Fluctuation relations for anomalous dynamics

Aleksei V. Chechkin\textsuperscript{1}, Rainer Klages\textsuperscript{2}

\textsuperscript{1} Institute for Theoretical Physics, Kharkov, Ukraine

\textsuperscript{2} Queen Mary University of London, School of Mathematical Sciences

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Outline

- ‘Normal’ fluctuation relations: motivation with some history

- Anomalous fluctuation relations: check transient fluctuation relations for three fundamental classes of anomalous stochastic processes

- Biological cell migration: brief outline and outlook towards checking these relations in experiments
two-dimensional fluid of soft particles under shear: measure the probability distribution \( \rho(\eta_t) \) of the entropy production rate \( \eta_t \sim P_{xyt} \) during time \( t \) in a nonequilibrium steady state

- ratio of the tails \( \rightarrow \) Second Law for small nonequ. systems
...with a groundbreaking idea

analytical argument (for $\rho(\eta t)$ in terms of the SRB measure) yielded the **steady state fluctuation relation**

\[ \ln \frac{\rho(\eta t)}{\rho(-\eta t)} = t\eta t \]

confirmed by computer simulations (for long enough $t$):

proof on basis of chaotic hypothesis by Gallavotti, Cohen (1995)
A second pioneering paper

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

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

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

*transient (Evans-Searles) fluctuation relation* (TFR)
Brownian particle in a harmonic trap dragged with constant velocity $v_\ast$ through a fluid:

- FRs can be checked in experiments!

Fluctuation relation for Langevin dynamics

**warmup**: check TFR for the overdamped Langevin equation

\[ \dot{x} = F + \zeta(t) \]  
(set all irrelevant constants to 1)

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

entropy production \( \xi_t \) is equal to (mechanical) work \( W_t = Fx(t) \)

with \( \rho(W_t) = F^{-1} \rho(x, t) \); remains to solve corresponding Fokker-Planck equation for initial condition \( x(0) = 0 \):

the position pdf is Gaussian,

\[ \rho(x, t) = \frac{1}{\sqrt{2\pi} \sigma_x^2} \exp \left( -\frac{(x-\langle x \rangle)^2}{2\sigma_x^2} \right) \]

straightforward:

(work) TFR holds if \( \langle W_t \rangle = \sigma_{W_t}^2/2 \)

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

see, e.g., van Zon, Cohen, PRE (2003)
TFRs for anomalous dynamics

**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:** polymer dynamics (Panja, 2010); biological cell migration (Dieterich et al., 2008)
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 \( K(t) \sim t^{-\beta} , \quad 0 < \beta < 1 \)

\( \rho(W_t) \sim \varrho(x, t) \) 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

\[ \langle \zeta(t)\zeta(t') \rangle \sim |t - t'|^{-\beta}, \ 0 < \beta < 1, \]

which is external, because there is no FDR2

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

\[ \langle W_t \rangle \sim t, \ \sigma_{W_t}^2 \sim t^{2-\beta} \]

yields the anomalous TFR

\[ \ln \frac{\rho(W_t)}{\rho(-W_t)} = C_\beta t^{\beta - 1} W_t \quad (0 < \beta < 1) \]

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

\[ \ln \frac{\rho(W_t)}{\rho(-W_t)} = \frac{C_\beta}{t^{1-\beta}} W_t \quad (0 < \beta < 1) \]

experiments on slime mold:


computer simulation on glassy lattice gas:

Sellitto, PRE (2009)

⇒ anomalous fluctuation relation important for glassy dynamics
Second type of anomalous dynamics: consider the Langevin equation
\[ \dot{x} = F + \zeta(t) \]
with white Lévy noise \( \rho(\zeta) \sim |\zeta|^{-1-\alpha} (\zeta \to \infty) , \, 0 \leq \alpha < 2 \)

**Examples of applications:** fluid dynamics (Solomon et al., 1993); Lévy flights for light (Barthelemy, 2008)

by solving the corresponding Fokker-Planck equation
\[ \frac{\partial \rho}{\partial t} = -F \frac{\partial \rho}{\partial x} + \frac{\partial^\alpha \rho}{\partial |x|^{\alpha}} \]

with Riesz fractional derivative
\[ \frac{\partial^\alpha \rho}{\partial |x|^{\alpha}} = \Gamma(1+\alpha) \frac{\sin(\alpha \pi/2)}{\pi} \int_0^\infty dy (\rho(x+y) - 2\rho(x) + \rho(x-y))/y^{1+\alpha} \]

and using the scaled variable \( w_t = W_t/(F^2 t) \) we recover
\[ \lim_{w_t \to \pm \infty} \frac{\rho(w_t)}{\rho(-w_t)} = 1 \]  
Touchette, Cohen, PRE (2007)

i.e., large fluctuations are equally possible
**TFR for time-fractional kinetics**

**Third type** of anomalous dynamics: via subordinated Langevin equation

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

with Gaussian white noise \( \zeta(u) \) and white Lévy stable noise \( \tau(u) > 0 \); leads to the time-fractional Fokker-Planck equation

\[
\frac{\partial \rho}{\partial t} = \frac{\partial^{1-\alpha}}{\partial t^{1-\alpha}} \left[ -\frac{\partial F}{\partial x} + \frac{\partial^2}{\partial x^2} \right] \rho
\]

with Riemann-Liouville fractional derivative

\[
\frac{\partial^\gamma \rho}{\partial t^\gamma} = \frac{\partial^m \rho}{\partial t^m} \left[ \frac{1}{\Gamma(m-\gamma)} \int_0^t dt' \frac{\rho(t')}{(t-t')^{\gamma+1-m}} \right] \text{ for } m - 1 < \gamma < m, \ m \in \mathbb{N}
\]

and \( \frac{\partial^\gamma \rho}{\partial t^\gamma} = \frac{\partial^m \rho}{\partial t^m} \) for \( \gamma = m \), which preserves a generalized FDR1

**examples of applications:** photo current in copy machines (Scher et al., 1975) and related systems modeled by

*Continuous Time Random Walk theory* (Metzler, Klafter, 2004)

for this dynamics we recover the conventional TFR
Outlook: Anomalous dynamics of cell migration

single biological cell crawling on a substrate; trajectory recorded with a video camera (Dieterich et al., 2008)

**movie:** MDCKF: $t=210\text{min}$, $dt=3\text{min}$
Position distribution function

- **two types**: wildtype and deficient one
- \( P(x, t) \to \text{Gaussian} \ (t \to \infty) \) and kurtosis
  \[ \kappa(t) := \frac{\langle x^4(t) \rangle}{\langle x^2(t) \rangle^2} \to 3 \ (t \to \infty) \]
  for Brownian motion (green lines, in 1d)
- **other solid lines**: fits from our model
- **also extracted**: mean square displacement, velocity autocorrelation fct.

\[ \Rightarrow \text{crossover from peaked to broad non-Gaussian distributions} \]
new experiments on **murine neutrophils** under **chemotaxis**

Schwab, Dieterich et al. (unpub.)

- **linear drift** in the direction of the gradient, \( < y(t) > \sim t \)
- \( msd(t) - < y(t) >^2 \sim t^\beta \) with same exponent \( \beta > 1 \) as in equilibrium \( \Rightarrow \) **fluctuation dissipation relation** 1
- data suggest an **anomalous fluctuation relation** of the type as obtained for generalized Langevin dynamics
The model

cell data fit by a fractional Klein-Kramers equation with external force $F(x)$ (Metzler, Sokolov, 2002):

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

with probability distribution $P = P(x, v, t)$, damping term $\kappa$, thermal velocity $v_{th}$ and Riemann-Liouville fractional derivative of order $1 - \alpha$

for $\alpha = 1$ ordinary Klein-Kramers equation recovered

analytical solutions yield correctly drift, msd, VACF and (for large enough $\kappa$ and $t$) the pdf's
TFR tested for three fundamental types of anomalous stochastic dynamics:

1. Gaussian stochastic processes with correlated noise:
   \[ \text{FDR2} \Rightarrow \text{FDR1} \Rightarrow \text{TFR} \]
   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 (cf. experiment by Wang et al., 2002)

outlook: work in progress on more generalized Gaussian processes and cell migration
References


- book on *Nonequilibrium statistical physics of small systems* currently in preparation (RK, Just, Jarzynski, Eds.; for 2012)

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Happy Birthday Denis!