Anomalous Transport and Fluctuation Relations: From Theory to Biology

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Outline

1. **Langevin dynamics:**

   from *Brownian motion* to *anomalous transport*

2. **Fluctuation relations:**

   from conventional ones generalizing the *2nd law of thermodynamics* to *anomalous* versions

3. **Non-Gaussian dynamics:**

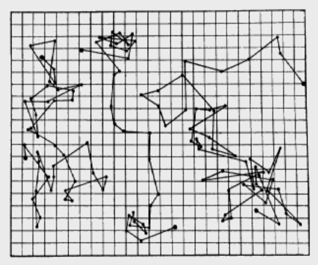
   check fluctuation relations for *time-fractional Fokker-Planck equations*

4. **Relation to experiments:**

   anomalous fluctuation relations in *glassy systems* and in *biological cell migration*

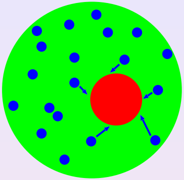
Theoretical modeling of Brownian motion

Brownian motion



Perrin (1913)

3 colloidal particles, positions joined by straight lines



$$m\dot{\mathbf{v}} = -\kappa \mathbf{v} + k\,\zeta(t)$$

Langevin equation (1908)

'Newton's law of stochastic physics'

velocity $\mathbf{v} = \dot{\mathbf{x}}$ of tracer particle in fluid

force on rhs decomposed into:

- viscous damping as Stokes friction
- random kicks of surrounding particles

modeled by Gaussian white noise

nb: Zwanzig's derivation (1973); breaking of Galilean invariance (Cairoli, RK, Baule, tbp)

Langevin dynamics

Langevin dynamics characterized by **solutions** of the Langevin equation; here in one dimension and focus on:

- mean square displacement (msd)

$$\sigma_x^2(t) = \langle (x(t) - \langle x(t) \rangle)^2 \rangle \sim t \quad (t \to \infty) \, ,$$

  where $\langle \ldots \rangle$ denotes an ensemble average

- position probability distribution function (pdf)

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

  (from solving the corresponding diffusion equation) reflects the Gaussianity of the noise

Generalized Langevin equation

Mori, Kubo (1965/66): generalize ordinary Langevin equation to

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

by using a time-dependent friction coefficient $\kappa(t) \sim t^{-\beta}$;
applications to polymer dynamics (Panja, 2010) and biological cell migration (Dieterich, RK et al., 2008)

solutions of this Langevin equation:

- position pdf is Gaussian (as the noise is still Gaussian)
- but msd $\sigma_x^2 \sim t^{\alpha(\beta)}$ $(t \to \infty)$ shows anomalous diffusion: $\alpha \neq 1$; $\alpha < 1$: subdiffusion, $\alpha > 1$: superdiffusion

The 1st term on the rhs defines a **fractional derivative**:

$$\frac{\partial^\gamma P}{\partial t^\gamma} := \frac{\partial^m}{\partial t^m}\left[\frac{1}{\Gamma(m-\gamma)}\int_0^t dt' \frac{P(t')}{(t-t')^{\gamma+1-m}}\right] \; , \; m-1 \leq \gamma \leq m$$

What is a fractional derivative?

letter from Leibniz to L'Hôpital (1695): $\frac{d^{1/2}}{dx^{1/2}} = ?$

one way to proceed: we know that for integers $n \geq m$

$$\frac{d^m}{dx^m} x^n = \frac{n!}{(n-m)!} x^{n-m} = \frac{\Gamma(n+1)}{\Gamma(n-m+1)} x^{n-m} ;$$

assume that this also holds for $m = 1/2$, $n = 1$

$$\Rightarrow \quad \boxed{\frac{d^{1/2}}{dx^{1/2}} x = \frac{2}{\sqrt{\pi}} x^{1/2}}$$

extension leads to the Riemann-Liouville fractional derivative, which yields power laws in Fourier (Laplace) space:

$$\frac{d^\gamma}{dx^\gamma} F(x) \leftrightarrow (ik)^\gamma \tilde{F}(k) , \ \gamma \geq 0$$

$\exists$ well-developed mathematical theory of **fractional calculus**

see Sokolov, Klafter, Blumen, Phys. Tod. (2002) for a short intro

Fluctuation-dissipation relations

Kubo (1966): two fundamental relations characterizing Langevin dynamics $m\dot{v} = -\int_0^t dt'\, \kappa(t-t')v(t') + k\, \zeta(t)$

1. fluctuation-dissipation relation of the 2nd kind (FDR2),

$$<\zeta(t)\zeta(t')>\sim \kappa(t-t')$$

   defines **internal noise**, which is correlated in the same way as the friction; if broken: **external noise**

2. fluctuation-dissipation relation of the 1st kind (FDR1),

$$<x>\sim \sigma_x^2$$

   implies that current and msd have the same time dependence

result: for generalized Langevin dynamics with correlated internal (FDR2) Gaussian noise **FDR2 implies FDR1**

Chechkin, Lenz, RK (2012)

Motivation: Fluctuation relations

Consider a (classical) 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)

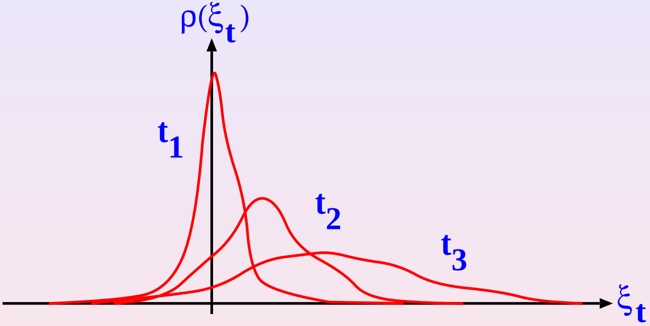
Evans, Cohen, Morriss, Searles, Gallavotti (1993ff)

why important? of *very general validity* and

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

Fluctuation relation and the Second Law

meaning of TFR in terms of the Second Law:



$t_1 < t_2 < t_3$

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

sample specifically the tails of the pdf (large deviation result)

Fluctuation relation for normal Langevin dynamics

check TFR for the overdamped Langevin equation

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

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 the corresponding Fokker-Planck equation for initial condition $x(0) = 0$

the position pdf is again Gaussian, which implies straightforwardly:

(work) TFR holds if $< x >= F\sigma_x^2/2$

hence **FDR1 $\Rightarrow$ TFR**

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

Fluctuation relation for anomalous Langevin dynamics

check TFR for overdamped generalized Langevin equation

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

both for internal and external power-law correlated Gaussian noise $\kappa(t) \sim t^{-\beta}$

1. internal Gaussian noise:

• as FDR2 implies FDR1 and $\rho(W_t) \sim \varrho(x,t)$ is Gaussian, it straightforwardly follows the existence of the transient fluctuation relation

for correlated **internal Gaussian noise** $\exists$ TFR

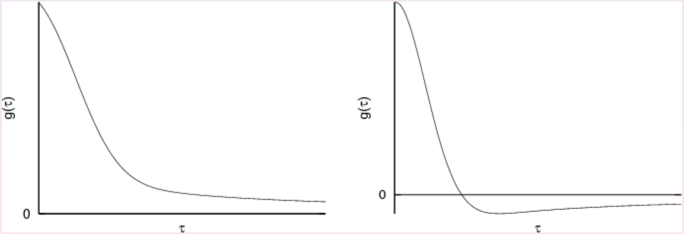
• diffusion and current may both be normal or anomalous depending on the memory kernel

Correlated external Gaussian noise

2. external Gaussian noise: break FDR2, modelled by the overdamped generalized Langevin equation

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

consider two types of Gaussian noise correlated by $g(\tau) = < \zeta(t)\zeta(t') >_{\tau = t - t'} \sim (\Delta/\tau)^\beta$ for $\tau > \Delta$, $\beta > 0$:



persistent **anti-persistent**

it is $< x >= Ft$ and $\sigma_x^2 = 2 \int_0^t d\tau (t - \tau) g(\tau)$

Results: TFRs for correlated external Gaussian noise

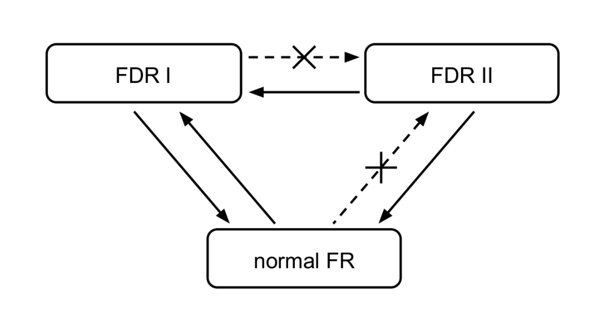
σ_x^2 and the fluctuation ratio $R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)}$ for $t \gg \Delta$ and $g(\tau) = < \zeta(t)\zeta(t') >_{\tau=t-t'} \sim (\Delta/\tau)^\beta$:

	persistent		**antipersistent** *	
β	σ_x^2	$R(W_t)$	σ_x^2	$R(W_t)$
$0 < \beta < 1$	$\sim t^{2-\beta}$	$\sim \frac{W_t}{t^{1-\beta}}$	*regime*	
$\beta = 1$	$\sim t \ln\left(\frac{t}{\Delta}\right)$	$\sim \frac{W_t}{\ln\left(\frac{t}{\Delta}\right)}$	*does not exist*	
$1 < \beta < 2$			$\sim t^{2-\beta}$	$\sim t^{\beta-1} W_t$
$\beta = 2$	$\sim 2Dt$	$\sim \frac{W_t}{D}$	$\sim \ln(t/\Delta)$	$\sim \frac{t}{\ln\left(\frac{t}{\Delta}\right)} W_t$
$2 < \beta < \infty$			$= const.$	$\sim t W_t$

* antipersistence for $\int_0^\infty d\tau g(\tau) > 0$ yields normal diffusion with generalized TFR; above antipersistence for $\int_0^\infty d\tau g(\tau) = 0$

Summary: FDR and TFR

relation between TFR and FDR I,II for **correlated Gaussian stochastic dynamics**: ('normal FR'= conventional TFR)



in particular:

FDR2 $\Rightarrow$ FDR1 $\Rightarrow$ TFR

$\nexists$ **TFR** $\Rightarrow$ $\nexists$ **FDR2**

Modeling non-Gaussian dynamics

- start again from overdamped Langevin equation $\dot{x} = F + \zeta(t)$, but here with **non-Gaussian** power law correlated noise

$$g(\tau) = < \zeta(t)\zeta(t') >_{\tau=t-t'} \sim (K_\alpha/\tau)^{2-\alpha} \;,\; 1 < \alpha < 2$$

- 'motivates' the non-Markovian Fokker-Planck equation

type A: $$\frac{\partial \varrho_A(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[F - K_\alpha D_t^{1-\alpha}\frac{\partial}{\partial x}\right]\varrho_A(x,t)$$

with Riemann-Liouville fractional derivative $D_t^{1-\alpha}$ (Balescu, 1997)

- two *formally similar* types derived from CTRW theory, for $0 < \alpha < 1$:

type B: $$\frac{\partial \varrho_B(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[F - K_\alpha D_t^{1-\alpha}\frac{\partial}{\partial x}\right]\varrho_B(x,t)$$

type C: $$\frac{\partial \varrho_C(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[F D_t^{1-\alpha} - K_\alpha D_t^{1-\alpha}\frac{\partial}{\partial x}\right]\varrho_C(x,t)$$

They model a *very different* class of stochastic process!

Properties of non-Gaussian dynamics

two important properties:

- **FDR1:** exists for type C but not for A and B
- **mean square displacement:**

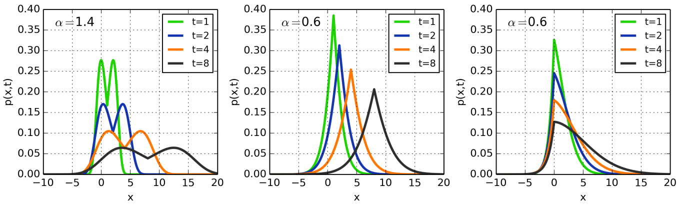
- type A: superdiffusive, $\sigma_x^2 \sim t^\alpha$, $1 < \alpha < 2$
- type B: subdiffusive, $\sigma_x^2 \sim t^\alpha$, $0 < \alpha < 1$
- type C: sub- or superdiffusive, $\sigma_x^2 \sim t^{2\alpha}$, $0 < \alpha < 1$

position pdfs: can be calculated approx. analytically for A, B, only numerically for C

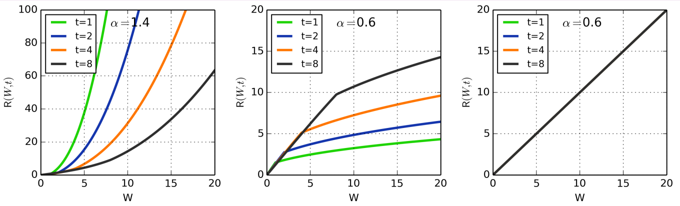
Probability distributions and fluctuation relations

type A type B type C

- **PDFs:**



- **TFRs:**



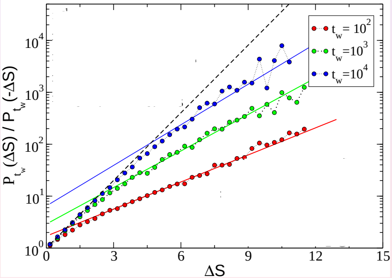
$$R(W_t) = \log \frac{\rho(W_t)}{\rho(-W_t)} \sim \begin{cases} c_\alpha W_t \,, & W_t \to 0 \\ t^{(2\alpha-2)/(2-\alpha)} W_t^{\alpha/(2-\alpha)} \,, & W_t \to \infty \end{cases}$$

Anomalous TFRs in experiments: glassy dynamics

$$R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{f}_\beta(\mathbf{t}) W_t$$

means by plotting R for different t the slope might change.

example 1: computer simulations for a binary Lennard-Jones mixture below the glass transition

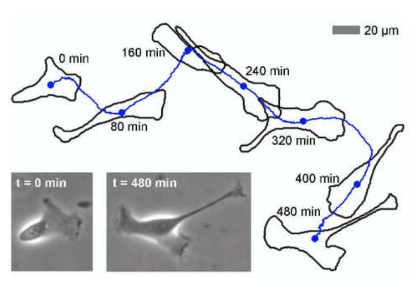


Crisanti, Ritort, PRL (2013)

similar results for other glassy systems (Sellitto, PRE, 2009)

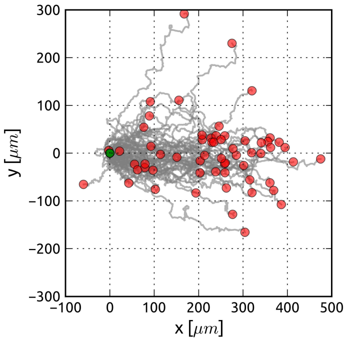
Cell migration without and with chemotaxis

example 2: single MDCKF cell crawling on a substrate; trajectory recorded with a video camera



Dieterich et al., PNAS (2008)

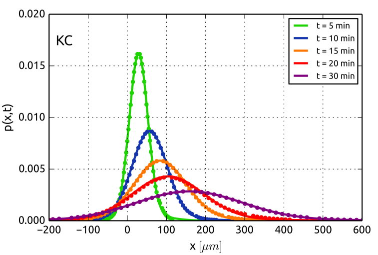
new experiments on murine neutrophils under chemotaxis:



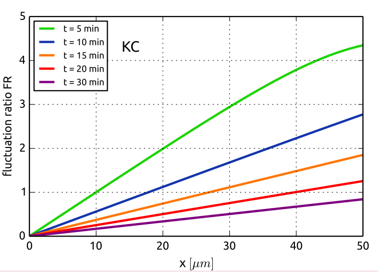
Dieterich et al. (tbp)

Anomalous fluctuation relation for cell migration

experim. results: position pdfs $\rho(x,t)$ are Gaussian



fluctuation ratio $R(W_t)$ is time dependent



$< x(t) > \sim t$ and $\sigma_x^2 \sim t^{2-\beta}$ with $0 < \beta < 1$: $\nexists$ FDR1 and

$$R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = \frac{W_t}{\mathbf{t}^{1-\beta}}$$

Dieterich et al. (tbp)

data matches to theory for persistent Gaussian correlations

Summary

- TFR tested for two generic cases of **non-Markovian correlated Gaussian stochastic dynamics**:
  1. **internal noise**:
     FDR2 implies the validity of the 'normal' work TFR
  2. **external noise**:
     FDR2 is broken; sub-classes of persistent and anti-persistent noise yield both anomalous TFRs
- TFR tested for three cases of **non-Gaussian dynamics**:
  breaking FDR1 implies again anomalous TFRs
- anomalous TFRs appear to be important for glassy ageing dynamics and for active biological cell migration

References

- A.V. Chechkin, F.Lenz, RK, J. Stat. Mech. L11001 (2012)
- A.V. Chechkin, RK, J. Stat. Mech. L03002 (2009)
- P.Dieterich et al., PNAS **105**, 459 (2008)