Markovian since Eq. (22) do not comply with the Chapmen-Kolmogorov equation

$$P(x,t+\Delta t) = \int P(x,t+\Delta t;y,t)P(y,t)dy,$$

which can be verified by direct substitution. Non-Markovity appears as a consequence of the existence of the memory about the past process. If for a Markovian process the future is uniquely determined by the present, then in the initial equation (13) the behavior of a particle in the next moment of time is, generally, dependent on the whole previous history starting from the very beginning of the motion, and the transition probability $P(x, t + \Delta t; y, t)$ does not depend on the time t only when $\Delta t \to 0$. In this connection the question of transition from Eq. (13) to the Fokker-Planck-type equation still remains to be solved. Indeed, the proposed method in Refs. 4) and 8) is based on the fractional Taylor series expansion of the transition probabilities in the Chapmen-Kolmogorov equation. Probably this problem may be solved by studying the waiting time probabilities and then writing down the equations similar to those used in Refs. 1) and 6).

From the velocity autocorrelation function the average kinetic energy of a particle $\langle E \rangle = \langle [v(t)]^2 \rangle$ can be obtained to be constant at large time, leading therefore (see Ref. 13)) to the Maxwellian distribution.

§4. Concluding remarks

Let us now summarize the results obtained. If we substitute the first derivative in the Langevin equation for the fractional one but use the same relationship for velocity and coordinate, then the solution possesses the same linear asymptotic behavior as the initial solution does. This means that taking into account the memory for the friction force and random force at the same moments of time does not affect the particle's motion at large times but only in the beginning of the motion. In a sense, this is quite reasonable, since a random source provides a particle with an additional energy, and friction results in its dissipation. At larger times, when the system arrives at the stable state, these two processes compensate each other, but only provided that they have the same duration.

The relationship between x and v in Eq. (10) means that the particle's motion equation written in the Newtonian form reads

$$\frac{d^{2\nu}x}{dt^{2\nu}} = \frac{d^{\nu}x}{dt^{\nu}} + F(t), \tag{23}$$

and is regarded as the most general one in the sense of memory calculation. Hence, every derivative with respect to time becomes fractional. Then anomalous properties of the diffusion arise from fractional integration of velocity, that is, from the assumption only part of instant velocities contribute to the final path.

The anomalous diffusion is also the result of the Langevin equation with a source that is a fractional derivative of the white noise. The autocorrelation function of such noise has a power time behavior [10)] and therefore appears to be a generalization of the flicker-noise (see Ref. 2)). Generally speaking, the fractional noise is nonstationary, but the nonstationary of the noise should not lead to a misunderstanding here. As we have mentioned above, our process can be regarded as stationary only in a wide sense (the corresponding transition probabilities depend uniquely upon the duration of the transition Δt) only for small Δt, that is for $\Delta t \ll t$. This lack of stationarity is an important and rather obvious property of anomalous diffusion, although it is not always given proper consideration. Here it is relevant to note the following. Normally, the Brownian motion can be described with two different stochastic processes. The Ornstein-Uhlenbeck process is strictly stationary but does not have independent increments. Moreover, its increments are not even uncorrelated. The Wiener process, which is the integrated Ornstein-Uhlenbeck process in the limit of intense friction and noise, has stationary independent increments, but is neither strictly stationary nor a wide-sense stationary. The process under investigation with a fractional derivative of the white noise seems to be an intermediate process that does not have stationary increments but is asymptotically stationary in a wide sense. The fractal nature of motion leads to the fact that even this kind of stationarity is observed only within short periods of time, which means that the process becomes quasistationary.

Finally, if the prehistory affects only the dissipative force acting on a particle, its behavior also becomes anomalous.

To conclude, we would like to note the following. Earlier the fractal Brownian motion was represented only as a Wiener stochastic process of fractional order. As shown in the present paper, the Ornstein-Uhlenbeck process with the fractional noise leads to similar results and allows to obtain more general probability distributions in an easier way, as compared to the path integrals. [12] The equations proposed can also be easily generalized by adding linear and nonlinear terms, and be used for calculation of various statistic characteristics of real stochastic dynamic systems.

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