Hitting Probability for Anomalous Diffusion Processes

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We present the universal features of the hitting probability $Q(x, L)$, the probability that a generic stochastic process starting at x and evolving in a box $[0, L]$ hits the upper boundary L before hitting the lower boundary at 0. For a generic self-affine process, we show that $Q(x, L) = Q(z = x/L)$ has a scaling $Q(z) \sim z^{\phi}$ as $z \to 0$, where $\phi = \theta/H$, H, and θ being the Hurst and persistence exponent of the process, respectively. This result is verified in several exact calculations, including when the process represents the position of a particle diffusing in a disordered potential. We also provide numerical support for our analytical results.

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The transfer of DNA, RNA, and proteins through cell membranes is key to understanding several biological processes [1]. A fundamental question concerns whether a polymer, once penetrated into the pore, will eventually complete its transit. The answer is naturally formulated in terms of the translocation coordinate $X(t)$, namely, the length of the translocated portion of the polymer at time t [2–4]. In absence of driving forces, the polymer dynamics is governed by thermal fluctuations. In this case, the translocation coordinate can be expressed as a stochastic process $X(t)$ that evolves in a box of size L (L being the polymer length), starting from some initial value $X(0) = x$, $0 < x < L$, and terminated upon touching either boundary for the first time (Fig. 1 left). It has been shown that excluded volume effects hinder the polymer dynamics, and the process $X(t)$ actually undergoes subdiffusion [3,5]. We define the hitting probability $Q(x, L)$ as the probability of exiting the domain through the boundary at L, which corresponds to the polymer completing the translocation.

More generally, the hitting probability $Q(x, L)$ of a particle undergoing anomalous (i.e., non-Brownian) diffusion allows addressing a variety of phenomena, such as the classical gambler's ruin problem in risk management [6,7], charge carriers transport in presence of disordered impurities [8], and the breakthrough of chemical species in site remediation [9], only to name a few. For Brownian diffusion, the hitting probability $Q(x, L) = x/L$ is easy to compute [6,7]. The goal of this Letter is to study $Q(x, L)$ for generic self-affine processes, beyond the Brownian world.

The sole length scale in the problem being L, $Q(x, L)$ depends only on the scaled variable x/L: $Q(x, L) = Q(x/L = z)$. For a Brownian motion, $Q(z) = z$ is linear. For a generic $X(t)$, $Q(z)$ is nontrivial (see, for example, Fig. 1 right). The central aim of this Letter is to determine the universal features associated with $Q(z)$ in these two cases: symmetric self-affine processes having a power-law scaling $X(t) \sim t^H$, with Hurst exponent $H > 0$; and a single particle diffusing in a disordered potential $V(X)$. The translocation process belongs to the former, whereas transport in quenched disorder to the latter.

We summarize here our main results, which are threefold: (i) For self-affine processes, we show that generically $Q(z) \sim z^{\phi}$ for small z, where $\phi = \theta/H$, and θ is the so-called persistence exponent [10] of the same process in a semi-infinite geometry; (ii) for a particle diffusing in a disordered potential $V(X)$, we provide an exact formula for $Q(x, L)$ valid for arbitrary $V(X)$, which incidentally allows computing the persistence exponent of particle dynamics for self-affine $V(X)$; (iii) the function $Q(z)$ is explicitly known for some anomalous diffusion processes. Amazingly, we find that these apparently different-looking formulae can be cast in the same superuniversal form, when expressed in terms of the exponent ϕ. This naturally

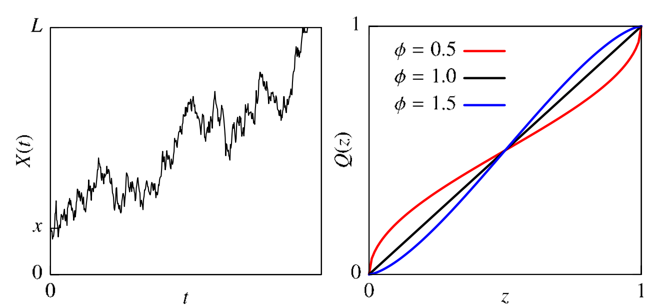

FIG. 1 (color online). Left. The evolution of a stochastic process initiated at $X(0) = x$ and terminated upon exiting from the box of size L. Right. The function $Q(z)$ as given by Eq. (8) for different values of the exponent ϕ.

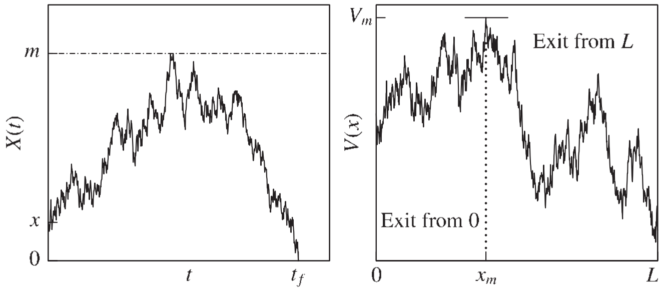

FIG. 2. Left. A stochastic process starting at x leaves the positive half axis for the first time at t_f; m denotes its maximum till t_f. Right. A self-affine disordered potential with maximum at x_m: when L is large, the diffusing particle, starting at $0 < x < L$, exits the box through 0 for $x < x_m$ and through L for $x > x_m$.

raises the question: how generic is this superuniversality? We provide numerical evidences that in some cases, superuniversality is violated, and we discuss its limit of validity.

Self-affine processes.—To compute $Q(x, L)$ in a box geometry, it is useful to relate it to another quantity associated with the same process $X(t)$ in a semi-infinite geometry $[0, \infty]$. Consider a process $X(t)$ in $[0, \infty]$, starting at x and absorbed at the origin for the first time at t_f. Let m denote the maximum of this process till t_f (see Fig. 2 left). Then, $1 - Q(x, L)$, the probability that the particle exits the box through the origin (and not through L), is precisely equal to the probability that the maximum m of the process in $[0, \infty]$ till t_f stays below L, i.e., the cumulative distribution of m, $\text{Prob}[m \le L|x]$, in the semi-infinite geometry. The distribution of m is, in turn, related to the distribution of the first-passage time t_f. Let $q(x, T) = \text{Prob}[t_f \ge T|x]$ denote the cumulative probability of t_f, which is also the survival probability of the particle starting at x in the semi-infinite geometry. For generic self-affine processes, $q(x, T) = q(x/T^H)$. For large T, $q(x, T) \sim T^{-\theta}$, where θ is the persistence exponent of the process [10]. This implies the scaling function $q(y) \sim y^{\theta/H}$ for small y [5]. Since $m \sim t_f^H$ for self-affine processes, then $Q(x, L) = 1 - \text{Prob}[m \le L|x] = \text{Prob}[m \ge L|x] \approx \text{Prob}[t_f \ge L^{1/H}|x] = q[x/L]$. This proves the scaling behavior anticipated before, namely, $Q(x, L) = Q(x/L)$, where $Q(z) = q(z)$. Moreover, since $q(y) \sim y^{\theta/H}$ for small y, we get $Q(z) \sim z^{\phi}$ for small z, with $\phi = \theta/H$. For Brownian motion, e.g., $H = 1/2$ and $\theta = 1/2$; hence, $\phi = 1$, in accordance with the exact result $Q(z) = z$. For the subclass of self-affine processes with stationary increments, the same exponent ϕ happens to describe the vanishing of the probability density close to an absorbing boundary [5].

Our general prediction $Q(z) \sim z^{\phi}$ for small z is explicitly verified for some self-affine processes where $Q(z)$ can be computed exactly, as discussed later. Moreover, we have numerically verified that this conjecture holds also for the fractional Brownian motion (fBm), i.e., a self-affine Gaussian process defined by the following autocorrelation function

$$\langle X(t_1)X(t_2)\rangle = \frac{1}{2}(t_1^{2H} + t_2^{2H} - |t_1 - t_2|^{2H}), \qquad (1)$$

with $0 < H < 1$ [11]. In [5], we have proposed fBm as a natural candidate for describing the dynamics of the translocation coordinate. The persistence exponent of fBm is known, $\theta = 1 - H$ [11], so that $\phi = (1 - H)/H$. An expedient algorithm for generating fBm paths is provided in [12]. The probability $Q(z)$ can be numerically computed as follows. Given a realization of the process starting from the origin, we record its minimum and maximum values for increasing time; the process is halted when $X_{\max} - X_{\min} \ge L$. If the last updated quantity is $X_{\min}$, the contribution to $Q(x, L)$ is 0 for $x \in (0, L - X_{\max})$ and 1 for $x \in (L - X_{\max}, L)$. In the opposite case, the contribution is 0 for $x \in (0, -X_{\min})$ and 1 otherwise. All simulations are performed by averaging over 10^6 samples. Figure 3 shows the agreement between numerical simulations and predicted scaling of $Q(z)$ for different values of H.

Disordered potential.—We next consider the stochastic motion of a single particle diffusing in a potential $V(X)$, starting at x. The dynamics is governed by the Langevin equation $\dot{X}(t) = f[X(t)] + \eta(t)$, where $X(0) = x$ and $f(X) = -dV(X)/dX$ is the force and $\eta(t)$ is a Gaussian white noise with $\langle \eta(t)\rangle = 0$ and $\langle \eta(t)\eta(t')\rangle = \delta(t - t')$. To compute $Q(x, L)$, we first write a differential equation satisfied by $Q(x, L)$, taking x as a variable and keeping L as fixed. During the small time interval $[0, \Delta t]$ at the beginning of the process, the particle moves from x to a new position $x + \Delta x$ at time Δt, where $\Delta x = f(x)\Delta t + \eta(0)\Delta t$, $\eta(0)$ being the noise that kicks in at time 0. Since the process is Markovian, the subsequent evolution does not know about the interval $[0, \Delta t]$; hence,

$$Q(x, L) = \langle Q[x + f(x)\Delta t + \eta(0)\Delta t, L]\rangle, \qquad (2)$$

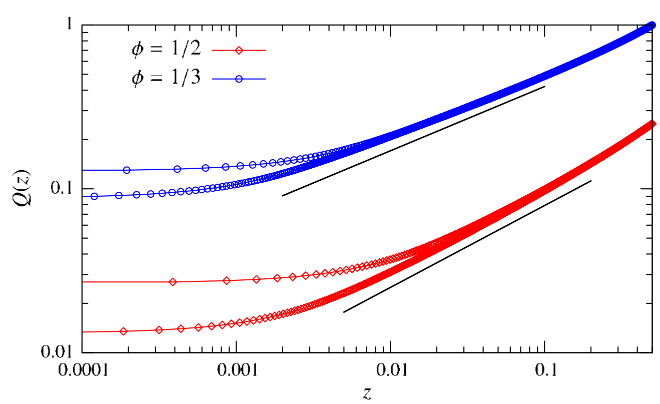

FIG. 3 (color online). Behavior of $Q(z)$ close to $z = 0$ for fBm processes. For $H = 2/3$ ($\phi = 1/2$), the size of the box is $L = 50, 200$; for $H = 3/4$ ($\phi = 1/3$), the size of the box is $L = 100, 300$. The continuum limit is reached when $L \to \infty$. The expected slopes are reported as solid lines. Data have been shifted to make visualization easier.

where $\langle\rangle$ denotes the average over the initial noise $\eta(0)$. Expanding the right-hand side of Eq. (2) as a Taylor series in powers of Δt, using $\langle\eta(0)\rangle = 0$ and $\langle\eta^2(0)\rangle = 1/\Delta t$ (delta correlated noise), yields $\frac{1}{2}Q''(x) + f(x)Q'(x) = 0$. Solving with boundary conditions $Q(0, L) = 0$ and $Q(L, L) = 1$ gives the exact result

$$Q(x, L) = \frac{\int_0^x e^{2V(x')}dx'}{\int_0^L e^{2V(x')}dx'}, \tag{3}$$

valid for arbitrary potential $V(X)$. For a potential-free particle, i.e., $V(X) = 0$, we recover the Brownian result, $Q(x, L) = x/L$.

Taking derivative with respect to x gives

$$p_{\rm eq}(x, L) = \frac{\partial}{\partial x}Q(x, L) = \frac{e^{2V(x)}}{\int_0^L e^{2V(x')}dx'}, \tag{4}$$

which can be interpreted as the equilibrium probability density of the particle to be at x in the presence of a potential $-V(X)$. When $V(X)$ is a realization of a disordered potential, it is natural to introduce $\overline{Q(x, L)}$, the disorder-averaged hitting probability. An example where we can explicitly determine $\overline{Q(x, L)}$ is the classical Sinai model, i.e., when the potential $V(X)$ is a trajectory of a Brownian motion in space, $V(X) \sim X^{1/2}$ [13]. For this model, $\overline{p_{\rm eq}(x, L)}$ can be computed exactly [14,15]

$$\overline{p_{\rm eq}(x, L)} = \frac{1}{\pi}\frac{1}{\sqrt{x(L-x)}}. \tag{5}$$

Thus, $\overline{Q(x, L)} = Q(z = x/L)$ again satisfies the generic scaling, with

$$Q(z) = \frac{2}{\pi}\arcsin(\sqrt{z}). \tag{6}$$

Close to the origin, $Q(z) \sim z^{\phi}$ with $\phi = 1/2$. On the other hand, in the Sinai potential, the particle evolves very slowly with time, $X \sim \ln^2(t)$ (showing a self-affine scaling in the variable $T = \log t$, with $H = 2$), and the survival probability decays as $1/\log t$, i.e., $T^{-\theta}$, with $\theta = 1$ [16,17]. Thus, $\theta/H = 1/2 = \phi$, in accordance with our general scaling prediction.

We consider next a generic self-affine potential, $V(X) \sim X^{H_V}$ [with $V(0) = 0$], the Sinai model being a special case with $H_V = 1/2$. We show that $\overline{p_{\rm eq}(x, L)}$ for such a potential is related to the probability density of the location x_m of the maximum of the potential $V(X)$ over $X \in [0, L]$. We rewrite Eq. (4) as $p_{\rm eq}(x, L) = [\int_0^L e^{2[V(x')-V(x)]}dx']^{-1}$, rescale variables $x' \to x'L$ and $x \to xL$, and use the self-affine property $V(xL) = L^{H_V}V(x)$ to obtain $p_{\rm eq}(x, L) = [\int_0^1 e^{2L^{H_V}[V(x')-V(x)]}dx']^{-1}$. For large L, using a steepest decent method, we see that, for each realization of the potential $V(X)$, $p_{\rm eq}(x, L) \simeq \delta(x - x_m)$, where x_m denotes the location where $V(X)$ is maximum. It follows that: (i) Integrating over x, we get, for each realization, $Q(x, L) \simeq \theta(x - x_m)$. Then, for any given realization, if x is to the left (right) of x_m, $Q(x, L) \simeq 0$ [respectively, $Q(x, L) \to 1$], and the particle exits the box through 0 (through L), as depicted in Fig. 2 (right). (ii) By averaging over the disorder, we get

$$\overline{p_{\rm eq}(x, L)} \simeq p_m(x, L) \tag{7}$$

where $p_m(x, L)$ is the probability density that the maximum of the potential $V(X)$ over [0, L] is located at x. For the Sinai model, e.g., the Lévy's arcsine law [6] implies $p_m(x, L) = 1/\pi\sqrt{x(L-x)}$. Thus, in this case, the relation (7) is verified by the exact result (5). However, the relation (7) holds for arbitrary self-affine potentials. Physically, Eq. (7) stems from $L \to \infty$ being equivalent to the zero temperature $T \to 0$ limit in a self-affine potential $-V(X)$ where the particle is at equilibrium, forcing the particle to the minimum of the potential $-V(x)$, or equivalently to the maximum x_m of $V(x)$.

Equation (7) relates the persistence or the survival probability of a particle in a disordered self-affine potential to the properties of the potential $V(X)$ itself. The disordered potential $V(X) \sim X^{H_V}$ [we assume $V(0) = 0$] can be regarded as a stochastic process, the space coordinate X playing the role of "time." So, the probability that $V(X)$ stays below (or above) the level $X = 0$ up to a distance L decays, for large L, as $L^{-\theta_V}$, where θ_V is the spatial persistence exponent [18] of $V(X)$. For the Sinai potential, e.g., $\theta_V = 1/2$. The exponents (H_V, θ_V) associated with $V(X)$ can be related to the corresponding exponents associated with the particle dynamics in the same potential. By Arrhenius' law for the activated dynamics, the time required for particles diffusing in $V(X)$ to overcome an energy barrier scales as $t \sim e^{V(X)}$. Using $V(X) \sim X^{H_V}$, then $X \sim T^{1/H_V}$, where $T = \log(t)$. Thus, the particle motion $X(T) \sim T^H$ is a self-affine process as a function of $T = \log(t)$, with Hurst exponent $H = 1/H_V$. Next, note that $p_m(x, L)$, the probability that the maximum of $V(X)$ occurs at x, coincides, when $x \to 0$, with the probability that $V(X) < 0$ up to a distance L; hence, $p_m(x \to 0, L) \propto L^{-\theta_V}$. On the other hand, based on our general argument, we expect $\overline{Q(x, L)} \sim (x/L)^{\phi}$ when $x \to 0$, where $\phi = \theta/H$. Then, $\overline{p_{\rm eq}(x, L)} \propto x^{\phi-1}/L^{\phi}$. Here, θ is the persistence exponent associated with the particle dynamics; i.e., the survival probability of the particle up to time $T = \log(t)$ decays as $\sim T^{-\theta}$. Matching powers of L from both sides of (7) provides the desired relation between temporal and spatial exponents $\theta = \theta_V H = \theta_V/H_V$. In the Sinai model, e.g., using $\theta_V = 1/2$ and $H_V = 1/2$, we get $\theta = 1$, in agreement with the exact result [16,17]. A potential satisfying $V''(X) = \xi(X)$, $\xi(X)$ being a white noise in space, is self-affine with $H_V = 3/2$. The exponent $\theta_V = 1/4$ is known exactly [19]. Thus, we predict that for this potential, the survival probability up to time t decays as $\sim(\log t)^{-\theta}$, with $\theta = 1/6$.

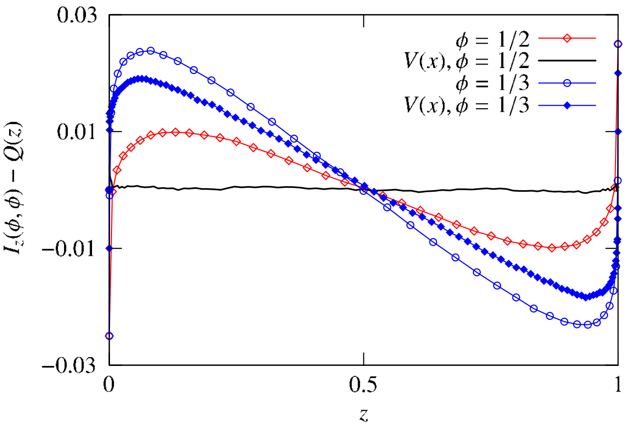

FIG. 4 (color online). The difference between Eq. (8) and simulated $Q(z)$. For fBm processes: $H = 2/3$ ($\phi = 1/2$) with box size $L = 200$, and $H = 3/4$ ($\phi = 1/3$), with box size $L = 300$. For fBm disordered potentials: $H_V = 2/3$ ($\phi = 1/3$), with box size $L = 10^4$. For comparison, we display also the Sinai model $H_V = 1/2$ ($\phi = 1/2$), with box size $L = 10^4$.

Superuniversality of $Q(z)$.—For some non-Brownian stochastic self-affine processes, the full function $Q(z)$ is known. For instance, Lévy Flights are Markovian superdiffusive processes whose increments obey a Lévy stable law of index $0 < \mu \leq 2$. The Hurst exponent is $H = 1/\mu$. By virtue of the Sparre Andersen theorem [20], the persistence exponent is $\theta = 1/2$, independent of μ. Hence, $\phi = \theta/H = \mu/2$ (see also [21]). The full function $Q(z)$ for Lévy Flights has been computed [22] and can be recast in an elegant form

$$Q(z) = I_z(\phi, \phi) = \frac{\Gamma(2\phi)}{\Gamma^2(\phi)} \int_0^z [u(1-u)]^{\phi-1} du, \qquad (8)$$

i.e., a regularized incomplete Beta function with a single parameter $\phi = \mu/2$. Clearly, $Q(z) \sim z^{\phi}$ as $z \to 0$, in agreement with our prediction. The formulae for Brownian motion (with $\phi = 1$) $Q(z) = z$ and for the Sinai model ($\phi = 1/2$) in (6) can also be expressed as (8). Moreover, the distribution of the maxima for a symmetric Lévy Flight is given by (5), by virtue of the Sparre Andersen theorem [20]. Hence, we expect the hitting probability (8) to apply also to particles diffusing in a Lévy Flight disordered potential, with $\phi = 1/2$. Finally, $Q(z)$ is known also for the Random Acceleration model, a non-Markovian process that is defined by $d^2X/dt^2 = \eta(t)$, with $\eta(t)$ as before. The motion starts at $X(0) = x$, with initial velocity $v(0) = 0$, and is superdiffusive, with $X \sim t^{3/2}$, i.e., $H = 3/2$. Its first-passage properties have been widely studied [19]. The persistence exponent is $\theta = 1/4$ so that $\phi = \theta/H = 1/6$. The full exit probability $Q(x, L)$ is computed in [23]. This formula can again be recast in the same superuniversal form (8), with $\phi = 1/6$.

Based on these special cases, we might conjecture that the full function $Q(z)$ for arbitrary anomalous doffusion processes has the superuniversal form (8), which depends only on ϕ. However, this turns out not to be the case, and we can show notable counterexamples. In Fig. 4, we compute $Q(z)$ for fBm self-affine processes and for particles diffusing in fBm disordered potentials, and display the numerical difference with respect to formula (8), with the appropriate exponent ϕ. We find that in neither case can $Q(z)$ be described by the superuniversal form (8).

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