Fluctuation relations for anomalous dynamics

Aleksei V. Chechkin[1], Rainer Klages[2]

1 Institute for Theoretical Physics, Kharkov, Ukraine

2 Queen Mary University of London, School of Mathematical Sciences

LDSG Workshop, UCL, 3 May 2011

Queen Mary University of London

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)

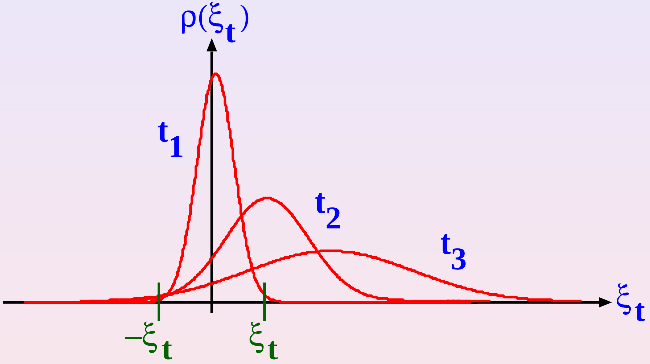
Evans et al. (1993/94); Gallavotti, Cohen (1995)

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 by experiments (Wang et al., 2002)

Fluctuation relation and the Second Law

meaning of TFR in terms of Second Law:



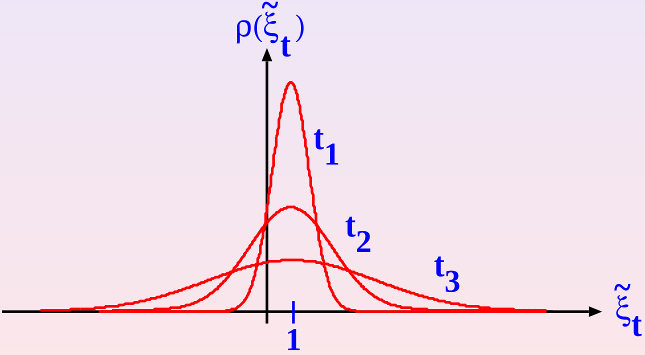
$t_1 < t_2 < t_3$

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

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

Fluctuation relation and scaling I

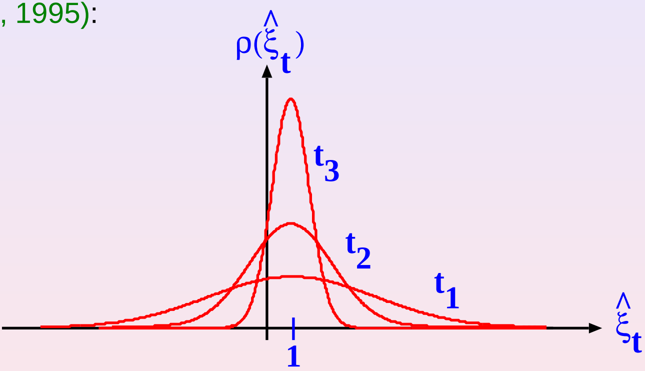
look at the pdf of the *scaled variable* $\tilde{\xi}_t = \frac{\xi_t}{<\xi_t>}$ for eliminating the drift (Touchette, Cohen, 2009):



$\Rightarrow \rho(\tilde{\xi}_t)$ is now centered at $\tilde{\xi}_t = 1$

Fluctuation relation and scaling II

look at pdf of the *scaled time average* $\hat{\xi}_t = \frac{\xi_t}{t < \xi_t >}$ (Gallavotti, Cohen, 1995):



$$\rho(\hat{\xi}_t) \to \delta(1-\hat{\xi}_t)\ (t\to\infty) \Rightarrow \frac{\xi_t}{t} \to < \xi_t > \geq 0\ (t\to\infty)$$

illustrates the Second Law again

A hierarchy of fluctuation relations

- there are steady state FRs, which are *formally* equivalent to the TFR (van Zon, Cohen, 2003; Gallavotti, Cohen, 1995)
- the Jarzynski work relation expresses the free energy difference between two equilibrium states in terms of the performed nonequilibrium work (Jarzynski, 1997)
- the Crooks relation is similar to the TFR but formulated in terms of forward and backward pdf's of entropy production (Crooks, 1999); the previous two FRs are derived from it
- there is another fluctuation relation by Seifert based on *stochastic thermodynamics* that implies all three (Seifert, 2005)

all these FRs have been tested in (computer and real) **experiments**, particularly for biomolecules (Ritort, 2003)

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

the position pdf is Gaussian,

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

easy to see:

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

i.e., $\exists$ 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 dynamics, where the mean square displacement $<\sigma_x^2>\sim t^\alpha$ does not grow linearly in time: $\alpha < 1$ subdiffusion, $\alpha > 1$ superdiffusion

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

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

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

$$< \sigma_x^2 >\sim t^{\beta}$$

by preserving **FDR1**,

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

for correlated internal Gaussian noise ∃ 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**

$\rho(W_t) \sim \rho(x, t)$ 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**

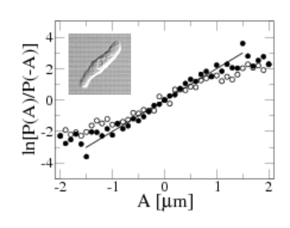
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{C}_\beta \mathbf{t}^{\beta-1} W_t \quad (0 < \beta < 1)$$

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

Relations to experiments

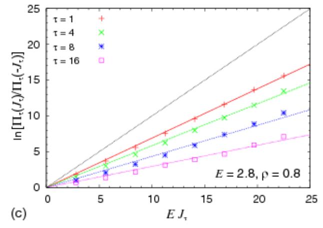
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \frac{\mathbf{C}_\beta}{\mathbf{t}^{1-\beta}} W_t \quad (0 < \beta < 1)$$

experiments on slime mold:



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

computer simulation on glassy lattice gas:



Sellitto, PRE (2009)

⇒ anomalous fluctuation relation important for glassy dynamics

TFR for Lévy flights

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); foraging of biological organisms (Vishwanathan, 1996)

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

$$\boxed{\lim_{w_t \to \pm\infty} \frac{\rho(w_t)}{\rho(-w_t)} = 1}$$ 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 $\frac{dx(u)}{du} = F + \zeta(u) \quad , \quad \frac{dt(u)}{du} = \tau(u)$
with Gaussian white noise $\zeta(u)$ and white Lévy stable noise $\tau(u) > 0$; leads to the time-fractional Fokker-Planck equation

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

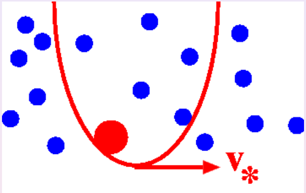
with Riemann-Liouville fractional derivative
$\frac{\partial^\gamma \rho}{\partial t^\gamma} = \frac{\partial^m}{\partial t^m} \left[\frac{1}{\Gamma(m-\gamma)} \int_0^t dt' \frac{\rho(t')}{(t-t')^{\gamma+1-m}} \right]$ for $m - 1 < \gamma < m \, , \, m \in \mathbb{N}$
and $\frac{\partial^\gamma \rho}{\partial t^\gamma} = \frac{\partial^m \rho}{\partial t^m}$ for $\gamma = m$

examples of applications: photo current in copy machines (?) (Scher et al., 1975), microsphere diffusion in cell membrane (?); cf. Metzler, Klafter (2004)

for this dynamics we recover the conventional TFR

TFR for a dragged particle

experiment by Wang et al., 2002: Brownian particle dragged through a fluid by a harmonic force with constant velocity v_*,



note: for this potential one needs to distinguish between *work and heat* for checking FRs (van Zon, Cohen, 2003)

in this case and for (total) work, same results obtained for (two plus one) types of anomalous dynamics as before

$\Rightarrow$ check anomalous FR experimentally for dragging particle through polymer gel?

Summary

- TFR tested for three fundamental types of **anomalous stochastic dynamics**:
  1. Gaussian stochastic processes with correlated noise:
     $$\boxed{\textbf{FDR2} \Rightarrow \textbf{FDR1} \Rightarrow \textbf{TFR}}$$
     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

question: anomalous TFRs of atoms in optical lattices?

Reference:

A.V. Chechkin, R. Klages, Fluctuation relations for anomalous dynamics, J. Stat. Mech. L03002 (2009)