Stochastic methods in Mathematical Modelling

Lecture 13. Anomalous random processes 1. Part 1.

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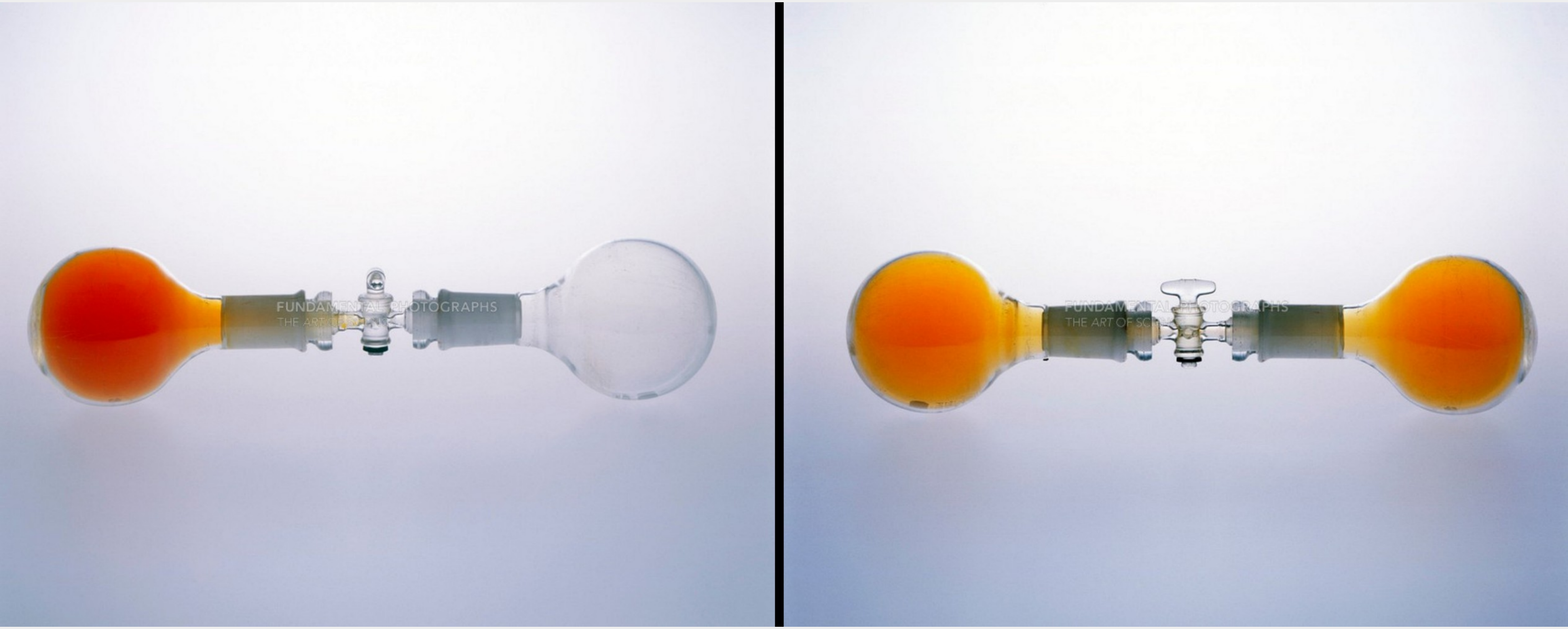
The plan of the lecture

1. Examples of Brownian and anomalous phenomena
Ergodicity, sub-, superdiffusion
2. CTRW model. Solution.
3. Fractional derivatives
4. Solution of subdiffusive fractional Fokker-Planck equation.
Mittag-Leffler and Fox H-functions

Diffusion



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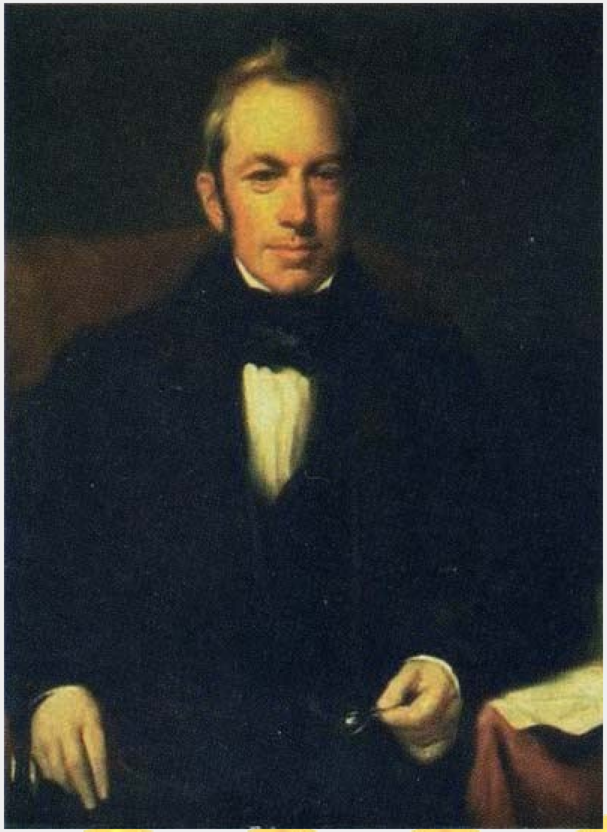
Diffusion

Jan Ingenhousz (1730-1799)

1785. Ingenhousz found that under a microscope the coal dust on the surface of alcohol moves erratically

Robert Brown (1773-1858)

1827. Brown sees that small lipid and starch organelles performing jittery motion known now as Brownian motion



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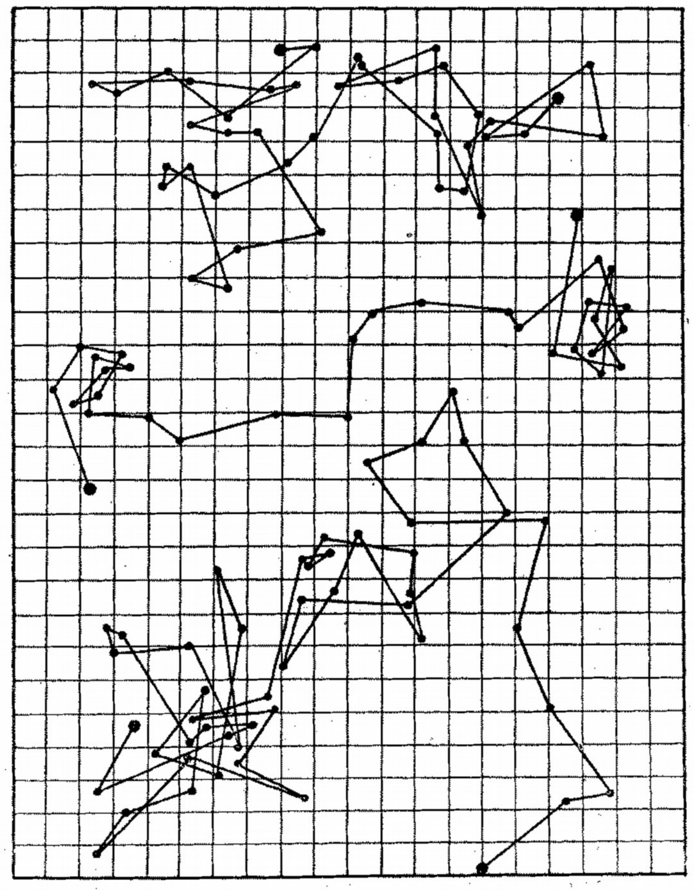
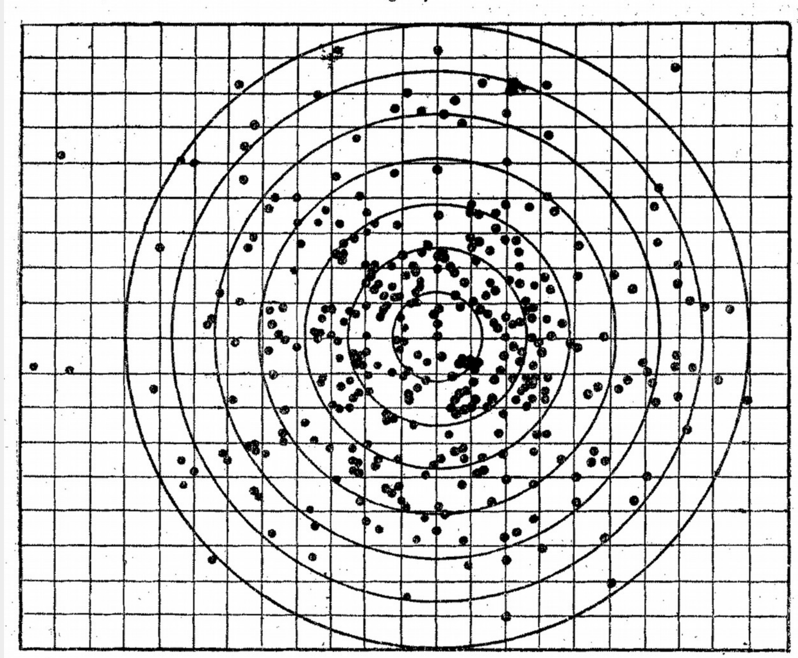
Perrin experiment. Brownian motion

Fig. 6.



$\Delta t = 30$ sec

Fig. 7.



$$P(r,\Delta t) = \frac{1}{(4\pi D\Delta t)^{d/2}} \exp\left(-\frac{r^2}{4D\Delta t}\right)$$

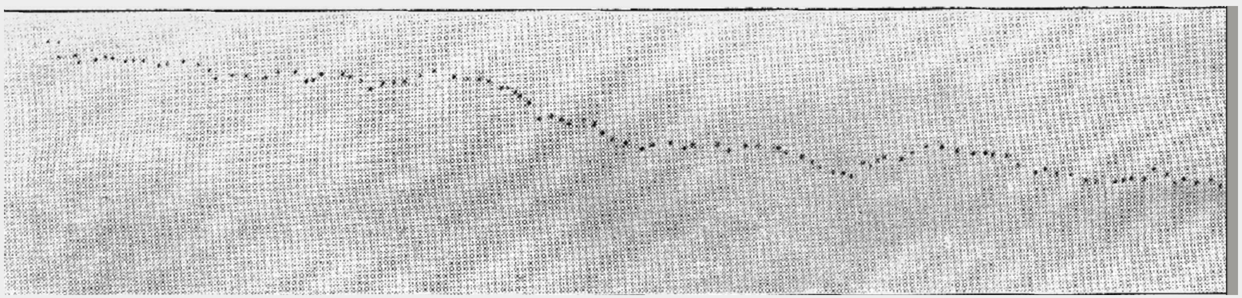
Einstein-(Smoluchowski) relation

$$D = \frac{k_B T}{m\eta} = \frac{R/N_A T}{m\eta}$$

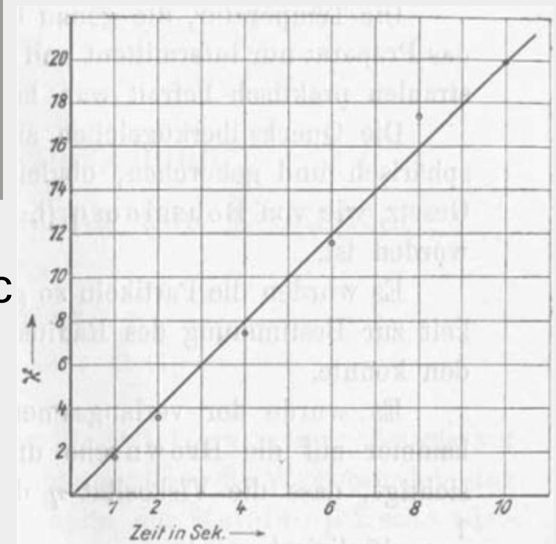
$$N_A = 7.05 \times 10^{23}$$

J Perrin, Comptes Rendus (Paris) 146 (1908) 967

Brownian motion II: single trajectory time series analysis



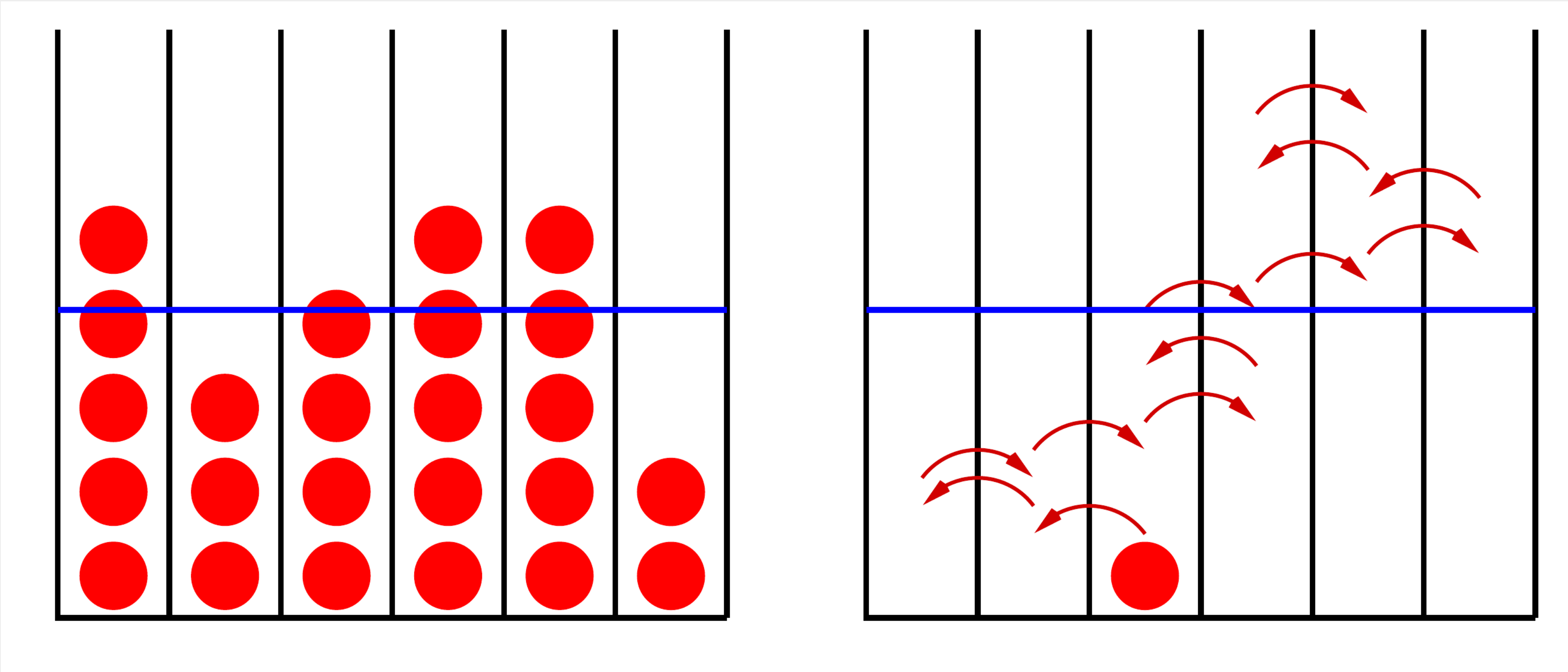
The stochastic, Brownian motion around the deterministic sedimentation with constant velocity
can be clearly distinguished



example for the time averaged
mean squared displacement versus time
(in seconds) from a single recorded
falling mercury droplet

I Nordlund, Z Physik (1914): $N_A = 5.91 \times 10^{23}$

Time versus ensemble averages: ergodic hypothesis



Ergodicity. Ensemble average = Time average:

$$\langle p_i \rangle = \lim_{N \to \infty} \frac{N_i}{N} \equiv \bar{p}_i = \lim_{t \to \infty} \frac{t_i}{t}$$

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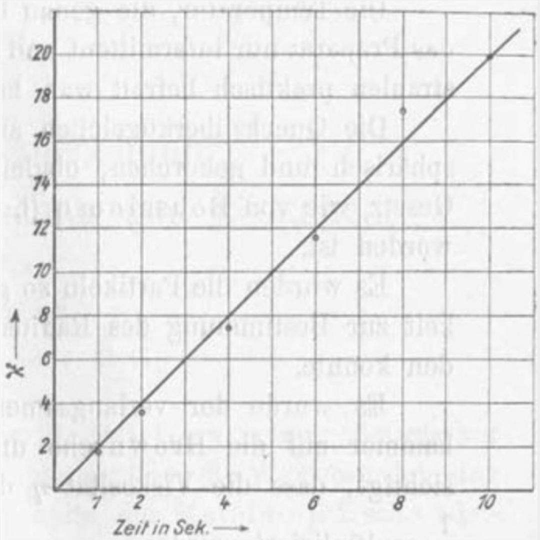
Extracting information from single trajectories

Ensemble average for normal diffusion

$$\langle x^2(t)\rangle = \int x^2 P(x,t)\,dx = 2D_1 t$$

Single particle trajectory time series x(t)

$$\overline{\delta^2(\Delta,T)} = \frac{\int_0^{T-\Delta} [x(t'+\Delta)-x(t')]^2\,dt'}{T-\Delta}$$



Normal diffusion: On average the number of jumps is proportional to the elapsed time

$$\langle [x(t+\Delta)-x(t)]^2\rangle = \langle \delta x^2\rangle n(t+\Delta,t) \simeq \frac{\langle \delta x^2\rangle}{\tau}\Delta$$

Single trajectory information equals ensemble information

$$\overline{\delta^2(\Delta,T)} \sim 2D_1\Delta = \lim_{T\to\infty}\overline{\delta^2}(\Delta,T),\ where\ D_1 = \frac{\langle \delta x^2\rangle}{2\tau}$$

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Normal vs Anomalous

Normal

$$\langle x^2(t) \rangle = 2 D_1 t$$

Anomalous

$$\langle x^2(t) \rangle \neq 2 K t$$

Mostly

$$\langle x^2(t) \rangle \sim K_\alpha t^\alpha$$

Superdiffusion α > 1
Subdiffusion α < 1

Could be more complicated (Sinai diffusion, for instance)

$$\langle x^2(t) \rangle \sim \log^\beta t$$

Reasons for anomality

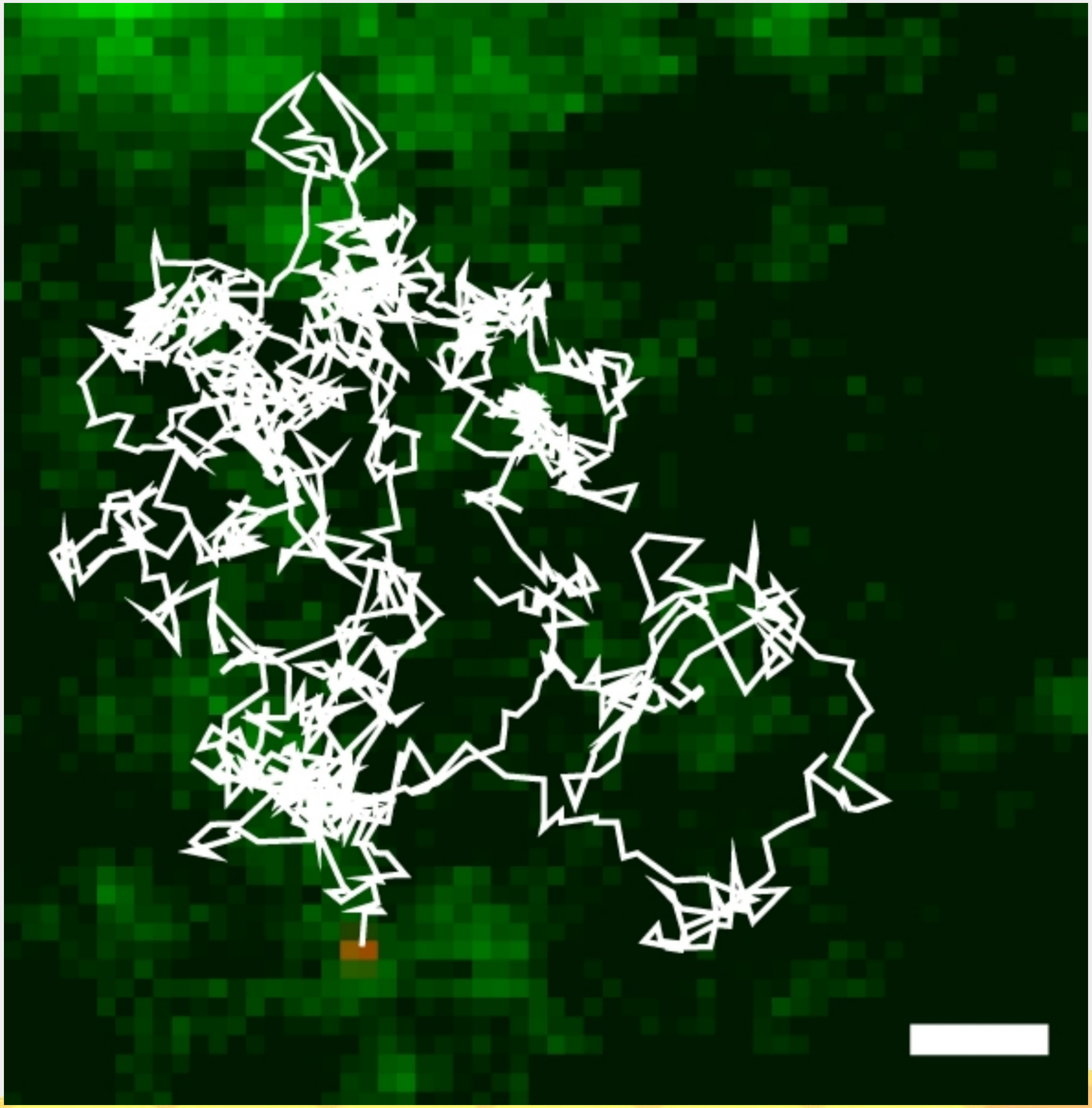
$$\langle x^2(t)\rangle \sim K_\alpha t^\alpha$$

1. Specific power-law distributions for jump lengths/waiting times (diverging second or first moments)

2. Correlations in jump directions

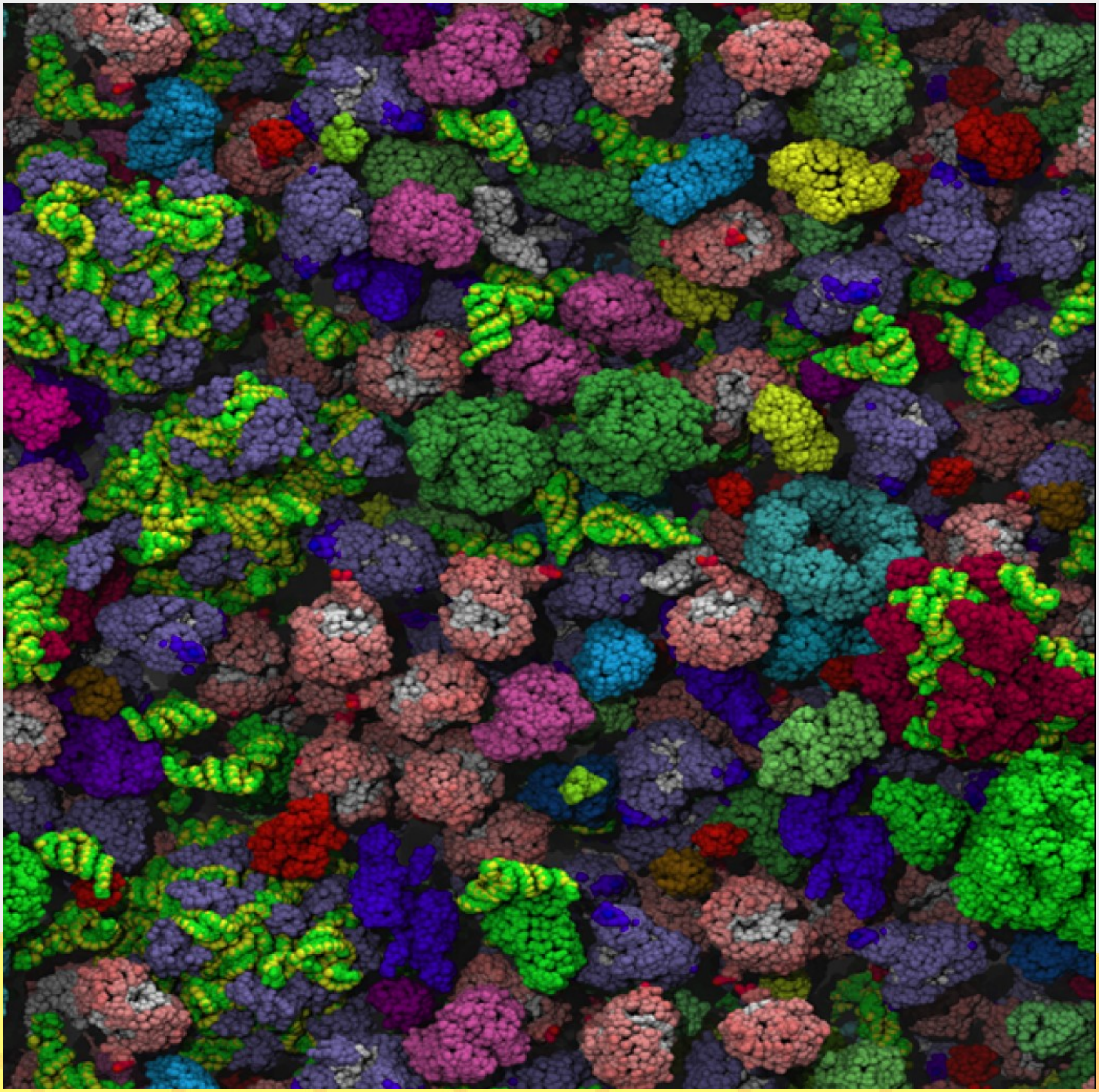
3. Specific geometry of the system (percolation cluster) or time evolution of parameters

Single particle tracking I



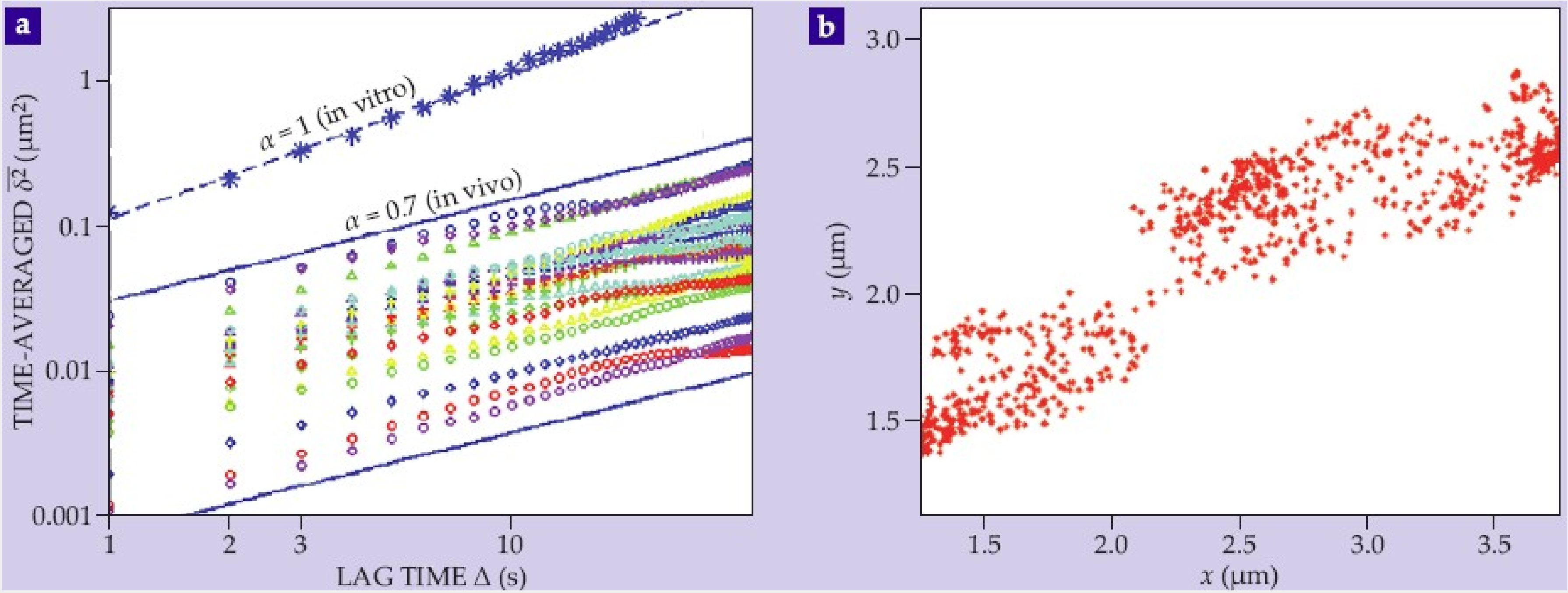
In living human embryonic kidney cells (scale bar: 1μm)
D. Krapf et al.

Inside of a cell



McGuee & AH Elcock, PLoS Comp Biol (2010)

Single particle tracking II



J.-H. Jeon et al. Phys. Rev. Lett. 106, 048103 (2011)

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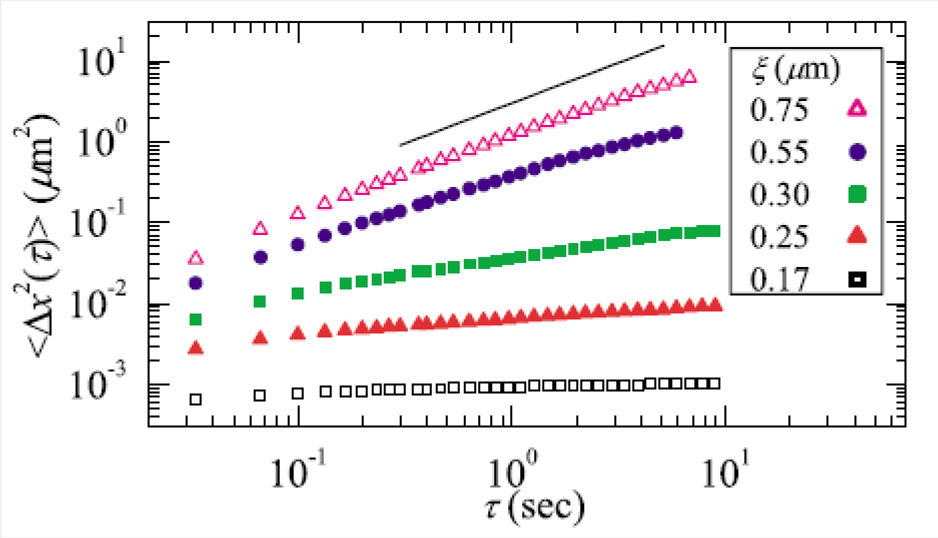
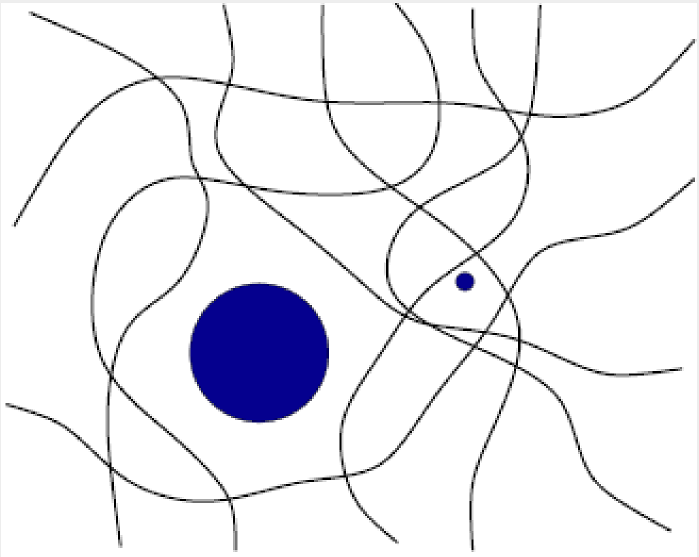
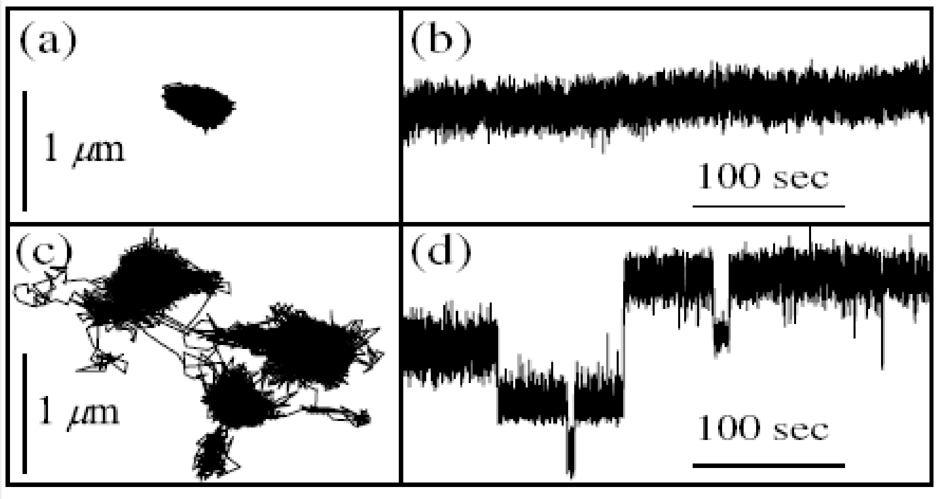
Actin net trapping experiment







ξ is a typical cell size

The ball size is 0.25 micrometers

Jump probability P ~ $\tau^{-1-\gamma}$

I.Y.Wong et al., Phys. Rev. Lett. 92, 178101 (2004)

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Travel adventures of a dollar bill

D Brockmann, Physics World (2010) https://www.wheresgeorge.com

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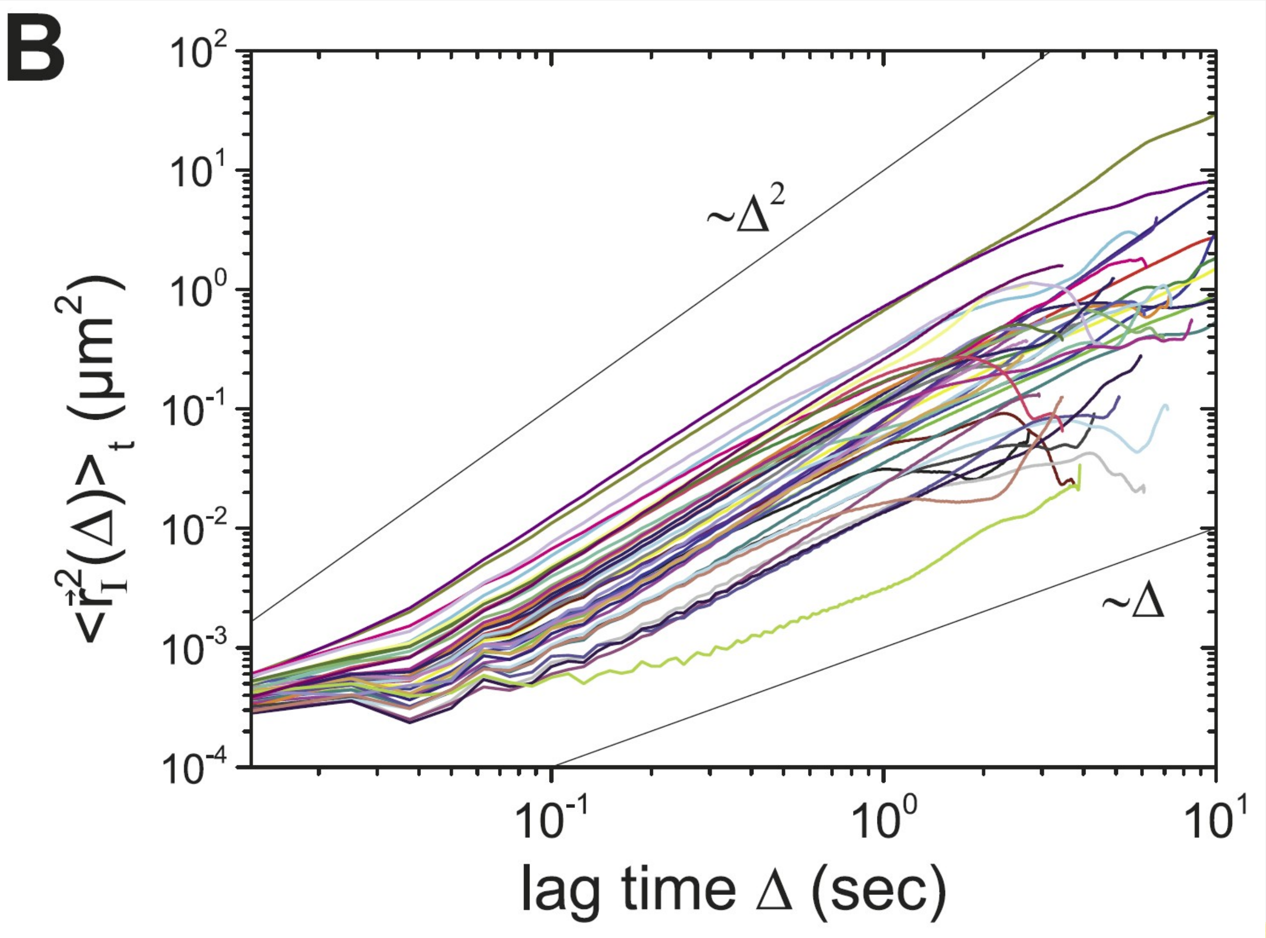
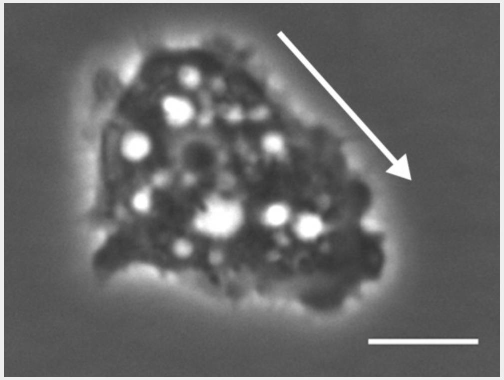
Superdiffusion in amoebae cells



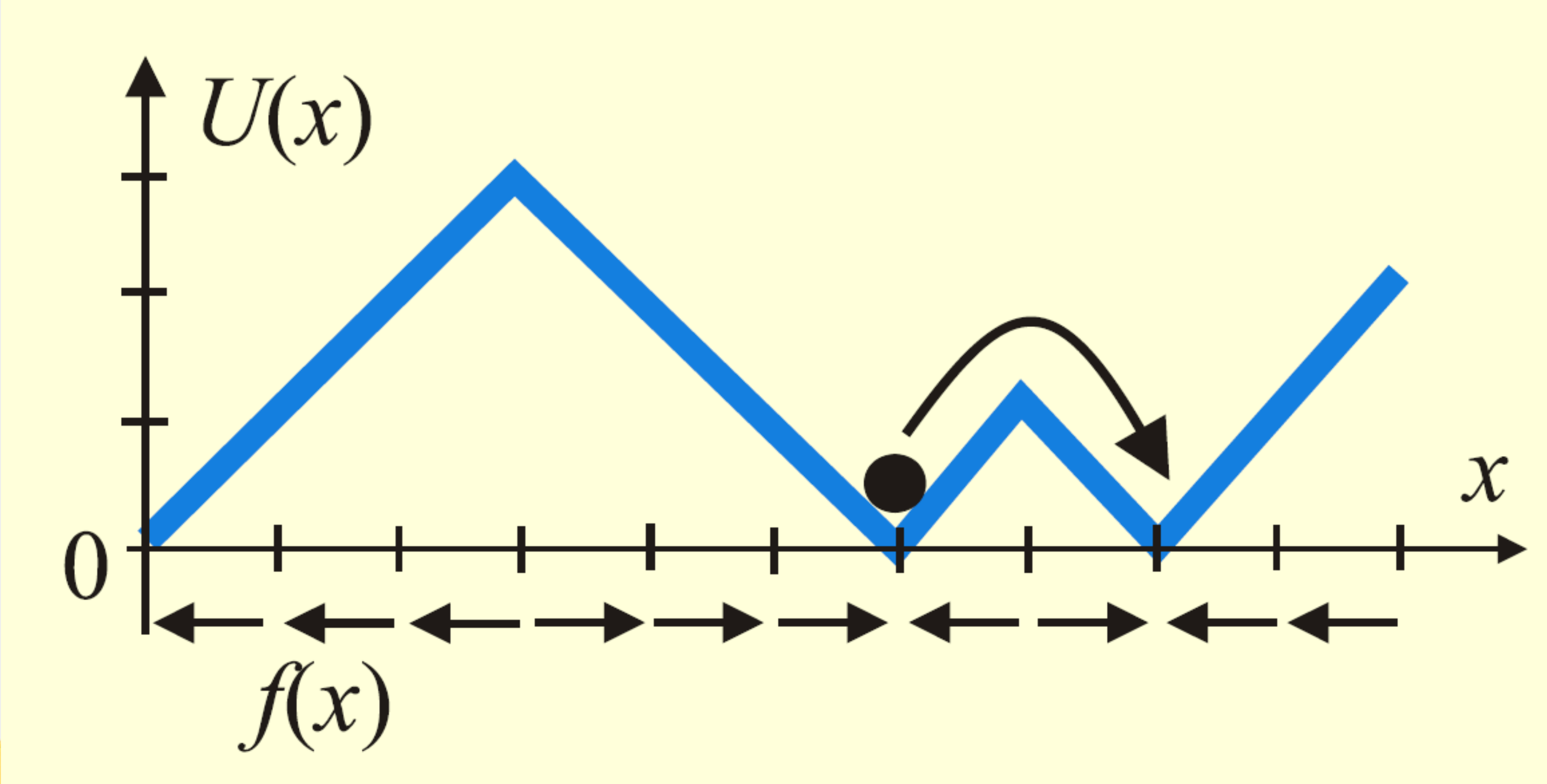


J.F. Reverey, J.H. Jeon et al. Scientific Reports 2015

Sinai diffusion

A simple random walk in a potential landscape
which is a simple random walk itself

$$\langle x^2(t) \rangle \sim \log^4 t$$



Continuous-Time Random Walk model (CTRW)

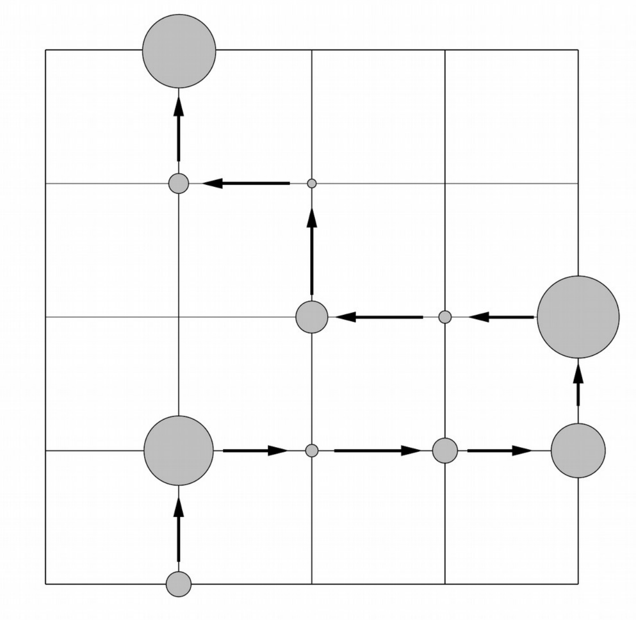
$$X(t) = X_0 + \sum_{i=1}^{N(t)} \Delta X_i$$

The lengths and waiting times (durations) of the jumps are drawn from φ(x,t)

Jump pdf $$\lambda(x) = \int dt\, \varphi(x,t)$$

Waiting time pdf $$w(t) = \int dx\, \varphi(x,t)$$

The concept of waiting times



Continuous-Time Random Walk model (CTRW)

$$X(t) = X_0 + \sum_{i=1}^{N(t)} \Delta X_i$$

Jump pdf

$$\lambda(x) = \int dt\, \varphi(x,t)$$

general jump-WT pdf $\varphi(x,t)$

Waiting time pdf

$$w(t) = \int dx\, \varphi(x,t)$$

General solution for the CTRW PDF

$$\boxed{P(k,s) = \frac{1-w(s)}{s} \frac{P_0(k)}{1-\varphi(k,s)}}$$

CTRW

$\lambda(x)$ is jump distribution

$$\lambda(x) = \int_0^t dt\, \psi(x,t)$$

$$w(t) = \int_{-\infty}^{+\infty} dx\, \psi(x,t)$$

$w(t)$ are waiting times

$$T = \int_0^\infty t\, w(t)\, dt$$

$$\Sigma^2 = \int_{-\infty}^{+\infty} x^2 \lambda(x)\, dx$$

could diverge

PDF of just arriving to (x,t):

1) $$\eta(x,t) = \int_{-\infty}^{+\infty} dx' \int_0^{t} \eta(x',t')\, \psi(x-x', t-t') + \underbrace{\delta(x)\delta(t)}_{P_0(x,\, t=0)}$$

2) $$P(x,t) = \int_0^t \eta(x,t')\, \Psi(t-t')$$

prob that we never moved in $t-t'$

3) $$\Psi(t) = 1 - \int_0^t dt'\, w(t')$$

PDF that we left

Fourier + Laplace (1),(2),(3)

$$\begin{cases} \Psi(s) = \dfrac{1}{s} - \dfrac{w(s)}{s} \\ P(k,s) = \eta(k,s)\,\Psi(s) \\ \eta(k,s) = \eta(k,s)\,\varphi(k,s) + P_0(k) \end{cases}$$

$$\Rightarrow P(k,s) = \frac{1-w(s)}{s}\,\frac{P_0(k)}{1-\varphi(k,s)}$$

if $\varphi(x,t) = w(t)\,\lambda(x)$

If τ & Σ^2 are finite $\Rightarrow$ Brownian motion

$$\left.\begin{aligned} w(t) &= \tau^{-1} e^{-t/\tau} \\ \lambda(x) &= \frac{1}{\sqrt{4\pi\sigma^2}}\, e^{-\frac{x^2}{4\sigma^2}} \end{aligned}\right\} \rightarrow \begin{aligned} w(s) &\sim 1 - s\tau + o(\tau^2) \\ \lambda(k) &\sim 1 - \sigma^2 k^2 + o(k^4) \end{aligned}$$

$$P(k,s) = \frac{P_0}{s + Dk^2}$$

$$P(k,s) = \frac{P_0}{s + Dk^2}$$

$$\downarrow$$

$$\underbrace{sP(k,s) - P_0}_{\mathcal{L}\left\{\frac{\partial P(k,t)}{\partial t}\right\}} = \underbrace{-Dk^2 P(k,s)}_{D\mathcal{F}\left\{\frac{\partial^2 P(x,s)}{\partial x^2}\right\}}$$

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

Long rests

$$\varphi(x,t) = w(t)\,\cancel{\lambda}(x)$$

$$w(t) \sim A\left(\frac{\tau}{t}\right)^{1+\alpha}, \quad t \gg \tau$$

Tauberian theorem

$$w(s) \sim 1 - (s\tau)^{\alpha}, \quad s \to 0$$

$$\lambda(k) \sim 1 - \sigma^2 k^2$$

$$\underbrace{P(k,s)}_{} = \frac{(s\tau)^{\alpha}}{s} \cdot \frac{P_0(k)}{1-\left(1-(s\tau)^{\alpha}\right)\left(1-\sigma^2 k^2\right)} \simeq \underbrace{\frac{P_0(k)/s}{1+K_\alpha s^{-\alpha} k^2}}_{}, \quad K_\alpha = \frac{\sigma^2}{\tau_\alpha}$$

$$\underbrace{s\,P(k,s) - P_0(k)}_{\mathcal{L}\left\{\frac{\partial P(x,t)}{\partial t}\right\}} = -K_\alpha s^{1-\alpha} \underbrace{k^2 P(k,s)}_{\mathcal{F}\left\{-\frac{\partial^2 P(x,s)}{\partial x^2}\right\}}$$

$$\mathcal{L}^{-1}\{s^{-p}P(x,s)\} = \underline{{}_0D_t^{-p}}\, P(x,t), \quad p \geq 0$$

$$P(x,s) - \frac{P_0(x)}{\underline{s}} = +K_\alpha s^{-\alpha} \frac{\partial^2 P(x,t)}{\partial x^2}$$

$sP - P_0$

$$\boxed{\frac{\partial P(x,t)}{\partial t} = {}_0D_t^{1-\alpha} \frac{\partial^2 P(x,t)}{\partial x^2}}$$

$${}_0D_t^{1-\alpha} P(x,t) = \frac{\partial}{\partial t}\, {}_0D_t^{-\alpha} P(x,t)$$

Riemann - Liouville derivative (operator)

fractional derivative

$${}_0D_t^{1-\alpha} P(x,t) = \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t \frac{P(x,t')}{(t-t')^{1-\alpha}}\, dt', \quad 0 < \alpha < 1$$

Long Rests: Fractional Diffusion Equation

$$\boxed{P(k,s)=\frac{1-w(s)}{s}\frac{P_0(k)}{1-\varphi(k,s)}}$$

Assume for *t* ->∞ $$w(t)\sim A\left(\frac{\tau}{t}\right)^{1+\alpha}$$

Assume that λ(x) has a finite variance

$$w(s)\sim 1-(s\,\tau)^{\alpha}$$

$$P(k,s)=\frac{P_0(k)/s}{1+K_\alpha k^2 s^{-\alpha}}$$

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Long Rests: Fractional Diffusion Equation

$$P(k,s)=\frac{P_0(k)/s}{1+K_\alpha k^2 s^{-\alpha}}$$

$$w(t)\sim A\left(\frac{\tau}{t}\right)^{1+\alpha}$$

λ(x) has
a finite variance

$$\frac{\partial P(x,t)}{\partial t}={}_0D_t^{1-\alpha}K_\alpha\frac{\partial^2}{\partial x^2}P(x,t),K_\alpha=\sigma^2/\tau^\alpha$$

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Fractional derivatives

Riemann-Liouville fractional derivative

$$ {}_0D_t^q P(x,t) = \frac{1}{\Gamma(1-q)} \frac{d}{dt} \int_0^t \frac{P(x,t')}{(t-t')^q} dt' \quad q<1 $$

$$ {}_aD_t^p P(t) = \frac{1}{\Gamma(n-p)} \frac{d^n}{dt^n} \int_a^t P(t')(t-t')^{n-p-1} dt', n-1 \le p < n $$

Examples

$$ {}_0D_t^\nu t^\mu = \frac{\Gamma(1+\mu)}{\Gamma(1+\mu-\nu)} t^{\mu-\nu} $$

$$ {}_0D_t^\nu 1 = \frac{1}{\Gamma(1-\nu)} t^{-\nu} $$

$$ {}_0D_t^\nu \mathrm{e}^t = \frac{t^{-\nu}}{\Gamma(1-\nu)} {}_1F_1(1, 1-\nu, t) $$

$$ {}_{-\infty}D_t^\nu \mathrm{e}^t = \mathrm{e}^t $$

Weyl fractional operator

Fractional derivatives

$$Df(x) = \frac{d f(x)}{dx} = I^{-1} f(x)$$

$$If(x) = \int_0^x f(x)\,dx = D^{-1} f(x)$$

$$D(Df(x)) = \frac{d^2 f(x)}{dx^2}$$

$$I(If(x)) = \int_0^x dx' \int_0^{x'} f(x'')\,dx''$$

$$(I^n f)(x) = \frac{1}{\underbrace{(n-1)!}_{\Gamma(n)}} \int_0^x (x-x')^{n-1} f(x')\,dx'$$

$$I^\alpha f(x) = \frac{1}{\Gamma(\alpha)} \int_0^x (x-x')^{\alpha-1} f(x')\,dx'$$

$$\alpha > 0$$

Riemann-Liouville integral

$$I^{\alpha}(I^{\beta}(x)) = I^{\alpha+\beta}(x)$$

$${}_{a}D_{t}^{p} f(t) = \left(\frac{d}{dt}\right)^{m+1} \int_{a}^{t} (t-\tau)^{m-p} f(\tau)\, d\tau$$

$$m \le p < m+1$$

Fractional derivatives

Riemann-Liouville fractional derivative

$$ {}_0D_t^q P(x,t) = \frac{1}{\Gamma(1-q)} \frac{d}{dt} \int_0^t \frac{P(x,t')}{(t-t')^q} dt' $$

q<1

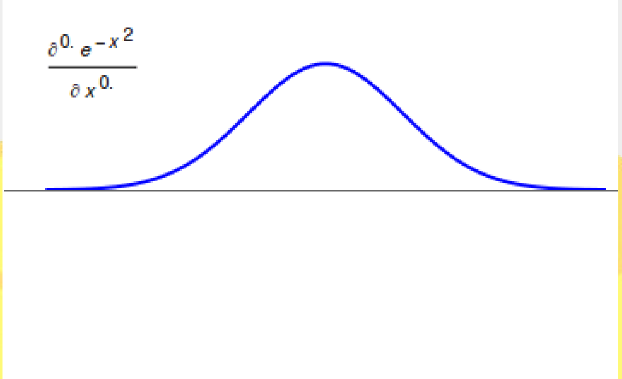
$$ \mathscr{L}\{{}_0D_t^{-q} f(t)\} = u^{-q} f(u) $$

q>0

$$ \mathscr{L}\{{}_0D_t^p f(t)\} = u^p f(u) - \sum_{j=0}^{n-1} u^j c_j $$

$$ c_j = \lim_{t \to 0} {}_0D_t^{p-1-j} f(t) $$

Example: a fractional derivative from a Gaussian changing from 0 to 1



Fractional derivatives

Weyl fractional derivative

$$\mathscr{F}\{\,_{-\infty}D_x^{\mu} f(x)\} = (\mathrm{i}k)^{\mu} f(k)$$

q<1

Grünwald-Letnikov fractional derivative: Finite element representation

$$f'(t) = \frac{df}{dt} = \lim_{h \to 0} \frac{f(t) - f(t-h)}{h}$$

$$f'''(t) = \frac{d^3 f}{dt^3} = \lim_{h \to 0} \frac{f(t) - 3f(t-h) + 3f(t-2h) - f(t-3h)}{h^3}$$

$$f^{(n)}(t) = \frac{d^n f}{dt^n} = \lim_{h \to 0} \frac{1}{h^n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} f(t - rh)$$

$$\binom{n}{r} = \frac{n(n-1)(n-2)\ldots(n-r+1)}{r!}$$

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Fractional derivatives

Grünwald-Letnikov fractional derivative: Finite element representation

$$f^{(n)}(t) = \frac{d^n f}{dt^n} = \lim_{h \to 0} \frac{1}{h^n} \sum_{r=0}^{n} (-1)^r \binom{n}{r} f(t - rh)$$

$$\binom{n}{r} = \frac{n(n-1)(n-2)\dots(n-r+1)}{r!}$$

$$f_h^{(p)}(t) = \frac{1}{h^p} \sum_{r=0}^{n} (-1)^k \binom{p}{r} f(t - rh)$$

$$\boxed{{}_aD_t^p f(t) = \lim_{\substack{h \to 0 \\ nh = t-a}} h^{-p} \sum_{r=0}^{n} (-1)^r \binom{p}{r} f(t - rh) = \lim_{\substack{h \to 0 \\ nh = t-a}} f_h^{(p)}(t)}$$

If we consider a class of functions f(t) having m + 1 continuous derivatives for t, then the Grünwald-Letnikov definition is equivalent to the Riemann-Liouville definition

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Solution of subdiffusive FFPE

$$\frac{\partial P(x,t)}{\partial t} = {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,t), K_\alpha = \sigma^2 / \tau^\alpha$$

$$\langle x^2(t) \rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)} t^\alpha$$

$$P(x,t) = \frac{1}{\sqrt{4K_\alpha t^\alpha}} H_{1,1}^{1,0}\left[\frac{|x|}{\sqrt{K_\alpha t^\alpha}}\middle| \begin{matrix}(1-\alpha/2, \alpha/2)\\(0,1)\end{matrix}\right]$$

$$\int_{-\infty}^{+\infty} 1 \cdot \cancel{x}^2 \, dx$$

$$\frac{\partial P}{\partial t} = {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2 P(x,t)}{\partial x^2} \qquad -\infty < x < \infty$$

Second moment

$$\frac{d\langle x^2(t)\rangle}{dt} = {}_0D_t^{1-\alpha} K_\alpha \underbrace{\int_{-\infty}^{+\infty} \frac{d^2 P(x,t)}{dx^2} x^2 \, dx}_{2} = {}_0D_t^{1-\alpha}(2K_\alpha) = \frac{2K_\alpha}{\Gamma(\alpha)} t^{\alpha-1}$$

$0 < \alpha \leq 1$

$$\langle x^2(t)\rangle = \frac{2K_\alpha}{\Gamma(\alpha+1)} t^\alpha$$

Fox H-functions

$$H_{pq}^{mn}(z) = H_{pq}^{mn}\left[z \middle| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right] = H_{pq}^{mn}\left[z \middle| \begin{matrix} (a_1, A_1), (a_2, A_2), \ldots, (a_p, A_p) \\ (b_1, B_1), (b_2, B_2), \ldots, (b_q, B_q) \end{matrix} \right] = \frac{1}{2\pi \mathrm{i}} \int_L \mathrm{d}s\, \chi(s) z^s$$

$$\chi(s) = \frac{\prod_1^m \Gamma(b_j - B_j s) \prod_1^n \Gamma(1 - a_j + A_j s)}{\prod_{m+1}^q \Gamma(1 - b_j + B_j s) \prod_{n+1}^p \Gamma(a_j - A_j s)}$$

Examples:

$$\mathrm{e}^{-z} = H_{01}^{10}\left[z \middle| \begin{matrix} \overline{} \\ (0,1) \end{matrix} \right]$$

$$\frac{1}{p + k^{2-\alpha}} = \frac{1}{p} \frac{1}{2-\alpha} H_{11}^{11}\left[\frac{k}{p^{\frac{1}{2-\alpha}}} \middle| \begin{matrix} \left(0, \frac{1}{2-\alpha}\right) \\ \left(0, \frac{1}{2-\alpha}\right) \end{matrix} \right]$$

Way to compute is to use the expansion for z → 0 under the set of conditions

$$H_{pq}^{mn}(z) = \sum_{h=1}^{m} \sum_{\nu=0}^{\infty} \frac{\prod_{j=1, j\neq h}^{m} \Gamma(b_j - B_j(b_h + \nu)/B_h)}{\prod_{j=m+1}^{q} \Gamma(1 - b_j + B_j(b_h + \nu)/B_h)} \frac{\prod_{j=1}^{n} \Gamma(1 - a_j + A_j(b_h + \nu)/B_h)}{\prod_{j=n+1}^{p} \Gamma(a_j - A_j(b_h + \nu)/B_h)} \times \frac{(-1)^\nu z^{(b_h + \nu)/B_h}}{\nu! B_h}$$

Fox H-functions

$$H^{mn}_{pq}(z) = H^{mn}_{pq}\left[z \middle| \begin{matrix} (a_p, A_p) \\ (b_q, B_q) \end{matrix} \right] = H^{mn}_{pq}\left[z \middle| \begin{matrix} (a_1, A_1), (a_2, A_2), \ldots, (a_p, A_p) \\ (b_1, B_1), (b_2, B_2), \ldots, (b_q, B_q) \end{matrix} \right] = \frac{1}{2\pi i} \int_L ds\, \chi(s) z^s$$

Pros and contras

Pros:

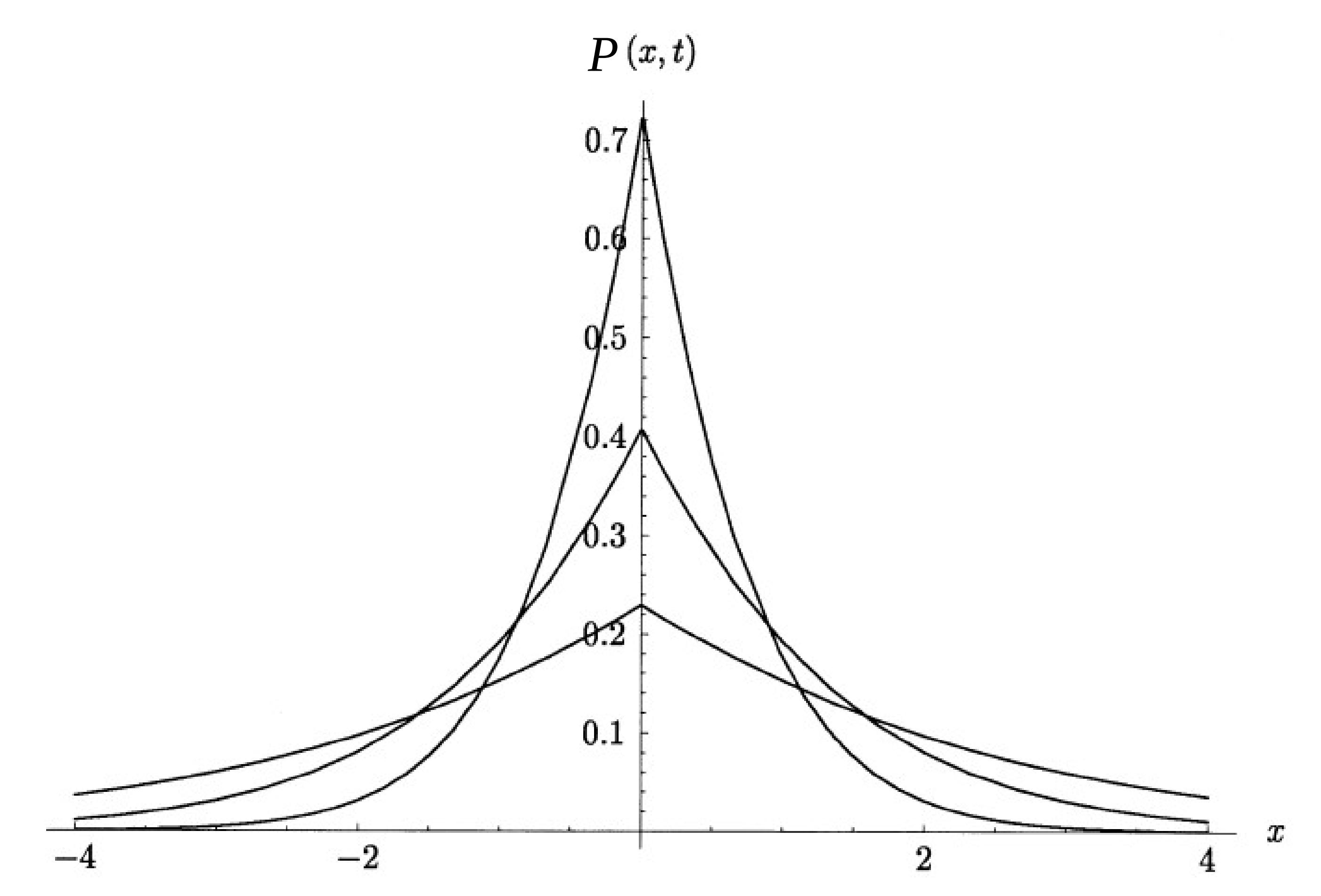
1. Perform integrations one cannot do otherwise
2. Analytical inverse Laplace transform
3. Always either $z \to 0$ or $z \to \infty$ expansion exists
4. Very helpful for equations with fractional derivatives

Contras

1. Not always possible to express a needed function as an *H*-function
2. Just by looking at coefficients we do not have a clue what the function is

Numerical results for subdiffusive FFPE

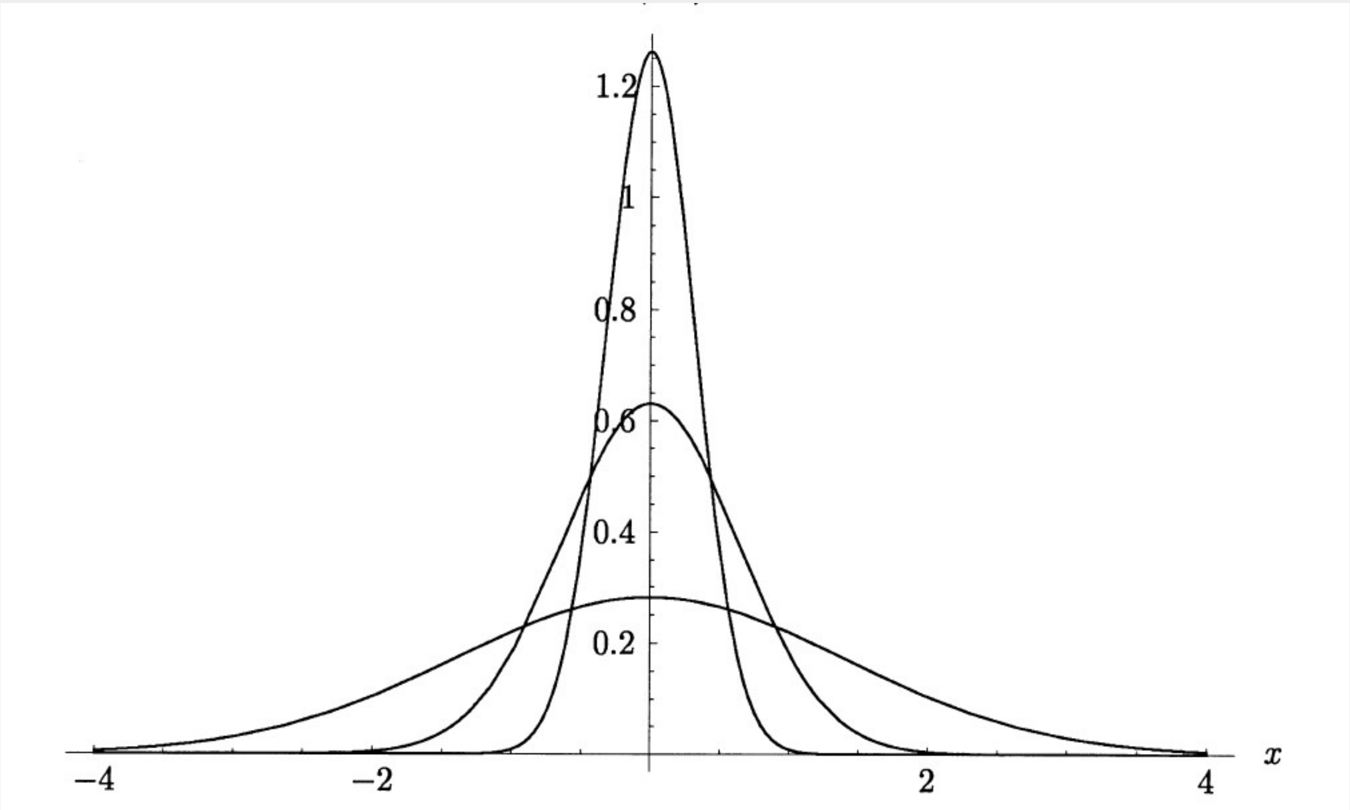
$$\frac{\partial P(x,t)}{\partial t} = {}_0D_t^{1-\alpha} K_\alpha \frac{\partial^2}{\partial x^2} P(x,t), K_\alpha = \sigma^2 / \tau^\alpha \quad \alpha = 0.5;\ t = 0.1,\ 1,\ 10$$



R. Metzler, J. Klafter, Phys. Rep. 2000

Reminder:
Numerical results for normal FPE

$$\frac{\partial P(x,t)}{\partial t} = K_2 \frac{\partial^2}{\partial x^2} P(x,t) \qquad t = 0.1,\ 1,\ 10$$



R. Metzler, J. Klafter, Phys. Rep. 2000

Literature

1. B.D. Hughes, Random Walks and Random Environments, Vol. 1 Random Walks, Clarendon Press, Oxford, 1995.
2. R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Physics reports 339, 1-77 (2000).
3. The restaurant at the end of the random walk: recent developments in the description of anomalous transport by fractional dynamics
R Metzler, J Klafter, Journal of Physics A: Math. and Gen. 37, R161 (2004)
4. Anomalous diffusion models and their properties: non-stationarity, non-ergodicity, and ageing at the centenary of single particle tracking
R Metzler, JH Jeon, AG Cherstvy, E Barkai, Physical Chemistry Chemical Physics 16, 24128-24164 (2014)

Literature.
Fractional derivatives and fractional differential equations

1. I. Podlubny, Fractional Differential Equations:
An Introduction to Fractional Derivatives, Fractional Differential Equations,
to Methods of Their Solution and Some of Their Applications. Elsevier, 1998.

2. Samko, S.; Kilbas, A.A.; Marichev, O. (1993). Fractional Integrals
and Derivatives: Theory and Applications. Taylor & Francis Books.

3. Publications of F. Mainardi

Fox H-functions:

1. A.M. Mathai, R.K. Saxena, H.J. Haubold, The H-Function
Theory and Applications, Springer, 2009.