Lévy Flights in Inhomogeneous Media

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We investigate the impact of external periodic potentials on superdiffusive random walks known as Lévy flights and show that even strongly superdiffusive transport is substantially affected by the external field. Unlike ordinary random walks, Lévy flights are surprisingly sensitive to the shape of the potential while their asymptotic behavior ceases to depend on the Lévy index μ. Our analysis is based on a novel generalization of the Fokker-Planck equation suitable for systems in thermal equilibrium. Thus, the results presented are applicable to the large class of situations in which superdiffusion is caused by topological complexity, such as diffusion on folded polymers and scale-free networks.

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Diffusion processes are ubiquitous in nature. A freely diffusive particle is characterized by a mean square displacement which increases linearly in time, $\langle X^2(t)\rangle \propto t$. However, a variety of interesting physical systems violate this temporal behavior. For example, the position $X(t)$ of a superdiffusive particle heuristically evolves as $X(t) \sim t^{1/\mu}$ with $0 < \mu < 2$. Superdiffusion has been observed in a number of systems ranging from early discoveries in intermittent chaotic systems [1], fluid particles in fully developed turbulence [2], to millennial climate changes [3], bacterial motion [4], and human eye movements [5].

Among the most successful theoretical concepts which have been applied to superdiffusive phenomena are random walks known as Lévy flights [6,7]. In contrast to ordinary random walks, the displacements Δx of a Lévy flight lack a well-defined variance, due to a heavy tail in the single step probability density. Lévy flights have paved the way towards a description of superdiffusive phenomena in terms of fractional Fokker-Planck equations (FFPE) [8].

Since many of the aforementioned systems evolve in inhomogeneous environments, it is crucial to understand the influence of external potentials on the dynamics. While in ordinary diffusive systems an external force is easily incorporated into the dynamics by a drift term in the corresponding Fokker-Planck equation (FPE) [9], the matter is more subtle in superdiffusive systems due to the nonlocal properties of the fractional operators involved. Depending on the underlying physical model, different types of FFPEs are appropriate [10], therefore the *ad hoc* introduction of fractional operators may lead to severe problems.

In cases where the external inhomogeneity can be represented by an additive force, considerable progress has been made in a generalized Langevin approach [11,12] which led to an FFPE in which deterministic and stochastic motion segregate into independent components. This approach, however, is suited only for systems in which such a segregation can be justified on physical grounds. Furthermore, it is valid only for systems far from thermodynamic equilibrium and fails in the large class of systems which obey Gibbs-Boltzmann thermodynamics, e.g., where superdiffusion is caused by the complex topology on which the process evolves, such as diffusion on folded polymers [13].

In this Letter, we investigate the impact of external potentials on this class of systems. Based on the paradigmatic case of a randomly hopping particle on a folded copolymer, we report a number of bizarre phenomena which emerge when Lévy flights evolve in periodic potentials and show that external potentials have a profound effect on the superdiffusive transport. This is in sharp contrast to generalized Langevin dynamics, which displays trivial asymptotic behavior, a possible reason why Lévy flights in periodic potentials have attracted little attention in the past. We demonstrate that even strongly superdiffusive Lévy flights are highly susceptible to periodic potentials. At low temperatures, they exhibit a significant dependence on the overall shape of the potential. The asymptotic behavior does not depend on the Lévy flight index μ, yet differs for various types of potentials (except in the ordinary diffusion limit). A perturbation analysis reveals a universal behavior for high temperatures. Finally, we show that in finite systems the effect of the potential on the generalized diffusion coefficient is least pronounced for intermediate values of μ. This is consistent with the observation that Lévy flights with $\mu \approx 1$ are particularly efficient in search processes [5,14]. The results we present are a first step towards an understanding of superdiffusive dynamics on topologically complex structures exposed to external inhomogeneities.

Let us begin with the dynamics of a particle performing an unbiased random walk in a homogeneous environment in continuous time. The probability $p(x, t)$ of finding the particle at a position x, given that it was initially at the origin, is governed by the master equation [9]

$$\partial_t p(x, t) = \int dy [w(x|y)\, p(y, t) - w(y|x)\, p(x, t)], \quad (1)$$

in which $w(x|y)$ is the probability rate of initiating a jump

$y \to x$. If this probability has a typical variance in distance, one may expand the right-hand side (rhs) of Eq. (1) in moments of $w(x|y)$ yielding the FPE for a freely diffusive particle, $\partial_t p = \Delta p$. However, when the rate asymptotically follows an inverse power law of distance, i.e., $w(x|y) \sim |x-y|^{-(1+\mu)}$ with $\mu < 2$, the variance of jump lengths diverges and the particle performs a superdiffusive walk known as a Lévy flight [6]. Inserting this rate into (1), the rhs defines the integral operator $\Delta^{\mu/2}$,

$$\Delta^{\mu/2} p(x,t) = \int dy \frac{[p(y,t) - p(x,t)]}{|x-y|^{1+\mu}}, \tag{2}$$

and Eq. (1) may be rewritten as

$$\partial_t p = D\Delta^{\mu/2} p. \tag{3}$$

The parameter D is the generalized diffusion coefficient. Up to a constant factor, the operator $\Delta^{\mu/2}$ is frequently referred to as the fractional Laplacian, because it represents a multiplication by $-|k|^\mu$ in Fourier space [8]. Equation (3) is solved by $p(x,t) = (Dt)^{1/\mu} L_\mu[x/(Dt)^{1/\mu}]$, where $L_\mu(z) = (2\pi)^{-1} \int dk \exp(ikz - |k|^\mu)$ is the symmetric Lévy stable law of index μ. The argument $x/t^{1/\mu}$ in L_μ reflects the superdiffusive behavior of the process. When $\mu = 2$ ordinary diffusion is recovered. In ordinary diffusion, a potential V is canonically introduced by a drift term $\beta \nabla V' p$ in the FPE. Thus, it may seem reasonable to formally allow for an external potential in a superdiffusive system by

$$\partial_t p = \beta \nabla V' p + \Delta^{\mu/2} p. \tag{4}$$

This FFPE has been studied extensively in the past [11,12]. It describes deterministic motion in a gradient field $F = -\beta V'$ subjected to Lévy stable white noise $\eta(t)$, i.e., $\dot{X} = -\beta V' + \eta(t)$. However, this approach introduces severe restrictions. Systems evolving according to (4) do not obey Gibbs-Boltzmann thermodynamics. The stationary state p_s, if it exists, is generally not $p_s \propto \exp(-\beta V)$ and depends on the tail parameter μ. Detailed balance is violated, and only in the diffusion limit ($\mu = 2$) can the parameter β be interpreted as an intensive inverse temperature. The asymptotics of Eq. (4) in periodic potentials is trivial. Rescaling the original coordinates $z = x/\gamma$, $\tau = t/\gamma^\mu$ with $\gamma \gg 1$ yields a form invariant FFPE in a new potential $\hat{V}(z) = \gamma^{\mu-2} V(\gamma z)$. The factor $\gamma^{\mu-2}$ implies that on large scales any bounded potential is insignificant to the dynamics, a possible explanation why Lévy flights in periodic potentials have attracted little attention in the past.

However, the generalized Langevin description is not appropriate for a variety of superdiffusive phenomena [10], as a segregation into deterministic and stochastic forces cannot be justified by the underlying physics. Consider the system depicted in Fig. 1. A particle is loosely attached to a polymer chain. Thermal activation causes the particle to jump between monomers. The heterogeneity of the polymer is accounted for by the potential $V(x)$ defined on chemical axis x. It is reasonable to assume that the rate $w(x \pm a|x)$ of making a transition between neighboring sites x and $x \pm a$ decreases with increasing potential at the target site and that it depends on the potential difference $\delta V_\pm = V(x \pm a) - V(x)$ in units of $k_B T = \beta^{-1}$. Both assumptions are accounted for by $w(x \pm a|x) \propto \exp[-\beta \delta V_\pm/2]$. If the polymer is in solution and subjected to fast conformational changes, regions of the chain that are distant along the chemical axis x of the polymer may come close in Euclidean space. Long distance transitions $x \to y$ may occur with a probability which follows an inverse power law of chemical distance $|x-y|^{-(1+\mu)}$ when $|x-y| \gg a$. The exponent μ is determined by the folding properties of the polymer, e.g., a Gaussian chain implies $\mu = 1/2$ [15]. The possibility of distant jumps along the chemical coordinate enhances the diffusion process considerably, and is believed to play a role in protein dynamics on DNA strands [16]. A jump process of this type can be modeled by a master equation (1), in which thermodynamic as well as geometric aspects need to be incorporated in the rate $w(x|y)$. The above reasoning suggests

$$w(x|y) \propto e^{-\beta[V(x)-V(y)]/2}/|x-y|^{1+\mu}. \tag{5}$$

In Ref. [17], a mean field theoretic treatment of the dynamics of the polymer chain also yields Eq. (5). Inserting the above rate into Eq. (1), we obtain

$$\partial_t p = e^{-\beta V/2} \Delta^{\mu/2} e^{\beta V/2} p - p e^{\beta V/2} \Delta^{\mu/2} e^{-\beta V/2}, \tag{6}$$

which is clearly different from the FFPE corresponding to generalized Langevin dynamics. Equation (6) obeys Gibbs-Boltzmann thermodynamics, $p_s \propto \exp(-\beta V)$ is the stationary solution, detailed balance is fulfilled, and β is a well-defined intensive inverse temperature for all $\mu \in (0, 2]$. Rescaling coordinates as above yields a potential $\hat{V}(z) = V(\gamma z)$ lacking the prefactor $\gamma^{2-\mu}$ which is present in the generalized Langevin scheme. Therefore, the effect of a bounded potential will have an effect on all scales. Note that, for $\mu = 2$, Eq. (6) reduces to the ordinary FPE. When $V \equiv 0$, the rhs is identical to $\Delta^{\mu/2} p$. Letting $\psi = \exp[-\beta V/2]\, p$, Eq. (6) can be recast into a fractional Schrödinger equation,

$$\partial_t \psi = -\mathcal{H} \psi, \tag{7}$$

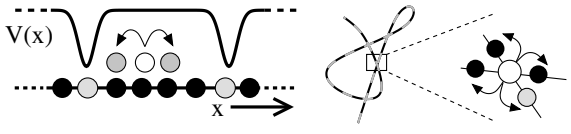

FIG. 1. A particle jumps randomly along a folded copolymer which consists of two types of periodically arranged monomers. Each monomer type has a different potential sketched qualitatively in the top left. Because of conformational changes of the chain, the particle can jump to a site close in Euclidean space yet distant in chemical coordinate x.

$$\mathcal{H} = -\Delta^{\mu/2} + U, \qquad U = e^{\beta V/2}\Delta^{\mu/2}e^{-\beta V/2}, \quad (8)$$

with an anomalous kinetic term $-\Delta^{\mu/2}$ and an effective potential U which depends on μ. A separation ansatz yields the associated stationary equation,

$$[E + \Delta^{\mu/2} - U]\psi(x) = 0, \quad (9)$$

for the spectrum E. Let us consider periodic potentials of wavelength $2\pi\lambda$, $V(x) = V(x + 2\pi\lambda n)$, with $n \in \mathbb{Z}$. Without loss of generality, we restrict ourselves to potentials with vanishing offset and unit variance. A Bloch ansatz $\psi_q(x) = e^{iqx}\theta(x)$ with $\theta(x) = \theta(x + 2\pi\lambda n)$ and $q \in [0, 1/\lambda]$ inserted into (7) in Fourier space yields

$$(E_{n,q} - E^0_{n,q} - \tilde{U}_0)\tilde{\theta}_n - \sum_{m\neq n}\tilde{U}_{n-m}\tilde{\theta}_m = 0. \quad (10)$$

In Eq. (10), $E_{n,q}$ are the eigenvalue bands labeled by the discrete band index n and the continuous Bloch phase q. The spectrum of the system for vanishing potential is given by $E^0_{n,q} = |n/\lambda - q|^\mu$. The Fourier coefficients of the periodic component of the eigenfunction and the effective potential are given by $\tilde{\theta}_n = 1/2\pi\lambda \int_{2\pi\lambda} dx\, \theta(x) \exp(-inx/\lambda)$ and $\tilde{U}_n = 1/2\pi\lambda \int_{2\pi\lambda} dx\, U(x) \exp(-inx/\lambda)$, respectively. The spectrum $E_{n,q}$ depends implicitly on β. In the high temperature limit, the eigenvalue bands merge to form a continuous spectrum. For nonvanishing β gaps between bands emerge. The band structure determines the relaxation properties of the system. For a comparison of different Lévy indices μ, it is more appropriate to compare the generalized crystal momentum defined as $\kappa_{n,q} = E^{1/\mu}_{n,q}$.

Figure 2 depicts the β dependence of the first few bands $\kappa_{n,q}$ for different potentials, each one reflecting a frequently encountered physical situation. In each panel ordinary diffusion is compared to enhanced diffusion with Lévy index $\mu = 1/2$. The band structure of ordinary diffusion ($\mu = 2$) in the cosine potential displays only one significant gap [18] contrasting the superdiffusive case in which the narrowing effect of individual bands is substantial [Fig. 2(A)]. The effect is even more pronounced in the square wave potential [Fig. 2(B)]. Band coupling leads to far more complex band structures when $\mu = 1/2$. The most striking difference occurs in the localized barrier (well) potentials, Figs. 2(C) and 2(D). In the example of copolymers discussed above, these cases describe situations in which the polymer consists mainly of a single type of monomer interspersed with small intervals of another type of monomer at a higher or lower potential, respectively. On one hand, the band structures are identical when $\mu = 2$, indicating that an ordinary diffusion process does not distinguish between barriers and wells. On the other hand, if $\mu = 1/2$, the band structures differ considerably; the shape of the potential has a profound impact on the band structure and thus on the dynamics of the system.

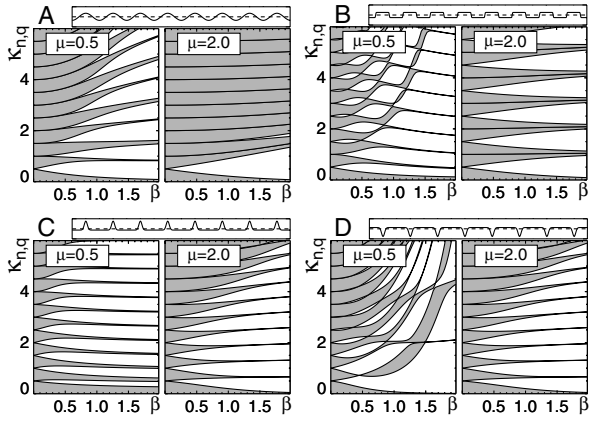

FIG. 2. Band structure $\kappa_{n,q}$ as a function of β for four different potentials. (A) A simple cosine potential $V \propto \cos(x/\lambda)$, (B) the square wave potential, and potentials given by $V \propto \pm[1 + \cos(x/\lambda)]^\gamma$. When $\gamma \gg 1$, the latter possess localized high potential barriers (C) or localized potential wells (D). A Lévy flight ($\mu = 1/2$) is compared to ordinary diffusion ($\mu = 2$).

The asymptotic behavior is governed by the lowest band of the spectrum, $n = 0$, and $q \ll \lambda^{-1}$. For $\beta = 0$, the system is freely superdiffusive. This yields $E^0_{0,q} = q^\mu$. When β is finite the q^μ dependence remains, i.e., $E_{0,q} \approx D(\beta)\, q^\mu$. The generalized diffusion coefficient $D(\beta)$ is reduced to a value less than unity; the process is slowed down by the potential. The high temperature regime can be investigated by expanding the effective potential U in (9) in powers of β. Neglecting all terms of order higher than $\mathcal{O}(\beta^3)$, we obtain

$$\tilde{U}_n = \frac{1}{\lambda^\mu}\left[\frac{\beta}{2}|n|^\mu\tilde{V}_n - \frac{\beta^2}{8}\sum_m \tilde{V}_{n-m}(|n|^\mu - 2|m|^\mu)\tilde{V}_m\right]. \quad (11)$$

Inserted into (10) yields in perturbation theory $E_{0,q} \approx q^\mu[1 - \beta^2 G_\mu(q)]$. As expected, $D(\beta)$ decreases quadratically with increasing β, i.e., $D(\beta) = 1 - \beta^2 G_\mu(q)$. The factor $G_\mu(q)$ is positive and depends on V and μ. It quantifies the effect on the asymptotics, the larger $G_\mu(q)$ the stronger the slowing down effect of the potential. We obtain

$$G_\mu(q) = \frac{1}{4}\sum_{m>0}|\tilde{V}_m|^2 g_\mu(q\lambda/m), \quad (12)$$

where

$$g_\mu(z) = \frac{1}{z^\mu}\left(\frac{1}{(1-z)^\mu - z^\mu} + \frac{1}{(1+z)^\mu - z^\mu} - 2\right). \quad (13)$$

Noting that $\sum_m |\tilde{V}_m|^2 = 1$, the asymptotic limit is

$$\lim_{q\to 0} G_\mu(q) = \begin{cases} 1 & \mu = 2 \\ 1/4 & 0 < \mu < 2. \end{cases} \quad (14)$$

The asymptotics are the same for any type of potential. In

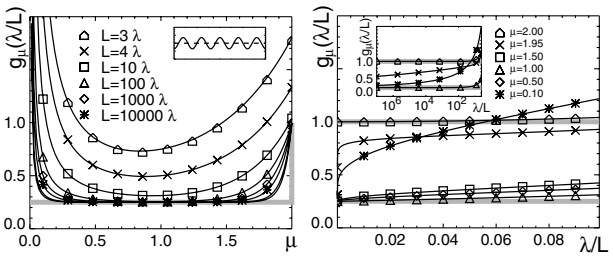

FIG. 3. The quantity $g_\mu(\lambda/L)$ in the high temperature regime as a function of Lévy index μ and fixed system size (left). The solid lines (symbols) depict the results obtained from perturbation theory (numerics). Thick gray lines indicate the asymptotic limit of $1/4$ (1) if $\mu < 2$ ($\mu = 2$). Viewed as a function of inverse relative system size λ/L for a set of values of μ (right) indicates that convergence to the limiting values is slowest when μ is small or slightly less than 2.

addition, the rhs of (14) is independent of μ with a discontinuity to a higher value on the margin $\mu = 2$.

The limit $q \to 0$ represents a system of infinite extent. In a finite system of size $2\pi L$, the Bloch phase acquires discrete values $q = n/L$ with $n \in \mathbb{N}$. The relaxation time is defined by the inverse of the lowest eigenvalue, obtained by (12) at $q = L^{-1} \ll \lambda^{-1}$. The result is shown in Fig. 3 for the cosine potential. In this case, Eq. (12) implies $G_\mu(1/L) = g_\mu(\lambda/L)$. On the left, g_μ is depicted as a function of μ for a number of system sizes. Surprisingly, the asymptotic limit is not attained uniformly on the μ interval $(0, 2]$. Even for very large systems g_μ exhibits a minimum at $\mu \approx 1$, as $\mu \to 0$ the factor g_μ diverges. Although small values of μ imply heavy tails in the transition probability, the potential strongly influences the dynamics in that range. We conclude that Lévy flights with intermediate values of μ are most robust when perturbed by an external field. This may explain why Lévy flights with $\mu \approx 1$ are the most efficient when employed in random search [14].

Finally, we investigate the effective generalized diffusion coefficient $D(\beta)$ in the low temperature regime. Since perturbation theory fails here, we must rely on the numerical diagonalization of (10). The result is depicted in Fig. 4. $D(\beta)$ is identical for all superdiffusive processes in a given potential. However, a comparison between potentials reveals a unique response of Lévy flights to each potential shown in the inset. The effect on $D(\beta)$ is least pronounced in the potential barrier system, intermediate for the cosine, and strongest in the potential well. In contrast, ordinary diffusion shows a decrease in $D(\beta)$ which is not only greater compared to all the other cases, but is independent of the shape of the potential. For small β, the results are consistent with those obtained from perturbation theory.

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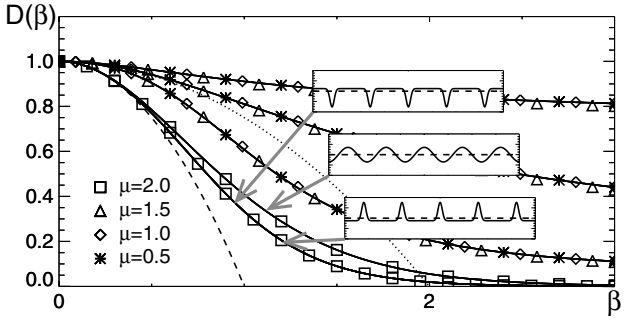

FIG. 4. The generalized diffusion coefficient $D(\beta)$ as a function of inverse temperature for a chosen set of Lévy indices (indicated by the symbols in the lower left) and the set of potentials depicted in the upper right. The data were obtained by numerical diagonalization of (10). The dotted ($\mu < 2$) and dashed ($\mu = 2$) curves indicate the result obtained by the perturbation expansion for small β.

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