Anomalous Fluctuation Relations

Aleksei V. Chechkin[1], Rainer Klages[2],
Peter Dieterich[3], Friedrich Lenz[2]

1 Institute for Theoretical Physics, Kharkov, Ukraine

2 Queen Mary University of London, School of Mathematical Sciences

3 Institute for Physiology, Technical University of Dresden, Germany

Small Systems far from Equilibrium, 17 October 2013

Queen Mary University of London

Outline

- **'Normal' fluctuation relations:**
  motivation and warm-up
- **Anomalous fluctuation relations:**
  check transient fluctuation relations for **correlated** Gaussian stochastic dynamics
- **Relations to experiments:**
  glassy dynamics, aging and cell migration

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:

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

Transient Fluctuation Relation (TFR)

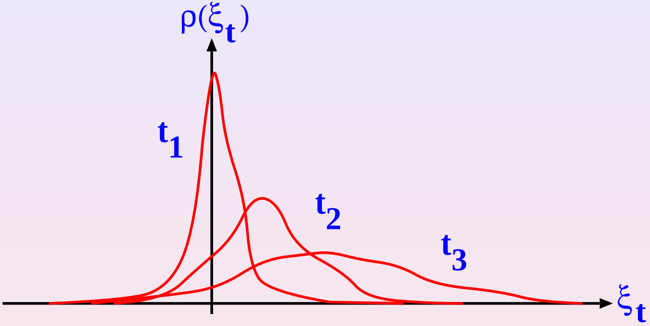
Evans, Cohen, Morriss (1993); Gallavotti, Cohen (1995)

why important? of *very general validity* and

1. generalizes the Second Law to small systems in nonequil.
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 Langevin dynamics

warmup: 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,

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

straightforward:

$$\boxed{\text{(work) TFR holds if } < x >= \sigma_x^2/2}$$

and $\boxed{\exists \text{ fluctuation-dissipation relation 1 } \textbf{(FDR1)} \Rightarrow \textbf{TFR}}$

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

Gaussian stochastic dynamics

goal: check TFR for Gaussian stochastic processes defined by the (overdamped) **generalized Langevin equation**

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

e.g., Kubo (1965)

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

such dynamics can generate **anomalous diffusion**:

$$\boxed{\sigma_x^2 \sim t^\alpha \text{ with } \alpha \neq 1 \; (t \to \infty)}$$

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

TFR for correlated internal Gaussian noise

consider two generic cases:

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

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

with non-Markovian (correlated) noise; e.g., $K(t) \sim t^{-\beta}$

solving the corresponding generalized Langevin equation in Laplace space yields

$$\boxed{\text{FDR2} \Rightarrow \text{‘FDR1’}}$$

and since $\rho(W_t) \sim \varrho(x,t)$ is Gaussian

$$\boxed{\text{‘FDR1’} \Rightarrow \text{TFR}}$$

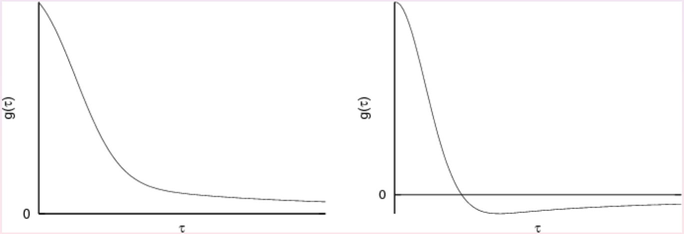
$$\boxed{\text{for correlated } \textbf{internal Gaussian noise} \; \exists \; \text{TFR}}$$

Correlated external Gaussian noise

2. external Gaussian noise for which there is **no FDR2**, modeled 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 $\sigma_x^2 = 2\int_0^t d\tau (t-\tau) g(\tau)$

TFRs for correlated external Gaussian noise I

persistent noise with $g(\tau) \sim (\Delta/\tau)^{\beta}$:

results for σ_x^2 and the fluctuation ratio $R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)}$

• $0 < \beta < 1$:

superdiffusion $\sigma_x^2 \sim t^{2-\beta}$ with anomalous TFR $R \sim \frac{W_t}{t^{1-\beta}}$

• $\beta = 1$:

weak superdiffusion $\sigma_x^2 \sim t \ln\left(\frac{t}{\Delta}\right)$ with weakly anomalous TFR $R \sim W_t / \ln\left(\frac{t}{\Delta}\right)$

• $1 < \beta < \infty$:

normal diffusion $\sigma_x^2 \sim 2Dt$ with $D = \int_0^\infty d\tau g(\tau)$ and anomalous (generalized) TFR $R \sim \frac{W_t}{D}$

TFRs for correlated external Gaussian noise II

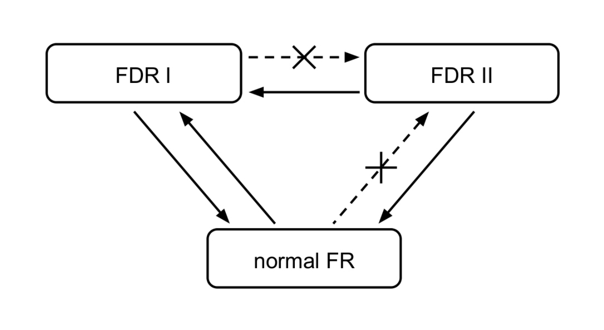
antipersistent noise:

$\int_0^\infty d\tau g(\tau) > 0$ yields normal diffusion with a generalized TFR for $t \gg \Delta$; for 'pure' antipersistent case with $\int_0^\infty d\tau g(\tau) = 0$:

- The regime $0 < \beta < 1$ does not exist (spectral density <0)
- $1 < \beta < 2$:
  subdiffusion $\sigma_x^2 \sim t^{2-\beta}$ with anomalous TFR $R \sim W_t t^{\beta-1}$
- $\beta = 2$:
  weak subdiffusion $\sigma_x^2 \sim \ln(t/\Delta)$ with anomalous TFR $R \sim W_t t / \ln(t/\Delta)$
- $2 < \beta < \infty$:
  localization $\sigma_x^2 = const.$ with anomalous TFR $R \sim W_t t$

FDR and TFR

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



in particular:

$$\boxed{\textbf{FDR2} \Rightarrow \textbf{FDR1} \Rightarrow \textbf{TFR}}$$

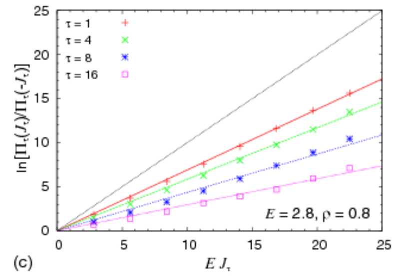
$$\boxed{\nexists\ \textbf{TFR} \Rightarrow \nexists\ \textbf{FDR2}}$$

Relations to experiments: A glassy lattice gas

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

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

example 1: computer simulations for glassy lattice gas with external field E

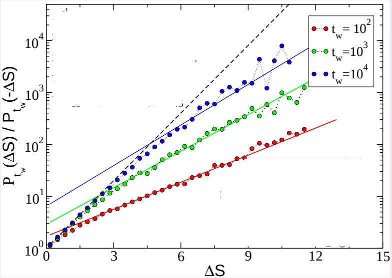


Sellitto, PRE (2009)

- slopes are decreasing with time

Aging systems

example 2: computer simulations for a binary Lennard-Jones mixture below the glass transition

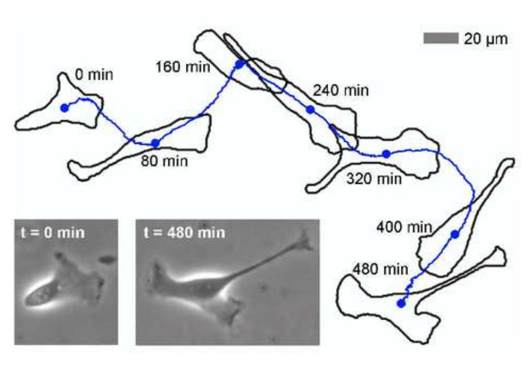


Crisanti, Ritort, PRL (2013)

- slopes are increasing with time
- convergence to the normal FR for small entropy production
- similar results for random orthogonal and Edwards-Anderson model

Biological cell migration

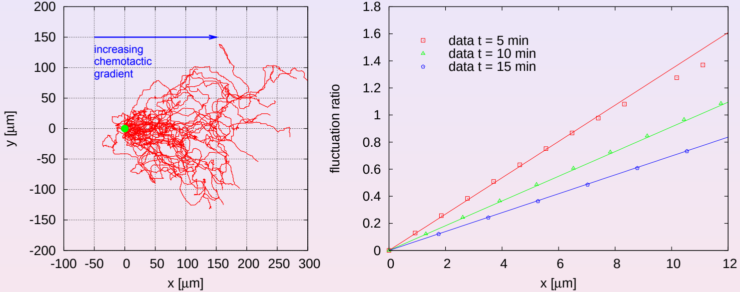
example 2: single biological cell crawling on a substrate; trajectory recorded with a video camera



Dieterich, RK et al., PNAS, 2008

Cell migration under chemical gradients

experiments on **murine neutrophils** under **chemotaxis**:



Dieterich et al. (2013)

- linear drift in the direction of the gradient, $< x(t) >\sim t$
- $\sigma_x^2 \sim t^\beta$ with $\beta > 1$ (long t): $\nexists$ FDR1
- modeling by a generalized Langevin equation with external noise and $0 < \beta < 1$ as discussed before

Summary

- TFR tested for two generic cases of **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
- anomalous TFRs appear to be important for glassy aging dynamics: cf. computer simulations on various glassy models and experiments on ('gelly') cell migration

References

- **A.V. Chechkin, F.Lenz, RK, J. Stat. Mech. L11001 (2012)**
- A.V. Chechkin, RK, J. Stat. Mech. L03002 (2009)
- RK, A.V. Chechkin, P.Dieterich, *Anomalous fluctuation relations* in: