Fractional kinetics

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Outline

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3. Continuous time random walk. Physical examples
4. Fractional kinetic equation. Fractional calculus
5. Super-diffusion and sub-diffusion
6. Strong anomalous diffusion
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St. Petersburg paradox (N. Bernoulli, 1713)

$$\left.\begin{array}{ccc} \text{Sequence} & \text{Win} & \text{Probability} \\ head & 1 & 1/2 \\ tail, head & 2 & 1/4 \\ 2\, tails, head & 2^2 & 1/8 \\ \cdots & \cdots & \cdots \\ N\, tails, head & 2^N & 1/2^{N+1} \\ \cdots & \cdots & \cdots \end{array}\right\} \begin{array}{c} \text{mean gain} \\ 1 \cdot \frac{1}{2} + 2 \cdot \frac{1}{4} + \cdots + 2^N \cdot \frac{1}{2^{N+1}} + \cdots \\ \text{diverges} \end{array}$$

Central Limit Theorem

$$X = \frac{1}{\sqrt{N}} \underbrace{(x_1 + \cdots + x_N)}_{\substack{\text{identically distributed} \\ \text{statistically independent} \\ P(x_j),\ \langle x_j \rangle = 0}} \quad \overset{N \gg 1}{\Longrightarrow} \quad \underbrace{P_G(X) = \frac{\exp\left(-X^2/(2\sigma)\right)}{\sqrt{2\pi\sigma}}}_{\substack{\text{Gaussian distribution} \\ \sigma = \langle x^2 \rangle}}$$

Lévy distribution

Identical normalized distributions

$$\begin{array}{ccccc} cx_3 & = & c_1x_1 & + & c_2x_2 \\ \uparrow & & \uparrow & & \uparrow \\ P(x_3) & & P(x_1) & & P(x_2) \end{array}$$

$$\int_{-\infty}^{\infty} P(x)dx = 1, \quad \widehat{P}(q) = \int_{-\infty}^{\infty} P(x)e^{iqx}dx$$

$$P(x_3) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} P(x_1)P(x_2)\delta\left(x_3 - \frac{c_1}{c}x_1 - \frac{c_2}{c}x_2\right) dx_1\, dx_2$$

$$e^{iqcx_3} \quad = \quad e^{iqc_1x_1} \quad \cdot \quad e^{iqc_2x_2}$$

$$\widehat{P}(cq) = \widehat{P}(c_1q)\widehat{P}(c_2q) \quad \longrightarrow \quad \ln\widehat{P}(cq) = \ln\widehat{P}(c_1q) + \ln\widehat{P}(c_2q)$$

Class of solutions

$$\ln P_\gamma(cq) = (cq)^\gamma, \quad \left(\frac{c_1}{c}\right)^\gamma + \left(\frac{c_2}{c}\right)^\gamma = 1$$

$\gamma = 2$ Gaussian distribution

$$\widehat{P}_\gamma(q) = \exp(-a|q|^\gamma)$$

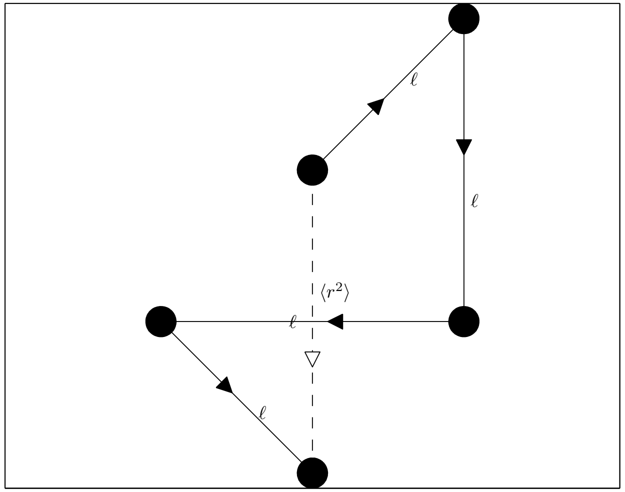
$0 < \gamma < 2$ Lévy distribution

$$P_\gamma(x) \sim |x|^{-\gamma-1}, \ |x| \gg 1$$

$$\langle x^m \rangle = \int_{-\infty}^{\infty} x^m P_\gamma(x) dx \quad \text{diverges for} \quad m \geqslant \gamma$$

$$\langle x^2 \rangle = \infty$$

Normal diffusion: gases, liquids, solids ...



$$\langle r^2 \rangle = C \underbrace{\ell^2}_{\substack{\textit{mean}\\ \textit{path}\\ \textit{length}}} \cdot \underbrace{N}_{\substack{\textit{number}\\ \textit{of jumps}}} \qquad N = \underbrace{\frac{t}{\tau}}_{\substack{\textit{mean time}\\ \textit{between}\\ \textit{collisions}\\ \textit{or jumps}}} \qquad \langle r^2 \rangle \sim \underbrace{\frac{\ell^2}{\tau}}_{\substack{\textit{diffusion}\\ \textit{coefficient}}} t$$

Continuous time random walk

Jump probability distribution function $\psi(\vec{r}, t)$

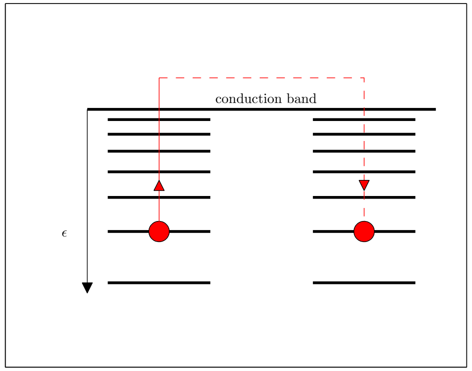
$$\ell^2 = \int_0^\infty \int_{\mathbb{R}^d} r^2 \psi(\vec{r}, t)\, d\vec{r}\, dt$$

$$\tau = \int_0^\infty \int_{\mathbb{R}^d} t\, \psi(\vec{r}, t)\, d\vec{r}\, dt$$

Simplification

$$\psi(\vec{r}, t) = \underbrace{w(t)}_{\substack{\textit{waiting time}\\ \textit{distribution}\\ \textit{function}}} \cdot \underbrace{\lambda(r)}_{\substack{\textit{step length}\\ \textit{distribution}\\ \textit{function}}}$$

Electrons in semi-conductors



Distribution of energy levels

$$\rho(\epsilon) = \rho_0 \exp\left(-\frac{\epsilon}{k\,T_0}\right)$$

Release rate

$$W(\epsilon) = W_0 \exp\left(-\frac{\epsilon}{k\,T}\right)$$

Waiting time distribution

$$w(t) \sim \int_0^\infty \rho(\epsilon) \exp\left(-W(\epsilon)\,t\right)\, W(\epsilon)\, d\epsilon = \int_{W_0}^0 \frac{d\epsilon}{dW} \rho(W) e^{-Wt} W\, dW$$

$$\epsilon = -kT \ln \frac{W}{W_0} \qquad \rho(W) = C\, W^{T/T_0} \qquad \frac{d\epsilon}{dW} = -\frac{kT}{W} \qquad \frac{T}{T_0} \equiv \gamma$$

$$w(t) \sim \int_0^{W_0} W^\gamma e^{-Wt}\, dW \quad \overset{t\gg 1, W=z/t}{\sim} \quad t^{-(1+\gamma)} \underbrace{\int_0^\infty z^\gamma e^{-z} dz}_{\text{const}}$$

Take a waiting time distribution function $\longrightarrow$ survival probability

$$w(t) = \frac{\gamma\tau_0^\gamma}{(\tau_0+t)^{\gamma+1}}, \quad \int_0^\infty w(t)\,dt = 1 \quad \longrightarrow \quad P(t) = 1 - \int_0^t w(t')\,dt' = \frac{\tau_0^\gamma}{(\tau_0+t)^\gamma}$$

Mean interval between jumps

$$\tau = \int_0^\infty t\,w(t)\,dt = \gamma\tau_0 \int_0^\infty \frac{t\,dt}{(\tau_0+t)^{\gamma+1}} \quad \begin{array}{lll} \nearrow & \mathit{finite} & \text{if} \quad \gamma > 1 \\ \searrow & \mathit{infinite} & \text{if} \quad \gamma \leqslant 1 \end{array}$$

Assume a step length distribution function

$$\lambda(x) = \exp(-x^2/(4\sigma^2))/\sqrt{4\pi\sigma^2}.$$

Probability distribution function of particles arriving at point x at time instant t

$$\eta(x,t) = \int_{-\infty}^\infty \int_0^\infty \eta(x',t')w(t-t')\lambda(x-x')\,dt'\,dx' + \delta(x)\delta(t)$$

Probability distribution for being in point x at time instant t

$$\rho(x,t) = \int_0^t \eta(x,t')\left[1 - \int_{t'}^t w(t''-t')\,dt''\right]\,dt'$$

Laplace transform | Fourier transform

$$\tilde{w}(s) = 1 - (s\tau_0)^\gamma,\ s \ll 1 \qquad\qquad \hat{\lambda}(k) = 1 - \sigma^2 k^2 + \mathcal{O}(k^4)$$

$$\hat{\tilde{\eta}}(k,s) = \frac{1}{1 - \tilde{w}(s)\hat{\lambda}(k)}$$

$$\hat{\tilde{\rho}}(k,s) = \frac{1 - \tilde{w}(s)}{s\left(1 - \tilde{w}(s)\hat{\lambda}(k)\right)} \sim \frac{(s\tau_0)^\gamma}{s\left[(s\tau_0)^\gamma + \sigma^2 k^2\right]} = \frac{1}{s(1 + K_\gamma s^{-\gamma} k^2)}$$

$$s\hat{\tilde{\rho}}(k,s) \ = \ K_\gamma(-k^2)s^{1-\gamma}\hat{\tilde{\rho}}(k,s) \ + \ 1$$

$$\downarrow \qquad\qquad\qquad \downarrow \qquad\qquad\qquad \downarrow$$

$$\frac{\partial \rho(x,t)}{\partial t} = K_\gamma \frac{\partial^2}{\partial x^2} \underbrace{{}_0\mathfrak{D}_t^{1-\gamma}\rho(x,t)}_{\substack{fractional \\ derivative}} + \delta(x)\delta(t)$$

Fractional calculus

Fractional integral

$$ {}_aD_t^{-\alpha} f(t) = \frac{1}{\Gamma(\alpha)} \int_a^t (t-t')^{\alpha-1} f(t') dt' \qquad 0 < \alpha < 1 $$

Fractional derivative

$$ {}_aD_t^{\alpha} f(t) = \frac{d^n}{dt^n} \, {}_aD_t^{\alpha-n} f(t) \qquad 0 < \alpha - n < 1 $$

Examples

$$ {}_0D_t^{\alpha} t^{\mu} = \tfrac{\Gamma(\mu+1)}{\Gamma(\mu-\alpha+1)} t^{\mu-\alpha} \qquad {}_0D_t^{\alpha} 1 = \tfrac{1}{\Gamma(1-\alpha)} t^{-\alpha} \qquad {}_0D_t^{\alpha} e^t = e^t \tfrac{\gamma(-\alpha,t)}{\Gamma(-\alpha)} $$

$$ {}_0D_t^{-1/2} e^t = \mathrm{erf}(\sqrt{t}) e^t \qquad {}_0D_t^{1/2} e^t = \mathrm{erf}(\sqrt{t}) e^t + \tfrac{1}{\sqrt{\pi t}} \qquad {}_0D_t^{-1/2} \ln t = 2\sqrt{\tfrac{\pi}{t}} [\ln(4t-2)] $$

$$ {}_0D_t^{1/2} \ln t = \tfrac{\ln(4t)}{\sqrt{\pi t}} \qquad \mathcal{L}\left[{}_0D_t^{-\alpha} f(t) \right] t^{-\alpha} \mathcal{L}\left[f(t) \right] \qquad \mathcal{F}\left[{}_{-\infty}D_t^{\alpha} f(t) \right] = (iw)^{\alpha} \hat{f}(w) $$

Riemann-Liouville operator

$$ {}_0\mathfrak{D}_t^{1-\gamma}\rho(x,t) = \frac{1}{\Gamma(\gamma)}\frac{\partial}{\partial t}\int_0^t \frac{\rho(x,t')}{(t-t')^{1-\gamma}}\,dt $$

$$ \langle x^2(t)\rangle = \int_{-\infty}^{\infty} x^2\rho(x,t)\,dx $$

$$ \widetilde{\langle x^2\rangle}(s) = \int_{-\infty}^{\infty} x^2\tilde{\rho}(x,s)\,dx \sim \left.\frac{\partial^2}{\partial k^2}\hat{\tilde{\rho}}(k,s)\right|_{k=0} \sim s^{-(1+\gamma)} $$

$$ \downarrow $$

Sub-diffusion

$$ \langle x^2\rangle(t) \sim t^{\gamma}, \quad 0<\gamma<1 $$

disordered systems

gels, glass forming systems

cell membranes, living cells (caging)

Continuous time random walk

Jump probability distribution function $\psi(\vec{r}, t) = \underbrace{\lambda(r)}_{\substack{step\ length\\ distribution}} \quad \underbrace{w(t)}_{\substack{waiting\ time\\ distribution}}$

$$\swarrow \qquad \searrow$$

$$\lambda \sim \frac{a^\gamma}{r^{\gamma+1}}, \quad \gamma = \frac{2}{\nu}, \quad r \gg 1 \qquad \longleftarrow \qquad \substack{super-diffusion\\ (Levy\ flight)} \qquad sub-diffusion$$

$$\frac{\partial n(x,t)}{\partial t} = D \underbrace{\frac{\partial^\gamma n}{\partial |x|^\gamma}}_{\substack{Riesz\ fractional\\ derivative}} \qquad \underbrace{\mathcal{F}\left[\frac{d^\gamma g(x)}{d|x|^\gamma}\right] = -|k|^\gamma \hat{g}(k),\ 1 < \gamma < 2}_{in\ k-space}$$

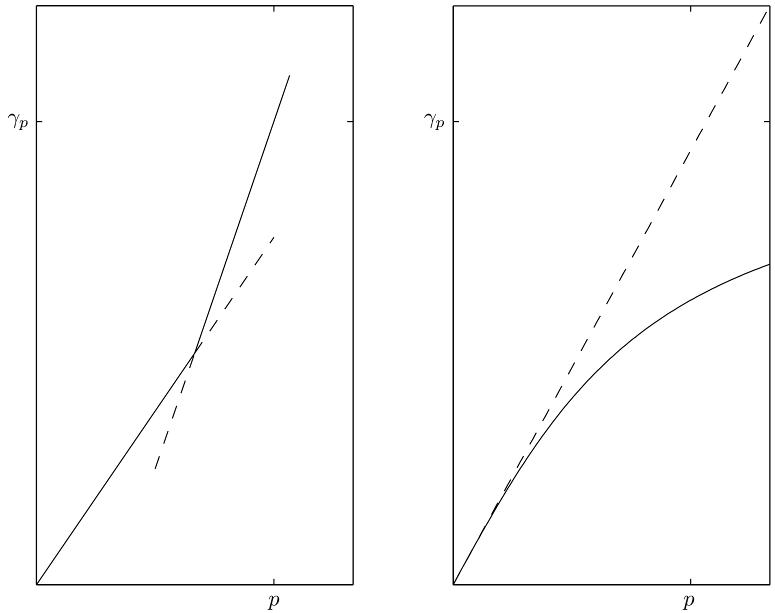
In x-space

$$\frac{\partial^\gamma n}{\partial |x|^\gamma} = -\frac{\sec(\pi\gamma/2)}{2\Gamma(2-\gamma)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{\infty} \frac{n(\zeta)}{|x-\zeta|^{\gamma-1}} d\zeta = -\frac{\sec(\pi\gamma/2)}{2\Gamma(-\gamma)} \int_{-\infty}^{\infty} \frac{n(\zeta) - n(x)}{|x-\zeta|^{\gamma+1}} d\zeta$$

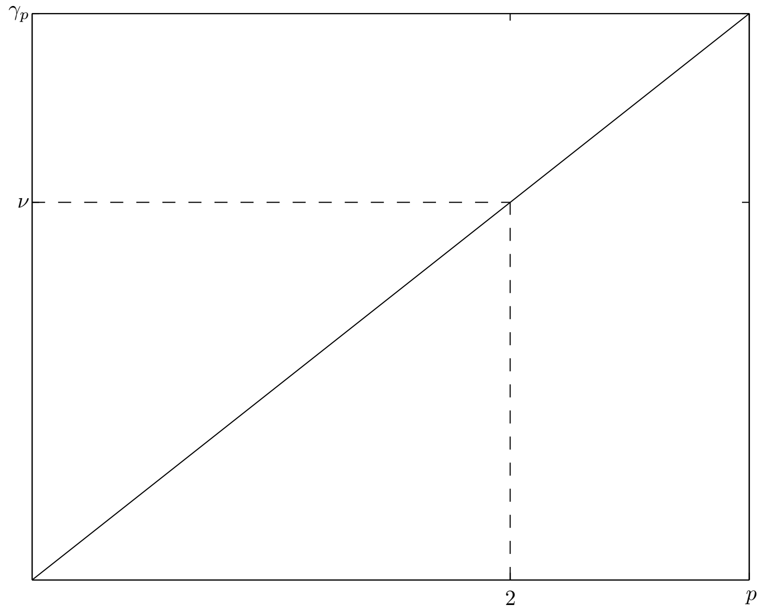
Strong anomalous diffusion

$$\langle x^p \rangle = \frac{1}{n} \sum_{n=1}^{N} |x_n(t)|^p \sim t^{\gamma_p}$$

large p characterize tails in the probability distribution



strong (multi-fractal) anomalous diffusion



weak (self-similar) anomalous diffusion

Alternative approach: generalized Langevin equation

$$m\frac{d^2x(t)}{dt^2} + \underbrace{\int_0^t \eta(t-t')\frac{dx(t')}{dt'}\,dt'}_{viscoelastic\ force} + \frac{\partial V(x,t)}{\partial x} = \underbrace{\xi(t)}_{\substack{fractional\\ Gaussian\\ noise}}$$

$$\eta(t) = \frac{\eta_\alpha}{\Gamma(1-\alpha)}\,t^{-\alpha}, \qquad \langle\xi(t)\xi(t')\rangle = k_B\,T\,\eta(|t-t'|) \qquad 0<\alpha<1$$

$$m\to 0:\ \langle\delta x^2(t)\rangle = \frac{2K_\alpha}{\Gamma(1+\alpha)}\,t^\alpha, \quad K_\alpha = \frac{k_B}{\eta_\alpha}\,T$$

Fractional Brownian motion

$$D(t) = \frac{K_\alpha}{\Gamma(1+\alpha)}\,t^{\alpha-1}$$

antipersistent velocity correlation

Transport in fluid flows

Anomalous diffusion $\quad \langle r^2 \rangle \sim t^{\nu/2} \qquad \nu \neq 2$

Effective diffusion coefficients

$$D_{ij} = \lim_{t\to\infty} \frac{1}{2t} \langle (x_i(t) - \langle x_i \rangle)\,(x_j(t) - \langle x_j \rangle)\rangle$$

Taylor, 1921

$$D_{ii} = \int_0^\infty \langle v_i\,(\vec{x}(t))\, v_i\,(\vec{x}(t+\tau))\rangle d\tau$$

Avellaneda and Majda, 1989

$$D_{ij} \text{ is finite if } \int \frac{1}{k^2} \left|\hat{\vec{v}}(\vec{k})\right|^2 dk < \infty$$

Richardson, 1926

$$\langle |\vec{x}_1(t) - \vec{x}_2(t)|^2 \rangle \sim t^3$$

Observations

- two dimensional flow in a rotating annulus {Solomon et al. 1993, 1994, Weaks et al. 1996}
- decaying two dimensional turbulence {Hansen et al. 1998}
- also: surface diffusion, animals' migration, living cells, wave turbulence, non-local transport in plasma, porous media

Reaction – super-diffusion (Lévy flight)

$$\partial_t n_j = \mathrm{D}_{ij}\ \mathfrak{D}_{|x|}^{\gamma_j} n_j + f_j(\mathbf{n}), \quad 1 < \gamma_j \leq 2,\ j = 1, \ldots, m.$$

Riesz derivative

$$\mathfrak{D}_{|x|}^{\gamma_j} e^{iq\xi} = -|q|^{\gamma_j} e^{iq\xi}.$$

Homogeneous steady state

$$\mathbf{f}(\mathbf{n}_0) = \mathbf{0}.$$

Hopf super-critical bifurcation via the kinetics sensitivity matrix trace ($\mu > 0$ super-criticality parameter)

$$F = \begin{pmatrix} F_{11} & F_{12} \\ F_{21} & -F_{11} + \epsilon^2 \mu \end{pmatrix} = F_0 + \epsilon^2 \begin{pmatrix} 0 & 0 \\ 0 & \mu \end{pmatrix}.$$

Multiple scales method

$$\mathbf{n}(x,t) = \mathbf{N}(\xi, t_0, \tau; \epsilon), \quad t_0 = t, \quad \tau = \epsilon^2 t,$$

$$\xi = \delta x, \quad \delta = \epsilon^{2/\min\{\gamma_1,\gamma_2\}}.$$

Analogue of complex Ginzburg-Landau equation

$$\frac{\partial A}{\partial \tau} = A + (1+\alpha i)\mathfrak{D}_{|\xi|}^{\min\{\gamma_1,\gamma_2\}} A \mp (1+\beta i) A|A|^2,$$

$$\alpha = \frac{F_{11}}{\sqrt{\det F_0}} \times \begin{cases} (d-1)/(d+1) & \gamma_1 = \gamma_2 = \gamma \\ \operatorname{sign}(\gamma_1 - \gamma_2) & \gamma_1 \neq \gamma_2 \,, \end{cases}$$

β and the sign of the cubic term depends on higher derivatives of $\mathbf{f}$.

Non-linear phase diffusion

Bifurcation at Benjamin-Feir domain boundary

$$0 < -(1+\alpha\beta) = \epsilon \ll 1.$$

Non-linear evolution of a general complex disturbance to the homogeneous oscillation solution

$$A = e^{-i\beta\tau_2/\epsilon^2} r(\tau_2, \xi_{1/\gamma}) e^{i\varphi(\tau_2, \xi_{1/\gamma})}$$

on the scales

$$\xi_{1/\gamma} = \epsilon^{1/\gamma}\xi, \qquad \tau_2 = \epsilon^2\tau$$

leads to an analogue of the Kuramoto-Sivashinsky equation (scaled)

$$\frac{\partial\varphi}{\partial\tau} = -\mathfrak{D}^{\gamma}_{|\xi|}\varphi - (\mathfrak{D}^{\gamma}_{|\xi|})^2\varphi + \frac{1}{2}\mathfrak{D}^{\gamma}_{|\xi|}\varphi^2 - \varphi\mathfrak{D}^{\gamma}_{|\xi|}\varphi.$$

Travelling shock waves

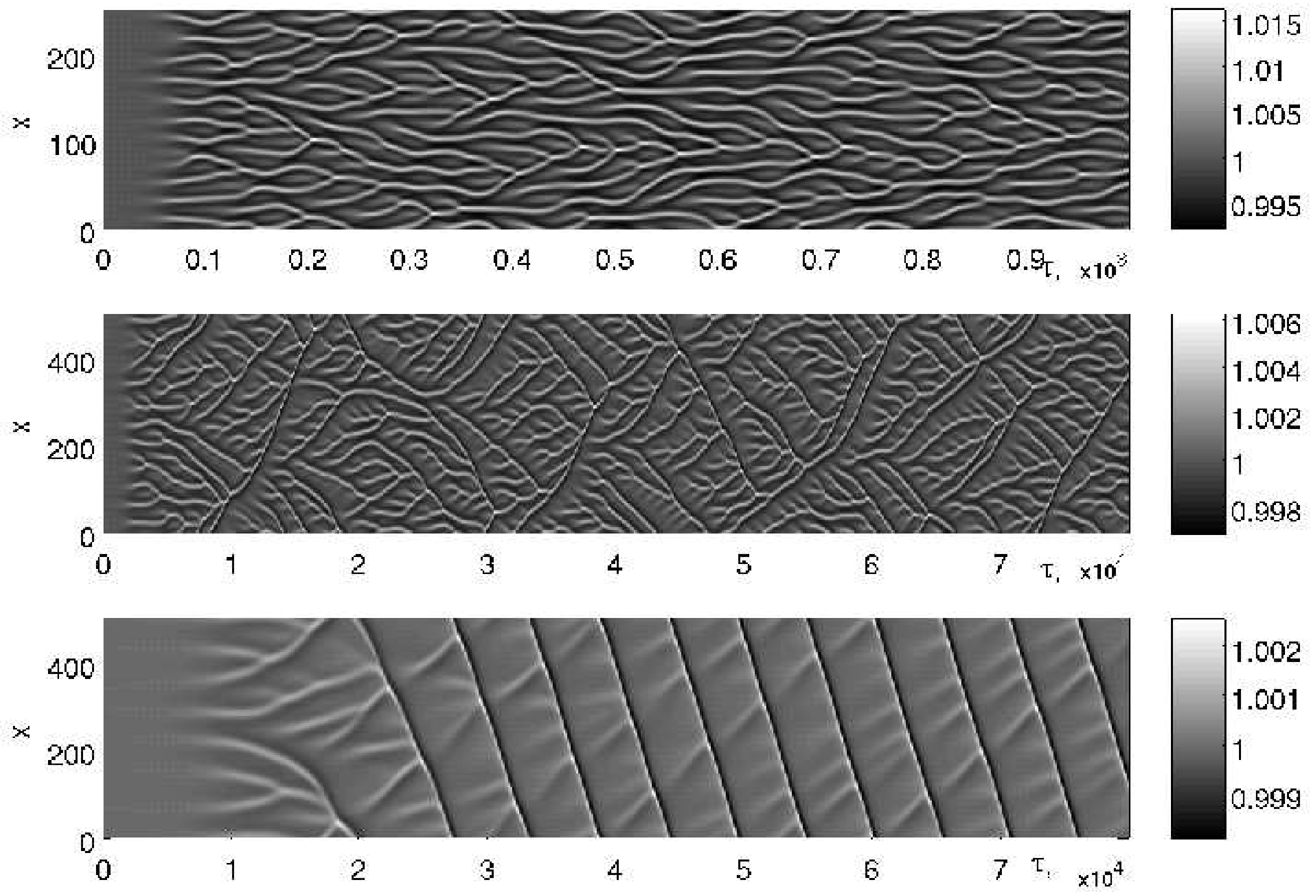


Figure 1

Phase to amplitude turbulence transition

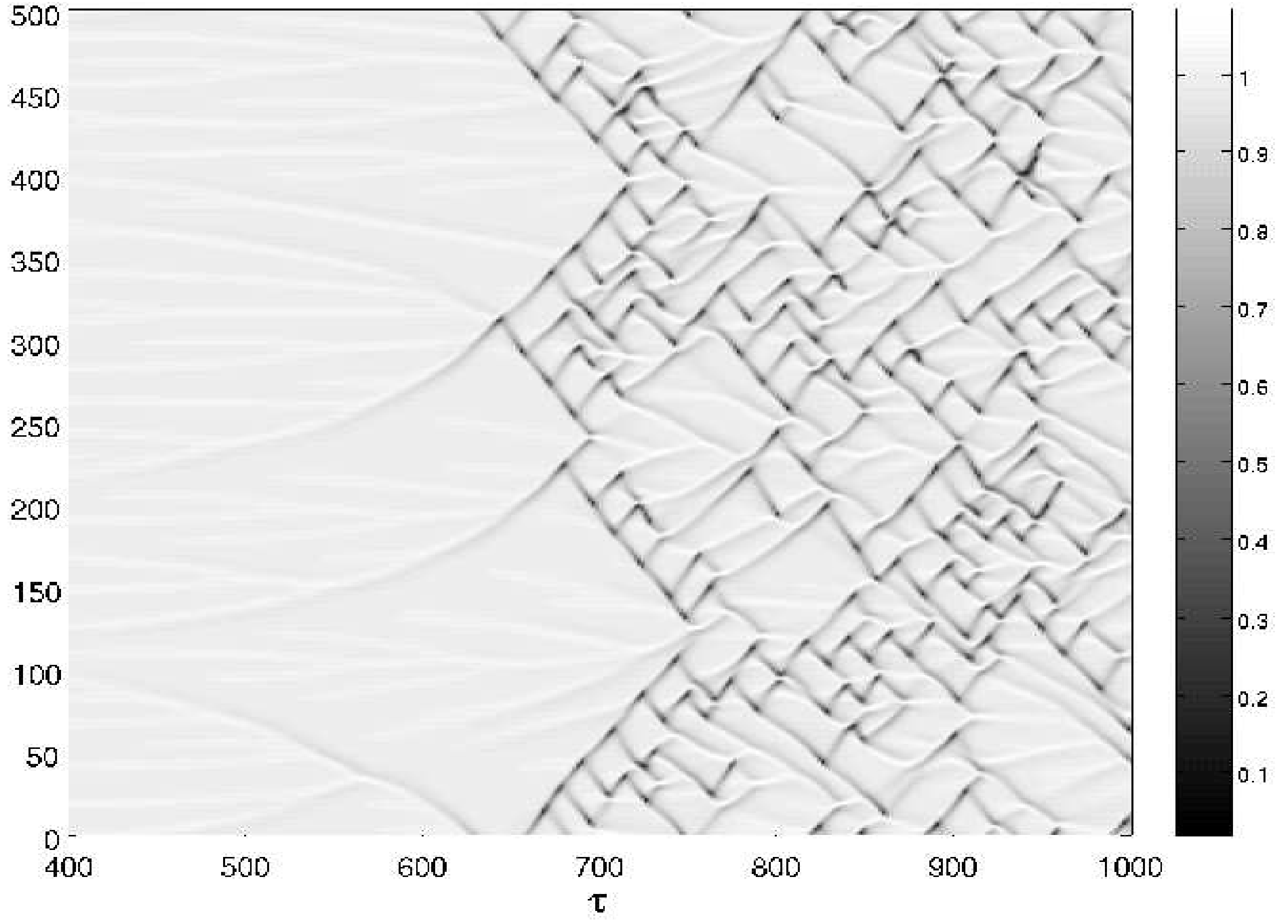


Figure 2

Amplitude turbulence regime

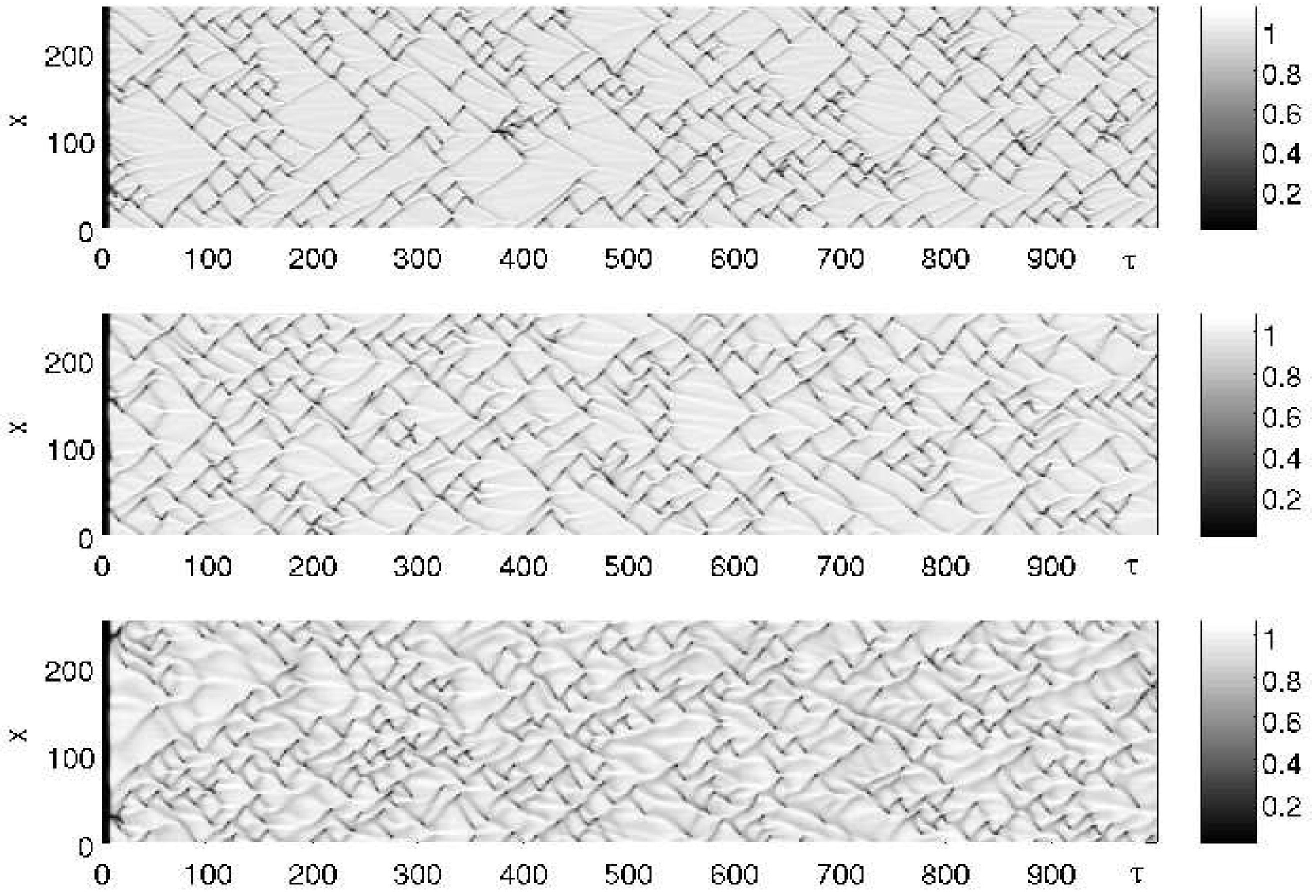


Figure 3

Reaction – sub-diffusion with aging: introduction

Continuous time random walk without reaction

$$\psi(\mathbf{r},t) = \mathrm{m}(\mathbf{r})w(t),$$

$$\mathcal{F}\mathrm{m}(\mathbf{q}) \sim \mathrm{I} - |\mathbf{q}|^2\sigma\mathrm{D}, \quad \mathcal{L}w(s) \sim 1 - \Gamma(1-\gamma)\tau_0^\gamma s^\gamma,$$

$$\partial_t \mathbf{n}(\mathbf{r},t) = \mathrm{D}\mathfrak{D}^{1-\gamma}\nabla^2\mathbf{n}(\mathbf{r},t), \quad 0 < \gamma < 1.$$

Decay concept

$$\partial_t \mathbf{n}(\mathbf{r},t,t') = -w(t-t')\mathbf{n}(\mathbf{r},t',t'),$$

Inclusion of linear kinetics

$$\mathbf{n}(\mathbf{r},t,t) = \int_\Omega \mathrm{m}(\mathbf{r}-\mathbf{r}') \int_0^t w(t-t')e^{\mathrm{M}(t-t')}\mathbf{n}(\mathbf{r}',t',t')dt'd\mathbf{r}'$$

(Nec & Nepomnyashchy, J. Physics A, 2007)

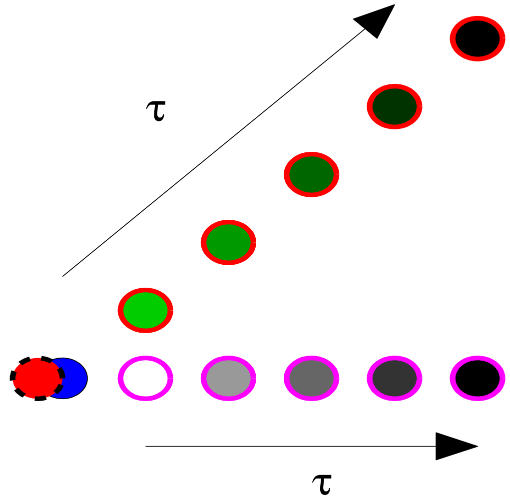
(Sokolov, Schmidt & Sagués, PRE, 2006)

Reaction – sub-diffusion with aging: problem formulation

Aging concept

$$\partial_t \mathbf{n}(\mathbf{r},t,t') = -W(t-t')\mathbf{n}(\mathbf{r},t,t'),$$

$$w(t-t') = W(t-t')\left(1 - \int_{t'}^{t} w(y-t')dy\right).$$

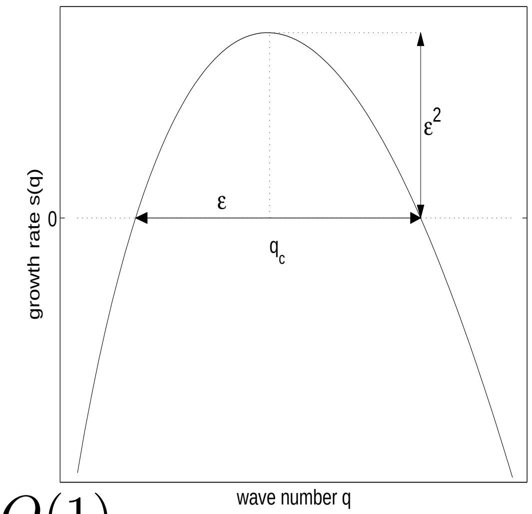


Inclusion of non-linear kinetics

$$\partial_t \mathbf{n}(\mathbf{r},t,t') = \left[-W(t-t')\mathrm{I} + \mathrm{M}(\boldsymbol{\rho})\right]\mathbf{n}(\mathbf{r},t,t'),$$

$$\boldsymbol{\rho}(\mathbf{r},t) = \int_0^t \mathbf{n}(\mathbf{r},t,t')dt', \quad \mathbf{r} \in \Omega, \quad 0 < t' < t < \infty,$$

$$\mathbf{n}(\mathbf{r},t,t) = \int_\Omega \mathrm{m}(\mathbf{r}-\mathbf{r}') \int_0^t W(t-t')\mathbf{n}(\mathbf{r}',t,t')dt'd\mathbf{r}'.$$



Possible bifurcation points

Turing (short wave instability) $q_c \sim O(1)$

Hopf (long wave limit) $q_c = 0.$

Outlook

1. Asymmetric fractional derivatives
2. Fractional derivatives of distributed order
3. Truncated Lévy flights
4. Lévy walks
5. Lévy walks in search processes
6. Multifractal random walks