Anomalous Langevin Dynamics, Fluctuation-Dissipation Relations and Fluctuation Relations

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Climate Fluctuations and Non-equilibrium Statistical Mechanics: An Interdisciplinary Dialogue

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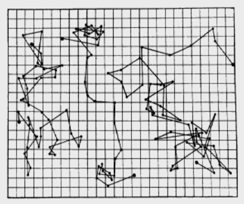
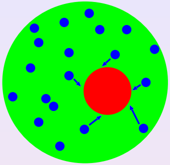
Outline

- **Standard Langevin dynamics:**
  very brief review for setting the scene
- **Generalized Langevin dynamics:**
  non-Markovian dynamics with memory generates anomalous diffusion; fluctuation-dissipation relations
- **Fluctuation relations:**
  test **(!)** of transient work fluctuation relation

Theoretical modeling of Brownian motion



Brownian motion (Perrin,1913)



'Newton's law of stochastic physics'

$$m\dot{\mathbf{v}} = -\kappa\mathbf{v} + k\,\zeta(t)$$ **Langevin equation (1908)**

for a tracer particle of velocity **v** immersed in a fluid

force on rhs decomposed into

- viscous damping as Stokes friction
- random kicks of surrounding particles modeled by Gaussian white noise

note: Kac-Zwanzig model (1965,1973) for derivation of this eq.

Langevin dynamics

solutions of the Langevin equation (in 1dim); here focus on:

- mean square displacement (msd)

$$\sigma_x^2 = \langle (x(t) - \langle x(t) \rangle)^2 \rangle \sim t \quad (t \to \infty) \,,$$

  where $\langle \ldots \rangle$ denotes an ensemble average

- position probability distribution function (pdf)

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

  (from solving the corresponding Fokker-Planck eq.)
  reflects the Gaussianity of the noise

Langevin dynamics for earth's surface temperature

from previous talk:

analogy between

stochastic energy balance equation

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

and Langevin equation (with field F)

$$m\dot{v} = -\kappa v + F + k\,\zeta(t)$$

mathematically identical

Generalized Langevin equation

Mori, Kubo (1965/66): generalize ordinary Langevin equation to

$$m\dot{v} = -\int_0^t dt' \, \kappa(t-t')v(t') + k\,\zeta(t)$$

by using a time-dependent friction coefficient $\kappa(t) \sim t^{-\beta}$;
cf. polymer dynamics (Panja, 2010) and biological cell migration (Dieterich et al., 2008ff)

solutions of this Langevin equation:

- position pdf is Gaussian (as the noise is still Gaussian)
- but for msd $\sigma_x^2 \sim t^{\alpha(\beta)}$ $(t \to \infty)$ with anomalous diffusion for $\alpha \neq 1$; $\alpha < 1$: subdiffusion; $\alpha > 1$: superdiffusion

(nb: the 1st term on the rhs defines a fractional derivative)

Fluctuation-dissipation relations

Kubo (1966): two fundamental relations characterizing Langevin dynamics

1. fluctuation-dissipation relation of the 2nd kind (FDR2),

$$< \zeta(t)\zeta(t') > \sim \kappa(t-t')$$

   defines **internal noise**, which is correlated in the same way as the friction; if broken: **external noise**

2. fluctuation-dissipation relation of the 1st kind (FDR1),

$$< x > \sim \sigma_x^2$$

   implies that current and msd have the same time dependence (linear response)

(nb: some technical subtleties neglected)

Implications of fluctuation-dissipation relations

- for generalized Langevin dynamics with power-law correlated internal (FDR2) Gaussian noise, $\kappa(t) \sim t^{-\beta}$, **FDR2 implies FDR1** (Chechkin, Lenz, RK, 2012)
- **see previous talk:** similar generalized Langevin dynamics used to model long-range memory effects in the earth's temperature dynamics
- **but:** modeling implies breaking of FDR2; meaningful?

$\Rightarrow$ **explore consequences of breaking/conserving FDR for fluctuation relations**

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:

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

Transient Fluctuation Relation (TFR)

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

note: ξ_t not necessarily identical to definition via stochastic thermodynamics (or Evans et al.)

Fluctuation relation for normal Langevin dynamics

check TFR for the overdamped Langevin equation

$$\dot{x} = F + \zeta(t) \qquad \text{(set all irrelevant constants to 1)}$$

for a particle at position x with constant field F and noise ζ.

entropy production ξ_t is equal to (mechanical) work $W_t = Fx(t)$
with $\rho(W_t) = F^{-1}\varrho(x,t)$; choose initial condition $x(0) = 0$ (!)

the position pdf is Gaussian which implies straightforwardly

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

hence **FDR1 $\Rightarrow$ TFR**

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

Fluctuation relation for anomalous Langevin dynamics

check TFR for overdamped generalized Langevin equation

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

both for internal and external power-law correlated Gaussian noise $\kappa(t) \sim t^{-\beta}$

1. internal Gaussian noise:

• as FDR2 implies FDR1 and $\rho(W_t) \sim \varrho(x,t)$ is Gaussian, it straightforwardly follows the existence of the transient fluctuation relation

for correlated **internal Gaussian noise** $\exists$ TFR

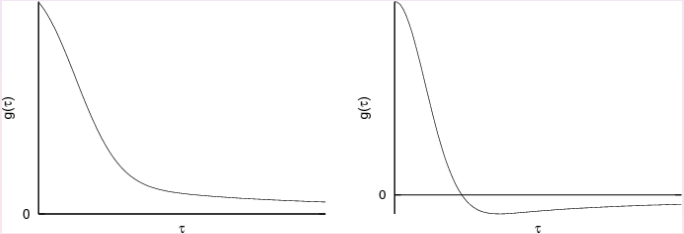
• diffusion and current may both be normal or anomalous depending on the memory kernel

Correlated external Gaussian noise

2. external Gaussian noise: break FDR2, modelled 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 $\sigma_x^2 = 2\int_0^t d\tau (t-\tau) g(\tau)$

Results: TFRs for correlated external Gaussian noise

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

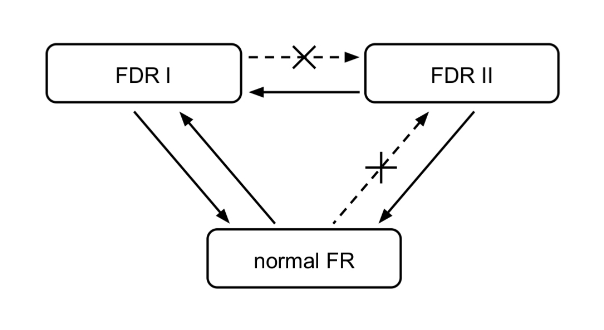
$g(\tau) =< \zeta(t)\zeta(t') >_{\tau=t-t'} \sim (\Delta/\tau)^\beta$:

	persistent		**antipersistent** *	
β	σ_x^2	$R(W_t)$	σ_x^2	$R(W_t)$
$0 < \beta < 1$	$\sim t^{2-\beta}$	$\sim \frac{W_t}{t^{1-\beta}}$	*regime*	
$\beta = 1$	$\sim t \ln\left(\frac{t}{\Delta}\right)$	$\sim \frac{W_t}{\ln\left(\frac{t}{\Delta}\right)}$	*does not exist*	
$1 < \beta < 2$			$\sim t^{2-\beta}$	$\sim t^{\beta-1} W_t$
$\beta = 2$	$\sim 2Dt$	$\sim \frac{W_t}{D}$	$\sim \ln(t/\Delta)$	$\sim \frac{t}{\ln\left(\frac{t}{\Delta}\right)} W_t$
$2 < \beta < \infty$			$= const.$	$\sim t W_t$

* antipersistence for $\int_0^\infty d\tau g(\tau) > 0$ yields normal diffusion with generalized TFR; above antipersistence for $\int_0^\infty d\tau g(\tau) = 0$

Summary: FDR and TFR

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



in particular:

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

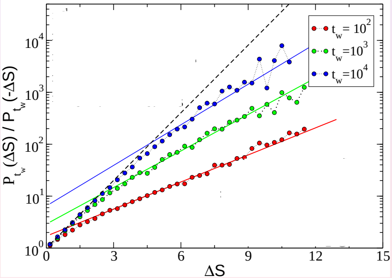
$\nexists$ **TFR** $\Rightarrow$ $\nexists$ **FDR2**: check in experiments?

Checking TFR in experiments

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

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

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



Crisanti, Ritort (2013); also Sellitto (2009)
similar results for chemotaxis of biological cells (Dieterich et al.)

Summary

- model long-range memory effects for stochastic climate dynamics by generalized Langevin equations?
- be careful of how you define your Langevin model with respect to fluctuation-dissipation relations:
  - is the physics modelled correctly in view of internal/external noise?
  - important consequences for (transient) fluctuation relation
- testing fluctuation relations for climate dynamics?

References

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