Reaction spreading in systems with Anomalous Diffusion

Angelo VULPIANI

Dept. of Physics, University of Rome "Sapienza", Italy
< angelo.vulpiani@roma1.infn.it >

Yerevan, Sept. 2016

SUMMARY

*** Diffusion Processes**

*** Standard Diffusion**

*** Anomalous Diffusion**:

a) *weak anomalous diffusion*

b) *strong anomalous diffusion*

*** Reaction- diffusion systems**:

a) *front propagation in presence of sub/super diffusion*

b) *reaction spreading on graphs*

A special thank to DAVIDE VERGNI

Thanks to:
Marcus Abel, Ken Andersen
Federico Bianco, Guido Boffetta
Raffaella Burioni, Patrizia Castiglione
Fabio Cecconi, Massimo Cencini
Sergio Chibbaro, Giuseppe Forte
Rosaria Mancinelli, Andrea Mazzino
Paolo Muratore- Ginanneschi, Maurizio Serva

A (short) review paper
F. Cecconi, D. Vergni and A. Vulpiani
Reaction Spreading in Systems With Anomalous Diffusion
Math. Model. Nat. Phenom. **11**, 107 (2016)

A diffusion (transport) process can be seen as:

* *From a Lagrangian point of view:*
A deterministic, or stochastic, rule for the time evolution $\mathbf{x}(0) \to \mathbf{x}(t) = \mathcal{S}^t \mathbf{x}(0)$, e.g.

A $\quad x(t+1) = x(t) + w(t) \ , \ \ w(t) = \textit{random variable}$

B $\quad x(t+1) = f(x(t)) \quad , \qquad f(x(t)) = \textit{chaotic map}$

C $\quad \dfrac{d\mathbf{x}}{dt} = \mathbf{u}(\mathbf{x}, t) + \sqrt{2D_0}\eta \quad , \qquad \eta(t) = \textit{white noise}$

* *From an Eulerian point of view:*
A rule for the time evolution of the PdF $\rho(\mathbf{x}, t)$, e.g. in the case **C**, for the incompressible flow $\nabla \cdot \mathbf{u} = 0$, one has the advection-diffusion equation (Fokker-Planck eq.)

$$\frac{\partial \rho}{\partial t} + (\mathbf{u} \cdot \nabla)\rho = D_0 \Delta \rho \ .$$

The typical scenario: Standard Diffusion

At large scale and asymptotically in time, usually one has the so called **standard diffusion** i.e. a Fick's law holds (just for simplicity we consider the case $<\mathbf{x}>=0$)

$$\frac{\partial \Theta}{\partial t} = \sum_{i,j} \mathcal{D}_{ij} \frac{\partial^2 \Theta}{\partial x_i \partial x_j}$$

and a Gaussian behavior.

Θ is the spatial coarse graining of ρ, and $\mathcal{D}_{ij}$ is the effective (eddy) diffusion tensor, depending (often in a non trivial way) from D_0 and the field $\mathbf{u}$:

$$\Theta(\mathbf{x}, t) \sim exp - \frac{1}{4t} \sum_{i,j} x_i [\mathcal{D}^{-1}]_{ij} x_j$$

$$< x_i(t) x_j(t) > \simeq 2\mathcal{D}_{ij} t \, .$$

QUESTIONS

* Is the standard diffusion generic?

* How violate the standard diffusion?

A) For incompressible velocity field $\nabla \cdot \mathbf{u} = 0$, if $D_0 > 0$ one has standard diffusion if the infrared contribution of $\mathbf{u}(\mathbf{x})$ is not "too large" (Majda-Avellaneda), i.e.

$$\int \frac{|\mathbf{V}(\mathbf{k})|^2}{k^2} d\mathbf{k} < \infty \tag{1}$$

where $\mathbf{V}(\mathbf{k})$ is the Fourier transform of $\mathbf{u}(\mathbf{x})$.

B) Standard diffusion is present if the lagrangian correlations decay fast enough (Taylor), i.e.

$$\int_0^\infty < v_L(t) v_L(0) > dt < \infty \tag{2}$$

where $v_L(t) = dx(t)/dt$ is the lagrangian velocity.

Anomalous diffusion is, somehow, a pathology: it is necessary the violate the hypothesis for the validity of central limit theorem.

EXAMPLES OF ANOMALOUS DIFFUSION:
Ex 1: Longitudinal diffusion in a random shear (Matheron and de Marsily): $\mathbf{u}(\mathbf{x}) = (U(y), 0)$, where $U(y)$ is a spatial random walk; it is possible to show that

$$< x(t)^2 > \sim t^{3/2} \ , \ \ \rho(x,t) \sim \frac{1}{t^{3/4}} \, exp - C\frac{x^4}{t^3} \ .$$

Ex 2: Levy walk

$$x(t+1) = x(t) + v(t)$$

where $v(t)$ is a random variable which can assume two values $\pm u_0$ for a duration T given by a random variable whose PdF is $\psi(T) \sim T^{-(\alpha+1)}$.

For $\alpha > 2$, one has the usual standard diffusion, on the contrary if $\alpha \leq 2$ one has a superdiffusion:

$$< x^2(t) > \sim t^{2\nu}$$

where

$$\nu = 1 \ , \ if \ \alpha < 1 \ , \ \nu = \frac{(3-\alpha)}{2} \ , \ if \ 1 < \alpha < 2 \ .$$

Ex 3: Lagrangian chaos in $2d$

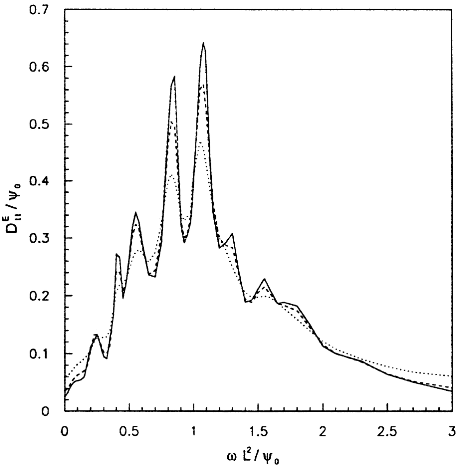
$$\frac{dx}{dt} = \frac{\partial \psi(x,y,t)}{\partial y} + \sqrt{2D_0}\,\eta_1 \ ,$$

$$\frac{dy}{dt} = -\frac{\partial \psi(x,y,t)}{\partial x} + \sqrt{2D_0}\,\eta_2 \ ,$$

where

$$\psi(x,y,t) = \psi_0 \sin\left(\frac{2\pi x}{L} + B \sin \omega t\right) \sin\left(\frac{2\pi y}{L}\right)$$

the term $B \cos \omega t$ represents the lateral oscillation of the rolls. For $B \neq 0$ one has chaos, generated by the mechanism of the homoclinic intersection.
The effective diffusion coefficient depends from D_0 and ω in a non trivial way.



Lagrangian chaos in $2d$: $\mathcal{D}_{11}$ vs ω (rescaled), $D_0/\psi_0 = 3 \times 10^{-3}$ (dotted curve); $D_0/\psi_0 = 10^{-3}$ (broken curve); $D_0/\psi_0 = 4 \times 10^{-4}$ (full curve).

Two different ways to have anomalous diffusion

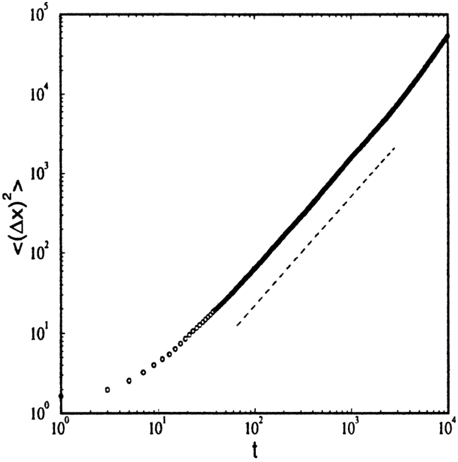
I) In the random shear flow the anomalous diffusion is due to the violation of (1) i.e. the infrared contributions are dominant.

II) In the Levy walk, the "violation" of the central theorem is due to the non integrable long tail of the velocity-velocity correlation function which determines, for $\alpha < 2$ (superdiffusion):

$$< v_L(t) v_L(0) > \sim t^{-\beta} \;\; , \;\; with \;\; \beta < 1 \, .$$

The same mechanism is present, for $D_0 = 0$ and special values of ω, in the Lagrangian chaos in the oscillating rolls.

An example of anomalous diffusion



Lagrangian chaos in 2d: $< x^2(t) >$ vs t, with $D_0 = 0$ and $\omega = 1.1$, the dashed line indicates $t^{1.3}$.

The result in the previous system is non an isolated case.
Such kind of mechanism is rather common in low dimensional symplectic chaotic systems, e.g. in the standard map

$$\theta_{t+1} = \theta_t + J_t \ , \ J_{t+1} = J_t + K \sin(\theta_{t+1})$$

for some peculiar values of K.

The long tail in the correlation function is due to the presence of (weakly unstable) ballistic trajectories.

SOME NATURAL QUESTIONS

* Does the value of the scaling exponent ν allow to determine the shape of $\rho(x,t)$?

* Is the scaling exponent ν (for $< x^2(t) >$) the unique relevant quantity?

In the standard diffusion one has $\nu = 1/2$ and a gaussian feature:

$$\Theta(x,t) \sim \frac{1}{t^{1/2}}\, exp - C\left(\frac{x}{t^{1/2}}\right)^2 \ ,$$

$$< |x(t)|^q > \sim t^{q/2}$$

Naively, in the case of anomalous diffusion, one could guess the simplest generalization:

$$\Theta(x,t) \sim \frac{1}{t^{\nu}} F_{\nu}\left(\frac{x}{t^{\nu}}\right) , \quad (3)$$

$$< |x(t)|^{q} > \sim t^{q\nu}$$

where $F_{\nu}(\,)$ is a suitable function, in the Gaussain case $F_{1/2}(z) = exp - Cz^2$.

The above scenario is called **weak anomalous diffusion**:
the exponent ν is sufficient to describe the scaling features, and the PdF has a scaling shape.

The existence of anomalous scaling in fully developed turbulence (and other phenomena) suggests that a more complex scenario can appear, namely

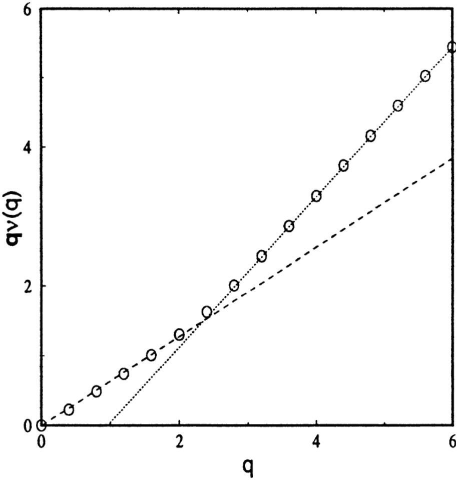
$$< |x(t)|^q >\sim t^{q\nu(q)}$$

where $\nu(q)$ is not constant.
In such a case called **strong anomalous diffusion** *the PdF cannot have a scaling structure* as in (3).

Are there non trivial examples of strong anomalous diffusion?

A first example: Lagrangian Chaos in Rayleigh-Benard convection; for $D_0 = 0$ for some values of ω, one has $\nu(q) \neq const$.

An example of strong anomalous diffusion



Lagrangian chaos in $2d$, $D_0 = 0$ and $\omega = 1.1$: $\nu(q)$ vs q, the dashed line corresponds to $0.65q$, the dotted line corresponds to $q - 1.04$ (Castiglione et al 1999).

The Lagrangian Chaos in Rayleigh-Benard convection is not an isolated case of strong anomalous diffusion (Pikovsky, Artuso, Cristadoro, Klages et al.)

Other examples:
* $1d$ intermittent maps
* Standard Map
* Levy walks

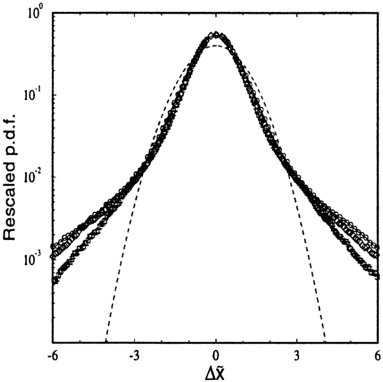
In particular it is rather common the following shape:

$$q\nu(q) \simeq q\nu(0) \ , \ for \ \ q < q^* \ ,$$

$$q\nu(q) \simeq q - const. \ , \ for \ q > q^* \ .$$

In some stochastic processes it is possible to derive, the above shape:

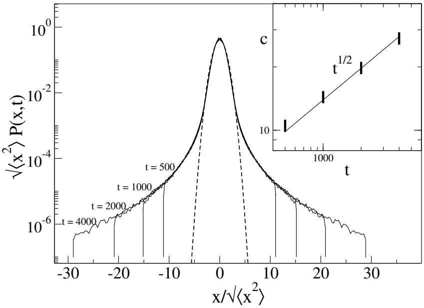
In presence of strong anomalous diffusion there is not a scaling structure of the PdF (Castiglione et al)



Lagrangian chaos in 2d, $D_0 = 0$ and $\omega = 1.1$: rescaled PdF: $p(x/t^{\nu(0)})$ vs $x/t^{\nu(0)}$ for three different times $(500, 1000, 2000)$.

Even in presence of standard diffusion, i.e. $< x^2(t) > \sim t$, the scenario can be not trivial (Forte et al)

For instance in the Levy walk with $\alpha > 2$ one has $\nu(2) = 1/2$, but the PdF does not rescale and $\nu(q) \neq 1/2$ for large values of q



Levy walk, $\alpha = 2.2$, rescaled PdF: $p(x/t^{\nu(2)})$ vs $x/t^{\nu(2)}$ for different times.

A NON ACADEMIC PROBLEM

RELATIVE DISPERSION IN TURBULENCE

The classical result of Richardson in the inertial range

$$< R^2(t) > \sim t^3$$

where $R(t) = |\mathbf{x}_1(t) - \mathbf{x}_2(t)|$. Now, a posteriori, this result is nothing but a simple consequence of the Kolmogorov scaling $\delta v(\ell) \sim \ell^{1/3}$.

What about the effect of intermittency for the relative diffusion? Two possible scenarios:

* Weak anomalous diffusion:

$$< R^p(t) > \sim t^{\frac{3}{2}p} \;;$$

* Strong anomalous diffusion:

$$< R^p(t) > \sim t^{\alpha(p)}$$

with $\alpha(p) \neq \frac{3}{2}p$.

From the multifractal model one has a prediction for $\alpha(p)$ in terms of $D(h)$ (Boffetta et al):

$$\alpha(p) = \inf_h \left[\frac{p + 3 - D(h)}{1 - h} \right] . \qquad (4)$$

It is remarkable that, even in presence of intermittency, the Richardson scaling $\alpha(2) = 3$ is exact; the (4) has been checked in synthetic turbulence, where the velocity field is random process with the proper statio-temporal statistical features (Boffetta et al) and in direct numerical simulation of the NS equations (Boffetta and Sokolov).

The simplest reaction-diffusion problem (FKPP 1937):
a system with standard diffusion and a reactive terms

$$\frac{\partial \theta}{\partial t} = D_0 \frac{\partial^2}{\partial x^2}\theta + \frac{1}{\tau} f(\theta) \ , \tag{5}$$

asymptotically one has a front propagation:

$$\theta(x,t) = F(x - v_f t)$$

where $F(-\infty) = 1$, $F(\infty) = 0$ and, if $f'' < 0$, the front speed is

$$v_f = 2\sqrt{D_0 f'(0)/\tau} \, .$$

$$\theta(x,t) \sim exp\Big[-\frac{(x - X_F(t))}{\zeta}\Big]$$

$$X_f(t) \simeq v_f t \ , \ \zeta = 8\sqrt{D_0\tau/f'(0)}$$

What happen in presence of anomalous diffusion?

For instance we can replace the (5) with

$$\frac{\partial\theta}{\partial t} = \mathcal{L}\theta + \frac{1}{\tau}f(\theta)$$

where $\mathcal{L}$ is linear operator such that, in absence of the reaction term, the diffusion is anomalous.

For the relative diffusion according to Richardson one has

$$\mathcal{L}\theta = \frac{1}{r^{d-1}}\frac{\partial}{\partial r}\left(K(r)r^{d-1}\frac{\partial}{\partial r}\theta\right) \ , \ K(r) \propto r^{4/3} \ .$$

There is class of systems where, in spite of the presence of the anomalous diffusion, the front propagation is always standard i.e. $X_F(t) \simeq v_f t$ **with a finite** v_f**, and** $\zeta = const.$

For instance if $\nu \neq 1/2$ and the PfD has the shape (which holds for the random shear and the random walk on a comb lattice):

$$\rho(x,t) \sim \frac{1}{t^{\nu}}\, exp - C\left(\frac{x}{t^{\nu}}\right)^{\frac{1}{1-\nu}}$$

the front propagation is standard (Mancinelli et al).

On the other hand, there are cases where the front propagation can be non standard, i.e.

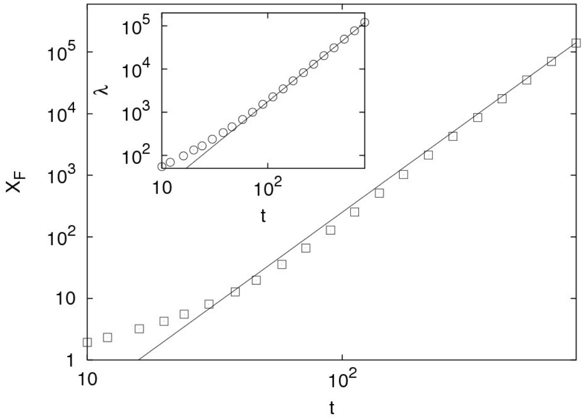
$$\theta(x,t) \sim exp\Big[- \frac{(x - X_F(t))}{\zeta(t)} \Big]$$

with

$$X_F(t) \sim t^{\gamma} \ , \ \zeta(t) \sim t^{\delta} \ with \ \delta = \gamma - 1 \ .$$

For instance in the Richardson reaction- diffusion equation one has

$$\gamma = 3 \ , \ \delta = 2 \ .$$



Front propagation in the Richardson reaction-diffusion equation: $X_F(t)$ vs t, in the insect $\zeta(t)$ vs t, the lines indicate the predictions $X_F(t) \sim t^3$, and $\zeta(t) \sim t^2$.

A simple argument

For the front propagation in presence of anomalous diffusion

* In absence of the reactive term

$$\rho(x,t) \sim \; exp - C\left(\frac{x}{t^{\nu}}\right)^{\alpha}$$

* In presence of the reactive term, at large x, $\theta(x,t) \ll 1$:

$$\theta(x,t) \sim \; exp\Big[- C\left(\frac{x}{t^{\nu}}\right)^{\alpha} + \frac{t}{\tau}\Big]$$

* The front position $X_F(t)$ is determined by the relation

$$-C\left(\frac{X_F}{t^{\nu}}\right)^{\alpha} + \frac{t}{\tau} = 0 \qquad \Longrightarrow$$

$$X_F(t) \sim t^{\delta} \quad , \quad \delta = \nu + \frac{1}{\alpha}$$

* If $\alpha = 1/(1-\nu)$ one has $\delta = 1$ even if $\nu \neq 1/2$

Sublinear front propagation in systems with subdiffusion (Serva et al 2016)

In order to have a sublinear front propagation it is necessary to have a $P(x,t)$ with very weak tails.

Subdiffusion in a process with memory, an anxious walker

$$x(t+1) = x(t) + \sigma(t)$$

$$\sigma(t) = signx(t) \;\; with \;\; probability = w(x,t)$$

$$\sigma(t) = -signx(t) \;\; with \;\; probability = 1 - w(x,t)$$

$$w(x,t) = \frac{1}{2 + \left(\frac{|x|}{t^{\lambda}}\right)^{\eta}}$$

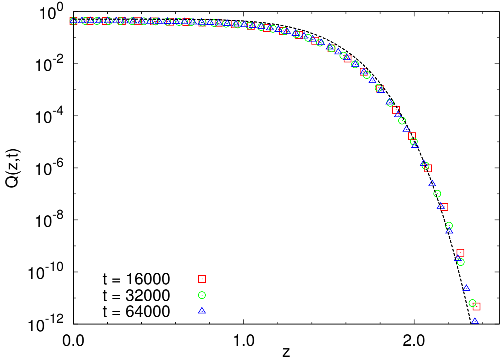
* If $|x| \ll t^{\lambda}$ we have the usual random walk
* If $\eta \to \infty$ we have the usual random walk

It is possible to show that

$$< x(t)^2 > \sim t^{2\nu} \quad , \quad \nu = min\left[\frac{1}{2}, \frac{\lambda\eta}{1+\eta}\right].$$

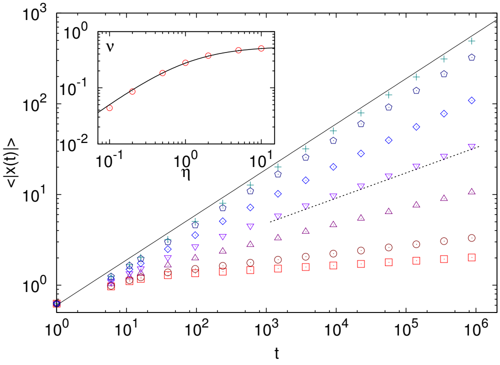
In addition in the bulk (i.e $|x|/t^{\nu}$ not too large) one has

$$\rho(x,t) \sim \frac{1}{t^{\nu}} exp - C\left(\frac{|x|}{t^{\nu}}\right)^{\eta+1} \quad .$$



PdF for $Q(z,t) = t^{\nu}\rho(x,t)$ vs $z = x/t^{\nu}$ the line indicates the prediction

$$\rho(x,t) \sim \frac{1}{t^{\nu}} exp - C\left(\frac{|x|}{t^{\nu}}\right)^{\eta+1}$$



Anomalous scaling at different η, from top to bottom $\eta = 10.0, 5.0, 2.0, 1.0, 0.5, 0.2$ and 0.1. In the inset ν vs η with the prediction

$$\nu = min\left[\frac{1}{2}, \frac{\lambda\eta}{1+\eta}\right].$$

Therefore it seems that

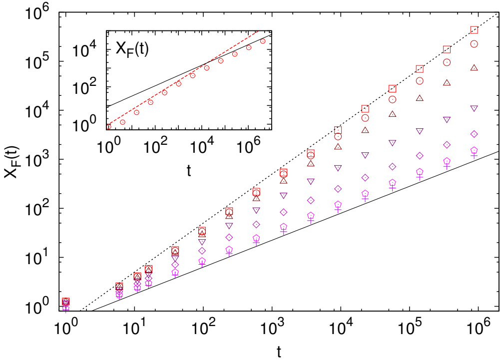
$$\delta = \frac{1 + \lambda\eta}{1 + \eta}$$

* The previous results are not enough for the asymptotic front behaviour but only for a transient which can be very long.
* Since the jump probability on the right (left) if $x > 0$ (< 0) goes to zero for $|x| > O(t^\lambda)$, the true asymptotic behaviour is

$$x_F(t) \sim t^\lambda$$

on the other hand there is a transient

$$x_F(t) \sim t^{\delta^*} \;\; with \;\; \delta^* = \frac{1 + \lambda\eta}{1 + \eta}$$



$X_F(t)$ vs t, with $\lambda = 0.55$, $\tau = 1$ at different η, from bottom to top $\eta = 10.0, 5.0, 2.0, 1.0, 0.5, 0.2$ and 0.1. In the inset, for $\eta = 1.0$, the preasymptotic behviour $X_F(t) \sim t^{\delta^*}$ and the asymptotic behaviour $X_F(t) \sim t^{\lambda}$.

Graphs in a nutshell:
A graph is a set of nodes $1, 2, 3, ..., N$ and links $\{A_{ij}\}$ among the nodes: $A_{ij} = 1$, if a link is present otherwise $A_{ij} = 0$.

Diffusion on a graph

$$* \ \ discrete \ \ time \qquad p_i(t+1) = \sum_j P_{j \to i} \, p_j(t)$$

$$* \ \ continuous \ \ time \qquad \frac{dp_i}{dt} = w \sum_{ij} D_{ij} p_j$$

where $P_{j \to i} > 0$ if $A_{ij} = 1$ (e.g. $P_{j \to i} = \frac{A_{ij}}{n_j}$);
$D_{ij} = A_{ij} - n_i \delta_{ij}$ is the Laplacian on the graph,
and $n_j = \sum_k A_{kj}$ is number of links of the node j.

3 different dimensions:

* Fractal dimension d_f:
Number of nodes in a ball of radius $\ell \sim \ell^{d_f}$

* Spectral dimension d_s: Prob(return after a time t) $\sim t^{-d_s/2}$

* Connectivity dimension d_l:
Number of different nodes touched by all the walks of t steps $\sim t^{d_l}$

Usually one has an anomalous (sub) diffusion

$$< x^2(t) > \sim t^{d_s/d_f} \ , \ \ d_s/d_f \leq 1$$

Reaction-diffusion on a graph

$$\frac{d\theta_i}{dt} = w \sum_{ij} D_{ij}\theta_j + \frac{1}{\tau} f(\theta_i)$$

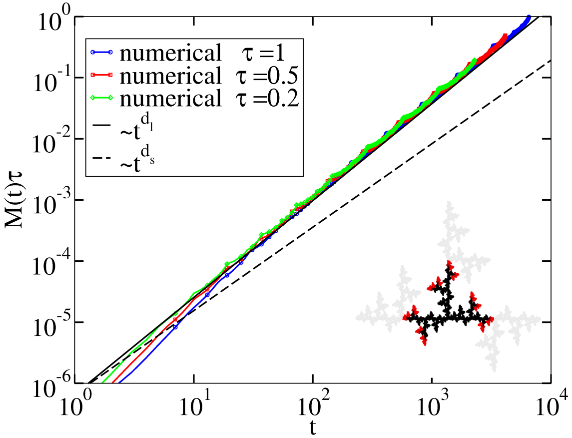
Consider an initial $\{\theta_i\}$ which is zero apart in a small set of nodes. On a regular lattice (e.g. square) with dimension $D = 1, 2$ or 3:

$$M(t) = \frac{1}{N} \sum_{i=1}^{N} \theta_i(t) \sim t^D \ .$$

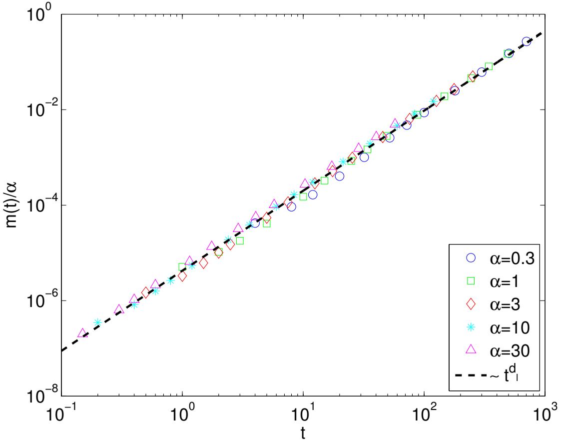
This corresponds to a linear growth of the "radius"

Numerical simulations on several graphs show

$$M(t) \sim t^{d_l}$$



$M(t)\tau$ vs t on a T fractal graph, with $w = 0.5$,
$d_l = \ln 3/\ln 2 \simeq 1.585$ and $d_s = 2\ln 3/\ln 5 \simeq 1.365$ (Burioni et al).



$M(t)/\alpha$ vs t ($\alpha = 1/\tau$) on a square percolating cluster ($p = p_c \simeq 0.595$), $d_l \simeq 1.67$ (Bianco et al).

An argument

$S_n(t)$ is the number of distinct sites visited by n independent random walkers, starting from the site 0, after t steps

$$S_n(t) = \sum_{j=0}^{N} (1 - C_{0j}(t)^n)$$

where $C_{0j}(t)$ is the probability that a walker starting from site 0 has not visited site j at time t. When the number of walkers is large ($n \to \infty$), $C_{0j}(t)^n$ tends to zero if site j has a nonzero probability of being reached in t steps. In this limit, $S_n(t)$ represents all the sites which have nonzero probability of being visited by step t and, $S_n(t) \sim t^{d_l}$. This is precisely the regime observed in the reaction spreading.

Summary

* Long time velocity correlations can induce anomalous diffusion: $< x^2(t) > \sim t^{2\nu}$ with $\nu > 1/2$.

* In the *strong anomalous diffusion* the exponent ν is not enough to describe the statistical features: $< |x(t)|^q > \sim t^{q\nu(q)}$ with $\nu(q) \neq const.$

* In the reaction/diffusion problem, the presence of the anomalous diffusion has non trivial consequences.
Depending on the system one can have different scenarios:
a) anomalous diffusion and standard front propagation;
b) anomalous diffusion and anomalous front propagation.

* In order to have a sublinear front propagation, i.e. $X_F \sim t^\delta$ with $\delta < 1$, it is necessary to have $\rho(x,t)$ with very weak tails (much smaller than those in a Gaussian PdF).

Some References

* K.Andersen, P. Castiglione, A. Mazzino and A. Vulpiani, Eur. J. Phys. B **18**, 447 (2000);
* R. Artuso and G. Cristadoro, Phys. Rev. Lett. **90**, 244101 (2003);
* F. Bianco, S. Chibbaro, D. Vergni and A. Vulpiani, Phys. Rev. E **87**, 062811 (2013);
* G. Boffetta, A.Celani A. Crisanti and A. Vulpiani, Phys. Rev. E **60**, 6734 (1999);
* G. Boffetta and I.M. Sokolov, Phys. Rev. Lett. **88**, 094501 (2002);
* R. Burioni, S. Chibbaro, D. Vergni and A. Vulpiani, Phys. Rev. E **86**, 055101(R) (2012);

* P. Castiglione, A. Mazzino, P. Muratore-Ginanneschi and A. Vulpiani, Physica D **134**, 75 (1999);
* F. Cecconi, D. Vergni and A Vulpiani, Math. Model. Nat. Phen. **11**, 107 (2016)
* G. Forte, F. Cecconi and A.Vulpiani, Eur. J. Phys. B **87**, 102 (2014);
* R.Klages, G.Radons and I.M.Sokolov (Editors) *Anomalous Transport* (Wiley-VCH, 2008);
* R. Mancinelli, D. Vergni and A.Vulpiani, Physica D **185**, 175 (2003).
* A. Pikovsky, Phys. Rev. A **43**, 3146 (1991).
* M. Serva, D. Vergni and A. Vulpiani, Phys. Rev. E **94**, 012141 (2016)