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Diffusion and annihilation reactions of Lévy flights with bounded long-range hoppings

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Abstract. A new kind of random walk named bounded Lévy flights (BLFs), where the step length is a bounded random variable, is proposed and their properties are studied with the aid of mean field and Monte Carlo techniques. BLFs are characterized by the Lévy exponent (σ) and the length of the longest possible flight (R_M). It is found that in one dimension (1D), the mean number of distinct sites visited by the walker (S_N) and the average square displacement ($\langle R_N^2 \rangle$) behave like $S_N \propto R_M^{d_s f(\sigma)} N^{d_s} (d_s = \frac{1}{2})$ and $\langle R_N^2 \rangle \propto R_M^{f(\sigma)} N^{\nu} (\nu = 1)$, where $f(\sigma)$ is a continuously tunable function of σ with $f(\sigma) \simeq 0.9 (\sigma < 0.1)$ and $f(\sigma) \simeq 0 (\sigma > 2)$. In addition, the long-time behaviour of annihilation reactions between BLFs, which react via exchange in 1D is found to be anomalous because the density of walkers (ρ_A) behaves like $d\rho_A/dt \simeq -R_M^{f(\sigma)} \rho_A^X$ with $X = 1 + (1/d_s) = 3 (t \to \infty)$ while, shortly after the beginning of the reaction, the classical behaviour $X = 2 (t \to 0)$ holds.

1. Introduction

Lévy flights (LFs) are random walks where the steps are not necessarily performed to next neighbours but the step length is a random variable with an infinite mean square displacement [1]. After this early work of Lévy, subsequent studies due to Mandelbrot [2], Montroll and West [3] and Shlesinger [4] have contributed to our understanding of the effects of arbitrarily long-range hoppings on diffusion. Recently, there has been considerable interest in the LF process including the study of the critical behaviour of self-avoiding LFs [5, 6], diffusion of LFs on fractals [7], the universality of node-avoiding and path-avoiding LFs [8], the LF approach to diffusion on a self-avoiding walk cross-links [9], etc. Very recently, Ott *et al* [10] have reported a very interesting experimental realization of the Lévy flight.

LFs are characterized by the Lévy exponent $0 < \sigma < 2$, that is the probability for a step to have a length greater than $r (P_{LF}(r))$ is assumed to behave like

$$P_{LF}(r) \propto r^{-\sigma} \qquad r \to \infty. \tag{1}$$

It is interesting to note that $0 < \sigma < 2$, leads to superdiffusive behaviour while the case $\sigma = 2$ corresponds to ordinary diffusion [6]. The distribution (1) has also been used to study the growth kinetic of a percolation cluster by the 'butterfly mechanism' [11, 12], where r is now the distance from the most recently added sick particle [11].

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Nevertheless, the butterfly flight is not an LF because the former moves on a fractal while the latter is a random walk on a Euclidean lattice.

The purpose of this work is to study the diffusion of LFs with bounded hoppings (BLFs), that is

$$P_{\mathrm{BLF}}(r) \propto r^{-\sigma} \qquad 0 < \sigma, r \leq R_{\mathrm{M}} \tag{2}$$

where R_{M} is the longest possible flight. Note that LFs are recovered in the limit $R_{\mathrm{M}} \to \infty, \sigma < 2$. while (1) is useful for the evaluation of the asymptotic ($r \to \infty$) properties of LFs [3, 6], in nature actual random walks necessarily perform bounded hoppings. Let us consider, for example, a molecule or an atom adsorbed on a surface site at temperature T. Such a particle can overcome the activation barrier for diffusion with probability $P \propto \mathrm{e}^{-E/kT}$ (E is the diffusion energy and k Boltzmann constant) and then travel over the surface a certain distance before becoming adsorbed again in another site. The travelled distance may depend on T, the details of the particle–surface interaction energy, the surface roughness, etc, but it is bounded to a certain maximum value R_{M}. Specifically, the dependence on both R_{M} and σ of the average number of distinct sites visited $\langle S_{\mathrm{N}} \rangle$ and the average square displacement $\langle R_N^2 \rangle$ of the BLF after N steps (flights) are studied by means of Monte Carlo simulations in one dimension (1D).

Furthermore, there is a growing interest in the study of diffusion-limited recombination reactions, of the type $\mathrm{A} + \mathrm{A} \to$ inert, between ordinary A-random walks. This kind of process is relevant in many areas of physics, chemistry and biology such as heterogeneous catalysis reaction kinetics, exciton annihilation in molecular crystals, particle–antiparticle annihilation in cosmology, etc [13–20]. It is found that the long-time behaviour of such reactions is anomalous because it is dominated by the spectral dimension of the substrata [13–18]. By contrast, little attention has been devoted to annihilation reactions via long-range interactions, such as exchange, in spite of their relevancy in solid state physics [21]. So, the present work also reports a combined mean-field and Monte-Carlo study of exchange mediated recombination reactions between BLFs in 1D.

2. Brief details on the simulation method

In order to perform the Monte Carlo simulations it is assumed that the probability of making a flight from x to $x \pm r (1 \leq r \leq R_{\mathrm{M}})$ is given by $\{C(R_{\mathrm{M}}, \sigma)(r^{-\sigma} - (r+1)^{-\sigma})\}/2$, where $C(R_{\mathrm{M}}, \sigma)$ is a normalization constant [5] (see also (2)). Both S_N and $\langle R_N^2 \rangle$ are evaluated up to 10^6 flights irrespective of the lattice size in order to avoid finite-size effects. Results are averaged over 5×10^2 samples for each pair of values (R_{M}, σ).

Annihilation reactions between BLFs have been carried out using 1D rings (periodic boundary conditions) of size $L = 10^4$. Simulations always start with fully filled samples, i.e. $\rho_{0\mathrm{A}} = 1$, where $\rho_{0\mathrm{A}}$ is the initial concentration of A-particles (BLFs) on the sample. Double occupancy of lattice sites is forbidden. The Monte Carlo time unit (t) is defined so that each BLF may be visited once, on average. Reactions are followed up to concentrations of about $\rho_{\mathrm{A}} \cong 5 \times 10^{-3}$, that is $t \cong 10^3$. During the process one has to select at random a BLF, the jumping direction and the jump length $R (R \leq R_{\mathrm{M}})$. In order to simulate the exchange reaction, the selected BLF moves sequentially in single steps and, if another BLF (the nearest) is found during such displacement, the reaction

takes place. So, both BLFs are removed from the sample and the process continues. Otherwise, the selected BLF is placed at a distance R form the starting position, i.e. one has a diffusion event without reaction. Results are typically averaged over 10^2–10^3 simulations.

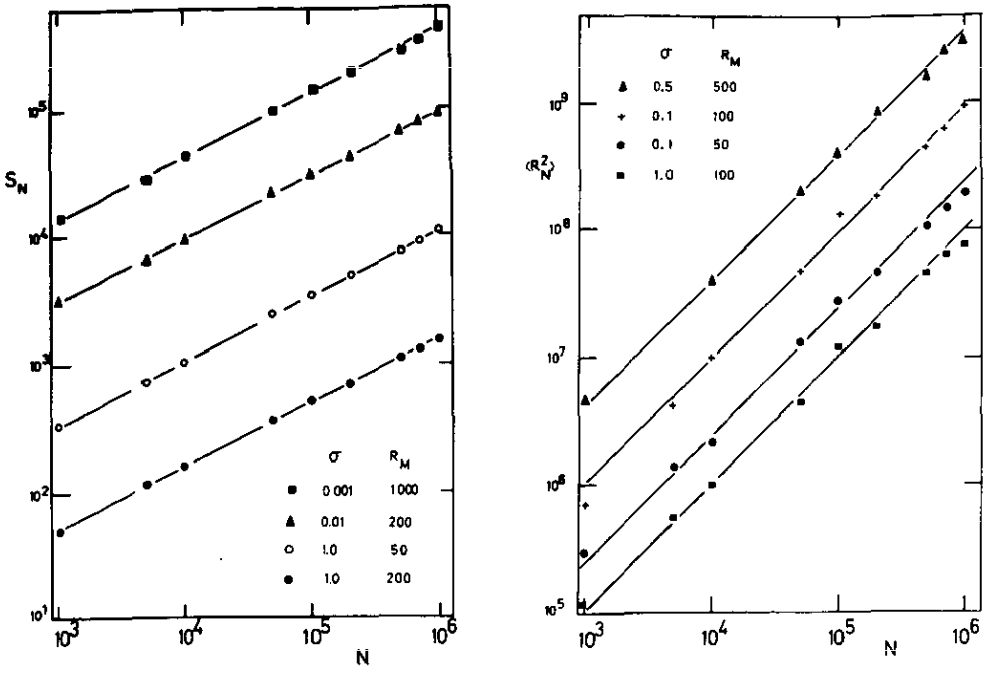

Figure 1. (*a*) and (*b*) log–log plots of S_N and $\langle R_N^2 \rangle$ against N, respectively. Data obtained using different values of both R_M and σ, as indicated in each figure. The straight lines have slope $d_s = \frac{1}{2}$ (*a*) and $\nu = 1$ (*b*), respectively.

3. Results and discussion

3.1. Diffusion of isolated BLFs

Figure 1(*a*) shows log–log plots of S_N agains N for different values of R_M and σ. These plots clearly suggest that S_N behaves like

$$S_N \propto F(R_M, \sigma) N^{d_s} \tag{3}$$

where $d_s = \frac{1}{2}$ is the random walk exponent of ordinary walkers in one dimension and $F(R_M, \sigma)$ is constant for fixed values of R_M and σ. On the other hand, log–log plots of $\langle R_N^2 \rangle$ against N (figure 1(*b*)) suggest the behaviour

$$\langle R_N^2 \rangle \propto \bar{F}(R_M, \sigma) N^{\nu} \tag{4}$$

where $\nu = 1$ is the exponent obtained for ordinary walkers in one dimension and $\bar{F}(R_M, \sigma)$ is constant for fixed values of R_M and σ. From figure 1 it follows that both

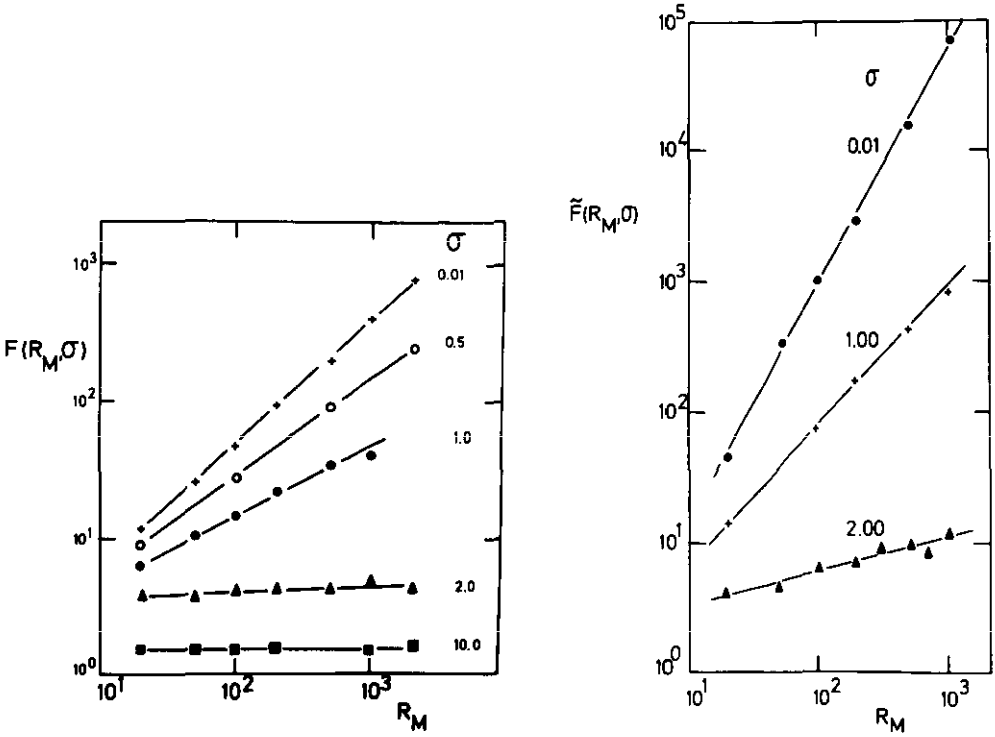

Figure 2. (*a*) and (*b*) log–log plots of $F(R_M,\sigma)$ and $\tilde{F}(R_M,\sigma)$ against R_M for different values of σ, respectively. More details in the text.

F and $\tilde{F}$ may change few orders of magnitude within the used range of R_M and σ values. In order to understand the dependence of these functions on the arguments it is useful to make log–log plots of F and $\tilde{F}$ against R_M (figures 2(*a*) and 2(*b*), respectively). The straight lines obtained suggest that the following behaviour should hold

$$F(R_M,\sigma) \propto R_M^{f(\sigma)} \tag{5a}$$

and

$$\tilde{F}(R_M,\sigma) \propto R_M^{\tilde{f}(\sigma)} \tag{5b}$$

where the exponents $f(\sigma)$ and $\tilde{f}(\sigma)$ are σ-dependent functions which have been evaluated by least-squares linear regression of the data points in figures 2(*a*) and 2(*b*), respectively. The error in the determination of both $f(\sigma)$ and $\tilde{f}(\sigma)$ is about 5% or less, as estimated from the observed fluctuations of the fitted values of the slopes using different number of data points. The dependence of $f(\sigma)$ on σ is shown in figure 3, and it follows that

$$f(\sigma) \simeq \begin{cases} (a)\ 0.9 & \sigma < 0.1 \\ (b)\ \text{crossover from } (a) \text{ to } (c) & 0.1 < \sigma < 2 \\ (c)\ 0 & \sigma > 2. \end{cases} \tag{6a}$$

The results obtained are also consistent with

$$f(\sigma) \cong (\tfrac{1}{2})\bar{f}(\sigma) \tag{6b}$$

within an error of 10% in the worst case ($\sigma \ll 1$). Nevertheless, as will be discussed after (8*b*), it is expected that (6*b*) should hold exactly.

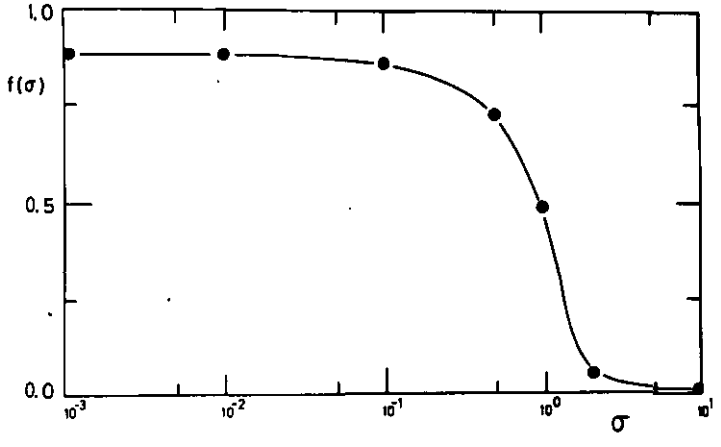

Figure 3. Semi-logarithmic plot of $f(\sigma)$ against σ. The estimated error in $f(\sigma)$ is less than 5%. More details in the text.

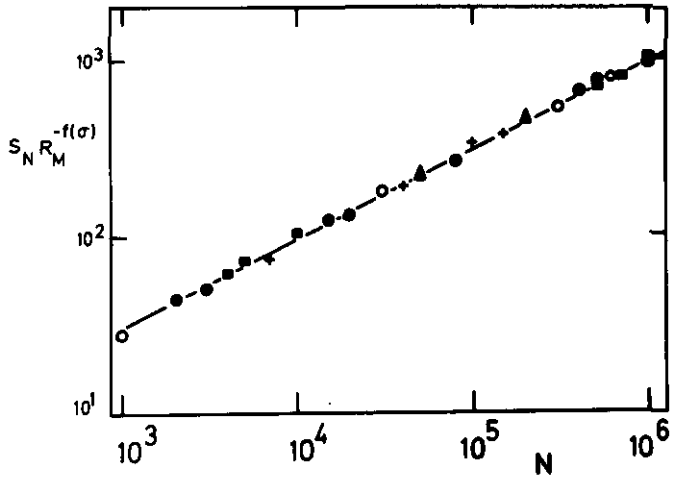

Figure 4. Log–log plot of $S_N R_M^{-f(\sigma)}$ against N, using $2 \times 10^1 \leq R_M \leq 2 \times 10^3$ and $10^{-3} \leq \sigma \leq 10^1$. More details in the text.

Therefore, using (5*a*) and (3) one expects that for BLFs the following behaviour should hold

$$S_N \propto R_M^{f(\sigma)} N^{d_s}. \tag{7}$$

So, a log–log plot of $S_N R_M^{-f(\sigma)}$ against N should give a single straight line with slope $d_s = \frac{1}{2}$ for all values of R_M and σ. This plot is shown in figure 4 where the excellent

collapse of the data suggests the validity of (7). A similar argument also holds for $\langle R_N^2 \rangle$ inserting (5*b*) in (4). So, defining $N' = R_M^{\bar{f}(\sigma)} N$ one has that (3) and (4) for BLFs can be rewritten as

$$S_{N'} \propto N'^{d_s} \tag{8a}$$

and

$$\langle R_{N'}^2 \rangle \propto N'^{\nu} \tag{8b}$$

respectively. That is, the behaviour of both S_N and $\langle R_N^2 \rangle$ is the same for both BLFs and ordinary walkers but using $R_M^{\bar{f}(\sigma)}$ as a scaling factor for the number of steps performed by BLFs. Note that replacing N' in (8*a*) one gets $S_N \propto R_M^{\bar{f}(\sigma)} N^{d_s}$, and comparing with (7) it follows that $f(\sigma) = \bar{f}(\sigma) d_s (d_s = \frac{1}{2})$. So, one expects that (6*b*) should hold exactly in order to be consistent with the scaling of the number of steps performed by the walker. It is also interesting to note that the exponent $\bar{f}(\sigma)$ of the scaling factor can be continuously tuned by a variation of the parameter σ. This behaviour is analogous to the observed in both the 'butterfly model' [11, 12] and the Fisher–Ma–Nickel model [22], because in both cases critical exponents can be continuously tuned by the parameter σ of the distribution (1).

3.2. Annihilation reactions between BLFs

Pointing now our attention to annihilation reactions, of the type A + A $\rightarrow$ inert, let us recall that for ordinary walkers the rate of reaction behaves like [13–16]

$$\frac{\mathrm{d}\rho_A}{\mathrm{d}t} \propto -\rho_A^X \tag{9a}$$

$$X = \begin{cases} 2 & t \Rightarrow 0 \\ 1 + 1/d_s & t \Rightarrow \infty \end{cases} \tag{9b}$$

where ρ_A is the concentration of A-walkers and X is the reaction order. Equation (8) can also be obtained for BLFs. In fact, defining the visitation efficiency $\epsilon \equiv \mathrm{d}S_N/\mathrm{d}t$ [13], assuming that $N \propto t$ and that the rate constant (K) behaves like $K \propto \epsilon$, from (7) it follows

$$\frac{\mathrm{d}\rho_A}{\mathrm{d}t} = -K\rho_A^2 \cong -\epsilon\rho_A^2 \propto -R_M^{f(\sigma)} t^{d_s - 1} \rho_A^2 \tag{10}$$

and then integrating (10) one has

$$\frac{\mathrm{d}\rho_A}{\mathrm{d}t} \propto -R_M^{f(\sigma)} \rho_A^X. \tag{11}$$

Therefore, for BLFs one expects that the same behaviour as that for ordinary walkers should hold but scaling the rate constant by a factor $R_M^{f(\sigma)}$, as it follows from the definition of ϵ and the assumed proportionality between K and ϵ. In order to test the validity of (10) Monte Carlo simulations of recombination reactions between A-BLFs in one dimension have been performed using standard techniques [15, 16]. For this purpose it is convenient to integrate (11), so one gets $(\rho_{0A}^{-(X-1)} - \rho_A^{-(X-1)}) \propto t$

where ρ_{0A} is the initial concentration of A-BLFs. Figure 5 shows a plot of $(\rho_{0A}^{-1} - \rho_A^{-1})$ against the Monte Carlo time. Shortly after the beginning of the reaction ($t < 100$) the plot exhibits a straight line behaviour with slope $X - 1 = 1$ in agreement with (9*b*). Nevertheless, for $t > 100$ one observes the crossover from the classical ($X = 2$) to the anomalous behaviour. So, for the latter the straight line obtained has a slope $X - 1 = 1/d_s (d_s = \frac{1}{2})$ as expected from (9*b*). Therefore, for short-time (high concentration regime) the reaction proceeds according to the classical prediction i.e. a typical second-order reaction, while for $t \Rightarrow \infty$ (low concentration regime) the BLFs actually 'feel' the 1D nature of the sample and the anomalous behaviour ($X = 3$) holds. Annihilation reactions of ordinary walkers in one dimension have already been studied in detail [13, 15] and the results are in agreement with the data shown in figure 5.

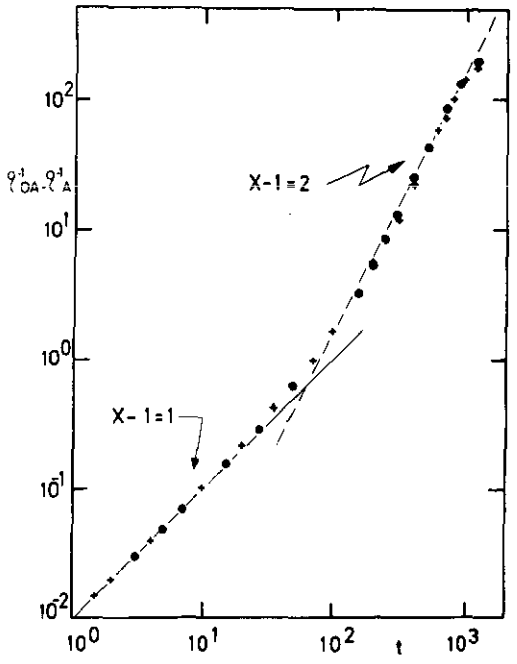

Figure 5. Log–log plot of $(\rho_{0A}^{-1} - \rho_A^{-1})$ against t for annihilation reactions between BLFs with $\rho_{0A} = 1.0 (+) \sigma = 10^{-1}, R_M = 10^2; (o) \sigma = 10^{-2}; R_M = 10^2$. The full (broken) line with slope $X - 1 = 1 (X - 1 = 2)$ has been drawn for comparison, respectively. More details in the text.

4. Conclusions and remarks

In this work, a new kind of random walk, the so-called bounded Lévy flights (BLFs), where the step length is a bounded random variable, is proposed and studied in one dimension. Both the mean number of distinct sites visited by the walker and the average square displacement of BLFs behave like ordinary walkers after a suitable

scaling of the number of steps performed by the walker. The scaling functions and exponents are evaluated.

Exchange mediated annihilation reactions between BLFs exhibit a crossover from the classical ($t \Rightarrow 0$, concentration $\rightarrow 1$, $X = 2$) to the anomalous ($t \Rightarrow \infty$, concentration $\rightarrow 0$, $X = 3$) behaviour, where X is the reaction order given by $X = 1 + d_s$ with $d_s = \frac{1}{2}$ for the former (d_s is the random walk exponent of BLFs in one dimension).

It should be interesting to study whether the behaviour observed in one dimension for annihilation reactions between BLFs also holds in higher dimensions and fractal media. In fact, recombination reactions between atoms and molecules is a topic of major interest in many fields such as biophysics, catalysis, exchange-dominated reactions in solids, etc. More work also has to be done in order to understand the role played by long-range interactions in recombination reactions.

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