Random walk in chemical space of Cantor dust as a paradigm of superdiffusion

Alexander S. Balankin,[1] Baltasar Mena,[2] C. L. Martínez-González,[1] and Daniel Morales Matamoros[3]
[1]*Grupo "Mecánica Fractal," Instituto Politécnico Nacional, México Distrito Federal 07738, Mexico*
[2]*Instituto de Ingeniería, Universidad Nacional Autónoma de México, México Distrito Federal, Mexico*
[3]*Instituto Mexicano del Petróleo, México Distrito Federal 07730, Mexico*
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We point out that the chemical space of a totally disconnected Cantor dust $K_n \subset E^n$ is a compact metric space C^n with the spectral dimension $d_s = d_\ell = n > D$, where D and $d_\ell = n$ are the fractal and chemical dimensions of K_n, respectively. Hence, we can define a random walk in the chemical space as a Markovian Gaussian process. The mapping of a random walk in C^n into $K_n \subset E^n$ defines the quenched Lévy flight on the Cantor dust with a single step duration independent of the step length. The equations, describing the superdiffusion and diffusion-reaction front propagation ruled by the local quenched Lévy flight on $K_n \subset E^n$, are derived. The use of these equations to model superdiffusive phenomena, observed in some physical systems in which propagators decay faster than algebraically, is discussed.

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Diffusion is one of the basic nonequilibrium transport phenomena [1–3]. It is, therefore, of fundamental relevancy in physics, chemistry, biology, and the social sciences [1–5]. Diffusive processes are closely tied with a random walk [6,7]. A random walk is a stochastic process in which particles move in a sequence of randomly directed steps of length ε and duration t_ε drawn from a specific probability distribution $p(\varepsilon,t_\varepsilon)$. The usual characterization of a random walker uses its mean-squared displacement, which for long enough times, asymptotically behaves as

$$\langle r^2 \rangle = \Xi_\gamma t^\gamma, \tag{1}$$

where Ξ_γ is the generalized diffusion constant and γ is the diffusion exponent [2,3]. Accordingly, diffusion processes are classified by analyzing the spread of the distance traveled by a random walker. In this way, a normal diffusion is well described in the theory of Brownian motion as a Gaussian process that is both local in space E^n and local in time t such that the propagator is $P(r,t) = (4\pi\,\Xi_1 t)^{-n/2} \exp(-r^2/4\Xi_1 t)$, and the mean-squared displacement (1) grows linearly in time ($\gamma = 1$).

The law of Brownian motion crucially relies on assumptions that the steps for the diffusing particle are small (with finite variance) and uncorrelated (Markovian nature of the underlying stochastic process). However, these assumptions do not hold for many complex systems in which diffusion also obeys the scaling relation (1) but with $\gamma \neq 1$. Diffusion processes with $\gamma \neq 1$ are termed as an anomalous diffusion and are called the subdiffusion if $\gamma < 1$ or the superdiffusion if $\gamma > 1$ [2–7]. Subdiffusion, for instance, appears in confined nanofilms [8], in charge carrier transport in amorphous semiconductors [9], and in the motion of a bead in a polymer network [10]. A classic example of superdiffusive phenomena is Richardson's observation that two particles moving in a turbulent fluid, which at time $t = 0$ are originally placed very close to each other, have a relative separation r at time t that follows relation (1) with $\gamma = 3$ [11]. Superdiffusion was also encountered in the light transport in disordered media [12,13], in diffusion of adsorbed molecules at liquid surfaces [14], in arrays of vortices in a rotating flow [15], in layered velocity fields [16], in the atmosphere [17], in geologic formations [18], and in the evolution of the stock markets [19] to name a few examples (see also Ref. [20]).

Although anomalous diffusion can be attributed to diverse reasons (see Refs. [2,21–28]), it is widely accepted that any subdiffusive process can be mapped into a random walk on a path-connected fractal, which serves as a general paradigm of anomalous subdiffusion [2–7]. Consequently, most approaches to anomalous diffusion on fractals exclude (explicitly or implicitly) the superdiffusive cases [27–39]. The random walk on a fractal embedded in E^n is governed by its topological dimension d, the fractal (metric) dimension $d < D \leqslant n$, the fractal dimension of shortest (minimum) pass $d_{\min}$, and the random walk dimension D_W [2–5]. The fractal dimension determines the number of sites $M \propto r^D$ within Euclidean distance r, whereas, the shortest path between two sites on the fractal (chemical distance) scales as $\ell \propto r^{d_{\min}}$, and the average number of random steps (s) needed to reach distance r scales as $s \propto r^{D_W}$ [3]. Accordingly, in the chemical space, $M \propto \ell^{d_\ell}$, where $d_\ell = D/d_{\min}$ is the chemical dimension of the fractal while $s \propto \ell^{d_W}$, where $d_W = D_W/d_{\min}$ [3–5]. For a regular random walk, the number of steps $s \propto t$, and so, the walk on a fractal obeys the scaling relation (1) with

$$\gamma = \frac{2}{D_W} = \frac{d_s}{D}, \tag{2}$$

where d_s is the spectral dimension of the fractal, whereas, the last equality is due to the Alexander and Orbach law $d_s = 2D/D_W = 2d_\ell/d_W$ (see, for review, Refs. [2–7]). For path-connected fractals, $1 \leqslant d_{\min} \leqslant D$, and so, $d \leqslant d_\ell \leqslant D \leqslant n$. For instance, for loopless Koch curves, $d_\ell = d_s = d = 1 < n$, and so, $D_W = 2D = 2d_{\min} > 2$, whereas, for fractals with $d_{\min} = 1$, such as Sierpinski gaskets and carpets, $d < d_\ell = D < n$, whereas, $D_W > 2$ and $d_s < D$ [40]. Diffusion on fractal trees with $d_s = D$ is normal, that is, $D_W = 2$ and $\gamma = 1$ [41].

Much effort has been expended in order to derive the function $P(r,t)$, giving the probability that a random walker stays at time t at a distance r from the origin. It is easy to understand that the exact propagator on a fractal with $D < n$

is a highly nonanalytic discontinuous function of $r \in E^n$ (see Ref. [30]). However, as shown in Ref. [30], we can define an analytic envelope of this propagator. Although there is no consensus about the explicit form of the propagator envelope, it is widely accepted that it can be expressed in the general form as $P(r,t) \propto t^{-d_s/2}\Phi(r^{2/\gamma}/t)$, where $r \in E^n$ and $\Phi(\xi)$ is a decreasing function of $\xi = r^{2/\gamma}/t$ [2–7]. Furthermore, the renormalization group arguments, Monte Carlo simulations, and some analytical models suggest that the propagator envelope on path-connected fractals has the following form:

$$P(r,t) \propto t^{-d_s/2}\left(\frac{r^{2/\gamma}}{t}\right)^{\alpha} \exp\left[-c\left(\frac{r^{2/\gamma}}{t}\right)^{\nu}\right], \qquad (3)$$

while the scaling exponents defined by different authors are given in Table I (notice that the analytic envelope can be defined for $r > t^{\gamma/2}$only). Somewhat different forms of $\Phi(\xi)$ for subdiffusion on path-connected fractals were suggested in Refs. [37–39]. Nonetheless, it should be pointed out that all propagators of subdiffusion on path-connected fractals decay at long distances faster than algebraically.

In contrast to the subdiffusion, the superdiffusion is more commonly associated with non-Gaussian jump-type processes, which violate the central limit theorem, such as the Lévy flights or walks (see Refs. [3–5]). Unlike ordinary random walks, which consist of independent random increments with a typical scale, single steps of the Lévy motion occur on all scales due to divergent moments of step length distributed according to a probability density function with the power-law asymptotic $p(\varepsilon) \propto |\varepsilon|^{-(\mu+1)}$, where $0 < \mu < 2$ is the Lévy index. For a Lévy flight, each step takes a unit time, whereas, for a Lévy walk, the time duration of a step is proportional to the length of the step, i.e., $t_\varepsilon \propto \varepsilon$. The step size statistic can be either imposed by an uncorrelated Lévy noise if the lengths of jumps are chosen randomly at each time step (annealed Lévy motion) or attributed to the medium topology (quenched Lévy motion). In the last case, the steps are strongly correlated due to a topological constraint (see, for review, Refs. [12,13,21,22]). Notice that the annealed and quenched Lévy motions lead to different classes of superdiffusion [21,22].

In this Brief Report, we suggest that superdiffusion can also be ruled by a Markovian random walk in the chemical space of totally disconnected Cantor dust embedded in the Euclidean space E^n such that the analytic envelope of the local propagator, averaged over all starting points on $K_n \subset E^n$, decays faster than algebraically.

Cantor dusts represent a class of self-similar totally discontinuous fractals with zero Lebesgue measure. Classic middle-third Cantor set K_1 is constructed by repeatedly removing the open middle third of a set of line segments starting from [0,1]. The points left over form a nowhere-dense subset of the real line $K_1 \subset [0,1]$, the fractal dimension of which is $D = \ln 2/\ln 3$ [40]. Furthermore, by dividing the line into k segments and removing, in each iteration, $m < k$ segments with probability $p(m)$, one can construct either a statistically self-similar Cantor set with $0 < D = \ln(k-m)/\ln k < 1$ if $p = 1$ or a multifractal Cantor set characterized by a continuum spectrum of the Rényi dimensions [42].

From a topological point of view, a fractal Cantor set is a zero-dimensional, bounded, perfect (every point is a limit point), uncountable, measurable compactum (without isolated points), which is unique up to a homeomorphism [43]. Furthermore, there is a one-to-one correspondence between the Cantor set and all points in the unit interval, although the Lebesgue measure of the Cantor set is zero and the measure of the unit interval is 1 [43]. Multidimensional Cantor dust $K_n \subset E^n$ is a generalization of the classical Cantor set $K_1 \subset [0,1]$ [40,44]. It can be either constructed in the same way as the Cantor set but starting from the n-dimensional unit cube $[0,1]^n$ or formed in E^n as the Cartesian product of n orthogonal Cantor sets with equal or different fractal dimensions D_i. The fractal dimension of Cantor dust $K_n \subset E^n$ is equal to $D = \sum_i^n D_i$ [40].

A noteworthy feature of any Cantor dust is that its chemical dimension coincides with the dimension of the embedding Euclidean space E^n, that is, $d_\ell = n > D$, whereas, the topological dimension of totally disconnected dusts is zero and $d_{\min} = D/n < 1$. Hence, we can define a Markovian random walk in the chemical space C^n with the Euclidean metric $\ell^2(X,Y) = \sum_1^n \ell_i^2$, where $\ell_i = (\widehat{x}_i - \widehat{y}_i)$ and, asymptotically, $\ell_i \propto (x_i - y_i)^{d_{\min}^{(i)}}$, whereas, $\widehat{x}_i, \widehat{y}_i$ and x_i, y_i denote the Cartesian coordinates of points $X, Y \in C^n$ in C^n and E^n, respectively. Furthermore, it was proved that every compact

TABLE I. Scaling exponents of the analytic envelope (3) of a propagator in different models of anomalous diffusion and their applicability to diffusion on different types of fractals. The symbol "?" means unknown.

Model	ν	α	Koch curves $d_{\min} = D$, $d_\ell = d_s = 1, n = 2$	Sierpinski gasket $d_{\min} = 1, d_\ell = D$	Cantor dust $d_\ell = n, d_s = n$
Normal diffusion	$1\ (D_W = 2)$	0	Not applicable		
A [29,30]	$1\ (D_W = 2+\theta)$	0	Best fit [36]	Poor fit [4]	Coincide with Eq. (5)
B [31]	$1/(D_W - 1)$	0	Not applicable	Better fit for long times	Not applicable
C [32]	$1/(D_W - 1)$	$(2D - D_W)/2(D_W - 1)$	Coincide with model B	Better fit for short times	Not applicable
D [33]	$1/(D_W - 1)$	$(d_s - D)/2(D_W - 1)$	Not applicable	?	Not applicable
E [34]	$1/(D_W - 1)$	$(1 - 2D + d_s)/2(D_W - 1)$	Not applicable	?	Not applicable
F [34]	$d_{\min}/(D_W - d_{\min})$	0	Coincide with model A	Coincide with model B	Coincide with Eq. (5)
Equation (5)	$\nu = 1, d_s = n,$ $D_W = 2D/n$	0	Not applicable		Superdiffusion

metric space is a continuous image of the Cantor set, that is, for each compact metric space C, there is a continuous map from the Cantor set onto C [45]. This permits the homeomorphic mapping of the random walk in C^n into the random walk on $K_n \subset E^n$ such that the Euclidean distance between two points $X,Y \in K_n \subset E^n$ is $r(X,Y) \propto \ell^{n/D}$ where $D = \sum_i^n d_{\min}^{(i)}$.

Another remarkable feature of Cantor dusts is that their spectral dimensions are determined by the degree of freedom of a point in the embedding space E^n, that is, $d_s = n = d_\ell$. Therefore, a Markovian random walk in the chemical space C^n is a Gaussian process characterized by the universal walk dimension $d_W = 2d_\ell/d_s = 2$. Hence, the random walk propagator in the chemical space of Cantor dust has the Gaussian form $P(r,t) = (4\pi\,\Xi_\ell t)^{-n/2} exp(-\ell^2/4\Xi_\ell t)$, and so, the Brownian motion in C^n is expected to obey the diffusion equation,

$$\frac{\partial P}{\partial t} = \Xi_\ell \ell^{1-n} \frac{\partial}{\partial \ell}\left(\ell^{n-1}\frac{\partial}{\partial \ell} P\right), \tag{4}$$

similar to the classic diffusion equation in E^n. The homeomorphic mapping from the chemical space of Cantor dust C^n into $K_n^D \subset E^n$ implies that the analytic envelope of the random walk propagator in E^n becomes non-Gaussian. Notice that the local propagator $P_j(r,t)$ on $K_n^D \subset E^n$ depends on the starting point j on the small distances r_j from j but obeys the universal asymptotic behavior for large distances $r_j \propto \ell^{1/d_{\min}} \propto r \gg t^{\gamma/2}$. Accordingly, the asymptotic behavior of the analytic envelope is independent of the starting point of the process on $K_n \subset E^n$ and has the form

$$P(r,t) \propto t^{-n/2} \exp\left[-c\left(\frac{r^{2D/n}}{t}\right)\right], \tag{5}$$

which resembles the asymptotic behavior of the propagator envelope on path-connected fractals [see Eq. (3)] rather than the propagator of the annealed Lévy motion because the step length distribution decays faster than algebraically. Notice that the local propagators of the quenched Lévy walk on Cantor graphs also do not display long tails [21,22]. However, if we first average the local propagators, which are explicitly dependent on the starting point, the asymptotic behavior of the averaged function obeys the algebraic decay such that the thermodynamic limit and the limit of long space and time do not commute [21,22]. This is typical of inhomogeneous systems (see, for review, Ref. [46]). So, one may expect that the asymptotic behavior of the average and of the local quantity can be different, even if the asymptotic behavior of $P_j(r,t)$ does not depend on j. This point requires special attention in further studies.

In the local case (5), the average of the walker's square displacement over the Cantor dust with the fractal measure $d^D r = r^{D-1} dr$ yields to the relation $\langle r^2 \rangle = \int r^2 P(r,t) r^{D-n} d^n r = \Xi_\gamma t^\gamma$ with the scaling exponent $\gamma = n/D = 1/d_{\min} > 1$. Furthermore, substituting $\ell \propto r^{d_{\min}}$ into Eq. (4), we get the diffusion equation,

$$\frac{\partial P}{\partial t} = \frac{n^2 \Xi_C}{D^2} r^{1-D} \frac{\partial}{\partial r}\left(r^{D(1-2/n)+1} \frac{\partial}{\partial r} P\right), \tag{6}$$

describing the superdiffusion on an isotropic Cantor dust embedded in E^n. Notice that, generally, Eqs. (5) and (6) do not hold for diffusion on the path-connected fractals, except for special cases, such as the loopless Koch curves with $d_{\min} = D$, which are homeomorphic to the closed interval $[0,1]$. Furthermore, taking into account that isotropic Cantor dusts are characterized by $d_s = d_\ell = n$, $d_{\min} = D/n$, and $D_W = 2d_{\min}$, one can see that Eq. (5) is consistent with the propagators of models A and F (see Table I) suggested in Refs. [29,30,35] from quite different physical arguments, but it differs from the propagators of models B–E (see Table I) suggested in Refs. [31–34] for random walks on the path-connected fractals. In fact, it is easy to understand that model A, developed in Ref. [30], implicitly states that $d_\ell = d$, whereas, to construct models B–E, it was explicitly or implicitly assumed that $d_{\min} = 1$, and so $d_\ell = D$, whereas, $d_s \leqslant D$. Consequently, models B–E provide better fits to the results of numerical simulations on the Sierpinski-type fractals (see Refs. [31–34]). Alternative models [37–39] are associated with non-Markovian random walks with a long-time memory.

It is pertinent to note that the Lagrangian approach, suggested in Ref. [35] (model F in Table I), implies that $D_e = D - D_W$, where D_e governs the scaling behavior of energy $e \propto r^{D_e}$. Physically, one expects that the energy is a nondecreasing function of r, and therefore, $D_e \geqslant 0$. Hence, the Lagrangian approach [35] is applicable for the random walk on the fractals with $D \geqslant D_W$ only. However, surprisingly, for some types of fractals with $D_W > D$, the propagator of model F coincides with propagators providing the best fits to numerical simulations of random walks on these fractals (see Table I), but the predicted values of $D_e < 0$ appear to be unphysical. Therefore, the coincidences of propagators derived in model F and models A and B for specific types of fractals with $D_W > D$ seem to be fortunate, rather than physically justified. On the other hand, for Cantor dust in E^n, the chemical and Lagrangian metrics coincide, that is, $\ell_L \propto r^{D_W/2} \propto r^{d_{\min}} \propto \ell$. Consequently, in this case, the propagator, derived within the Lagrangian approach, coincides with Eq. (5) for the superdiffusion on the Cantor dust obeying the scaling behavior (1) with the scaling exponent $\gamma = n/D > 1$. Accordingly, the Lévy flight, ruled by the random walk in the chemical space of Cantor dust, is characterized by the energy scaling with $D_e = D - D_W = (n-2)d_{\min} \geqslant 0$ in the Euclidean space of $n \geqslant 2$, but $D_e < 0$ in the case of $n = 1$. Notice, in this context, that a Lévy flight on $K_1 \subset [0,1]$ is recurrent (returns to the origin infinitely many times), whereas, if $n \geqslant 3$, a Lévy flight on a Cantor dust is transient (some parts of the dust remain unvisited).

Accordingly, a superdiffusive phenomenon in a physical system can be associated with annealed or quenched Lévy motion (walk or flight) such that the propagator displays either algebraic or faster decay at longer distances. Although in both cases, the mean-squared displacement behaves as (1) with $\gamma > 1$, the difference in propagator asymptotics permits distinguishing between two kinds of superdiffusion for a specific system. In this context, we note that the authors of Ref. [47] have emphasized that the tail of the Richardson propagator is not algebraic and, thus, question the relevance of the Lévy motion for the superdiffusion observed in Ref. [11]. The model suggested in this Brief Report permits avoiding the contradiction pointed out in Ref. [47]. In fact, Eqs. (5) and (6) are converted into the equations originally used to describe

the Richardson superdiffusion (see Ref. [11]) if we set $n = 3$ and $D = n/3$, that, in E^3, corresponds to the random walk in the chemical space of Cantor dust with $D = 1$, whereas, $d = 0$, $d_{\min} = 1/3$, and $D_W = 2/3$ such that $\gamma = 3$, but the propagator has the form of Eq. (5).

The superdiffusion equation (6) can be generalized for a random walk on an anisotropic Cantor dust treated as the Cartesian product of n orthogonal Cantor sets of different dimensions $0 < D_i < 1$ $(i = 1,2,\ldots,n)$ such that the shortest paths along the Cartesian axes are characterized by $d_{\min}^{(i)} = D_i$, whereas, $D = \sum_i^n D_i$ and $D_W = (2/n)\sum_1^n d_{\min}^{(i)} = 2D/n$. It is a straightforward matter to see that, in the Cartesian coordinates (x_i), the equation of superdiffusion has the form

$$\frac{\partial P}{\partial t} = \sum_i^n \frac{\Xi_i}{\left(d_{\min}^{(i)}\right)^2} x_i^{1-d_{\min}^{(1)}} \frac{\partial}{\partial x_i}\left(x_i^{1-d_{\min}^{(i)}} \frac{\partial}{\partial x_i} P\right), \qquad (7)$$

where Ξ_i is the diagonal tensor of the diffusion coefficients. It is interesting to note that, if $\Xi_i/(d_{\min}^{(i)}) = \Xi$ for all Cartesian directions, then Eq. (8) can be rewritten in the form $\partial P/\partial t = \Xi_i \Delta_H P$, where Δ_H is the Hausdorff Laplacian introduced in Ref. [48] in the context of fractal continuum flow.

Equation (6) describes how the analytic envelope of probability density varies in time according to the spatial behavior of individuals on an isotropic Cantor dust. To account for individuals appearing and disappearing at any occupied point of the dust, in Eq. (6), we can include logistic term $\propto (1 - P)P$ for production, commonly employed in biological applications (see Refs. [49]). The solution of Eq. (6) with the additional term on the right hand side describes the propagation of the diffusion-reaction front in the Cantor dust. This solution should obey the general form of traveling fronts (see Ref. [50]). In particular, the Hamilton-Jacobi method (see Ref. [51]) yields that the speed of the traveling front in an isotropic Cantor dust increases in time as $V \propto t^{1/d_{\min}-1}$, that is, the superdiffusion produces the acceleration of reaction-diffusion fronts in Cantor dusts with $d_{\min} < 1$. Accordingly, we noted that acceleration of chemical waves observed in a Belousov-Zhabotinsky reaction in a quasi-two-dimensional chaotic flow [52] can be described within the framework of our model, rather than using a model with a heavy tailed propagator. In fact, in the experiments of Ref. [52], it was found that the superdiffusion exponent $\gamma = 1.3 \pm 0.1$ is independent of the Lévy index $0.7 \leqslant \mu \leqslant 1.6$ as is expected in the case of the random walk in the chemical space of Cantor dust in contrast to the strong dependence of the front acceleration rate on the Lévy index expected (see Ref. [52]) in models with the propagator having a power-law asymptotic behavior.

Summarizing, we have introduced a model of a random walk in the chemical space of Cantor dust. The mapping of the random walk in C^n into $K_n \subset E^n$ defines the local quenched Lévy flight on the Cantor dust with a constant step duration independent of the Euclidean length of single steps. The asymptotic of an analytic envelope of the local propagator, averaged over all admissible starting points on $K_n \subset E^n$, displays a stretched exponential decay at longer distances. This permits explaining the superdiffusion with the propagator decaying at longer distances faster than algebraically as observed in some physical systems. Hence, a random walk in the chemical space of Cantor dust can be considered as a paradigm of superdiffusion without a long-tailed asymptotic of propagator. The equations, describing superdiffusion with the stretched exponential decay of the propagator envelope, are derived. The acceleration of reaction-diffusion fronts in Cantor dusts is predicted.

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