Fractional Langevin equation

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We investigate fractional Brownian motion with a microscopic random-matrix model and introduce a fractional Langevin equation. We use the latter to study both subdiffusion and superdiffusion of a free particle coupled to a fractal heat bath. We further compare fractional Brownian motion with the fractal time process. The respective mean-square displacements of these two forms of anomalous diffusion exhibit the same power-law behavior. Here we show that their lowest moments are actually all identical, except the second moment of the velocity. This provides a simple criterion that enable us to distinguish these two non-Markovian processes.

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Diffusion is one of the basic nonequilibrium phenomena. Normal diffusion is well described in the theory of Brownian motion as a Gaussian process that is both local in space and time. It is characterized by a mean-square displacement that is asymptotically linear in time, $\langle x^2\rangle = 2Dt$, where D is the diffusion constant [1]. However, a growing number of experimental observations show that more complex processes, in which the mean-square displacement is not proportional to t, also occur in nature. Anomalous diffusion has for instance been seen in micelle systems [2], two-dimensional rotating flows [3], porous glasses [4], actine networks [5], but also on capillary surface waves [6], in strongly coupled dusty plasmas [7], and more recently in intracellular transport [8]. Anomalous diffusion finds its dynamical origin in nonlocality, either in space or in time (for a recent review see [9]). A well-known example of a process that is nonlocal in space is Lévy stable motion, for which the mean-square displacement is actually infinite due to the occurrence of very long jumps [10]. In this paper we focus on processes that are nonlocal in time and whence show memory effects. Specifically, we shall discuss and compare fractional Brownian motion (FBM) [11] and the fractal time process (FTP) [12]. These two forms of anomalous diffusion are fundamentally different (see below). Yet, they are difficult to tell apart experimentally, since both yield a mean-square displacement of the form $\langle x^2\rangle \propto t^{\alpha}$, $\alpha \neq 1$. It is for instance still an open question whether the long-range correlations observed in nucleotide sequences [13–15] are to be interpreted in terms of FBM or FTP-type DNA walks [16]. In this paper we aim at providing a simple criterion that permits to distinguish between these two non-Markovian processes.

The very difference between FBM and FTP is best illustrated by looking at their diffusion equations. The solution of the diffusion equation for FBM [17]

$$\frac{\partial}{\partial t}P_{\mathrm{FBM}}(x,t) = \alpha D t^{\alpha-1}\frac{\partial^2}{\partial x^2}P_{\mathrm{FBM}}(x,t), \tag{1}$$

is easily found to be the Gaussian distribution $P_{\mathrm{FBM}}(x,t) = \exp(-x^2/4Dt^{\alpha})/[4\pi D t^{\alpha}]^{1/2}$. FBM thus describes Gaussian transport. It is important to note that Eq. (1) is thereby local in time (there is no memory kernel). The non-Markovian character is expressed through a time-dependent diffusion constant, $D_{\alpha}(t) = \alpha D t^{\alpha-1}$. In contradistinction, the diffusion equation for FTP [18]

$$\frac{\partial}{\partial t}P_{\mathrm{FTP}}(x,t) = \frac{D}{\Gamma(\alpha-1)}\int_0^t \frac{d\tau}{(t-\tau)^{2-\alpha}}\,\frac{\partial^2}{\partial x^2}P_{\mathrm{FTP}}(x,\tau) \tag{2}$$

contains a memory kernel and the distribution function $P_{\mathrm{FTP}}(x,t)$ is hence non-Gaussian. The solution of Eq. (2) is given by $P_{\mathrm{FTP}}[x,z] = \exp(-|x|z^{\alpha/2}/D^{1/2})/[2D^{1/2}z^{1-\alpha/2}]$ in Laplace z space. In time, $P_{\mathrm{FTP}}(x,t)$ has been expressed in closed form in terms of a Fox function [19] or a one sided Lévy stable distribution [20]. By introducing further the Riemann-Liouville fractional derivative $(-1<\lambda<0)$ [21]

$$\frac{\partial^{\lambda} f(t)}{\partial t^{\lambda}} = \frac{1}{\Gamma(-\lambda)}\int_0^t \frac{f(\tau)\,d\tau}{(t-\tau)^{\lambda+1}}, \tag{3}$$

Eq. (2) can be rewritten as a fractional diffusion equation [22]

$$\frac{\partial}{\partial t}P_{\mathrm{FTP}}(x,t) = D\,\frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\,\frac{\partial^2}{\partial x^2}P_{\mathrm{FTP}}(x,t). \tag{4}$$

Both Eqs. (1) and (4) reduce to the normal diffusion equation when $\alpha = 1$.

We begin our discussion of FBM by introducing a fractional Langevin equation. It is worthwhile to point out that the Langevin and the phase-space descriptions of Brownian motion are no longer fully equivalent in the non-Markovian regime of interest here. As recently discussed by Calzetta *et al.* [25], the Langevin equation contains more information and thus appears more fundamental. We then apply this fractional Langevin equation to study in some detail the anomalous diffusion of a free particle coupled to a fractal heat bath. In particular, we evaluate the first two moments of both the position and the velocity of the particle, which we express in terms of Mittag-Leffler functions. Finally, we compare with the results obtained recently for FTP by Metzler and Klafter for $0<\alpha<1$ [23] and by Barkai and Silbey for $1<\alpha<2$ [24] by using a fractional Klein-Kramers equation. We find that FBM and FTP satisfy the same generalized Einstein relation. Moreover, their lowest moments are all equal, except the second moments of the velocity.

We examine the dynamics of the Brownian particle with a microscopic random-matrix model. Random-matrix theory has already been successfully applied in the context of anomalous diffusion in Refs. [27–29]. The relaxation of a system coupled to a complex environment is expected to be insensitive to the details of the interaction. The process may then be described within a statistical approach where the interaction is modeled by a random operator [26]. We thus consider a system S weakly coupled to a fractal heat bath B via a random-matrix interaction [29,30]. The coupling is chosen linear in the position x of the system. The generic form of the Hamiltonian is given by

$$H=H_S\otimes\mathbb{1}_B+\mathbb{1}_S\otimes H_B+x\otimes V, \tag{5}$$

where $H_S=p^2/2M+U(x)$ is the Hamiltonian of the system, H_B describes the bath and V is a centered Gaussian random band matrix. It is assumed that initially the system and the bath are uncorrelated and that the latter is in thermal equilibrium at temperature $\beta=(kT)^{-1}$. The variance of the random interaction is further taken to have the form [29]

$$\overline{V_{ab}^2}=A_0\frac{|\varepsilon_a-\varepsilon_b|^{\alpha-1}}{[\rho(\varepsilon_a)\rho(\varepsilon_b)]^{1/2}}\exp\left[-\frac{(\varepsilon_a-\varepsilon_b)^2}{2\Delta^2}\right]. \tag{6}$$

Here ε_a's denote the eigenenergies of the bath Hamiltonian ($H_B|a\rangle=\varepsilon_a|a\rangle$), A_0 is the strength of the coupling, Δ the bandwidth, and $\rho(\varepsilon)$ is the density of states of the bath, which is locally written as $\rho(\varepsilon)=\rho_0\exp(\beta\varepsilon)$. As shown in [29], the variance (6) gives rise to subdiffusion when $\alpha<1$ and to superdiffusion when $1<\alpha<2$. The coupling to the bath is characterized by the bath correlation function that is defined as $K(t)=\langle\tilde{V}(t)\tilde{V}(0)\rangle_B=K'(t)+iK''(t)$. Here $\tilde{V}(t)=\exp(iH_Bt)V\exp(-iH_Bt)$ and $\langle\cdots\rangle_B$ denotes the average thermal. After performing the average over the random-matrix ensemble, $\overline{K}(t)$ is found to be simply the Fourier transform of the variance $\overline{V_{ab}}^2$ with respect to ε_b. In the following we consider the limit of high temperature and large bandwidth, $1\ll\Delta\ll kT$. Using the variance (6) we then obtain

$$\overline{K'}(t)=2A_0\Gamma(\alpha)\cos\left(\frac{\alpha\pi}{2}\right)t^{-\alpha},\quad \overline{K''}(t)=\frac{\beta}{2}\frac{d\overline{K'}}{dt}. \tag{7}$$

We see that the time dependence of $\overline{K}(t)$ follows an inverse power law. This presence of a long tail leads to long-time correlation effects in the dynamics of the Brownian system [29]. Note that for $\alpha=1$, the Fourier transform of Eq. (6) reads $\overline{K'}(t)=2\pi A_0\delta(t)$ and normal Brownian motion is recovered. The generalized Langevin equation that corresponds to the random-matrix Hamiltonian (5) can easily be derived with the method presented in Ref. [31]. In the limit of weak coupling this leads to

$$M\ddot{x}(t)+M\int_0^t\gamma(t-\tau)\dot{x}(\tau)d\tau+U'(x)=\xi(t), \tag{8}$$

where $\xi(t)$ is a Gaussian random force with mean zero and variance $\langle\xi(t)\xi(0)\rangle=\overline{K'}(t)$, and $\gamma(t)$ is a damping kernel that obeys $MkT\gamma(t)=\overline{K'}(t)$. This last relation is often referred to as the second fluctuation-dissipation theorem [33]. Remark that the Langevin equation is completely determined by the real part $\overline{K'}(t)$ of the bath correlation function. Furthermore, in the limit of weak coupling, the dynamics described by the Hamiltonian (5) is Gaussian and one can show that the corresponding diffusion equation is precisely given by Eq. (1). Using again the fractional derivative (3), we may rewrite Eq. (8) in the form of a fractional Langevin equation. We obtain

$$M\ddot{x}(t)+M\gamma_\alpha\frac{\partial^{\alpha-1}}{\partial t^{\alpha-1}}\dot{x}(t)+U'(x)=\xi(t), \tag{9}$$

where we have defined $\gamma_\alpha=\pi A_0\beta/[M\sin(\alpha\pi/2)]$. The fractional Langevin equation (9) describes both subdiffusion for $0<\alpha<1$ and superdiffusion for $1<\alpha<2$ [34]. As a simple application of the fractional equation (9), we now concentrate on the free particle and accordingly set $U(x)=0$. In this case, the solution of the Langevin equation is easily obtained by applying Laplace transform techniques [32]. We find

$$x(t)=x_0+v_0B_v(t)+\int_0^tB_v(t-\tau)\xi(\tau)d\tau, \tag{10}$$

where (x_0,v_0) are the initial coordinates of the particle and $B_v(t)=\int_0^tC_v(t')dt'$ is the integral of the (normalized) velocity autocorrelation function $C_v(t)=\langle v(t)v\rangle/\langle v^2\rangle$. The Laplace transform of $C_v(t)$ is given by

$$C_v[z]=\frac{1}{z+\gamma[z]}=\frac{1}{z+\gamma_\alpha z^{\alpha-1}}, \tag{11}$$

where $\gamma[z]$ is the Laplace transform of the damping kernel. Equation (11) is known as the first fluctuation-dissipation theorem [33]. By taking the inverse Laplace transform, the velocity autocorrelation function can be written as

$$C_v(t)=E_{2-\alpha}(-\gamma_\alpha t^{2-\alpha}). \tag{12}$$

Here we have introduced the Mittag-Leffler function $E_\alpha(t)$, which is defined by the series expansion [35]

$$E_\alpha(t)=\sum_{n=0}^{\infty}\frac{t^n}{\Gamma(\alpha n+1)}. \tag{13}$$

The function $E_\alpha(t)$ reduces to the exponential when $\alpha=1$. The asymptotic behavior of the Mittag-Leffler function (13) for short and long times is respectively given by $\sim\exp(t)$ and $\sim-[t\Gamma(1-\alpha)]^{-1}$, $0<\alpha<1$ and $1<\alpha<2$ [36]. For the velocity autocorrelation function (12) this yields a typical stretched exponential behavior at short times

$$C_v(t)\sim\exp\frac{-\gamma_\alpha t^{2-\alpha}}{\Gamma(3-\alpha)},\quad t\ll\frac{1}{(\gamma_\alpha)^{1/\alpha}}, \tag{14}$$

and an inverse power-law tail at long times

$$C_v(t) \sim \frac{t^{\alpha-2}}{\gamma_\alpha \Gamma(\alpha-1)}, \quad t \gg \frac{1}{(\gamma_\alpha)^{1/\alpha}}. \tag{15}$$

The result (15) has already been obtained in Ref. [29], where it has been shown to induce the ''whip-back'' effect. After time integration, we finally get from Eq. (12)

$$B_v(t) = t\, E_{2-\alpha,2}(-\gamma_\alpha t^{2-\alpha}), \tag{16}$$

where we have used the generalized Mittag-Leffler function $E_{\alpha,\beta}(t)$ defined as [35]

$$E_{\alpha,\beta}(t) = \sum_n^\infty \frac{t^n}{\Gamma(\alpha n+\beta)}. \tag{17}$$

In the long-time limit, the generalized Mittag-Leffler function satisfies $E_{\alpha,\beta}(t) \sim -[t\,\Gamma(\beta-\alpha)]^{-1}$. Accordingly, $B_v(t)$ exhibits a decay of the form

$$B_v(t) \sim \frac{t^{\alpha-1}}{\gamma_\alpha \Gamma(\alpha)}, \quad \text{when} \quad t \to \infty. \tag{18}$$

We emphasize that the solution (10) of the fractional Langevin equation in the force-free case is completely specified by the knowledge of the function $B_v(t)$.

Let us now turn to the evaluation of the lowest moments of the position and the velocity of the free particle. The mean displacement and the mean-square displacement are readily deduced from Eq. (10). We find

$$\langle x \rangle = x_0 + v_0 t\, E_{2-\alpha,2}(-\gamma_\alpha t^{2-\alpha}) \underset{t\to\infty}{\sim} \frac{v_0}{\gamma_\alpha} \frac{t^{\alpha-1}}{\Gamma(\alpha)} \tag{19}$$

and

$$\langle x^2 \rangle = \frac{2kT}{M} t^2 E_{2-\alpha,3}(-\gamma_\alpha t^{2-\alpha}) \underset{t\to\infty}{\sim} \frac{2kT}{\gamma_\alpha M} \frac{t^\alpha}{\Gamma(1+\alpha)}. \tag{20}$$

In the last equation, thermal initial conditions have been assumed ($x_0=0$, $v_0^2=kT/M$). In addition, one may easily verify that $\langle x \rangle^2$, $\langle x^2 \rangle$, and $C_v(t)$ satisfy the general Green-Kubo relation

$$\langle x^2 \rangle - \langle x \rangle^2 = \frac{2kT}{M} \int_0^t dt' \int_0^{t'} d\tau\, C_v(\tau), \tag{21}$$

which is known from linear response theory [33]. In a similar way, one can compute the first and second moments of the velocity from the time derivative of Eq. (10). This results in

$$\langle v \rangle = v_0 E_{2-\alpha}(-\gamma_\alpha t^{2-\alpha}) \underset{t\to\infty}{\sim} \frac{v_0}{\gamma_\alpha} t^{\alpha-2}, \tag{22}$$

and

$$\langle v^2 \rangle = v_0^2 [E_{2-\alpha}(-\gamma_\alpha t^{2-\alpha})]^2 + \frac{kT}{M}\{1-[E_{2-\alpha}(-\gamma_\alpha t^{2-\alpha})]^2\}. \tag{23}$$

We observe that $\langle v^2 \rangle$ decays like $(t^{\alpha-2})^2$ for large t. A common remarkable property of the above calculated mean values is their slow relaxation towards equilibrium as given by the (generalized) Mittag-Leffler function. This has to be contrasted with normal Brownian motion where all this quantities display an exponential decay. Let us now discuss the generalized Einstein relation that relates driven and free process [37]. We consider a particle initially at rest ($x_0=v_0=0$) and seek the mean position $\langle x \rangle_F$ as a function of an externally applied constant force $U(x) = -xF\theta(t)$. From the Langevin equation we easily find

$$\frac{d\langle x \rangle_F}{dt} = \frac{F}{M} \int_0^t C_v(t')\, dt', \tag{24}$$

where the velocity autocorrelation function $C_v(t)$ is given by Eq. (12). Equation (24) together with the Green-Kubo relation (21) for $\langle x^2 \rangle_0$ in the force-free case, then yields the generalized Einstein relation for FBM

$$\langle x \rangle_F = \frac{F}{2kT} \langle x^2 \rangle_0. \tag{25}$$

It is interesting to note that the validity of the Einstein relation (25) has been recently verified experimentally [38,39].

We now come to the comparison of FBM with FTP. Barkai and Silbey have investigated superdiffusive FTP with a fractional Klein-Kramers equation that they inferred from a generalized Rayleigh model [24]. For the free particle, a direct comparison [40] between their results and our Eqs. (19)–(25) shows that the mean displacement (19), the mean-square displacement (20), the velocity's first moment (22), and the velocity autocorrelation function (12) are identical for the two processes. This means, in particular, that FBM and FTP satisfy the same Green-Kubo relation (21). Moreover, both FBM and FTP obey the same generalized Einstein relation (25). Although FBM and FTP are fundamentally different processes, we thus notice that they share strikingly common features. However, the second moments of the velocity are different. For convenience, we quote their equation (2.18) that reads (in our notation)

$$\langle v^2 \rangle_{\mathrm{FTP}} = v_0^2 E_{2-\alpha}(-2\gamma_\alpha t^{2-\alpha}) + \frac{kT}{M}\{1-E_{2-\alpha}(-2\gamma_\alpha t^{2-\alpha})\}. \tag{26}$$

We see that for FTP, the second moment of the velocity relaxes asymptotically like $t^{\alpha-2}$. This is in sharp contrast to the FBM result Eq. (23) that exhibits a much faster decay. It is also worth noting that Eqs. (22) and (26) reduce to the same (exponential) expression for $\alpha=1$. On the other hand, subdiffusive FTP has been studied by Metzler and Klafter by using a fractional Klein-Kramers equation derived from a non-Markovian generalization of the Chapman-Kolmogorov equation. A comparison with their results for the force-free case leads to similar conclusions as in the superdiffusive regime. Many experiments on anomalous diffusion have measured either the mean-square displacement [5–8] or the generalized Einstein relation [38,39]. However, the latter do not allow to distinguish FBM and FTP, as we have just shown. In contrast, the variance of the velocity offers a clear distinction between these two processes as exemplified by Eqs. (23) and (26). This result could stimulate ongoing experiments on anomalous diffusion [41].

In summary, we have investigated FBM within a generic random-matrix approach and introduced a fractional Langevin equation that applies for both subdiffusion and superdiffusion. The Langevin approach thus provides a unified treatment of anomalous diffusion. We have further studied the anomalous dynamics of a free particle coupled to a fractal heat bath and performed a comparison between FBM and FTP. We have found that these completely different forms of non-Markovian anomalous diffusion share many common characteristics. In particular, they satisfy the same generalized Einstein relation and their lowest moments are all equal with the exception of the second moment of the velocity.

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