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

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Outline

focus on **deterministic random walks on the line**

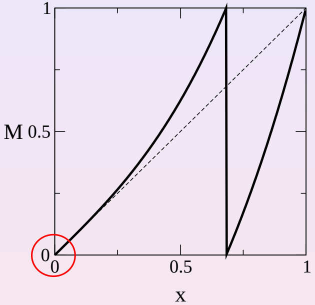
two lectures:

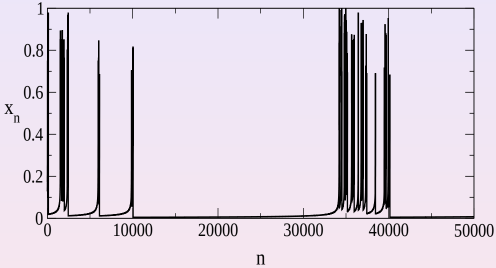
1. **Normal deterministic diffusion**
   two methods for two maps: Taylor-Green-Kubo and escape rate approach

2. **Anomalous (deterministic) diffusion**
   subdiffusion in a weakly chaotic map: CTRW theory and a fractional diffusion equation; fluctuation relations for anomalous stochastic processes

Pomeau-Manneville map

brief reminder: $x_{n+1} = M(x_n) = x_n + a x_n^z \mod 1 \, , \ z \geq 1$





weakly chaotic dynamics with stretched exponential instability and infinite invariant measure for $z > 2$

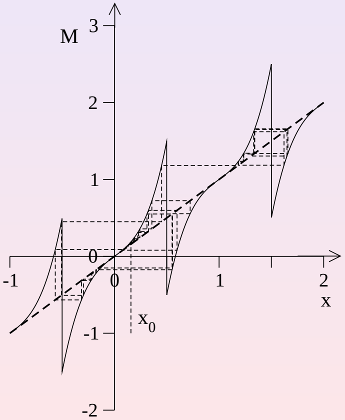
model deterministic diffusion with this map - **two questions:**

- Which type of diffusion do we get?
- How to quantify with respect to parameter variation z, a?

A subdiffusive intermittent map

lift map subdiffusively

Geisel, Thomae (1984); Zumofen, Klafter (1993)



mean square displacement

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

if $\alpha \neq 1$ **anomalous diffusion**

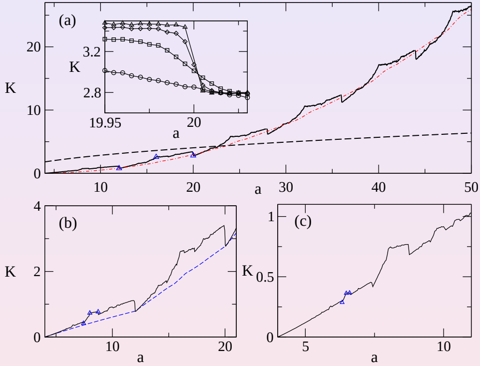
here:

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

goal: calculate the 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, RK et al. (2005)

- ∃ fractal structure
- $K(a)$ conjectured to be discontinuous 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: need $w(t), \lambda(x)$ (Klafter, Geisel, 1984ff)

sketch:

- $w(t)$ calulated from $w(t) \simeq \varrho(x_0) \left| \frac{dx_0}{dt} \right|$ with density of initial positions $\varrho(x_0) \simeq 1$, $x_0 = x(0)$; for waiting times $t(x_0)$ solve the continuous-time approximation of the PM-map
$x_{n+1} - x_n \simeq \frac{dx}{dt} = ax^z , \quad x \ll 1$ with $x(t) = 1$

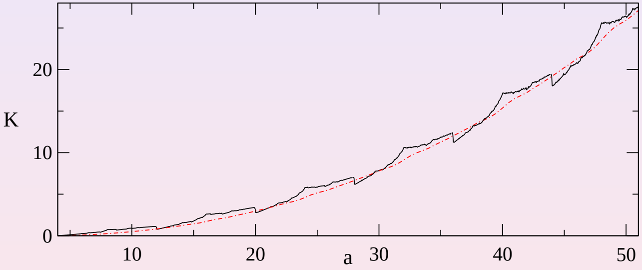
- (revised) ansatz for jumps:
$$\lambda(x) = \frac{p}{2}\delta(|x| - \ell) + (1 - p)\delta(x)$$
with average jump length ℓ and escape probability p

CTRW machinery . . . yields exactly

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

Anomalous random walk solution

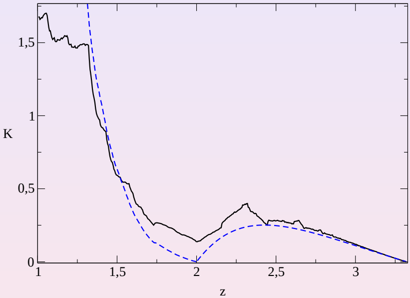
define average jump length $\ell := < |M(x) - x| >_{\varrho_0 = 1}$:
for $z = 3$ we get $K(a) \sim a^{5/2}$



CTRW yields **anomalous drunken sailor solution**, which correctly describes the coarse scale behaviour of $K(3, a)$

Dynamical phase transition to anomalous diffusion

compare CTRW approximation (blue line) with simulation results for $K(z,5)$:



$\exists$ **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

For the lifted **PM map** $M(x) = x + ax^z \bmod 1$, the MW equation in long-time and large-space asymptotic form reads

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

LHS is the Laplace transform of the Caputo fractional derivative

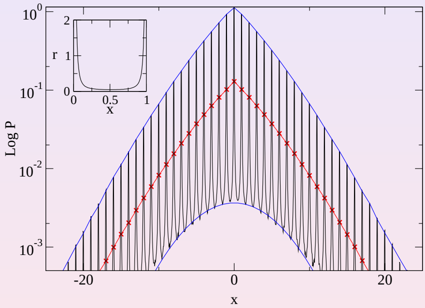
$$\frac{\partial^\gamma \varrho}{\partial t^\gamma} := \begin{cases} \frac{\partial \varrho}{\partial t} & \gamma = 1 \\ \frac{1}{\Gamma(1-\gamma)} \int_0^t dt' (t-t')^{-\gamma} \frac{\partial \varrho}{\partial t'} & 0 < \gamma < 1 \end{cases}$$

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

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

Deterministic vs. stochastic density

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



- fine structure due to density on the unit interval $r = \varrho_n(x)$ $(n \gg 1)$ (see inset)
- Gaussian and non-Gaussian envelopes (blue) reflect intermittency (Korabel, RK et al., 2007)

Motivation: Fluctuation relations

Consider a particle system evolving from some initial state into a nonequilibrium steady state.

Measure the probability distribution $\rho(\xi_t)$ of entropy production ξ_t during time t:

$$\ln \frac{\rho(\xi_t)}{\rho(-\xi_t)} = \xi_t$$

transient fluctuation relation (TFR)

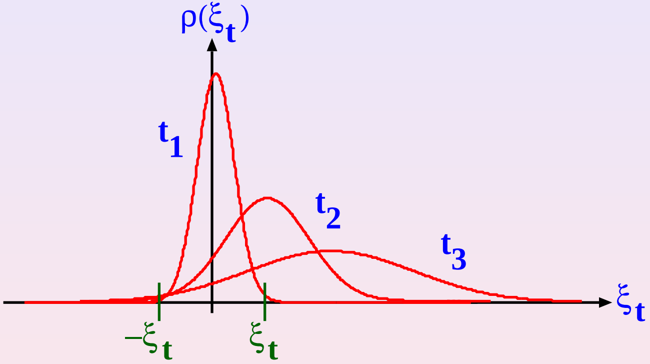
Evans et al. (1993/94); Gallavotti, Cohen (1995)

why important? Of *very general validity* and

1. generalizes the Second Law to small noneq. systems
2. yields nonlinear response relations
3. connection with fluctuation dissipation relations
4. can be checked in experiments (Wang et al., 2002)

Fluctuation relation and the Second Law

meaning of TFR in terms of Second Law:



$t_1 < t_2 < t_3$

$$\boxed{\rho(\xi_t) = \rho(-\xi_t)\exp(\xi_t)} \geq \rho(-\xi_t)\ (\xi_t \geq 0)\ \Rightarrow <\xi_t> \geq 0$$

goal: sample specifically the tails of the pdf...

Fluctuation relation for Langevin dynamics

check TFR for the overdamped Langevin equation

$$\dot{x} = F + \zeta(t) \qquad \text{(set all irrelevant constants to 1)}$$

with constant field F and Gaussian white noise $\zeta(t)$.

entropy production ξ_t is equal to (mechanical) work $W_t = Fx(t)$ with $\rho(W_t) = F^{-1}\varrho(x,t)$; remains to solve corresponding Fokker-Planck equation for initial condition $x(0) = 0$:

the position pdf is Gaussian,

$$\varrho(x,t) = \frac{1}{\sqrt{2\pi\sigma_x^2}} \exp\left(-\frac{(x - <x>)^2}{2\sigma_x^2}\right)$$

not difficult to see:

TFR holds if $< W_t >= \sigma_{W_t}^2/2$

and $\exists$ fluctuation-dissipation relation 1 **(FDR1)** $\Rightarrow$ **TFR**

see, e.g., van Zon, Cohen, PRE (2003)

TFRs for anomalous dynamics

FRs widely verified for 'Brownian motion-type' dynamics; only specific violations (Harris et al., 2006; Evans et al., 2005)

goal: check TFR for three fundamental types of anomalous diffusion

First type: Gaussian stochastic processes defined by the (overdamped) *generalized Langevin equation* (Kubo, 1965)

$$\int_0^t dt' \dot{x}(t') K(t - t') = F + \zeta(t)$$

with Gaussian noise $\zeta(t)$ and a suitable memory kernel $K(t)$

examples of applications: generalized elastic model (Taloni, 2010); polymer dynamics (Panja, 2010); biological cell migration (Dieterich et al., 2008)

TFR for correlated internal Gaussian noise

split this class into two cases:

1. internal Gaussian noise defined by the **FDR2**

$$< \zeta(t)\zeta(t') > \sim K(t-t') \, ,$$

which is correlated by $K(t) \sim t^{-\beta}$, $0 < \beta < 1$

$\rho(W_t) \sim \varrho(x,t)$ is Gaussian; solving the generalized Langevin equation in Laplace space yields **subdiffusion**

$$\sigma_x^2 \sim t^\beta$$

by preserving **FDR1** which implies

$$< W_t > = \sigma_{W_t}^2/2$$

for correlated internal Gaussian noise $\exists$ TFR

TFR for correlated external Gaussian noise

2. consider overdamped generalized Langevin equation

$$\dot{x} = F + \zeta(t)$$

with correlated Gaussian noise defined by

$$< \zeta(t)\zeta(t') > \sim |t - t'|^{-\beta} \;,\; 0 < \beta < 1 \;,$$

which is external, because there is **no FDR2**

$\rho(W_t) \sim \varrho(x,t)$ is again Gaussian but here with **superdiffusion** by **breaking FDR1**:

$$< W_t > \sim t \quad , \quad \sigma^2_{W_t} \sim t^{2-\beta}$$

yields the **anomalous TFR**

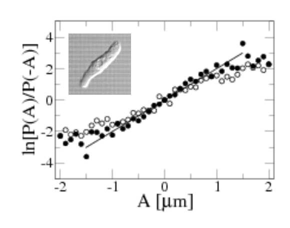
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{C}_\beta \mathbf{t}^{\beta-1} W_t \quad (0 < \beta < 1)$$

note: pre-factor on rhs *not equal to one* and *time dependent*

Relations to experiments

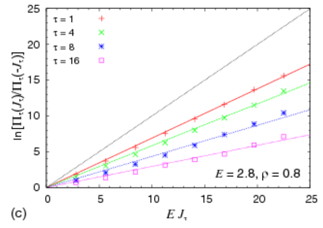
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \frac{\mathbf{C}_\beta}{\mathbf{t}^{1-\beta}} W_t \quad (0 < \beta < 1)$$

experiments on slime mold:



Hayashi, Takagi, J.Phys.Soc.Jap. (2007)

computer simulation on glassy lattice gas:



Sellitto, PRE (2009)

$\Rightarrow$ anomalous fluctuation relation important for glassy dynamics

TFR for other anomalous stochastic processes

- consider the Langevin equation

$$\dot{x} = F + \zeta(t)$$

with white Lévy noise $\varrho(\zeta) \sim \zeta^{-1-\alpha}\ (\zeta \to \infty)\ ,\ 0 \le \alpha < 2\ ,$
breaking FDR1; solving a space-fractional Fokker-Planck eq. yields (cf. Touchette, Cohen (2007))

$$\lim_{w \to \pm\infty} g_t(w) = \lim_{w \to \pm\infty} \frac{\rho(W_t = wF^2 t)}{\rho(W_t = -wF^2 t)} = 1$$

i.e., large fluctuations are *equally possible*

- consider the subordinated Langevin equation

$$\frac{dx(u)}{du} = F + \zeta(u) \quad , \quad \frac{dt(u)}{du} = \tau(u)$$

with Gaussian white noise $\zeta(u)$ and white Lévy stable noise $\tau(u) > 0$, which **preserves** a generalized **FDR2**
by solving the corresponding time-fractional Fokker-Planck eq. the conventional TFR is recovered

Anomalous fluctuation relations: summary

- TFR tested for three fundamental types of **anomalous stochastic dynamics**:
  1. Gaussian stochastic processes with correlated noise:
     FDR2 $\Rightarrow$ FDR1 $\Rightarrow$ TFR
     TFR holds for internal noise, mild violation for external one
  2. strong violation of TFR for space-fractional (Lévy) dynamics
  3. TFR holds for time-fractional dynamics
- same results obtained for a particle confined in a harmonic potential dragged by a constant velocity

Back to the beginning

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

⇒ theory of nonequilibrium statistical physics starting from microscopic chaos?

Some open questions

- Irregular diffusion coefficients in billiards C^1 but not C^2? real experiments?
- Escape rate theory for anomalous diffusion?
- Exact method for calculating parameter-dependent anomalous diffusion coefficient?
- Check superdiffusive Pomeau-Manneville map
- Discontinuous diffusion coefficient for PM map?
- Anomalous fluctuation relations $\leftrightarrow$ weak chaos $\leftrightarrow$ nonlinear response $\leftrightarrow$ fluctuation-dissipation relations $\leftrightarrow$ experiments?

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References

- **CTRW for map:**

  N. Korabel et al., Phys. Rev. E **75**, 036213 (2007)

- **anomalous fluctuation relations:**

  A.V. Chechkin, RK, J. Stat. Mech. L03002 (2009)

more general background info: