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

Nonequilibrium Processes, Obergurgl, 1st September 2011

Queen Mary University of London

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

A pioneering paper...

VOLUME 71, NUMBER 15 PHYSICAL REVIEW LETTERS 11 OCTOBER 1993

Probability of Second Law Violations in Shearing Steady States

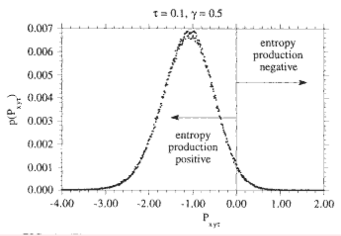
Denis J. Evans
Research School of Chemistry, Australian National University, Canberra, Australian Capital Territory 2600, Australia

E. G. D. Cohen
The Rockefeller University, 1230 York Avenue, New York, New York 10021

G. P. Morriss
School of Physics, University of South Wales, Kensington, New South Wales, Australia
(Received 26 March 1993)

We propose a new definition of natural invariant measure for trajectory segments of finite duration for a many-particle system. On this basis we give an expression for the probability of fluctuations in the shear stress of a fluid in a nonequilibrium steady state far from equilibrium. In particular we obtain a formula for the ratio that, for a finite time, the shear stress reverses sign, violating the second law of thermodynamics. Computer simulations support this formula.

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



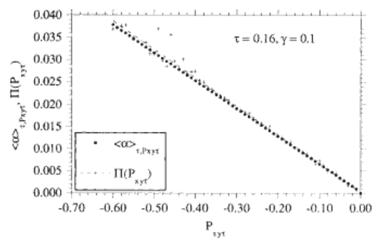
- ratio of the tails → **Second Law** for small nonequ. systems

...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

PHYSICAL REVIEW E VOLUME 50, NUMBER 2 AUGUST 1994

Equilibrium microstates which generate second law violating steady states

Denis J. Evans and Debra J. Searles
Research School of Chemistry, The Australian National University, Canberra, Australian Capital Territory 0200, Australia
(Received 8 November 1993)

For reversible deterministic *N*-particle thermostatted systems, we examine the question of why it is so difficult to find initial microstates that will, at long times under the influence of an external dissipative field and a thermostat, lead to second law violating nonequilibrium steady states. We prove that the measure of those phases that generate second law violating phase space trajectories vanishes exponentially with time.

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 (Evans-Searles) fluctuation relation (TFR)

Yet a third one...

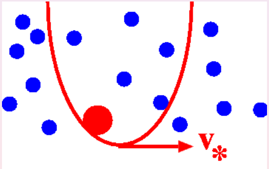
VOLUME 89, NUMBER 5 PHYSICAL REVIEW LETTERS 29 JULY 2002

Experimental Demonstration of Violations of the Second Law of Thermodynamics for Small Systems and Short Time Scales

G. M. Wang,[1] E. M. Sevick,[1] Emil Mittag,[1] Debra J. Searles,[2] and Denis J. Evans[1]
[1]*Research School of Chemistry, The Australian National University, Canberra ACT 0200, Australia*
[2]*School of Science, Griffith University, Brisbane QLD 4111, Australia*
(Received 4 March 2002; published 15 July 2002)

We experimentally demonstrate the fluctuation theorem, which predicts appreciable and measurable violations of the second law of thermodynamics for small systems over short time scales, by following the trajectory of a colloidal particle captured in an optical trap that is translated relative to surrounding water molecules. From each particle trajectory, we calculate the entropy production/consumption over the duration of the trajectory and determine the fraction of second law–defying trajectories. Our results show entropy consumption can occur over colloidal length and time scales.

Brownian particle in a harmonic trap dragged with constant velocity v_* through a fluid:



- FRs can be checked in experiments!

work on related concepts: Jarzynski (1997), Crooks (1999), Seifert (2005); experiments by Ciliberto (1998), Ritort (2002).

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:

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

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)

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

$\rho(W_t) \sim \varrho(x,t)$ 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 ∃ 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**

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

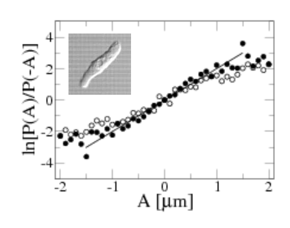
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \mathbf{C}_\beta \mathbf{t}^{\beta-1} W_t \quad (0 < \beta < 1)$$

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

Relations to experiments

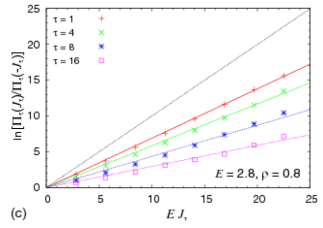
$$\ln \frac{\rho(W_t)}{\rho(-W_t)} = \frac{C_\beta}{t^{1-\beta}} W_t \quad (0 < \beta < 1)$$

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); 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

$$\boxed{\lim_{w_t \to \pm\infty} \frac{\rho(w_t)}{\rho(-w_t)} = 1}$$ 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 $\gamma = m$, which **preserves** a generalized **FDR1**

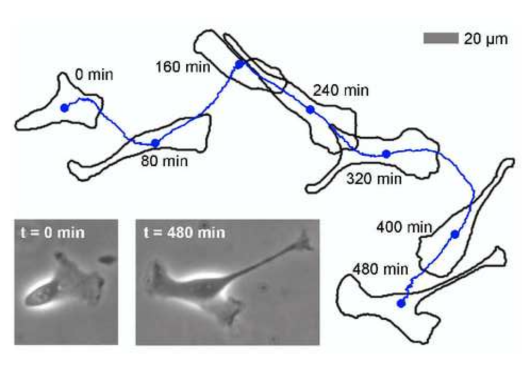
examples of applications: photo current in copy machines (Scher et al., 1975) and related systems modeled by *Continuous Time Random Walk theory* (Metzler, Klafter, 2004)

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=210min, dt=3min



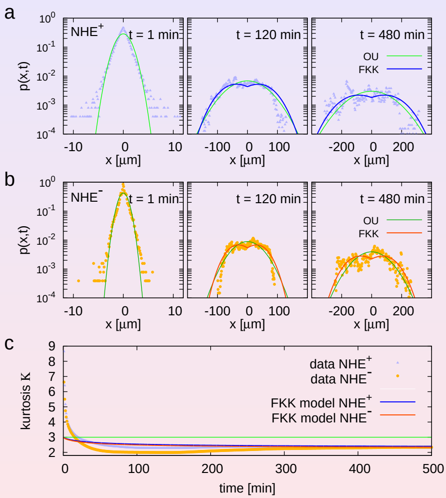
Position distribution function

- **two types:** wildtype and deficient one
- $P(x,t) \to$ Gaussian $(t \to \infty)$ and kurtosis

$$\kappa(t) := \frac{<x^4(t)>}{<x^2(t)>^2} \to 3 \ (t \to \infty)$$

for Brownian motion (green lines, in 1d)

- **other solid lines:** fits from our model
- **also extracted:** mean square displacement, velocity autocorrelation fct.

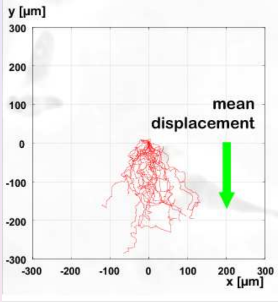


$\Rightarrow$ crossover from peaked to broad **non-Gaussian distributions**

Cell migration under chemical gradients

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 $\Rightarrow \nexists$ 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 κ, 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 κ and t) the pdf's

Anomalous fluctuation relations: summary

- TFR tested for three fundamental types of **anomalous stochastic dynamics**:
  1. Gaussian stochastic processes with correlated noise:

     FDR2 $\Rightarrow$ FDR1 $\Rightarrow$ 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

- A.V. Chechkin, RK, *Fluctuation relations for anomalous dynamics*, J. Stat. Mech. L03002 (2009)
- P. Dieterich et al., *Anomalous dynamics of cell migration*, PNAS **105**, 459 (2008)
- book on **Nonequilibrium statistical physics of small systems** currently in preparation (RK, Just, Jarzynski, Eds.; for 2012)

Happy Birthday Denis!