Anomalous Fluctuation Relations

Aleksei V. Chechkin\textsuperscript{1}, Rainer Klages\textsuperscript{2}, Peter Dieterich\textsuperscript{3}, Friedrich Lenz\textsuperscript{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

Mathematics for the Fluid Earth
Newton Institute, Cambridge, 30 October 2013
‘Normal’ fluctuation relations: motivation and warm-up for ordinary Langevin dynamics

Anomalous fluctuation relations: check transient fluctuation relations for correlated Gaussian stochastic dynamics

Relations to experiments: glassy dynamics and cell migration
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 $\xi_t$ during time $t$:

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

**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 nonequilibrium
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:

\[ \rho(\xi_t) = \rho(-\xi_t) \exp(\xi_t) \geq \rho(-\xi_t) (\xi_t \geq 0) \Rightarrow \langle \xi_t \rangle \geq 0 \]
Mathematics for the Fluid Earth

Langevin equation (‘Newton’s law of stochastic physics’) used to model the dynamics of the earth’s surface temperature $T$:

linearized energy-balance equation derived as

$$C \dot{T} = -\frac{1}{S_{eq}} T + F + k \zeta(t)$$

K.Rypdal (2012)

with heat capacity $C$, equilibrium climate sensitivity $S_{eq}$, (solar) radiative influx $F$ and Gaussian white noise $\zeta$ of strength $k$

note: even a long-range memory generalization proposed

Rypdal, Rypdal (2013)

*(many thanks to N. Watkins for pointing these refs. out to me)*
**Fluctuation relation for Langevin dynamics**

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

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

(set all irrelevant constants to 1)

for a particle at position \( x \) with constant field \( F \) and noise \( \zeta \).  

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 \( \langle x \rangle = \sigma_x^2/2 \)

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

\[ \sigma_x^2 \sim t^\alpha \quad \text{with} \quad \alpha \neq 1 \ (t \to \infty) \]

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

\[
\text{FDR2} \Rightarrow \text{‘FDR1’}
\]

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

\[
\text{‘FDR1’} \Rightarrow \text{TFR}
\]

for correlated **internal Gaussian noise** \ Exist TFR
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

\[ g(\tau) = \langle \zeta(t)\zeta(t') \rangle_{\tau=t-t'} \sim (\Delta/\tau)\beta \text{ for } \tau > \Delta, \beta > 0: \]

**persistent**

\[ \langle x \rangle = Ft \]

\[ \sigma_x^2 = 2 \int_0^t d\tau (t - \tau)g(\tau) \]

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

results for $\sigma_x^2$ 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 $R \sim \frac{W_t}{\ln \left( \frac{t}{\Delta} \right)}$

• $1 < \beta < \infty$:
  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 \( \sigma_x^2 = \text{const.} \) with anomalous TFR \( R \sim W_t t \)
relation between TFR and FDR I,II for **correlated Gaussian stochastic dynamics**: (‘normal FR’= conventional TFR)

in particular:

FDR2 $\Rightarrow$ FDR1 $\Rightarrow$ TFR

$\not\exists$ TFR $\Rightarrow$ $\not\exists$ FDR2
Relations to experiments: glassy dynamics

\[ R(W_t) = \ln \frac{\rho(W_t)}{\rho(-W_t)} = f_\beta(t) W_t \]

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)
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**:

- **linear drift** in the direction of the gradient, \( < x(t) > \sim t \)
- \( \sigma_x^2 \sim t^{\beta} \) with \( \beta > 1 \) (long \( t \)): \( \not\exists \) FDR1
- modeling by a **generalized Langevin equation** with external noise and \( 0 < \beta < 1 \) as discussed before

Dieterich et al. (2013)
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