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Pseudochaos and Stable-Chaos in Statistical Mechanics and Quantum Physics

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From normal to anomalous deterministic diffusion (II): Anomalous deterministic diffusion

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From normal to anomalous deterministic diffusion
Part 2: Anomalous deterministic diffusion

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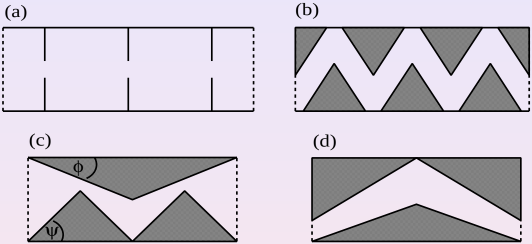
Reminder

two parts:

1. **Normal deterministic diffusion:**
   simple maps and billiards, dynamical systems theory, and zeolites
2. **Anomalous deterministic diffusion:**
   some slightly more complicated maps, ergodic and stochastic theory, and cell migration

Polygonal billiard channels

instead of convex scatterers, look at polygonal ones:



- **weak chaos:** dispersion of nearby trajectories $\Delta(t)$ grows weaker than exponential (Zaslavsky, Usikov, 2001)
- **pseudochaos:** algebraic dispersion $\Delta \sim t^{\nu}$, $0 < \nu$ (Zaslavsky, Edelman, 2002); above: special case $\nu = 1$

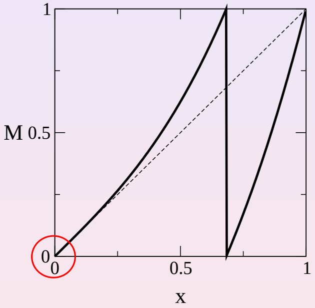
'highly non-trivial' parameter dependence of diffusion in simulations (→ Rondoni); relation to piecewise isometries (→ Vivaldi) and to ergodic theory (→ Artuso, Gutkin, Prosen)

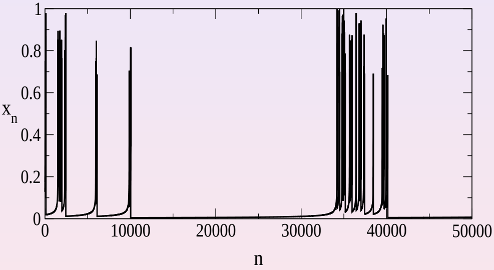
(∃ review about pseudochaotic diffusion in book by R.K., 2007)

Intermittency in the Pomeau-Manneville map

consider the nonlinear one-dimensional map

$$x_{n+1} = M(x_n) = x_n + a x_n^z \mod 1 \, , \; z \geq 1 \quad , \quad a = 1$$





phenomenology of **intermittency**: long periodic *laminar phases* interrupted by *chaotic bursts*; here due to an indifferent fixed point, $M'(0) = 1$ (Pomeau, Manneville, 1980)

$\Rightarrow$ map not hyperbolic ($\nexists N > 0$ s.t. $\forall x \forall n \geq N \; |(M^n)'(x)| \neq 1$)

From ergodic to infinite ergodic theory

choose a 'nice' *observable* $f(x)$:

• for $1 \leq z < 2$ it is $\sum_{i=0}^{n-1} f(x_i) \sim n \ (n \to \infty)$

Birkhoff's theorem: if M is ergodic then $\frac{1}{n} \sum_{i=0}^{n} f(x_i) = < f >_\mu$

• but for $2 \leq z$ we have the **Aaronson-Darling-Kac theorem**,

$$\frac{1}{a_n} \sum_{i=0}^{n-1} f(x_i) \xrightarrow{d} \mathcal{M}_\alpha < f >_\mu \quad (n \to \infty)$$

$\mathcal{M}_\alpha$: random variable with normalized *Mittag-Leffler* pdf

for M it is $a_n = n^\alpha$, $\alpha := 1/(z-1)$; integration wrt to Lebesgue measure m suggests

$$\frac{1}{n^\alpha} \sum_{i=0}^{n-1} < f(x_i) >_m \sim < f(x) >_\mu$$

note: for $z < 2$, $\alpha = 1$ $\exists$ absolutely continuous invariant measure μ, and we have an equality; for $z \geq 2$ $\exists$ infinite invariant measure, and it remains a *proportionality*

Defining weak chaos quantities

This motivates to define a **generalized Ljapunov exponent** as

$$\Lambda(M) := \lim_{n\to\infty} \frac{\Gamma(1+\alpha)}{n^\alpha} \sum_{i=0}^{n-1} < \ln \left| M'(x_i) \right| >_m$$

(*stretched* exponential instability) and analogously a **generalized KS entropy**,

$$h_{KS}(M) := \lim_{n\to\infty} -\frac{\Gamma(1+\alpha)}{n^\alpha} \sum_{w\in\{W_i^n\}} \mu(w) \ln \mu(w)$$

For a piecewise linearization of M one can show analytically

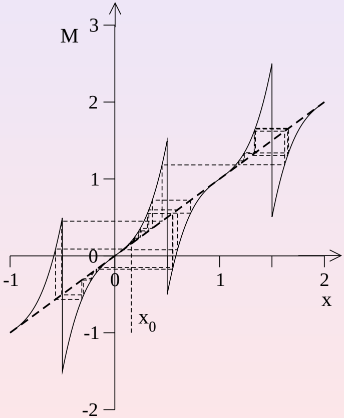
$$h_{KS}(M) = \Lambda(M)$$

see **Rokhlin's formula**, which generalizes *Pesin's theorem* to intermittent dynamics (Howard, RK, 2009)($\rightarrow$ Korabel)

open question: escape rate approach for anomalous deterministic diffusion?

An intermittent map with anomalous diffusion

continue map by $M(-x) = -M(x)$ and $M(x+1) = M(x) + 1$:
(Geisel, Thomae, 1984; Zumofen, Klafter, 1993)



deterministic random walk on the line; classify diffusion in terms of the mean square displacement

$$\langle x^2 \rangle = K\, n^{\alpha} \; (n \to \infty)$$

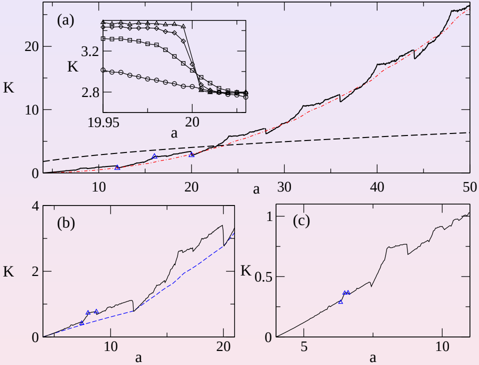
if $\alpha \neq 1$ one speaks of **anomalous diffusion**; here one finds

$$\alpha = \begin{cases} 1, & 1 \leq z \leq 2 \\ \frac{1}{z-1} < 1, & 2 < z \end{cases}$$

focus on generalized diffusion coefficient $K = K(z, a)$

Parameter dependent anomalous diffusion

$K(z = 3, a)$ for $M(x) = x + ax^3$ from computer simulations:



Korabel, R.K. et al., 2005

- $\exists$ *fractal structure*
- $K(a)$ conjectured to be *discontinuous* (inset) on dense set
- comparison with *stochastic theory*, see dashed lines

CTRW theory I: Montroll-Weiss equation

Montroll, Weiss, Scher, 1973:

master equation for a stochastic process defined by *waiting time distribution* $w(t)$ and *distribution of jumps* $\lambda(x)$:

$$\varrho(x,t) = \int_{-\infty}^{\infty} dx' \lambda(x-x') \int_0^t dt'\, w(t-t')\, \varrho(x',t') + \\ +(1-\int_0^t dt' w(t'))\delta(x)$$

structure: jump + no jump for particle starting at $(x,t)=(0,0)$

$\hat{\text{F}}$ourier-$\tilde{\text{L}}$aplace transform yields Montroll-Weiss eqn (1965)

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

with mean square displacement $\tilde{\langle x^2(s)\rangle} = -\left.\frac{\partial^2 \hat{\tilde{\varrho}}(k,s)}{\partial k^2}\right|_{k=0}$

CTRW theory II: application to maps

apply CTRW to maps (Geisel, Klafter, 1984ff): need $w(t), \lambda(x)$

- continuous-time approximation for the PM-map

$$x_{n+1} - x_n \simeq \frac{dx}{dt} = ax^z , \quad x \ll 1$$

solve for $x(t)$ with initial condition $x(0) = x_0$, define jump as $x(t) = 1$, solve for $t(x_0)$ and compute $w(t) \simeq \varrho_{in}(x_0) \left| \frac{dx_0}{dt} \right|$ by assuming uniform density of injection points, $\varrho_{in}(x_0) \simeq 1$

- (revised) ansatz for jumps:

$$\lambda(x) = \frac{p}{2}\delta(|x| - \ell) + (1 - p)\delta(x)$$

with jump length ℓ, escape probability
$p := 2(\frac{1}{2} - x_c)$, $M(x_c) := 1$
CTRW machinery . . . yields exactly

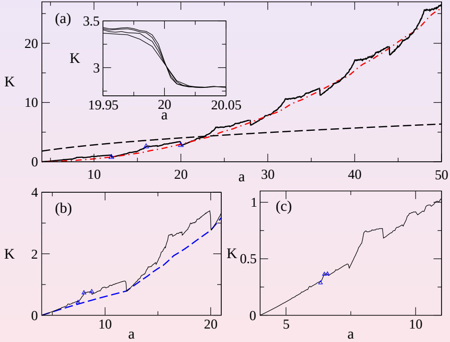
$$K = p\ell^2 \begin{cases} \frac{a^\gamma \sin(\pi\gamma)}{\pi\gamma^{1+\gamma}}, & 0 < \gamma < 1 \\ a\frac{\gamma-1}{\gamma}, & \gamma \geq 1 \end{cases} \quad , \quad \gamma := 1/(z-1) \, , \, z > 1$$

Dynamical crossover in anomalous diffusion

define average jump length:

$\ell_1 :=< |M(x) - x| >_{\varrho_0=1,escape} \quad \Rightarrow K \sim a^{5/2} \quad$ for $\ell_1 \gg 2$

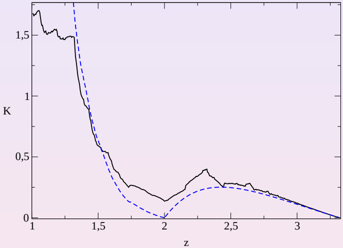
$\ell_2 :=< |[M(x)]| >_{\varrho_0=1,escape} \quad \Rightarrow K \sim p(a) \quad$ for $\ell_2 \ll 2$

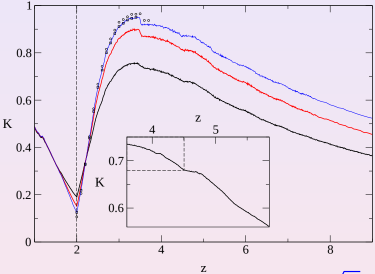


- $\exists$ dynamical crossover between small and large a
- $\exists$ same crossover in periodic Lorentz gas (R.K., Dellago, 2002) and in maps of previous talk

Phase transition from normal to anomalous diffusion

now $K(z,5)$; left fig.: compare CTRW approximation (blue line, with integer jump length ℓ_2) with simulation results





right fig. with $K(z,a)$ for fixed height $h(z,a) := M(1/2) = \sqrt{3}$ after different simulations times shows more clearly:

$\exists$ full suppression of diffusion due to logarithmic corrections

$$<x^2>\sim \begin{cases} n/\ln n, n < n_{cr} \text{ and } \sim n, n > n_{cr}, & z < 2 \\ n/\ln n, & z = 2 \\ n^\alpha/\ln n, n < \tilde{n}_{cr} \text{ and } \sim n^\alpha, n > \tilde{n}_{cr}, & z > 2 \end{cases}$$

Time-fractional equation for subdiffusion

Montroll-Weiss equation for PM map in long-time and -space asymptotic form reads

$$s^\gamma \hat{\tilde{\varrho}} - s^{\gamma-1} = -\frac{p\ell^2 a^\gamma}{2\Gamma(1-\gamma)\gamma^\gamma} k^2 \hat{\tilde{\varrho}}$$

LHS is the Laplace transform of the Caputo fractional derivative

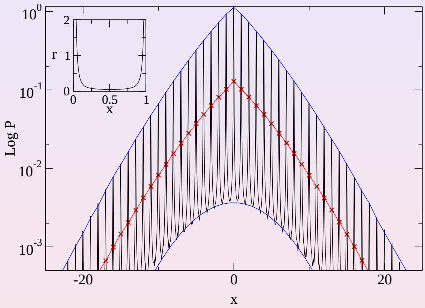
$$\frac{\partial^\gamma \varrho}{\partial t^\gamma} := \begin{cases} \frac{\partial \varrho}{\partial t} & \gamma = 1 \\ \frac{1}{\Gamma(1-\gamma)} \int_0^t dt' (t-t')^{-\gamma} \frac{\partial \varrho}{\partial t'} & 0 < \gamma < 1 \end{cases}$$

transforming the Montroll-Weiss eq. back to real space yields the time-fractional diffusion equation

$$\boxed{\frac{\partial^\gamma \varrho(x,t)}{\partial t^\gamma} = K \frac{\Gamma(1+\alpha)}{2} \frac{\partial^2 \varrho(x,t)}{\partial x^2}}$$

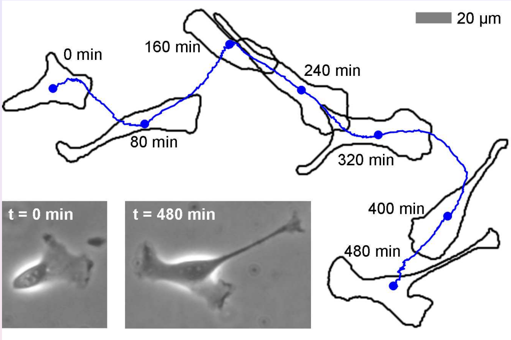
Comparison with simulations

fractional diffusion equation can be solved exactly; compare with simulation results for $P = \varrho_n(x)$:



- *Gaussian and non-Gaussian envelopes* (blue) reflect intermittency
- *fine structure* due to density on the unit interval $r = \varrho_n(x)$ $(n \gg 1)$ (see inset)

Application: dynamics of migrating cells



(Dieterich, R.K. et al., 2008)

single biological cell crawling on a substrate:

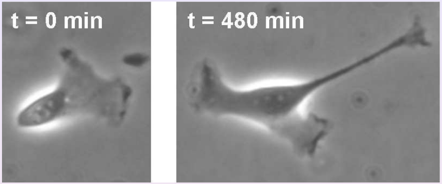
$\exists$ **Brownian motion** in terms of **Langevin dynamics**

$$\boxed{\dot{\mathbf{v}} + \kappa \mathbf{v} = \sqrt{\zeta}\, \xi(t)} \quad ?$$

Our cell types and how they migrate

MDCK-F (Madin-Darby canine kidney) cells

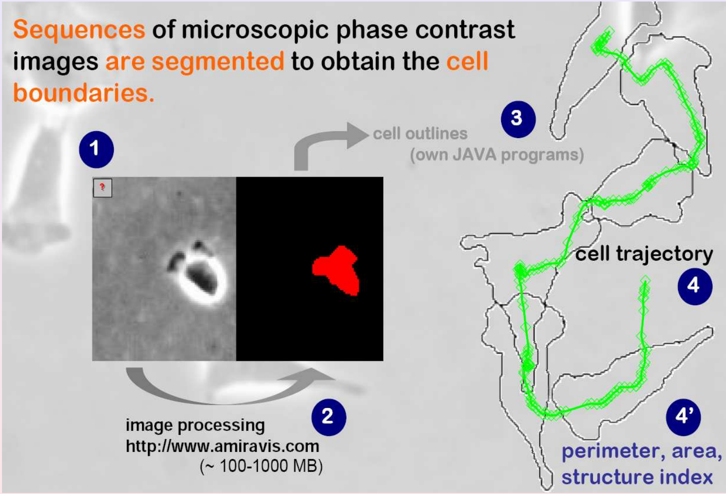
two types: wildtype (*NHE*$^+$) and NHE-deficient (*NHE*$^-$)



movie: NHE+: t=210min, dt=3min

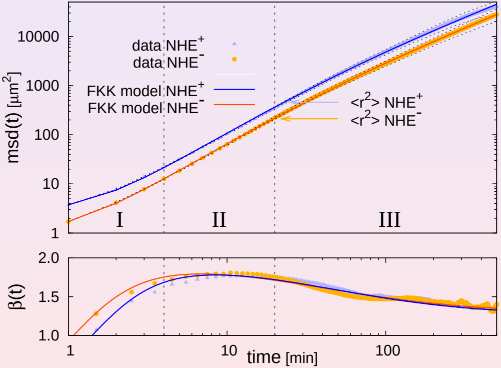
note:
the *microscopic origin* of cell migration is a **highly complex process** involving a huge number of proteins and signaling mechanisms in the *cytoskeleton*, which is a complicated *biopolymer gel* – we do not consider this here!

Measuring cell migration



Experimental results I: mean square displacement

- $msd(t) := <[\mathbf{x}(t) - \mathbf{x}(0)]^2> \sim t^\beta$ with $\beta \to 2\ (t \to 0)$ and $\beta \to 1\ (t \to \infty)$ for Brownian motion; $\beta(t) = d \ln msd(t) / d \ln t$
- *solid lines:* (Bayes) fits from our model



anomalous diffusion if $\beta \neq 1\ (t \to \infty)$: here superdiffusion

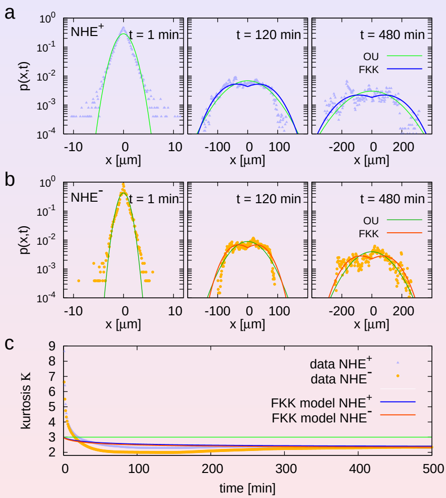
Experimental results II: position distribution function

- $P(x,t) \to$ Gaussian $(t \to \infty)$ and kurtosis

$$\kappa(t) := \frac{<x^4(t)>}{<x^2(t)>^2} \to 3 \ (t \to \infty)$$

for Brownian motion (green lines, in 1d)

- *other solid lines:* fits from our model; parameter values as before



$\Rightarrow$ crossover from peaked to broad non-Gaussian distributions

The model

- **Fractional Klein-Kramers equation** (Barkai, Silbey, 2000):

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}[vP] + \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}}\kappa\left[\frac{\partial}{\partial v}v + v_{th}^2\frac{\partial^2}{\partial v^2}\right]P$$

with probability distribution $P = P(x, v, t)$, damping term κ, thermal velocity $v_{th}^2 = kT/m$ and *Riemann-Liouville fractional (generalized ordinary) derivative* of order $1-\alpha$

for $\alpha = 1$ Langevin's theory of Brownian motion recovered

- **analytical solutions** for $msd(t)$ and $P(x, t)$ can be obtained in terms of special functions (Barkai, Silbey, 2000; Schneider, Wyss, 1989)

- **4 fit parameters** v_{th}, α, κ (plus another one for short-time dynamics)

Possible physical interpretation

- **physical meaning of the fractional derivative?**

fractional Klein-Kramers equation can *approximately* be related to generalized Langevin equation of the type

$$\dot{v} + \int_0^t dt' \, \kappa(t-t')v(t') = \sqrt{\zeta}\, \xi(t)$$

e.g., Mori, Kubo, 1965/66

with time-dependent friction coefficient $\kappa(t) \sim t^{-\alpha}$

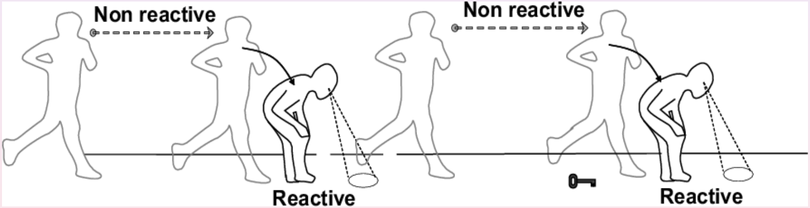
cell anomalies might originate from *soft glassy behavior* of the cytoskeleton gel, where power law exponents are conjectured to be universal (Fabry et al., 2003; Kroy et al., 2008)

Possible biological interpretation

- **biological meaning of anomalous cell migration?**

experimental data and theoretical modeling suggest *slower diffusion for small times* while *long-time motion is faster*

compare with intermittent optimal search strategies of foraging animals (Bénichou et al., 2006)



note: ∃ current controversy about *modeling the migration of foraging animals* (albatross, fruitflies,...); work on foraging bumblebees in progress (Lenz, R.K. et al.)

Summary

nonequilibrium conditions →

		equilibrium	nonequilibrium steady states	nonequilibrium non-steady states
microscopic	dynamical systems	ergodic hypothesis	**microscopic chaos** strong	weak
↓	statistical mechanics	Gibbs ensembles	**complexity** fractal SRB measures	infinite measures
macroscopic	thermodynamics	thermodynamic properties	**deterministic transport** normal	anomalous

⇒ general theory of nonequilibrium statistical physics starting from **weak** microscopic chaos?

Acknowledgements and literature

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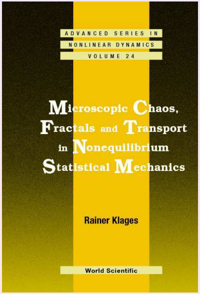
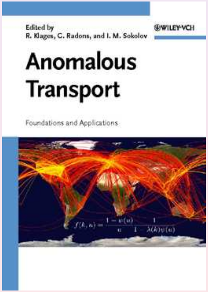
background information to:

Part 1



Part 2



and for cell migration: Dieterich et al., PNAS **105**, 459 (2008)