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 $\mu$. 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, fluid particles in fully developed turbulence, to millennial climate changes, bacterial motion and human eye movements.

Among the most successful theoretical concepts which have been applied to superdiffusive phenomena is a class of random walks known as Lévy flights. In contrast to ordinary random walks, the displacements $\Delta x$ of a Lévy flight lack a well defined variance, due to a heavy tail in the single step probability density. Lévy flight models have paved the way towards a description of superdiffusive phenomena in terms of fractional Fokker-Planck equations (FFPE). 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) the matter is more subtle in superdiffusive systems due to the non-local properties of the fractional operators involved. Depending on the underlying physical model, different types of FFPEs are appropriate, therefore the ad hoc introduction of fractional operators may lead to severe problems.

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. Counterintuitively, the asymptotic behavior does not depend on the Lévy flight index $\mu$, 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 $\mu$. This is consistent with the observation that Lévy flights with $\mu \approx 1$ are particularly efficient in search processes. The results present 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

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

in which $w(x|y)$ is the probability rate of initiating a jump $y \rightarrow x$. If this probability has a typical variance in distance one may expand the 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. Inserting this rate into (1) the rhs defines the integral operator...
\[ \Delta^{\mu/2} p(x, t) = \int dx \left[ p(y, t) - p(x, t) \right]/|x - y|^{1+\mu}, \]

and Eq. (1) may be rewritten as

\[ \partial_t p = D \Delta^{\mu/2} p. \] (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 [3]. This simple spectral property of the operator is the reason why fractional evolution equations are frequently introduced in the Fourier domain. However, the position representation, Eq. (2), along with Eq. (1), provides a more intuitive picture of the dynamics and emphasizes the essential fact that \( \Delta^{\mu/2} \) is defined by a non-local integral kernel which decreases algebraically with distance. Eq. (3) is solved by \( p(x, t) = (D t)^{\mu/2} L_\mu (x/(D t)^{1/2}) \) where \( L_\mu(z) = (2\pi)^{-1} \int dk \exp(ikz - |k|^\mu) \) is the symmetric Lévy stable law of index \( \mu \). The argument \( x/(D t)^{1/2} \) in \( L_\mu \) 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 \( \beta V \) in the FPE. Thus, it may seem reasonable to formally allow for an external potential in a superdiffusive system as

\[ \partial_t p = \beta V p + \Delta^{\mu/2} p. \] (4)

This type of FFPE has been studied extensively in the past [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 several restrictions. Systems evolving according to (4) do not obey ordinary 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 \( \mu \). Detailed balance is violated, and only in the diffusion limit (\( \mu = 2 \)) can the parameter \( \beta \) be interpreted as an intensive inverse temperature.

The asymptotics of Eq. (4) in periodic potentials is trivial. Rescaling the original coordinates \( x, t \rightarrow z = x/\gamma, \tau = t/\gamma^\mu \) with \( \gamma \gg 1 \) yields a form invariant FFPE in a new potential \( \hat{V}(z) = \gamma^{\mu-2} V(\gamma z) \). The factor \( \gamma^{\mu-2} \ll 1 \) implies that on large spatiotemporal 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 \( \delta V_k = V(x + a) - V(x) \) in units of \( k_B T = \beta^{-1} \). Both assumptions are accounted for by: \( w(x \pm a|x| \propto \exp(-\beta \delta V_k/2) \). 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 \( x \rightarrow y \) 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 \( \mu \) is determined by the folding properties of the polymer, e.g. a Gaussian chain implies \( \mu = 1/2 \) [15]. The possibility of initiating 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,

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

\[ \partial_t p = e^{\beta V/2} \Delta^{\mu/2} e^{-\beta V/2} p - p e^{\beta V/2} \Delta^{\mu/2} e^{-\beta V/2}, \] (6)

which is clearly different from the FFPE corresponding to generalized Langevin dynamics. Eq. (6) obeys Gibbs-Boltzmann thermodynamics, \( p_s \propto \exp(-\beta V) \) is the stationary solution, detailed balance is fulfilled, and \( \beta \) 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 pre-factor \( \gamma^{2-\mu} \) 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 \( \psi(x, t) = \exp[-\beta V(x)/2] p(x, t) \), Eq. (6) can be recast into a fractional Schrödinger equation,

\[ \partial_t \psi = -\mathcal{H} \psi \] (7)

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

with an anomalous kinetic term \(-\Delta^{\mu/2}\) and an effective potential \( U \) which depends on \( \mu \). A separation ansatz yields the
The band structure determines the relaxation properties of the system. For a comparison of different Lévy indices spectrum, for non-vanishing 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 $E_{0,q}^0 = q^\mu$. When $\beta$ is finite the $q^\mu$-dependence remains, i.e. $E_{0,q} \approx D(\beta) q^\mu$. The generalized diffusion coefficient $D(\beta)$, however, is reduced to a value less than unity; the process is slowed down when a potential is present. The high temperature regime can be investigated by expanding the effective potential $U$ in $q^\mu$ powers of $\beta$. Neglecting all terms of order higher than $O(\beta^3)$ we obtain

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

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

![Figure 2](image)

Figure 2: Bandstructure $\kappa_{n,q}$ as a function of $\beta$ 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 ($\mu = 2$).

associated stationary equation,

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

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 (9) in Fourier space yields

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

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 contrasting the superdiffusive case in which the narrowing effect of individual bands is substantial (Fig. 2A). The effect is even more pronounced in the square wave potential (Fig. 2B). Band coupling leads to far more complex band structures when $\mu = 1/2$. The most striking difference occurs in the localized barrier (well) potentials, Fig. 2C(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. In a system containing barriers, a particle located at any given position may initiate a distant jump with a probability which is decreased by the concentration of energetically unfavorable target positions. In the repetitive barrier potential this is low, so the process is not considerably affected. In Fig. 2D the particle is likely to be trapped in a potential well. The probability of initiating a distant transition to another energetically favorable state is low and the repetitive well potential slows down the dispersion dramatically.

![Figure 3](image)

Figure 3: The quantity $g_\mu(\lambda/L)$ in the high temperature regime as a function of Lévy index $\mu$ 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 $\lambda/L$ for a set of values of $\mu$ (right) indicates that convergence to the limiting values is slowest when $\mu$ is small or slightly less than 2.
$\beta^2 G_\mu(q)$. As expected, the generalized diffusion coefficient $D(\beta) = 1 - \beta^2 G_\mu(q)$ decreases quadratically with increasing $\beta$. The factor $G_\mu(q)$ is positive and depends on $V$ and $\mu$. It quantifies the effect on the asymptotics, the larger $G_\mu(q)$ the stronger the slowing down effect of the potential. We obtain

$$G_\mu(q) = \frac{1}{4} \sum_{m=0} \bar{|V_m|}^2 g_\mu(q \lambda/m) \quad \text{where}$$

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

(13)

Noting that $\sum_m |V_m|^2 = 1$ the asymptotic limit is

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

(14)

The asymptotics are the same for any type of potential. In addition, the rhs of (14) is independent of $\mu$ with a discontinuity to a higher value on the margin $\mu = 2$.

The limit $q \to 0$ represents an idealized system of infinite extent. In a finite 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 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, $g_\mu$ is depicted as a function of $\mu$ for a number of system sizes. Surprisingly, the asymptotic limit is not attained uniformly on the $\mu$-interval $(0,2]$. Even for very large systems $g_\mu$ exhibits a minimum at an intermediate value $\mu \approx 1$. Interestingly, as $\mu \to 0$ the factor $g_\mu$ diverges. Although small values of $\mu$ are equivalent to heavy tails in the transition probability, the potential strongly influences the dynamics in that range. We conclude that Lévy flights with intermediate values of $\mu$ 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.

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 (13). The result is depicted in figure 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 $\beta$ the results are consistent with those obtained from perturbation theory as indicated by the dotted ($\mu < 2$) and dashed ($\mu = 2$) lines.

In this Letter we have shown that Lévy flights are substantially affected by external inhomogeneities, a feature generic to topologically induced superdiffusion, absent in popular generalized Langevin models, yet crucial for the understanding of physical applications such as protein search on DNA strands and random motion on complex networks.

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