Critical Exponent of the Fractional Langevin Equation

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We investigate the dynamical phase diagram of the fractional Langevin equation and show that critical exponents mark dynamical transitions in the behavior of the system. For a free and harmonically bound particle the critical exponent $\alpha_c = 0.402 \pm 0.002$ marks a transition to a nonmonotonic underdamped phase. The critical exponent $\alpha_R = 0.441\ldots$ marks a transition to a resonance phase, when an external oscillating field drives the system. Physically, we explain these behaviors using a cage effect, where the medium induces an elastic type of friction. Phase diagrams describing the underdamped, the overdamped and critical frequencies of the fractional oscillator, recently used to model single protein experiments, show behaviors vastly different from normal.

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Anomalous subdiffusion $\langle x^2 \rangle \sim t^\alpha$ with $0 < \alpha < 1$ is found in diverse physical systems ranging from charge transport in disordered semiconductors, and quantum dots, to relaxation dynamics of proteins and diffusion of mRNA in live *E. coli* cells to name a few examples [1–8]. On the stochastic level, anomalous diffusion and relaxation is modeled using the fractional Fokker-Planck-Kramers equations [1,2,8–10], and the fractional Langevin equation [2,4,11–17]. For example recent single molecule experiments on protein dynamics [4,11] revealed anomalous Mittag-Leffler relaxation. The recorded anomalous behavior: the distance between an electron donor and acceptor pair within the protein, bounded by a harmonic force, was successfully modeled by the fractional Langevin equation (FLE) [4,11].

For the standard Langevin equation with white noise, the well-known underdamped and overdamped phases and the critical frequency yield a dynamical phase diagram of the motion. In this manuscript fractional over and underdamped behaviors are investigated, which exhibit rich behaviors vastly different from the normal case. The most surprising result is the appearance of a critical exponent for the FLE: $\alpha_c \approx 0.402$. For $\alpha < \alpha_c$ the overdamped behavior totally disappears, and the decay to equilibrium is never monotonic. We will interpret this behavior in terms of a cage effect, and show that similar critical behaviors are found also for a particle free of deterministic external forces, and for the response of the system to an external time dependent field. Thus critical exponents control fractional dynamics. Contrary to expectation, our work shows that the transition between normal diffusion and relaxation $\alpha = 1$ to the strongly anomalous case $\alpha \to 0$, is not a smooth transition.

The FLE is a generalized Langevin equation [2,18] with a power-law memory kernel [2,4,11–17]

$$m \frac{d^2 x(t)}{dt^2} = F(x) - \bar{\gamma} \int_0^t \frac{1}{(t - t')^\alpha} \frac{dx}{dt'} dt' + \xi(t), \quad (1)$$

where $\bar{\gamma} > 0$ is a generalized friction constant, $F(x)$ is an external force field, $0 < \alpha < 1$ is the fractional exponent, and $\xi(t)$ is a stationary, fractional Gaussian noise [2,19] satisfying the fluctuation-dissipation relation [2]

$$\langle \xi(t) \rangle = 0, \qquad \langle \xi(t)\xi(t') \rangle = k_B T \bar{\gamma} |t - t'|^{-\alpha}. \quad (2)$$

The FLE Eq. (2) can be derived from the Kac-Zwanzig model of a Brownian particle coupled to an harmonic bath [17]. And recently the nontrivial fractional Kramers escape problem for the FLE was solved [15]. Another convenient way to write Eq. (1) is

$$m\ddot{x} = F(x) - \bar{\gamma}\Gamma(1 - \alpha) \frac{d^\alpha x}{dt^\alpha} + \xi(t), \quad (3)$$

where the fractional derivative [1] is defined in the Caputo sense $\frac{d^\alpha f(t)}{dt^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t - t')^{-\alpha} [df(t')/dt'] dt'$. In recent years, fractional calculus was shown to describe many physical systems [1,8].

The normalized correlation function

$$C_x(t) = \frac{\langle x(t)x(0) \rangle}{\langle x(0)^2 \rangle}, \quad (4)$$

for a harmonic force field $F(x) = -m\omega^2 x$, was used to describe single protein dynamics [4,11], so we will first focus on this experimentally measured quantity. Thermal initial conditions are used $\langle \xi(t)x(0) \rangle = 0$, $\langle x(0)^2 \rangle = k_B T / m\omega^2$ and $\langle x(0)v(0) \rangle = 0$. We assume that $\alpha = p/q$, where $q > p > 0$ are integers and p/q is irreducible (i.e., not equal to some other l/n, where $l < p$ and $n < q$ are integers). Using the convolution theorem and Eq. (3), the Laplace transform of $C_x(t)$ is

$$\hat{C}_x(s) = \frac{s + \gamma s^{(p/q)-1}}{s^2 + \gamma s^{(p/q)} + \omega^2}, \quad (5)$$

where $\gamma = \frac{1}{m} \bar{\gamma}\Gamma(1 - \alpha)$. We rewrite Eq. (5) as

$$\hat{C}_x(s) = \frac{(s + \gamma s^{(p/q)-1})\hat{Q}(s)}{\hat{P}(s)} \quad (6)$$

with

$$\hat{Q}(s) = \frac{(s^2 + \omega^2)^q + (-1)^{q-1} \gamma^q s^p}{s^2 + \gamma s^{(p/q)} + \omega^2}, \quad (7)$$

and

$$\hat{P}(s) = (s^2 + \omega^2)^q + (-1)^{q-1}\gamma^q s^p. \quad (8)$$

By finding the $2q$ zeros of $\hat{P}(a_k) = 0$, a_k with $k = 1, \ldots 2q$, and using analysis of poles in the complex plane we invert Eq. (5) and obtain an explicit analytical solution for $C_x(t)$ [20]. Defining the constants $A_k = 1/d\hat{P}(s)/ds|_{s=a_k}$ and $\tilde{B}_{mj}$ by the expansion $\hat{Q}(s) \times (s + \gamma s^{p/q-1}) = \sum_{m=0}^{2q-1}\sum_{j=0}^{q-1}\tilde{B}_{mj}s^{m-j/q}$, the solution is

$$C_x(t) = \sum_{m=0}^{2q-1}\sum_{j=0}^{q-1}\sum_{k=1}^{2q} a_k^m \tilde{B}_{mj} A_k t^{j/q} E_{1,1+(j/q)}(a_k t), \quad (9)$$

where $E_{\eta,\mu}(y)$ is a generalized Mittag-Leffler function [1]. The solution Eq. (9) is valid provided that all the a_ks are distinct, otherwise a critical behavior is found which is soon discussed. We see that finding the solution to the problem is equivalent to finding the zeros of the polynomial $\hat{P}(s)$, once these zeros are found one can investigate and plot the solution with a program like MATHEMATICA. For example, for $\alpha = 1/2$ Eq. (9) reads

$$C_x(t) = \sum_{k=1}^{4}[(-\gamma^2 + \omega^2 a_k + a_k^3)A_k e^{a_k t} + \gamma\omega^2 A_k t^{1/2} E_{1,(3/2)}(a_k t)], \quad (10)$$

where a_k are nonidentical solutions of $\hat{P}(s) = (s^2 + \omega^2)^2 - \gamma^2 s = 0$.

The $t \to \infty$ asymptotic behavior is found using the exact solution Eq. (9)

$$C_x(t) \sim \frac{\gamma}{\omega^2\Gamma(1-\alpha)} t^{-\alpha} \quad (11)$$

or with Tauberian theorems [21]. Hence for very long times $C_x(t)$ always decays monotonically. However, for shorter times the picture is very different. In Fig. 1, the analytical solution for $C_x(t)$ with $\alpha = 1/2$ is plotted for various ω using natural units $\gamma = 1$. Three types of behaviors exist (i) Monotonic decay of the solution—Fig. 1(a). (ii) Nonmonotonic decay of the solution with no zero crossing $C_x(t) \geq 0$ Fig. 1(b). (iii) When the frequency ω becomes large $C_x(t)$ exhibits nonmonotonic decay with zero crossings, Fig. 1(c). Similar types of behaviors are found also for other parameter set.

Our goal now is to clarify the phase diagram of the dynamics of the fractional oscillator. For $\alpha = 1$, the regular damped oscillator, $\omega_c = \gamma/2$ defines the critical frequency which marks the transition between overdamped and underdamped motion. For the fractional oscillator $0 < \alpha < 1$ the identification of a single critical frequency is not possible, and we use three definitions for critical frequencies where the dynamics of the system undergoes a transition in its behavior. For the normal case $\alpha = 1$, the critical frequency ω_c is found when two zeros of $\hat{P}(s)$ coincide, i.e., an appearance of a pole of a second order for $\hat{C}_x(s)$. Similarly, for the $0 < \alpha < 1$ case we define ω_c as a critical

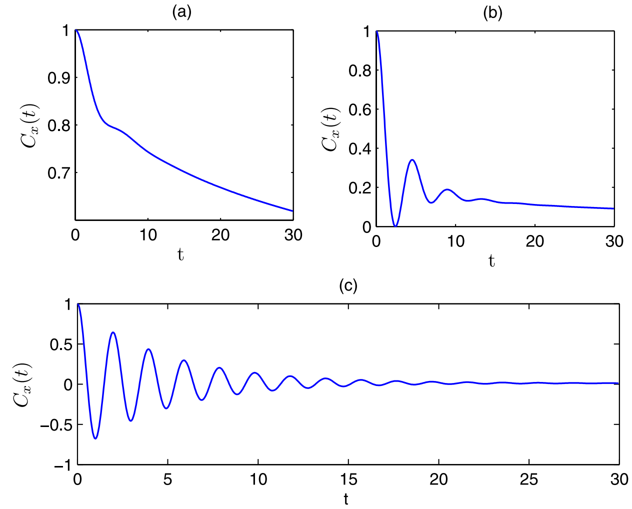

FIG. 1 (color online). The correlation function $C_x(t)$ versus t with $\alpha = 1/2$ and natural units $\gamma = 1$. Three types of solutions are presented (a) $\omega = 0.3$ and the correlation function decays monotonically. (b) The critical frequency $\omega = \omega_z \approx 1.053$ where the transition between motion with and without zero crossing, namely $C_x(t) = 0$ for a single point in time. (c) For larger frequency $\omega = 3$ we observe nonmonotonic decay with zero crossing.

point for which not all the zeros of $\hat{P}(s)$ are distinct and as a result for such ω_c Eq. (9) is not valid. The second approach is to take the minimal frequency ω_z at which the solution $C_x(t)$ crosses the zero line. Finally, we will investigate the minimal frequency ω_m at which $C_x(t)$ is no longer a monotonically decaying function. Only for the regular damped oscillator $\alpha = 1$, we have $\omega_c = \omega_z = \omega_m$.

Equations (5) and (9) are used now to investigate the phase diagram of the motion. By its definition, at the critical frequency ω_c a pole of second order in Eq. (5) is found. It is easy to see that for such ω_c two conditions must be satisfied, $\hat{P}(s) = 0$ and $d\hat{P}(s)/ds = 0$. These two conditions lead to the following relation for ω_c

$$\omega_c = \frac{1}{2^{1/(2-\alpha)}}\sqrt{(2-\alpha)\alpha^{\alpha/(2-\alpha)}}\gamma^{1/(2-\alpha)}, \quad (12)$$

which is valid only for even q or even $(q + p)$, where $\alpha = p/q$. For odd q and even p, the critical point ω_c does not exist at all. Similar to Eq. (12) we find from dimensional analysis

$$\omega_z = \kappa_z(\alpha)\gamma^{1/(2-\alpha)}, \qquad \omega_m = \kappa_m(\alpha)\gamma^{1/(2-\alpha)}, \quad (13)$$

where $\kappa_z(\alpha)$ and $\kappa_m(\alpha)$ depend only on α. By investigating the exact analytical solution Eq. (9) for various α and $\gamma = 1$ we obtain the functions $\kappa_z(\alpha)$ and $\kappa_m(\alpha)$. The resulting phase diagram of the fractional oscillator is presented in Fig. 2.

From the phase diagram Fig. 2 a very interesting result emerges. For $\alpha < \alpha_c \approx 0.4$ the solution is never decaying monotonically. For such α an oscillatory behavior is always found even if the frequency of the binding harmonic field $\omega \to 0$. In this sense the solution is always underdamped. Thus we find a critical exponent α_c which marks a pronounced transition in the behaviors of the solutions of the fractional oscillator. We also note that for α near α_c we find $\kappa_m(\alpha) \propto (\alpha - \alpha_c)^{1/2}$, which describes the boundary between the monotonic and nonmonotonic phases. Note that the phase diagram Fig. 2 also exhibits some expected behaviors: as we increase ω we find a critical line above which the solutions are nonmonotonic and exhibit zero crossing (similar to usual underdamped behavior) and for $\alpha = 1$ the three critical frequencies ω_c, ω_z and ω_m are identical.

A physical explanation for the phase diagram is based on the cage effect. For small α the friction force induced by the medium is not just slowing down the particle but also causing the particle a rattling motion. To see this consider the FLE Eq. (3) in the limit $\alpha \to 0$

$$m\ddot{x} + m\gamma(x - x_0) + m\omega^2 x \approx \xi(t), \tag{14}$$

where x_0 is the initial condition. Equation (14) describes harmonic motion and the "friction" γ in this $\alpha \to 0$ limit yields an elastic harmonic force. In this sense the medium is binding the particle preventing diffusion but forcing oscillations. In the opposite limit of $\alpha \to 1$

$$m\ddot{x} + m\gamma\dot{x} + m\omega^2 x \approx \xi(t) \quad \text{when } \alpha \to 1, \tag{15}$$

the usual damped oscillator with noise is found. So from Eq. (14) for $\alpha \to 0$ an oscillating behavior is expected, even when $\omega \to 0$ which can be explained by the rattling motion of a particle in the cage formed by the surrounding particles. This behavior manifests itself in the nonmonotonic oscillating solution we have found in our phase diagram

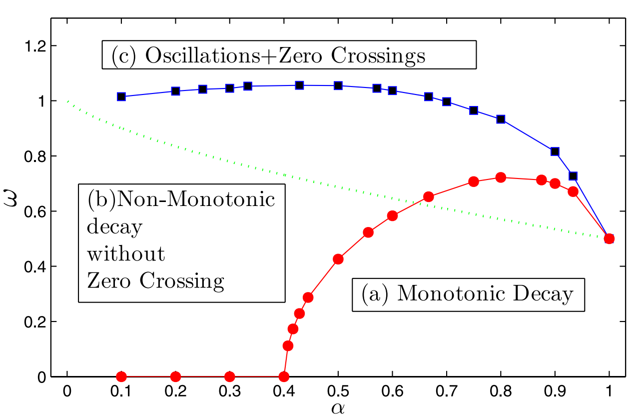

FIG. 2 (color online). The phase diagram of the fractional oscillator. Phase (a) monotonic decay of the correlation function $C_x(t)$, phase (b) nonmonotonic decay without zero-crossing and (c) oscillations with zero crossings. The boundary between (b) and (c) is $\omega_z = \kappa_z(\alpha)$ (solid line + squares), the boundary between (a) and (b) is $\omega_m = \kappa_m(\alpha)$ (solid line + circles). For $\alpha < \alpha_c \simeq 0.402$, the phase of monotonic decay disappears, namely, we do not find overdamped behavior. The dotted curve is the critical line ω_c given by Eq. (12). All the curves are calculated for $\gamma = 1$. For $\alpha = 1$, $\omega_c = \omega_z = \omega_m = \gamma/2$.

Fig. 2 when $\alpha \to 0$. Our finding that α_c marks a non smooth transition between normal friction $\alpha \to 1$ and elastic friction $\alpha \to 0$ is certainly a surprising result which could not be anticipated without our mathematical analysis.

To find accurate values of α_c we used also a method based on the Bernstein theorem [21]. According to the theorem if and only if a function $f(t)$ is positive then for any integer n, $0 \le (-1)^n[d^n\hat{f}(s)/ds^n]$, where $\hat{f}(s)$ is the Laplace pair of $f(t)$. To see when $C_x(t)$ is decaying monotonically, we investigate the positivity of its derivative. Using Bernstein's theorem inspecting the $n = 150$ order derivatives gives the exact lower bound $\alpha_c \ge 0.394$, while the method using exact solution for $C_x(t)$ gives $\alpha_c = 0.402 \pm 0.002$. Further we can show that the critical exponent is not equal to 0.4, and hence it seems a nontrivial number. We now show that the critical exponent α_c is important for other physical quantities.

The mean square displacement $\langle x^2(t)\rangle$ for the force free particle $F(x) = 0$ is now investigated. We consider averages over the noise and thermal initial conditions $\langle v^2\rangle|_{t=0} = k_B T/m$. The analytical solution for this case was found already in [10,12] and is given by $\langle x^2(t)\rangle = 2(k_b T/m)t^2 E_{2-\alpha,3}(-\gamma t^{2-\alpha})$. We find that for $\alpha < \alpha_c$ $\langle x^2(t)\rangle$ is nonmonotonic, while for $\alpha > \alpha_c$ it is monotonic. The nonmonotonic behavior of $\langle x^2(t)\rangle$ for small α is a manifestation of a cage effect. Our finding that the same critical exponent α_c describes both the phase diagram of the fractional harmonic oscillator and also the fluctuations of a particle free of an external force field, emphasizes the generality of our results. Although not explored here in detail, the same α_c is likely to describe motion in any binding potential field, since it is the medium inducing the oscillations. We note that our results can be derived also from the fractional Kramers equation [10,22] and hence are not limited to the FLE.

The response of a system to an oscillating time dependent field naturally leads to the phenomena of resonances, when the frequency of the external field matches a natural frequency of the system. The response of subdiffusing systems to such time dependent fields was the subject of intensive research [23–25]. In particular fractional approach to subdiffusion naturally leads to anomalous response functions commonly found in many systems, e.g., the Cole-Cole relaxation [9,26]. Here we investigate the response of a particle in a harmonic force field, as found in the experiments [4,11], to a time dependent force $F_0\cos(\Omega t)$ using Eq. (3). In the long time limit, using the stationarity of the process we find

$$\langle x\rangle \sim \frac{\mathcal{F}_0}{m} R(\Omega)\cos[\Omega t + \theta(\Omega)] \qquad t \to \infty, \tag{16}$$

where the response function is

$$R(\Omega) = |[\omega^2 + \gamma(-i\Omega)^\alpha - \Omega^2]^{-1}|, \tag{17}$$

which was derived already in [27] using a different model. As well known for the normal case $\alpha = 1$ a resonance is

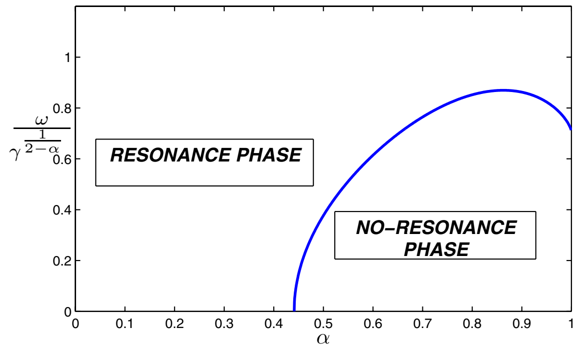

FIG. 3 (color online). Phase diagram of the response of the system to a oscillating time dependent force field. Two simple behaviors are found either a resonance exists or not. For $\alpha < \alpha_R = 0.441\ldots$ a resonance exists for any binding harmonic field and any friction.

found when the friction is weak, namely, a peak in $R(\Omega)$ is observed when $\omega > \gamma/\sqrt{2}$. On the other hand if the damping is strong $\omega < \gamma/\sqrt{2}$ the peak is not found. The simple phase diagram describing the response of the fractional system is shown in Fig. 3, where a resonance phase means a phase with a peak in the response function. For α smaller than a critical exponent $\alpha_R = 0.441\ldots$ one always detects a resonance, even if $\omega \to 0$. This is clearly a manifestation of the cage effect and it clearly shows that the critical exponent α_R marks a dynamical transition of the response of the system to an external force field.

Many works consider the overdamped approximation to anomalous diffusion, which means that Newton's acceleration term is neglected, $m = 0$ in Eq. (1). This approximation must be used with care. As we showed when $\alpha < \alpha_c$ the exact solution of the FLE always exhibits a nonmonotonic decay of $C_x(t)$, while the overdamped approximation gives a monotonic decay. And according to our results when $\alpha < \alpha_R$ resonances always appear in the response of the system to an external oscillating field, which are not found with the overdamped approximation. In this sense the overdamped approximation fails when α is smaller than the critical exponents of the system. This is in complete contrast to the usual Langevin equation with white noise, where the overdamped approximation captures the main features of the dynamics. This striking difference between the FLE and the usual Langevin equation stems from the fact that for the FLE the dissipative memory induces oscillations, as mentioned.

In conclusion, critical exponents mark sharp transitions in the behaviors of systems with fractional dynamics. The critical exponents describe a wide range of physical behaviors: the correlation function $C_x(t)$ of a particle bounded by a harmonic field, the mean square displacement of the free particle, and the response of the system to an external oscillating field. Thus these critical exponents are clearly very important and general in the description of the anomalous kinetics. The phase diagrams we obtained are related to a cage effect, where for small enough α the medium induces oscillations in the dynamics of the particle. Thus the fractional dynamics is profoundly different from the dynamics described by the Langevin equation with white noise.

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