Diffusion regimes in Lévy flights with trapping

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Abstract

The diffusion of a walk in the presence of traps is investigated. Different diffusion regimes are obtained considering the magnitude of the fluctuations in waiting times and jump distances. A constant velocity during the jump motion is assumed to avoid the divergence of the mean squared displacement. Using the limit theorems of the theory of Lévy stable distributions we have provided a characterization of the different diffusion regimes. © 1999 Elsevier Science B.V. All rights reserved.

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1. Introduction

There are many physical situations where diffusion takes place under the presence of traps, trapping diffusion. Examples are found in electronic conduction in amorphous semiconductors and quasicrystals [1], atomic diffusion in glass like materials [2], tracer diffusion in living polymers [3], and more [4,5]. The existence of traps is generally modeled through a probability density of waiting times between successive steps in the walk, continuous-time random walks (CTRW) [5]. The theory of CTRW has been extensively developed in the literature, using the generating function methods [5] or simple statistical reasoning [4]. The existence of a wide distribution of waiting times leads to a subdiffusive regime where the mean squared displacement grows slower than time. On the other hand, there are physical situations where the time between successive jumps may be considered constant, but the distribution of jump distances is wide [4–7] (Lévy flights) [6].

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Lévy flights are also observed in a large variety of phenomena, for instance in chaotic dynamical systems [7,8], turbulent [9,10] flow and self-gravitating systems [11]. The existence of a wide distribution of jump distances leads to a superdiffusive regime, where the mean squared displacement grows faster than time. Moreover, Lévy flights generates fractal structures in space [6]. Nevertheless, more complex behaviors are expected in systems where both the distribution of waiting times and jump distances are wide. For instance, Schulz [12] studied an anomalous Drude model for transport properties of quasicrystals. He assumed that the walks move with an anomalous speed \( v_t \sim t^\sigma \) between collisions, and a power law \( p(\tau) \sim \tau^{-1-\mu} \) distribution of time between collisions. In this way, he obtained the phase diagram \((\mu, \sigma)\) of the system, which is divided in different regions. While the anomalous velocity may mimic the existence of traps, it is introduced artificially and cannot be derived from a Hamiltonian. In [13], Klafter et al. introduced a stochastic description of anomalous transport phenomena and found different behavior of the mean square displacement of CTRW. Zumofen and Klafter [8] studied a one-dimensional map which exhibits intermittent chaotic behavior with coexisting laminar and localized phases, and analyzed them in terms of Lévy statistics.

A more consistent approach was presented by Klafter and Zumofen [14]. They studied the diffusion in a Hamiltonian system in terms of the CTRW formulation, and considered wide distributions of waiting times and jump distances. However, they did not provide a complete characterization of the different diffusion regimes that may be obtained. In a recent letter Fogedby [15] considered Lévy flights in the presence of a quenched isotropic random force field studying the interplay between the built in superdiffusive behavior of the Lévy flights and the pinning effect of the random environment.

In the present work we study the behavior of a random walk in the presence of traps. Disorder is introduced in an annealed way, through power law distributions of waiting times \( p(\tau) \sim \tau^{-1-\mu} \) and jump distances \( p(x) \sim x^{-1-\nu} \). We use simple statistical reasoning close to the approach developed by Bouchaud and Georges [4] instead of that of the work by Klafter and Zumofen [14], which use the CTRW formulation. The present formalism contains as a fundamental tool the theory of Lévy stable distributions, introduced by Lévy [16] and developed by other authors [17,18].

2. The model

We consider a random walk on a lattice, such that the particle has to wait for a time \( \tau_w \) on each site before performing the next jump. The waiting time is a random variable independently chosen at each new jump according to a distribution \( p(\tau_w) \). We also assume that the waiting time is not correlated to the length of the jump \( x \), which is distributed according to \( p(x) \). The diffusion process will be characterized by the scattering function \( F(k,t) \), the Fourier transform of the diffusion front. Other properties like the diffusion front and the mean squared displacement can be derived from this
function. For instance, the mean squared displacement is given by

\[ \langle x^2(t) \rangle = -\frac{\partial^2 F}{\partial k^2} \bigg|_{k=0} . \]

(1)

Let \( N \) be the number of steps performed by a walker during time \( t \). \( N \) is, in general, a random variable which depends on the duration of the jumps and waiting times. The scattering function can thus be expressed as a sum over all possible jumps during time \( t \)

\[ F(k,t) = \int dN F(k,N)P(N,t) , \]

(2)

where \( F(k,t) \) is the scattering function of the same problem, but considering regular duration of the jumps and no waiting time and \( P(N,t) \) stands for the probability distribution of \( N \) jumps at a fixed time \( t \).

2.1. Mean squared displacement after \( N \) steps

The total displacement after \( N \) steps is given by

\[ X_N = \sum_{i=1}^{N} x_i . \]

(3)

In the right-hand side we have a sum of mutually independent random variables with the common distribution \( p(x) \), with zero mean. The limit distribution for large \( N \) will be a stable Lévy distribution [17,18], i.e.

\[ X_N \overset{\text{d}}{=} l^* N^{1/\alpha} u \]

(4)

where \( \overset{\text{d}}{=\text{ denotes that random variables in both sides have the same distribution, \( l^* \)

is a characteristic value and \( u \) follows the symmetric Lévy distribution \( L_{x,0}(u) \). The canonical (Fourier transform) representation of Lévy stable laws is (for \( \alpha \neq 1 \))

\[ \text{FT}[\mathcal{L}_{x\beta}](k) = \exp \left[ -|k|^\alpha \left( 1 + \frac{k}{|k|} i \beta \tan \frac{\pi}{2} \right) \right] , \]

(5)

where \( \alpha \) and \( \beta \) are real numbers defined in the intervals \( 0 < \alpha \leq 2 \) and \( -1 \leq \beta \leq 1 \). The case \( \alpha = 2 \) and \( \beta = 0 \) corresponds with the Gaussian distribution, which decays faster than any power law for large arguments. On the contrary, all Lévy distributions, except the Gaussian, have the asymptotic behavior for \( u \gg 1 \) [17,18]

\[ L_{x\beta}(u) \sim u^{-1-\alpha} . \]

(6)

Then, from Eqs. (4) and (5) it follows that

\[ F(k,N) = \exp[ -([k]l^*)^\alpha N] , \]

(7)

If \( p(x) \) has finite variance \( \sigma \) then \( l^* = \sigma \) and \( \alpha_c = 2 \). If \( p(x) \approx l^*_0 |x|^{-1-\mu} \), with \( 0 < \mu < 2 \) then \( l^* \sim l_0 \) and \( \alpha_c = \mu \).
Fig. 1. The phase diagram ($\alpha_w, \alpha_x$). The behavior in the different regions is as follows: I. normal diffusion; II. LTT with exponent $\alpha_x$ and superdiffusion; III. LTT with exponent $\alpha_w$ (a) superdiffusive, (b) normal diffusion; IV. LTT with exponent $\alpha_x$ and ballistic motion; V. LTT with exponent $\alpha_w$, (a) superdiffusive, (b) and (c) subdiffusive. See text for a detailed description.

2.2. Number of steps after time $t$

On the other hand, the number of steps after time $t$ is given by

$$t = \sum_{i=1}^{N} \tau_{wi} + \sum_{i=1}^{N} \tau_{xi},$$

(8)

where $\tau_{xi}$ are the duration of the jumps. If we assume that during the jump motion the walker moves continuously at a constant velocity $v$ and changes directions at random then $\tau_x = v^{-1}|x|$ and $p(\tau_x) = 2v|\tau|/v$. In the right-hand side of Eq. (8) we have two sums of independent random variables, with common distribution $p(\tau_w)$ and $p(\tau_x)$, respectively. The limit distributions for large $N$ will follow Lévy distributions [17,18], i.e.

$$t = \tau N + \tau_w^* N^{1/\alpha_w} u_1 + \tau_x^* N^{1/\alpha_x} u_2,$$

(9)

where $u_1$ and $u_2$ follows the Lévy distribution $L_{\alpha_1}(u_1)$ and $L_{\alpha_2}(u_2)$, respectively. The first term in the right-hand side appears only if $p(\tau_w)$ or $p(\tau_x)$ have finite mean, and $\tau$ is given by the sum of the finite means. If $p(\tau_w)$ has finite variance $\sigma$ then $\tau_w^* = \sigma$ and $\alpha_w = 2$, while if $p(\tau_w) \approx \tau_w^{-\alpha_w-1-\mu}$ ($0 < \mu < 2$) then $\tau_w^* \sim \tau_0$ and $\alpha_w = \mu$. If $p(\tau_x)$ has finite variance $\sigma$ then $\tau_x^* = \sigma$ and $\alpha_x = 2$, while if $p(\tau_x) \approx \tau_x^{-\alpha_x-1-\mu}$ ($0 < \mu < 2$) then $\tau_x^* \sim \tau_0$ and $\alpha_x = \mu$. From Eqs. (2), (7) and (9) it follows that

$$F(k,t) = \int \int du_1 du_2 L_{\alpha_1}(u_1) L_{\alpha_2}(u_2) \exp[-(kl^*)^\mu]N,$$

(10)

where the functional dependence of $N$ with $u_1$, $u_2$ and $t$ is determined from Eq. (9). Next we analyze the behavior of the scattering function, defined through this expression, for different values of $\alpha_x$ and $\alpha_w$. With this purpose we have divided the corresponding phase diagram in five regions, as it is illustrated in Fig. 1.
3. Results

In region I both the distribution of waiting times and jump distances have finite variance. Hence, the random variables $u_1$ and $u_2$ will follow a Gaussian distribution. For large $N$, we can therefore neglect the last two terms in the right-hand side of Eq. (9), obtaining $N \approx t/\tau$. Then Eq. (10) reduces to

$$F(k,t) = \exp\left[-\frac{(|k|\tau)^2}{\tau}\right].$$

Moreover, using Eq. (1) one obtains

$$\langle x^2(t) \rangle \sim t .$$

We thus find normal or classical diffusion in this region: the scattering function decays exponentially with time and the mean squared displacement grows proportional to time.

In region IV the distribution of jump distances is quite wide, and even wider than the distribution of waiting times. Hence, it is expected that the third term in Eq. (9) gives the major contribution, thus obtaining $N \approx (t/\tau)^{x_1} u_2^{-x_2}$. Substituting this result in Eq. (10), and expanding the exponential inside the integral, one obtains

$$F(k,t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{F(1+n\tau_k)} \left( \frac{t}{\tau_k} \right)^{nx_1} ,$$

where $\tau_k = \tau_1^*/|k|\tau$. This series has an infinite radius of convergence and, therefore, can be taken as a series expansion for the scattering function in this region. For small times ($t \ll \tau_k$) the scattering function follows a stretched exponential decay, with stretched exponent $x_1$. On the contrary, for $t \gg \tau_k$ the relaxation becomes slower than an exponential. Taking $L_{x_1}(u_1) \sim u_1^{-1-x_1}$, from Eq. (10) it follows that $F(k,t) \sim t^{-x_1}$. Hence, for long times the scattering function follows a long time tail (LTT), with an exponent $x_1$ smaller than one. In this case, the mean squared displacement determined from Eqs. (1) and (13) is not finite. This is a consequence of the divergence of the second moment of the distribution of jump distances. Nevertheless, the total displacement at time $t$ cannot be larger than $vt$ and, therefore, there is a cutoff $k_c \sim t^{-1}$ for small values of $k$. Thus, to avoid the divergence of the mean squared displacement we evaluate Eq. (1) in $k = k_c$ instead of $k = 0$. In this way we obtain

$$\langle x^2(t) \rangle \sim t^2 , \text{ in IV}.$$

The motion of the walk is in this case of ballistic type. The behavior in this region has been investigated by different authors, which consider random walk motion due to a periodic potential [14].

In region V we can use a similar reasoning as in region IV, but in this case the dominant term will be the second one, associated to huge fluctuations in the waiting time. In this way we obtain

$$F(k,t) = \sum_{n=0}^{\infty} \frac{(-1)^n}{F(1+n\tau_w)} \left( \frac{t}{\tau_k} \right)^{nx_2} ,$$
where \( \tau_k = \tau_*^k |k|^{1/\alpha} \). This expression is similar to Eq. (13). Besides, the asymptotic behaviors for short and long times are the same, replacing \( \alpha \) by \( \alpha_* \). The main difference is observed in the \( k \)-dependence of the relaxation time \( \tau_k \), which is manifested in the temporal dependence of the mean squared displacement,

\[
\langle x^2(t) \rangle \sim \begin{cases} 
t^{2-\alpha+\alpha_*}, & \text{in Va and Vb;} \\
t^{\alpha_*}, & \text{in Vc.} 
\end{cases}
\] (16)

The difference between region Va and Vb is that, in the former the mean squared displacement grows faster than time and, therefore, the system is in a superdiffusive regime, while in the second one it grows slower than time and the system is in a subdiffusive regime. In region Vc there is also a subdiffusive regime, which has been investigated by different authors, using the generating function formulation [5] or simple statistical reasoning [4]. However, in region Vc \( \alpha > 2 \) and, therefore, the spatial trajectories of the walk will not be self-similar as in regions Va and Vb.

In region II and III the fluctuations in jump distances and waiting times, respectively, are still Lévy type, but are not so strong as in regions IV and V, respectively. In these cases one cannot neglect the first term in the right-hand side of Eq. (9) and, hence, there is some reminiscent of normal diffusion behavior.

In region II the distribution of jump distances is wider than the distribution of waiting times, and both have finite mean. We thus expect that the third term in the right-hand side of Eq. (9) gives the major contribution to the fluctuations in \( N \), and the second one may be neglected. Even with this simplification we cannot solve Eq. (9) analytically, however the following asymptotic behaviors are obtained

\[
N \approx \begin{cases} 
t/\tau, & u \ll u_*(t), \\
(t/\tau_*)^{\alpha_*}, & u \gg u_*(t), 
\end{cases}
\] (17)

where \( u_*(t) \sim (t/\tau)^{\alpha_*} \). For small times, substituting Eq. (17) in Eq. (10) one obtains

\[
F(k,t) = \exp\left[-(kl)^{\gamma_*} t/\tau\right].
\] (18)

The relaxation for small times is the exponential like in the normal diffusion case, region I. However the mean squared displacement does not grow linearly with time,

\[
\langle x^2(t) \rangle \sim t^{2-\alpha}, \quad \text{in II},
\] (19)

but is characteristic of a superdiffusion regime. For long times, from Eqs. (10) and (17), and the asymptotic expansion for large arguments of Lévy distributions in Eq. (6), it follows that \( F(k,t) \sim t^{-\gamma_*} \). For long times the scattering function decays slower than an exponential following a power tail, like in region IV, but with a larger exponent.

In region III we can use a similar reasoning as in region II, but now neglecting the fluctuations in the jump distances in relation to the fluctuations in the waiting times. Again, even with this simplification we cannot solve Eq. (9) analytically, however the following asymptotic behaviors are obtained:

\[
N \approx \begin{cases} 
t/\tau, & u \ll u_*(t), \\
(t/\tau_*)^{\alpha_*}, & u \gg u_*(t), 
\end{cases}
\] (20)
where now \( u_x(t) \sim (t/\tau)^{x_c} \). For small times, substituting Eq. (20) in Eq. (10) one obtains an exponential relaxation as in Eq. (18). However, the characteristic exponent \( x_0 \) can be now larger than two leading to different behaviors for the mean squared displacement,

\[
\langle x^2(t) \rangle \sim \begin{cases} t^{1-x_0}, & \text{in } \text{IIIa}, \\ t, & \text{in } \text{IIIb}. \end{cases}
\]  

(21)

Hence, in subregions IIIa and IIIb we found superdiffusion and normal diffusion behavior, respectively. For long times, from Eqs. (10) and (20), and the asymptotic expansion for large arguments of Lévy distributions in Eq. (6), it follows that \( F(k,t) \sim t^{-x_0} \). For long times the scattering function decays slower than an exponential following a power tail, like in region V, but with a larger exponent.

4. Summary and conclusions

In summary we have investigated the diffusion behavior in the whole plane \((x, t)\), which has been divided in five regions considering the magnitude of the fluctuations in waiting times and jump distances. A constant velocity during the jump motion was assumed to avoid the divergence of the mean squared displacement. Using as a fundamental tool the limit theorems of the theory of Lévy distributions we have provided a characterization of the different diffusion regimes.

We conclude that the diffusion behavior cannot be just classified as normal diffusion, superdiffusion and subdiffusion. This classification only takes into account the temporal dependence of the scattering function for short times, while the long time decay may be different. For instance, in regions II and IIIa we have similar superdiffusive regimes, but the long time behavior is determined by the distribution of jump distances, in the first case, and by the distribution of waiting times in the second one.

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