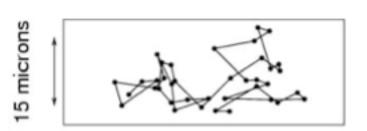
Anomalous diffusion and Nonlinear Fokker-Planck equations

Evaldo M. F. Curado Centro Brasileiro de Pesquisas Físicas Rio de Janeiro, RJ, Brazil

Collaborators: Fernando D. Nobre, Veit Schwammle

random walk

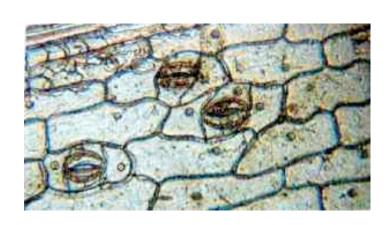




Brownian motion

Robert Brown (botanist) - 1827





http://www.brianjford.com/wbbrownc.htm

A

BRIEF ACCOUNT

OF

MICROSCOPICAL OBSERVATIONS

Made in the Months of June, July, and August, 1827,

ON THE PARTICLES CONTAINED IN THE POLLEN OF PLANTS;

AND

ON THE GENERAL EXISTENCE OF ACTIVE
MOLECULES

IN ORGANIC AND INORGANIC BODIES.

BY

ROBERT BROWN,

F.R.S., HON. M.R.S.E. AND R.I. ACAD., V.P.L.S.,

MEMBER OF THE ROYAL ACADEMY OF SCIENCES OF SWEDEN, OF THE ROYAL SOCIETY OF DENMARK, AND OF THE IMPERIAL ACADEMY NATURE CURIOSORUM; CORRESPONDING MEMBER OF THE ROYAL INSTITUTES OF FRANCE AND OF THE NETHERLANDS, OF THE IMPERIAL ACADEMY OF SCIENCES AT ST. PETERSBURG, AND OF THE ROYAL ACADEMIES OF PRUSSIA AND BAVARIA, ETC.



R. Brown, Edinb. New Philos. J. 5 (1828) 358-371

rw -> normal diffusion (1 dimension):

$$\frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P(x,t)}{\partial^2 x}$$

$$P(x,t) = \frac{1}{(4\pi Dt)^{1/2}} \exp\left[-\frac{(x-x_0)^2}{4Dt}\right]$$

$$< x(t) > = x_0 ; < (x(t) - x_0)^2 > = 2Dt$$

Einstein Relation : $D = \mu k_B T$

$$P(x,t) = t^{-1/2}g(x^2/t) \Rightarrow \sigma^2 \sim t$$

Linear Fokker-Planck equation:

$$\frac{\partial P(x,t)}{\partial t} = \left(\frac{\partial \{F(x)P(x,t)\}}{\partial x}\right) + D\frac{\partial^2 P(x,t)}{\partial x^2}$$
$$F(x) = -\frac{d\phi}{dx}$$

$$P(x,t)\big|_{x\to\pm\infty} = 0; \quad \frac{\partial P(x,t)}{\partial x}\big|_{x\to\pm\infty} = 0; \quad F(x)P(x,t)\big|_{x\to\pm\infty} = 0 (\forall t)$$

$$\int_{-\infty}^{\infty} dx \ P(x,t) = \int_{-\infty}^{\infty} dx \ P(x,t_0) = 1 \quad (\forall t)$$

H-theorem and FP equation

$$F = U - TS ; U = \int_{-\infty}^{\infty} dx \, \phi(x) P(x, t) ; S = -k_B \int_{-\infty}^{\infty} dx \, P(x, t) \ln P(x, t)$$

BG

$$\frac{dF}{dt} = \frac{\partial}{\partial t} \left(\int_{-\infty}^{\infty} dx \, \phi(x) P(x,t) + k_B T \, \int_{-\infty}^{\infty} dx P(x,t) \ln P(x,t) \right)$$

$$= \int_{-\infty}^{\infty} dx \, \left\{ \phi(x) + k_B T [\ln P(x,t) + 1] \right\} \left(\frac{\partial P(x,t)}{\partial t} \right) \longrightarrow \text{FPE}$$

$$\left(\frac{dF}{dt} \le 0\right)$$

H-theorem is valid for linear FPE "and" BG entropy => relation between FPE and BG entropy?

general solution Fokker-Planck equation

ullet dependence on time \longrightarrow F(x) = -kx

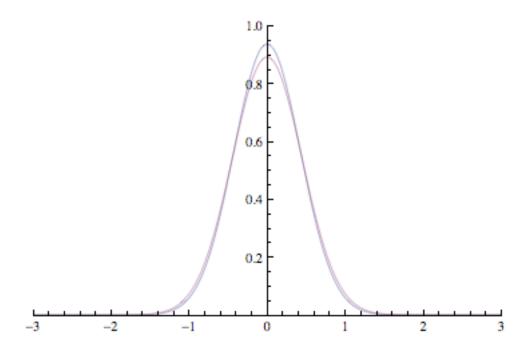
$$P(x,t) = \frac{1}{\sqrt{2\pi D(1 - e^{-2t})/k}} e^{-\frac{kx^2}{2D(1 - e^{-2t})}}$$

ullet normal diffusion $\ (t<<1)$

$$P(x,t) = \frac{1}{\sqrt{4\pi Dt/k}} e^{-\frac{kx^2}{4Dt}} \longrightarrow \langle (x - \langle x \rangle)^2 \rangle = \frac{2Dt}{k}$$

•
$$t >> 1$$
 \longrightarrow $\langle (x - \langle x \rangle)^2 \rangle = \frac{D}{k}$ $\left(P(x) = \frac{1}{\sqrt{2\pi D/k}} e^{-\frac{kx^2}{2D}} \right)$

(BG entropy



anomalous diffusion

$$<(x(t)-x_0)^2> \sim t^{\gamma} \qquad (\gamma \neq 1)$$

- ullet subdiffusive $(\gamma < 1)$
- superdiffusive $(\gamma > 1)$

anomalous diffusion -> subdiffusion

$$<(x(t)-x_0)^2> \sim t^{\gamma}$$
 ($\gamma<1:$ Subdiffusion)

- existence of "traps" in space, where the particles stay for a certain time, with a broad distribution of released time
- conductivity of disordered ionic chains
- photocopiers, laser printers
- random walks on fractal substrates
- diffusion in convective rolls
- diffusion of contaminants in groundwater
- diffusion of proteins across cell membranes, etc

subdiffusion - exemples

 photocopiers, laser printers: transport of electrons or holes in amorphous semiconductors in an electric field

PHYSICAL REVIEW B

VOLUME 12, NUMBER 6

15 SEPTEMBER 1975

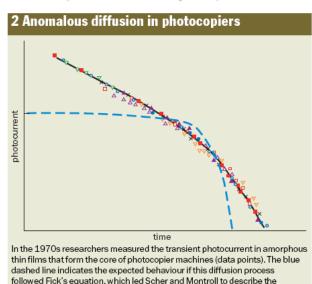
Anomalous transit-time dispersion in amorphous solids

Harvey Scher

Xerox Webster Research Center, 800 Phillips Road, Webster, New York 14580

Elliott W. Montroll

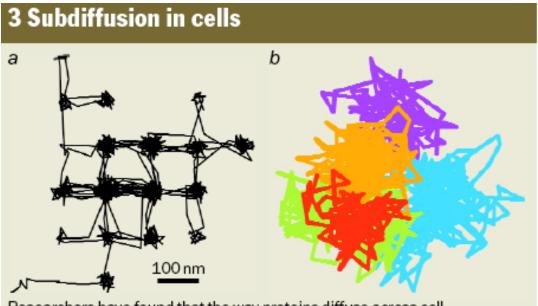
Institute for Fundamental Studies,* Department of Physics and Astronomy, University of Rochester, Rochester, New York 14627
(Received 13 January 1975)



process using broad distributions of waiting times. Both axes are logarithmic. This became the best known example of anomalous subdiffusion in nature. From H Scher and E Montroll 1975 *Phys. Rev.* B **12** 2455–2477

subdiffusion

diffusion of proteins across cell membranes



Researchers have found that the way proteins diffuse across cell membranes can be described by anomalous diffusion that is slower than the normal case. (a) This is a simulation of such a random walk, which shows a 2 ms timeframe over which a protein "hops" between 120 nm² compartments thought to be formed by the cell's cytoskeleton. (b) The experimental trajectories of proteins in the plasma membrane of a live cell (shown in a 0.025 ms timeframe) provide evidence for this trapping nature, as shown by the different colours. The long residence times in these compartments is thought to be the origin of the anomalous behaviour.

anomalous diffusion -> superdiffusion

$$<(x(t)-x_0)^2> \sim t^{\gamma}$$
 ($\gamma>1:$ Superdiffusion)

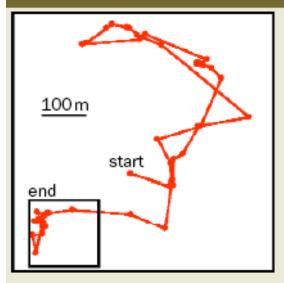
- existence of long range (in time) correlations present in the velocity of the tracer particle, Levy flights, nonlinear effects, etc.

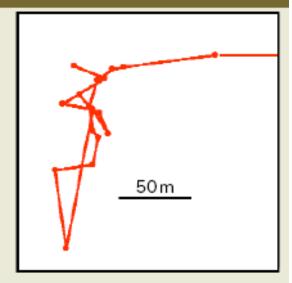
- diffusion of micelles in salted water
- Richardson diffusion in turbulent fluids
- flight of albatrosses
- bacteria, plankton, jackals, spider monkeys
- it seems that superdiffusion superates normal BM as a strategy for finding randomly located food, etc.

anomalous diffusion -> superdiffusion

spider monkeys

4 Superdiffusion in monkey behaviour





The typical trajectories of spider monkeys in the forest of the Mexican Yucatan peninsula display steps with variable lengths, which correspond to a diffusive process that is faster than that of normal diffusion. An example of such a trajectory is shown on the left. A magnified part of it is shown on the right; this image looks qualitatively similar to the larger-scale trajectory, which is an important property of Lévy walks. Similar behaviour is found in the foraging habits of other animals, and could mean that anomalous diffusion offers a better search strategy than that of normal diffusion.







→ modifications in linear diffusion equation

nonlinear Fokker-Planck equation

Porous media equation (M. Muskat - 1937)

$$\rightarrow \frac{\partial P(x,t)}{\partial t} = D \frac{\partial^2 P^{\nu}(x,t)}{\partial x^2}$$

$$\langle (x - \langle x \rangle)^2 \rangle \sim t^{\frac{2}{\nu+1}}$$

- A. R. Plastino and A. Plastino, Physica A 222 (1995) 347;
 - C. Tsallis and Bukman D. J., PRE 54 (1996) R2197

$$\frac{\partial P(x,t)}{\partial t} = \left(-\frac{\partial \{F(x)P(x,t)\}}{\partial x} + D\frac{\partial^2 P^{\nu}(x,t)}{\partial x^2} \right)$$

$$F(x) = -\frac{d\phi}{dx}$$

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial \{F(x)P(x,t)\}}{\partial x} + D\frac{\partial^2 P^{\nu}(x,t)}{\partial x^2}$$

$$F(x) = -\frac{d\phi}{dx}$$

stationary solution $(\nu = 2 - q)$

$$P(x) = C[1 - \beta(1 - q)\phi(x)]^{1/(1-q)}$$

$$\beta = (1/D)[C^{q-1}/(2-q)]$$
 (C is a positive constant)

same distribution that maximizes Tsallis entropy with the external constraint $\phi(x)$!

NLFPE <-> Tsallis entropy!

master equation -> NL Fokker-Planck equation

$$\frac{\partial P(n,t)}{\partial t} = \sum_{m=-\infty}^{\infty} \left[P(m,t) w_{m,n}(t) - P(n,t) w_{n,m}(t) \right]$$

 nonlinear transition rates -> nonlinear Fokker-Planck equations

$$\omega_{m,n}(t) \to \omega_{m,n}(P,t)$$

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial \{F(x)\Psi[P(x,t)]\}}{\partial x} + \frac{\partial}{\partial x} \left\{ \Omega[P(x,t)] \frac{\partial P(x,t)}{\partial x} \right\}$$

nonlinear Fokker-Planck equation

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial \{F(x)\Psi[P(x,t)]\}}{\partial x} + \frac{\partial}{\partial x} \left\{ \Omega[P(x,t)] \frac{\partial P(x,t)}{\partial x} \right\}$$

$$\Omega[P]>0$$

$$\Psi[P]>0$$

$$F(x)=-\frac{d\phi}{dx}$$

$$\Omega[P]=\mathrm{const.}$$

$$\Gamma[P]=\mathrm{const.}$$

$$\Gamma[P]=\mathrm{const.}$$

$$\Omega[P] = a[P]b[P] ; \quad \Psi[P] = a[P]P$$

$$\int_{-\infty}^{\infty} dx \ P(x,t) = \int_{-\infty}^{\infty} dx \ P(x,t_0) = 1 \qquad (\forall t)$$

$$a[P] = \mathrm{const.}$$
 $\Omega[P] = \mathrm{const.}$

$$a[P] = \text{const.}$$

$$a[P] = {\rm const.}$$

$$\Omega[P] = DP^{\mu-1}$$
 NLFPE – Plastino and

Plastino, Physica A 1995

master equation -> NLFPE

EMFC & FD Nobre, PRE 2003, FD Nobre, EMFC & G Rowlands, Physica A 2004

H-theorem

$$S[P] = \int_{-\infty}^{\infty} g[P(x,t)] dx$$

$$g(0) = g(1) = 0$$

$$\frac{d^2g}{dP^2} \le 0$$

$$g[P] = -P \ln P$$

$$F_G = U - \frac{1}{\beta} S ;$$

$$F_G=U-rac{1}{eta}\;S\;; \qquad U=\int_{-\infty}^{\infty}dx\;\phi(x)P(x,t) \ g[P]\propto P^q$$
 Tsallis

$$g[P] \propto P^q$$

$$-\frac{1}{\beta} \frac{d^2 g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]} \quad \Rightarrow \quad \frac{dF}{dt} \le 0$$

$$\frac{dF}{dt} \le 0$$

NLFPE <-> entropy

$$-\frac{1}{\beta}\frac{d^2g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]}$$

$$\downarrow$$
 entropy
$$\qquad \qquad \text{FPE}$$

TD Frank, PH Chavanis, FD Nobre, EMFC, etc

connection between entropy and Fokker-Planck equations

stationary state of the NLFPE

$$\mathcal{I}[P(x,t)] = S[P] + \alpha \left(1 - \int_{-\infty}^{\infty} dx \; P(x,t)\right) + \beta \left(U - \int_{-\infty}^{\infty} dx \; \phi(x) P(x,t)\right)$$

$$\frac{d\mathcal{I}}{dP} = 0 \implies \text{same pdf of the stationary state ->}$$

$$\text{equivalent to MaxEnt (S)}$$

families of FPEs <-> entropies

$$-\frac{1}{\beta}\frac{d^2g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]} \qquad \text{relation entropy <-> FPE}$$

same ratio $\frac{\Omega[P]}{\Psi[P]}$ same entropy!

let us consider the classes of FPEs satisfying

$$\Omega[P] = a[P]b[P] ; \quad \Psi[P] = a[P]P$$

$$\frac{d^2g[P]}{dP^2} = -\beta \, \frac{b[P]}{P}$$
 Schwammle V, Nobre FD, EMFC, PRE 2007 Schwammle V FMFC, Nobre FD, EPIB 2007

Freedom for functional a[P]

Schwammle V, EMFC, Nobre FD, EPJB 2007

NLFPEs <-> Boltzmann-Gibbs entropy

$$\frac{d^2g[P]}{dP^2} = -\beta \frac{b[P]}{P}$$

$$b[P] = D$$

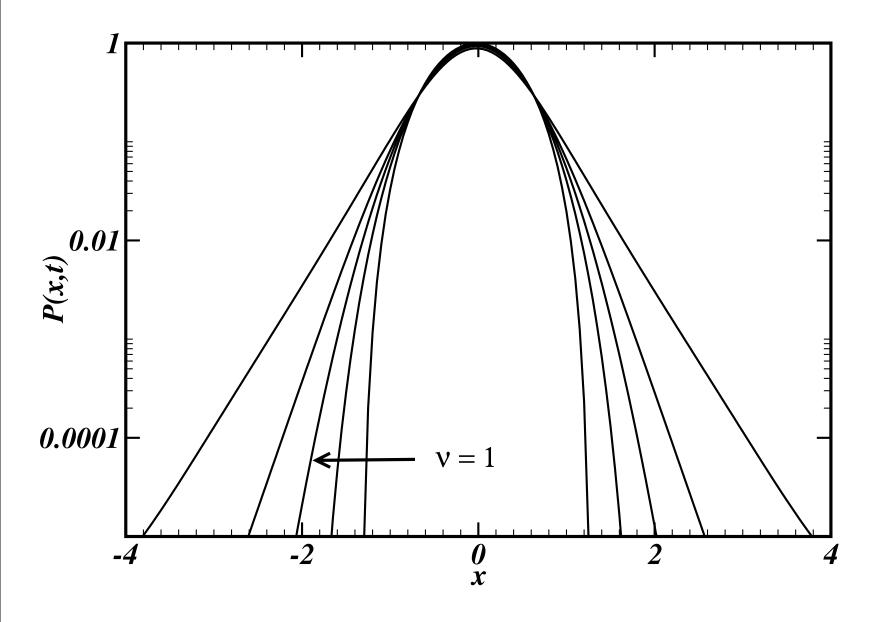
$$\beta = k_B/D$$

$$\frac{dg}{dP} = -\beta D \ln P + C \quad \Rightarrow \quad g[P] = -k_B P \ln P$$

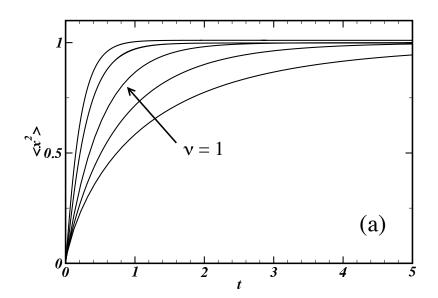
$$S = -k_B \int P(x) \ln P(x) dx$$
 if $a[P] \propto P^{\nu-1}$

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left(F(x)P(x,t)^{\nu} \right) + D\frac{\partial}{\partial x} \left(P(x,t)^{\nu-1} \frac{\partial P(x,t)}{\partial x} \right)$$

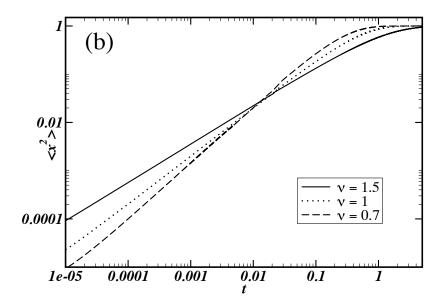
$$\nu=1$$
 Iinear Fokker-Planck equation



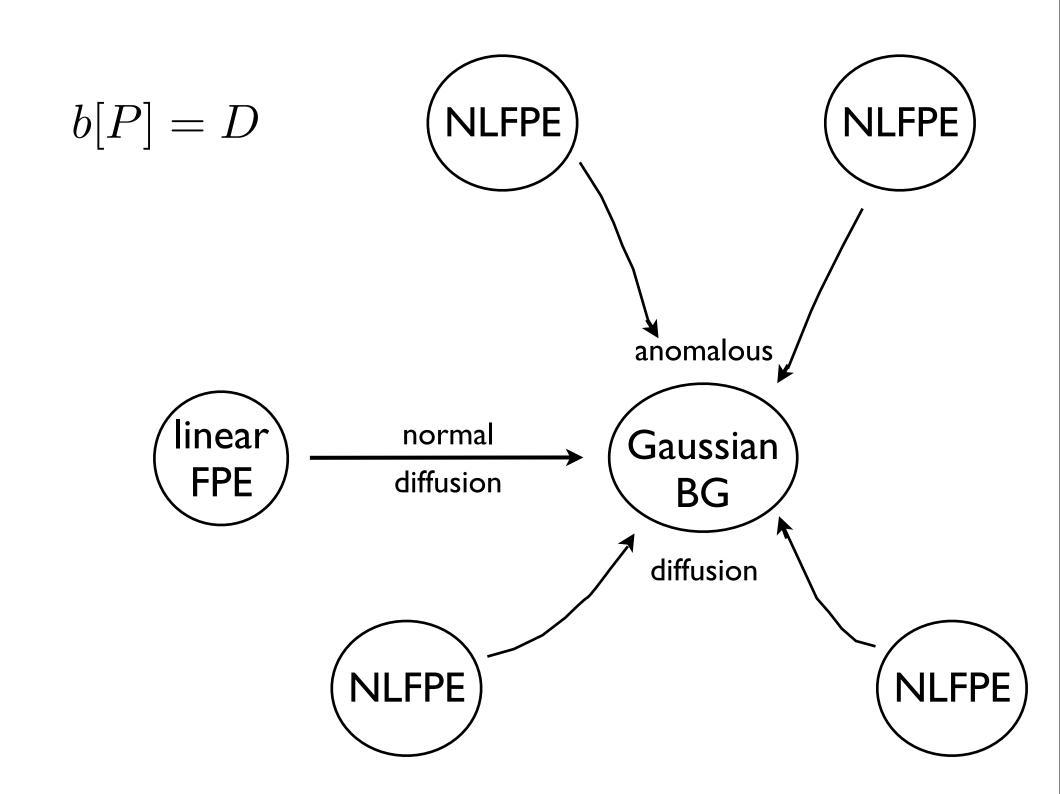
$$F(x) = -kx$$
 $t = 0.1$ $P(x,0) = \delta(x)$ $\nu = 0.7, 0.9, 1, 1.1, 1.25$



$$\nu = 0.5, 0.7, 1, \\ 1.25, 1.5$$



$$\langle x^2 \rangle \sim \left(\frac{2}{\nu^2}\right) t^{\frac{2}{\nu+1}}$$



NLFPEs <-> Tsallis entropy

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial \{F(x)\Psi[P(x,t)]\}}{\partial x} + \frac{\partial}{\partial x} \left\{ \Omega[P(x,t)] \frac{\partial P(x,t)}{\partial x} \right\}$$

$$\Omega[P] = a[P]b[P] ; \quad \Psi[P] = a[P]P$$

$$\frac{d^2g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]} = -\beta \frac{b[P]}{P}$$

$$\frac{d^2g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]} = -\beta \, \frac{b[P]}{P} \qquad b[P(x,t)] = D\nu P(x,t)^{\nu-1}$$

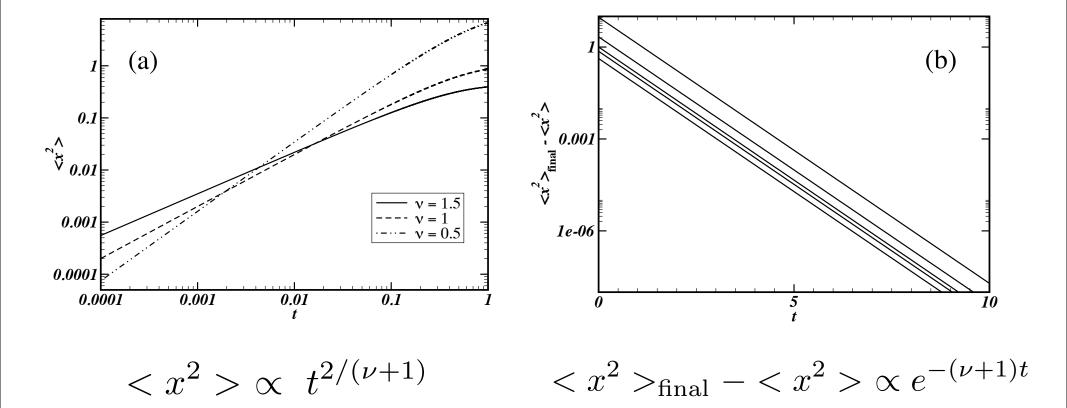
$$g[P] = -\frac{\beta D}{\nu - 1} P^{\nu} + CP \Rightarrow g[P] = k_B \frac{P - P^{\nu}}{\nu - 1}$$
if $a[P] \propto P^{\mu - 1}$



$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left(F(x)P(x,t)^{\mu} \right) + D\frac{\partial}{\partial x} \left(P(x,t)^{\mu+\nu-2} \frac{\partial P(x,t)}{\partial x} \right)$$

a)
$$\mu=1$$
 (NLFPE - Plastino&Plastino1995)

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left(F(x)P(x,t) \right) + D\frac{\partial}{\partial x} \left(P^{\nu-1}(x,t) \frac{\partial P(x,t)}{\partial x} \right)$$

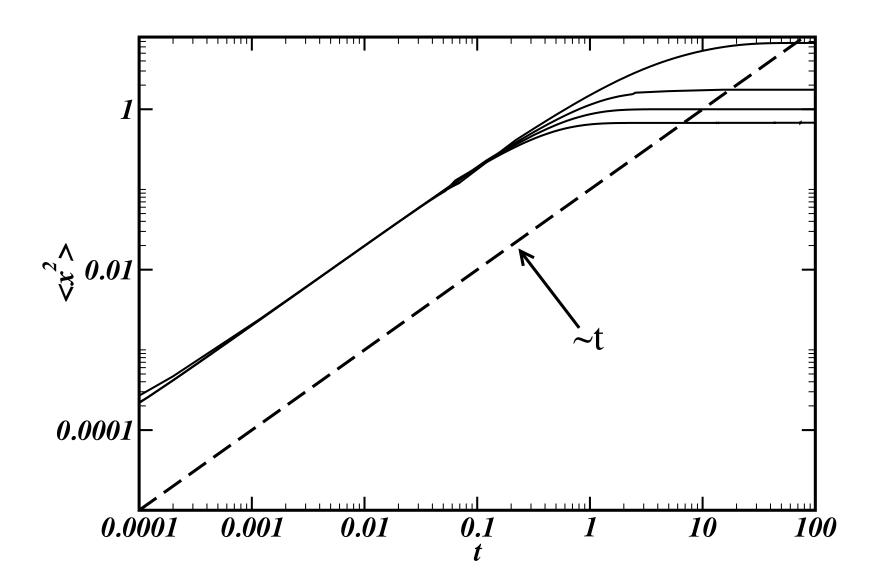


Nonlinear FPE -> normal diffusion

b)
$$\nu = 2 - \mu \ (\mu \neq 1)$$

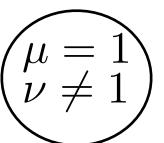
$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x} \left(F(x)P(x,t)^{\mu} \right) + D \frac{\partial^2 P(x,t)}{\partial x^2}$$

stationary solution -> q-Gaussian



 $\mu = 0.7, 1, 1.2, 1.5$

NLFPE



$$b[P(x,t)] = D\nu P(x,t)^{\nu-1}$$

anomalous diffusion q-Gaussian

$$\left(\begin{array}{c} \mu \neq 1 \\ \nu = 2 - \mu \end{array} \right)$$

normal

diffusion

q-Gaussian

anomalous diffusion

$$\mu \neq 1$$

$$\nu \neq 1$$

V. Schwammle, EMFC, FD Nobre EPJB (2009) in press

non-orthodox constraints

$$U = \int_{-\infty}^{\infty} dx \, \phi(x) \Gamma[P(x,t)]$$

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial}{\partial x} \left(\Psi[P] \underbrace{\frac{\partial}{\partial x} \left(\phi(x) \chi[P] \right)}_{F(x)} \right) + \frac{\partial}{\partial x} \left(\Omega[P] \frac{\partial P}{\partial x} \right)$$

$$\chi[P] = \frac{d\Gamma[P]}{dP} \qquad -\frac{1}{\beta} \frac{d^2 g[P]}{dP^2} = \frac{\Omega[P]}{\Psi[P]}$$

$$P(x) = C[1 - \beta(1 - q)\phi(x)]^{1/(1-q)}$$

- conclusions curious situations:
- nonlinear FPEs -> Gaussian as stationary state -> same distribution obtained from Boltzmann-Gibbs entropy -> anomalous diffusion
- nonlinear FPEs -> q-Gaussian as stationary states -> same distribution obtained from Tsallis entropy -> normal diffusion.