Fluctuation dissipation and response in out of equilibrium systems

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Outline

- Modified Fluctuation Dissipation Theorems (MFDTs) for Non Equilibrium Steady State (NESS)

- Fluctuation Theorem for systems driven out of equilibrium by a random force.

Modified Fluctuation Dissipation Theorems (MFDT)

Motivation: Test in an experiment the new FDT for an out of equilibrium system

Outline :

- MFDT Three formulations: 1) Lagrangian FDT
  2) Frenesy FDT
  3) Generalized FDT
- Langevin dynamics
- Experimental realisation
- Results

Fluctuation Dissipation Theorem (FDT)

In equilibrium FDT takes the form :

$$-R(t-s) = \frac{1}{k_B T}\partial_s C(t-s)$$

Observable $O_t(\theta)$ of the dynamical process θ and its conjugated variable h

Correlation function

$C(t-s) = < O_t \, O_s >$

Response function to a delta perturbation of h

$R(t-s) = < \frac{\delta O_s}{h} >$

Langevin Dynamics

$$\nu \dot{x} = -\partial_x U(x) + G + \eta$$

with $< \eta(t)\eta(t') >= 2k_B T \nu \delta(t - t')$

G non conservative force

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G non conservative force

with $G = 0$ equilibrium FDT holds

Langevin Dynamics

$$\nu\dot{x} = -\partial_x U(x) + G + \eta$$

with $< \eta(t)\eta(t') >= 2k_B T \nu \delta(t - t')$

G non conservative force

with $G = 0$ equilibrium FDT holds

with $G \neq 0$ the system is driven into
a non equilibrium steady state **(NESS)**
where equilibrium FDT does not hold

Modified Fluctuation Dissipation Theorem (MFDT) for NESS

R. Chetrite, G. Falkovich, and K. Gawedzki, J. Stat. Mech.P08005 (2008).

$$-R^L(t,s) = \frac{1}{k_B T}\partial_s C^L(t,s)$$

R^L and C^L are measured in the Lagrangian frame moving at mean local velocity $v_0(\theta)$

The new observable $O(t,\theta)$ evolves according to :

$$\partial_t O(t,\theta) + v_0(\theta)\cdot\nabla O(t,\theta) = 0$$

MFDT for NESS

The MFDT in the lagrangian frame,

$$R^L(t,s) = -\frac{1}{k_B T}\partial_s C^L(t,s),$$

can also be written in the laboratory frame, replacing ∂_s in FDT with the convective derivative $\partial_s + \nabla \cdot v_0(\theta)$

MFDT becomes:

$$R(t-s)\ k_B T = \partial_s C(t-s) - b(t-s)$$

where

$$b(t-s) = < O(t,\theta) v_0(\theta(s)) \partial_\theta O(s,\theta) >$$

MFDT for NESS

The MFDT in the lagrangian frame,

$$R^L(t,s) = -\frac{1}{k_B T}\partial_s C^L(t,s),$$

can also be written in the laboratory frame, replacing ∂_s in FDT with the convective derivative $\partial_s + \nabla \cdot v_0(\theta)$

MFDT becomes: This is the equality that we want to test

$$R(t-s)\ k_B T = \partial_s C(t-s) - b(t-s)$$

where

$$b(t-s) = < O(t,\theta) v_0(\theta(s)) \partial_\theta O(s,\theta) >$$

MFDT for NESS

In experiments is much safe to use the integral form :

$$\chi(t-s)\ k_B T = [C(0) - C(t-s)] - B(t-s)$$

$\chi(t-s)$ is the integrated response and

$$B(t-s) = \int_0^s b(t-t')dt'$$

We test this equality on the Langevin dynamics

$$\gamma \dot{x} = -\partial_x U(x) + G + \eta$$

with $< \eta(t)\eta(t') >= 2k_B T \nu \delta(t-t')$

$G = constant \neq 0$ non conservative force

Experiment with optical trap

Let us consider first the case with $U = 0$

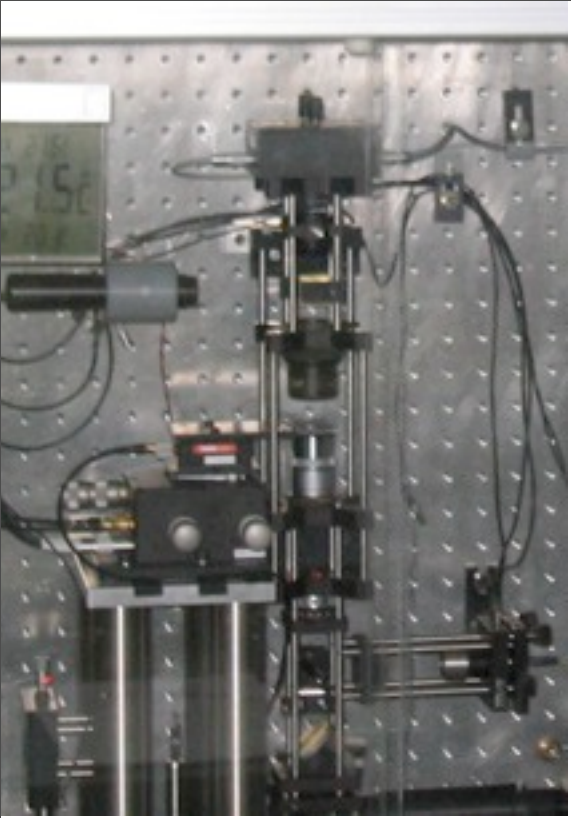
$$\nu \dot{x} = G + \eta$$

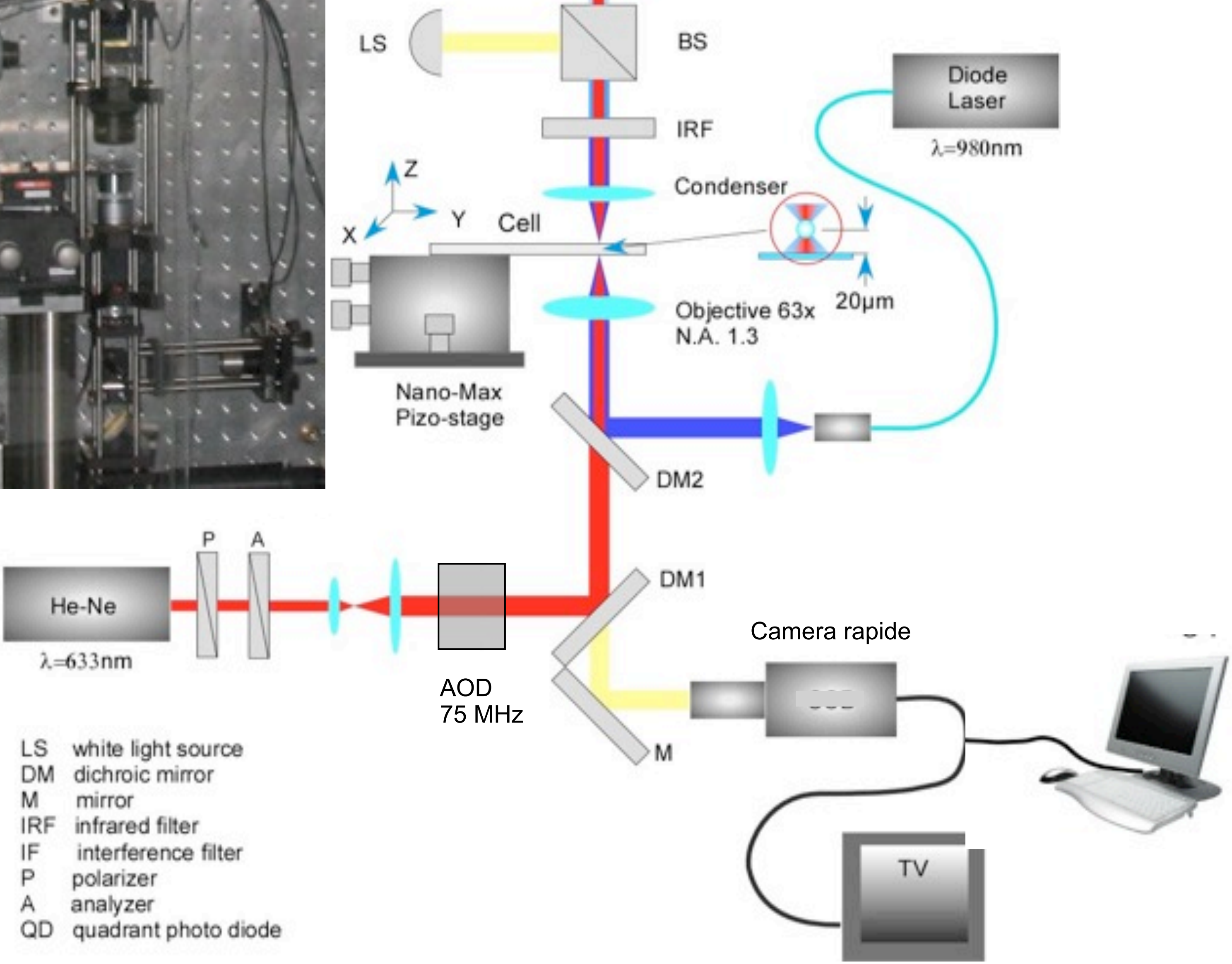
$G = constant \neq 0$ non conservative force

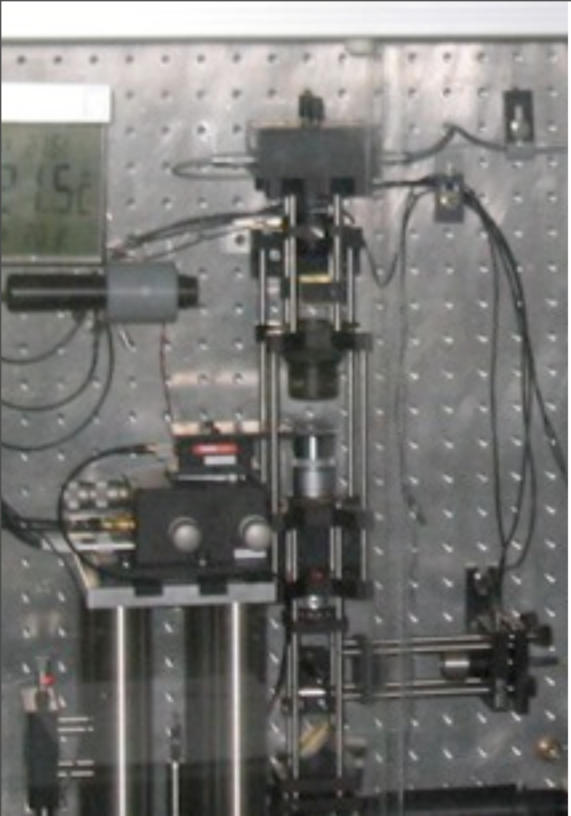
We use a Bownian particle confined in an optical trap

The experimental set up

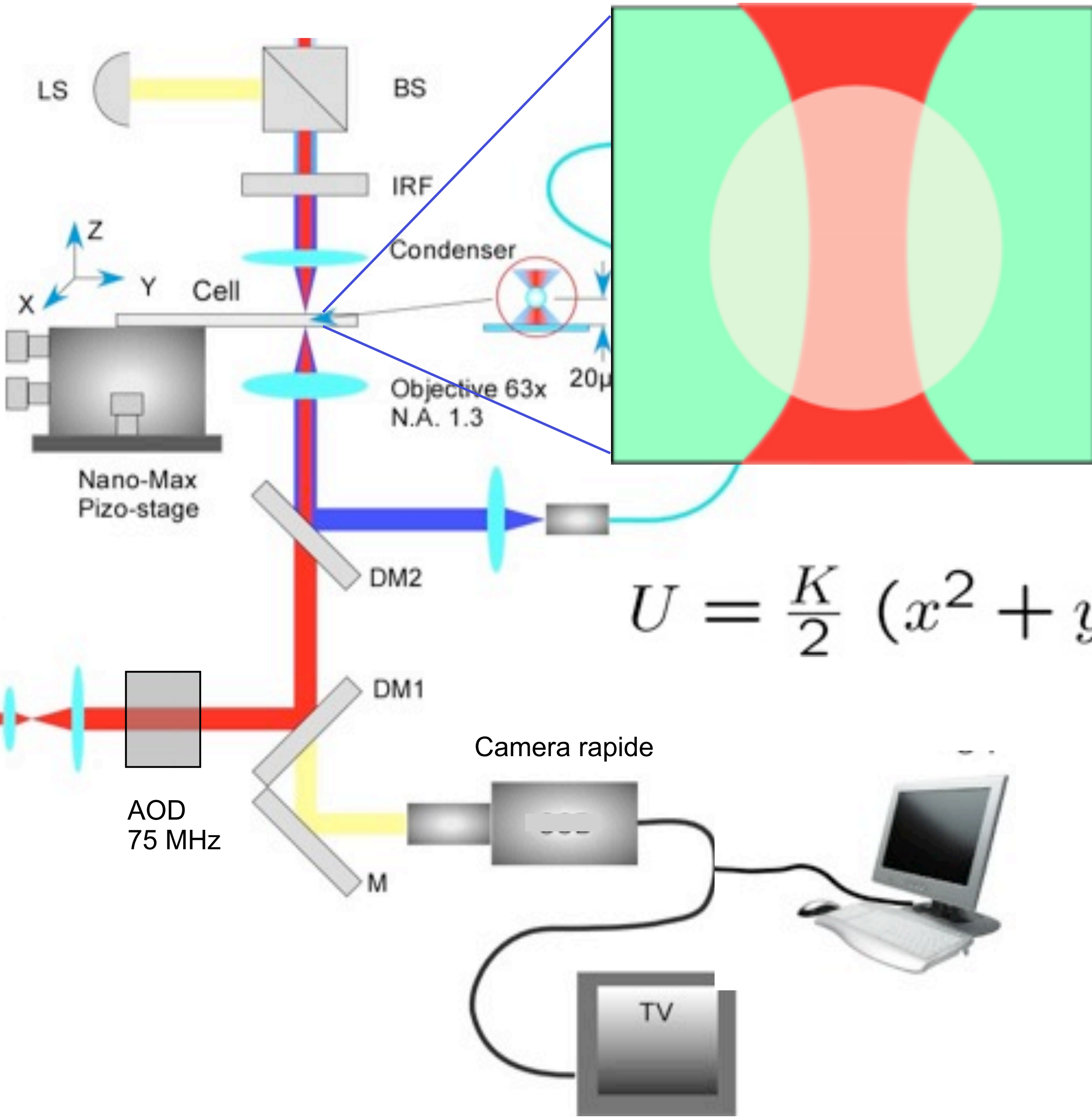
Optical traps





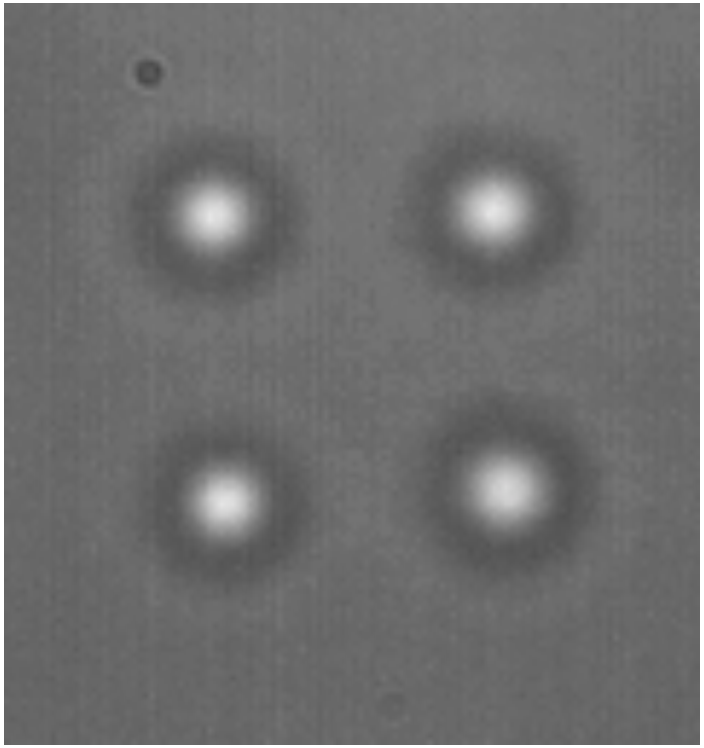


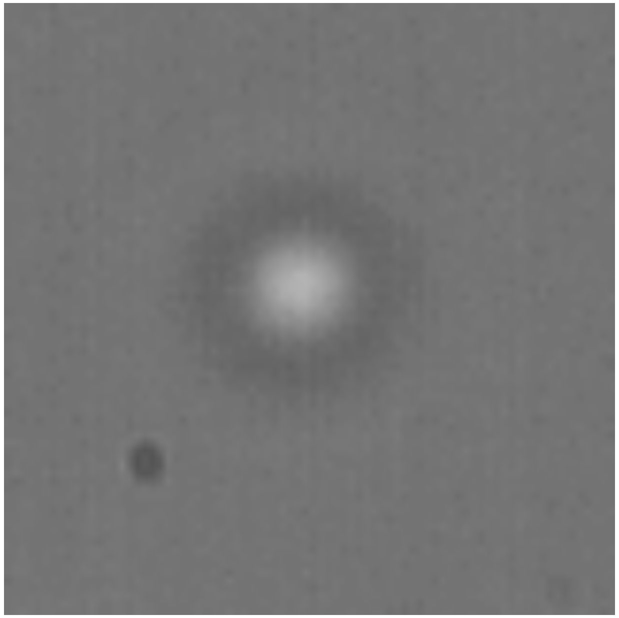
Optical traps

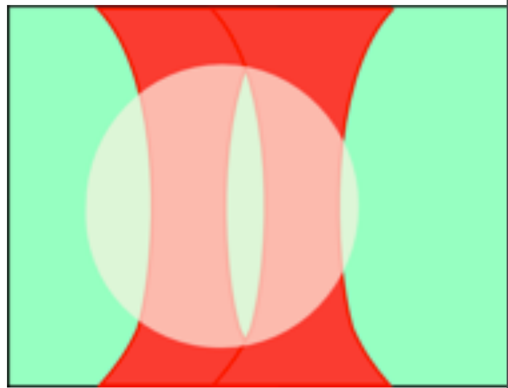


$$U = \frac{K}{2}\left(x^2 + y^2\right)$$

Examples of traps







The Kramer rate is

$$r_k = \tau_o^{-1} \exp(-\frac{\delta U}{k_B T})$$

Experiment with optical trap

Let us consider first the case with $U = 0$

$$\nu \dot{x} = G + \eta$$

$G = constant \neq 0$ non conservative force

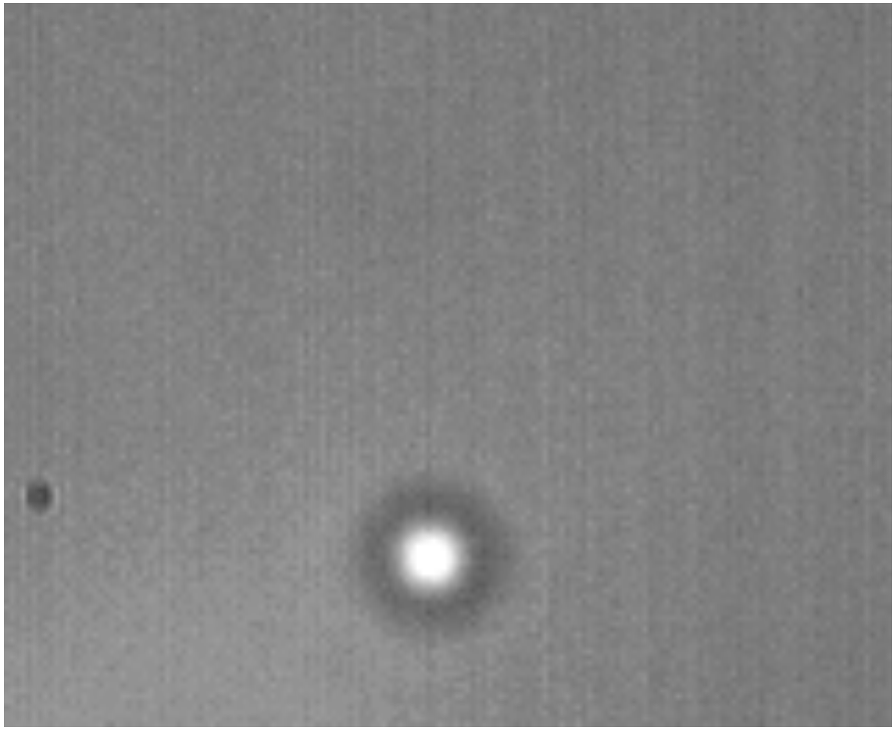
The motion of the particle is confined on a circle of radius a

$$x = a\ \theta \quad \text{with} \quad 0 \leq \theta \leq 2\pi$$

This is achieved by a circular sweeping of the laser beam

How G is obtained ?

Particle motion with U=0

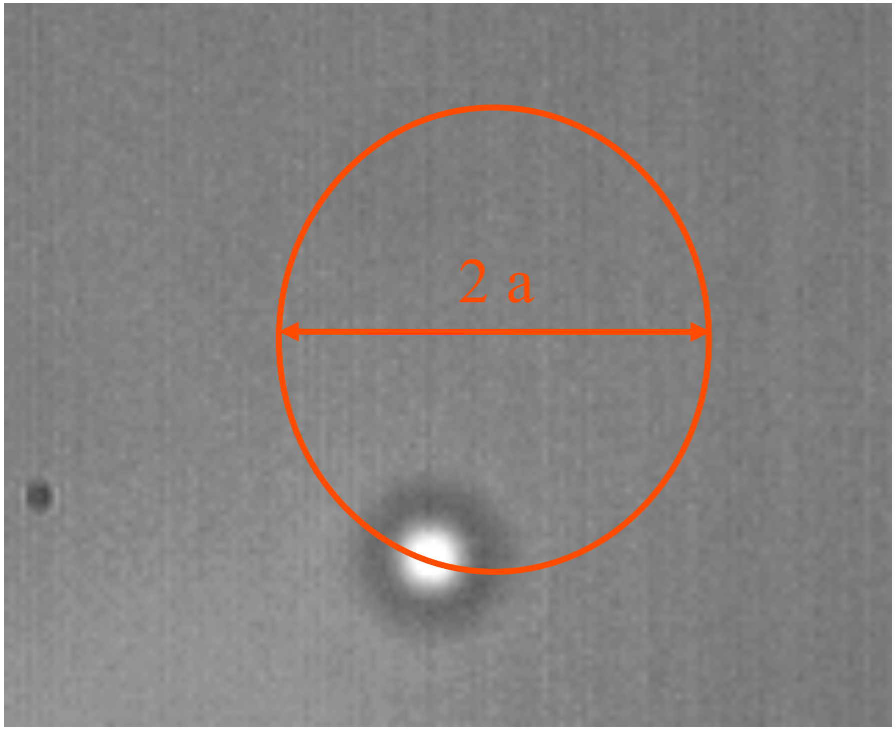


$$\nu \; a \; \dot{\theta} = G + \eta$$

$$\nu = 6\pi \; r \; \mu$$

$$v_0 = < \dot{\theta} > = G/\nu$$

Particle motion with U=0



$$\nu \; a \; \dot{\theta} = G + \eta$$

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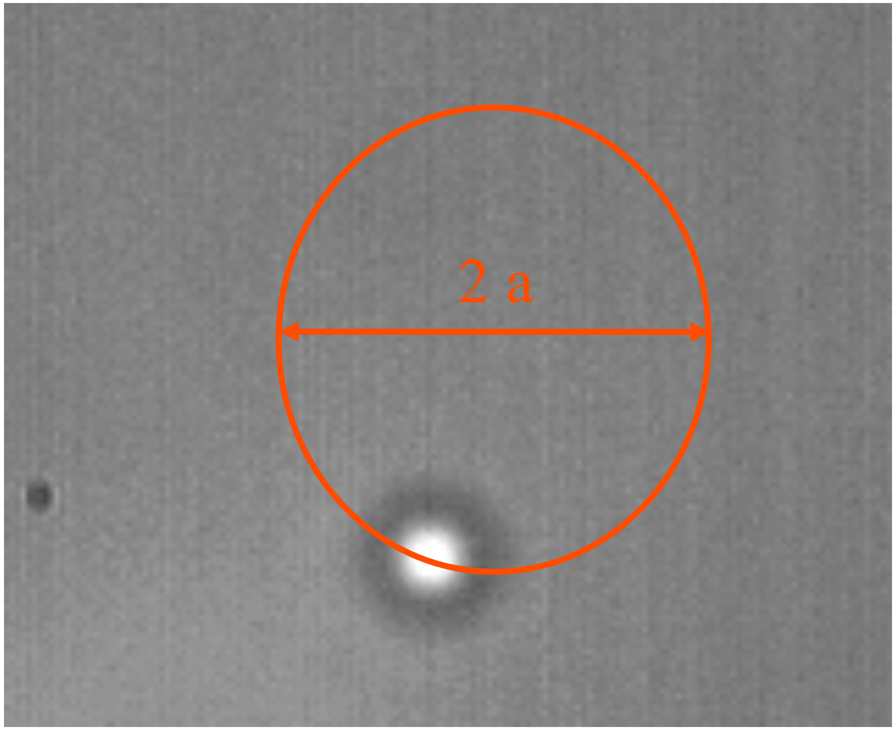
$$v_0 = \langle \dot{\theta} \rangle = G/\nu$$

Particle motion with U=0



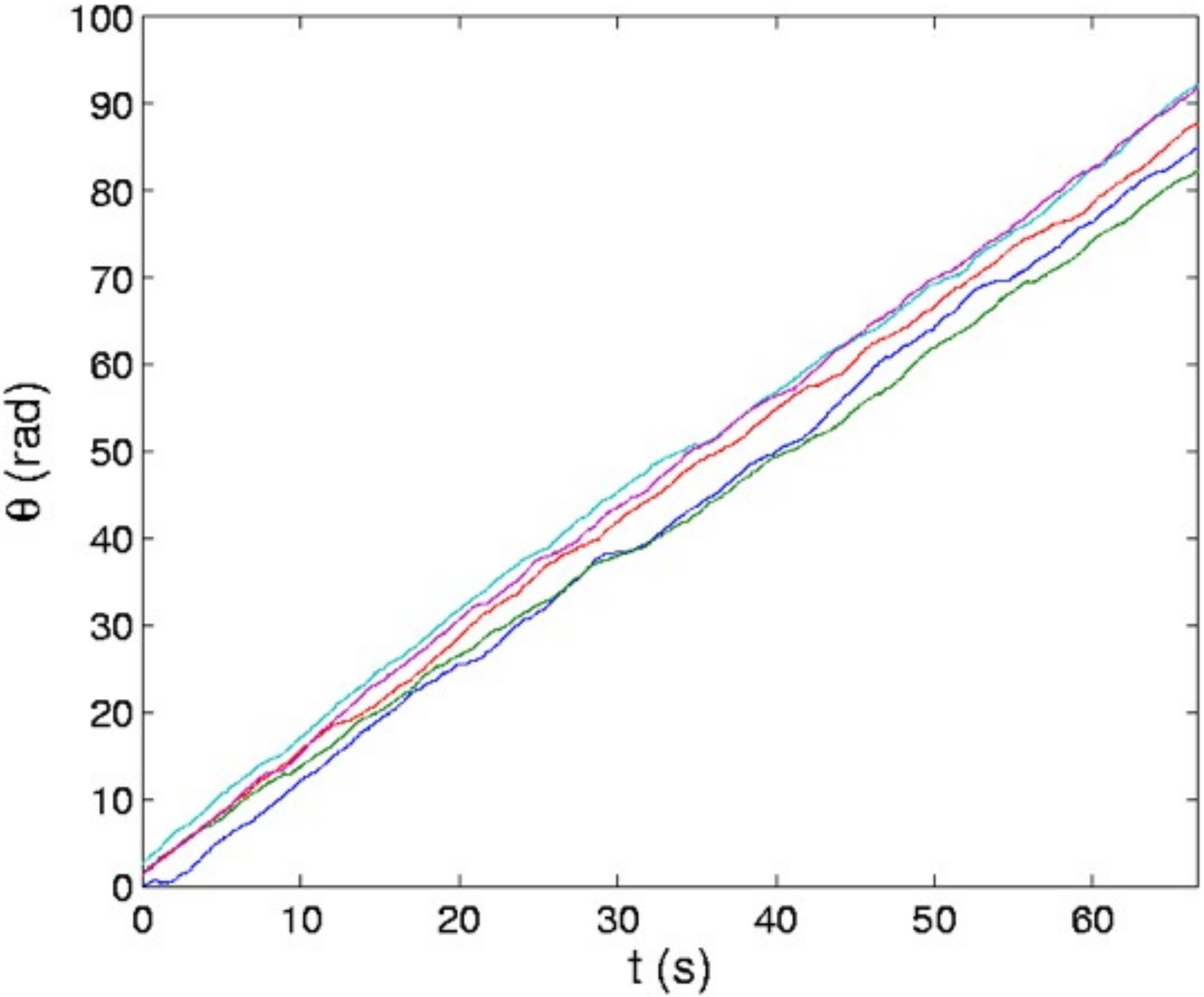
$$\nu \; a \; \dot{\theta} = G + \eta$$

$$\nu = 6\pi \; r \; \mu$$

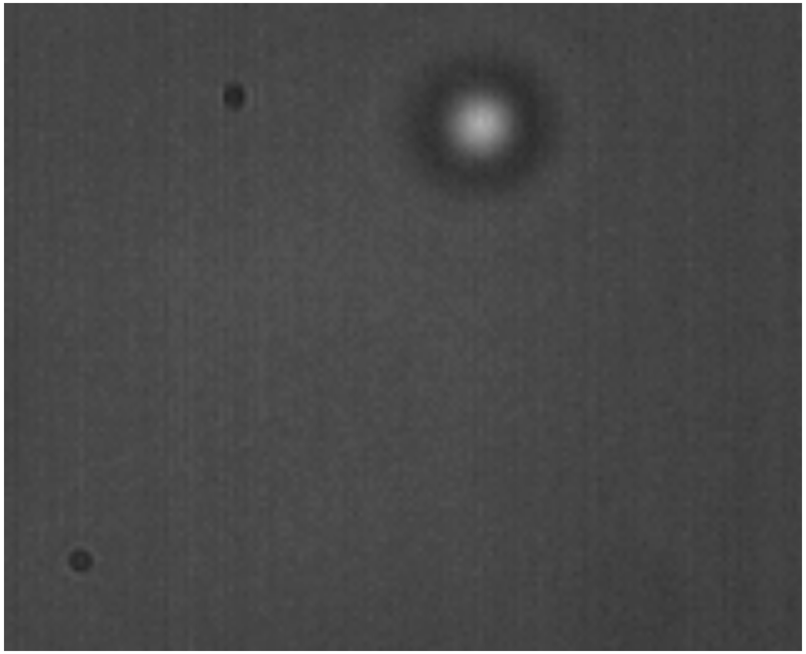
$$v_0 = < \dot{\theta} > = G/\nu$$

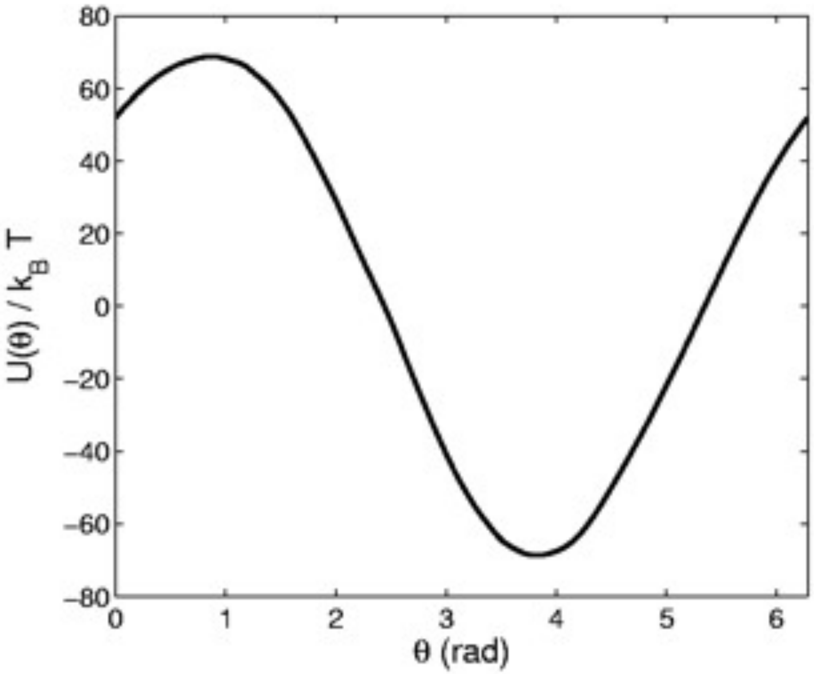
$a = 4.5\mu m$, $r = 1\mu m$, $\mu = 10^{-3} Pa$ s

We obtain $G = 6.60 \; 10^{-14} N$ from the measure of $v_0 = 0.85 rad/s$


θ (rad)
t (s)
0
10
20
30
40
50
60
70
80
90
100
0
10
20
30
40
50
60

Particle motion with potential





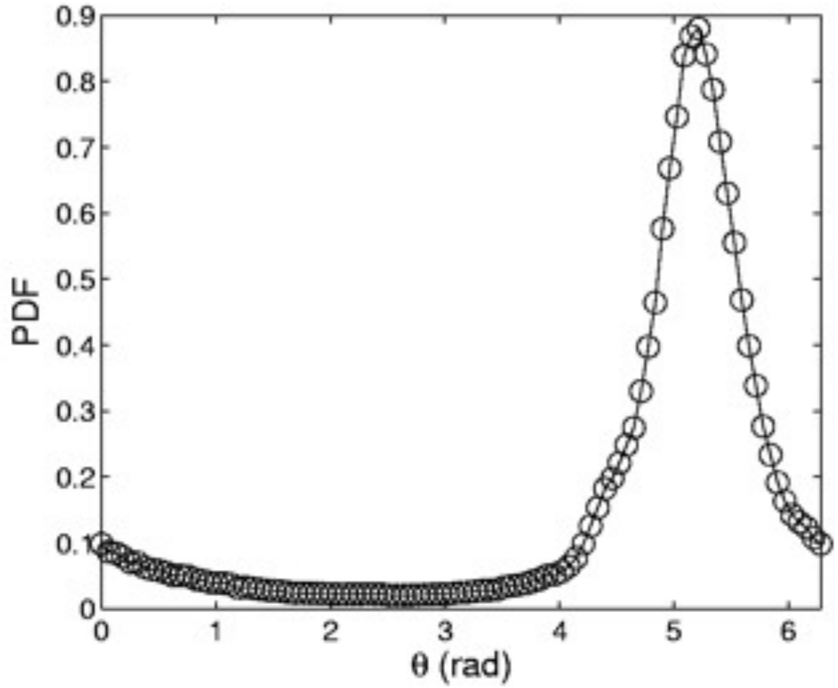
Periodic potential $U = A\sin(\theta + \varphi)$

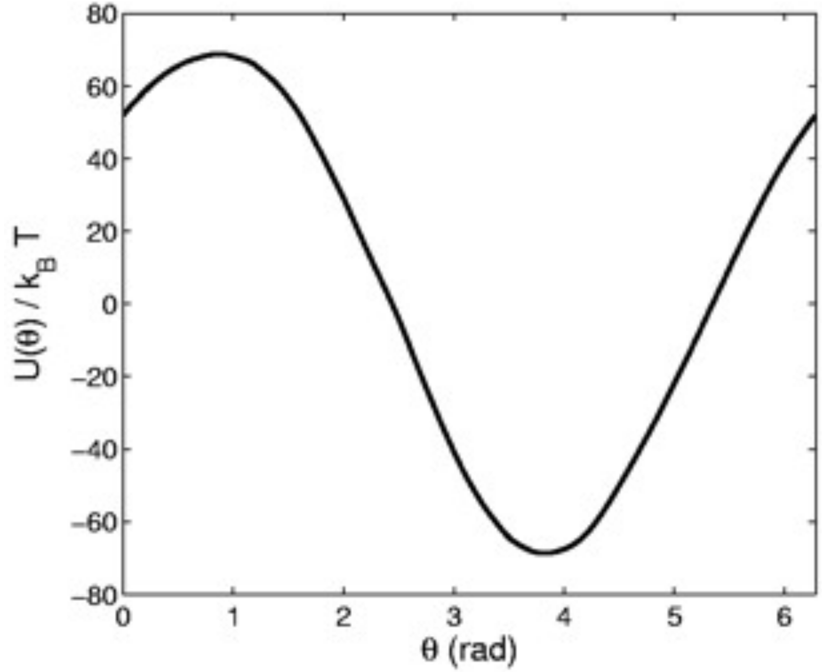
$$\nu\ a^2\ \dot{\theta} = -\partial_\theta U(\theta) + F + \eta\ a$$

$F = G\ a\ =$ constant non conservative torque

The potential U is produced by a modulation (5%) of the laser intensity

PDF of the particle position

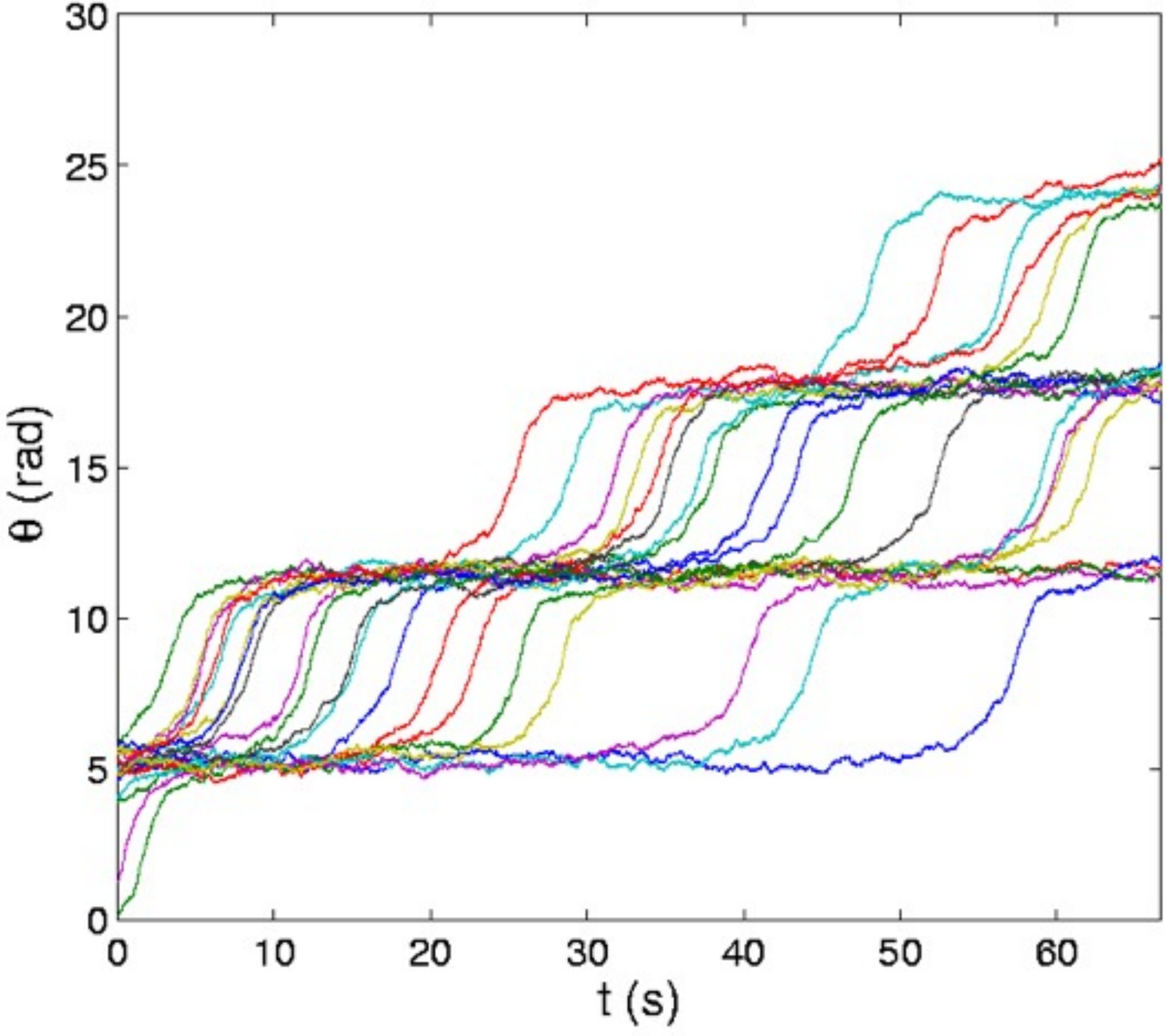




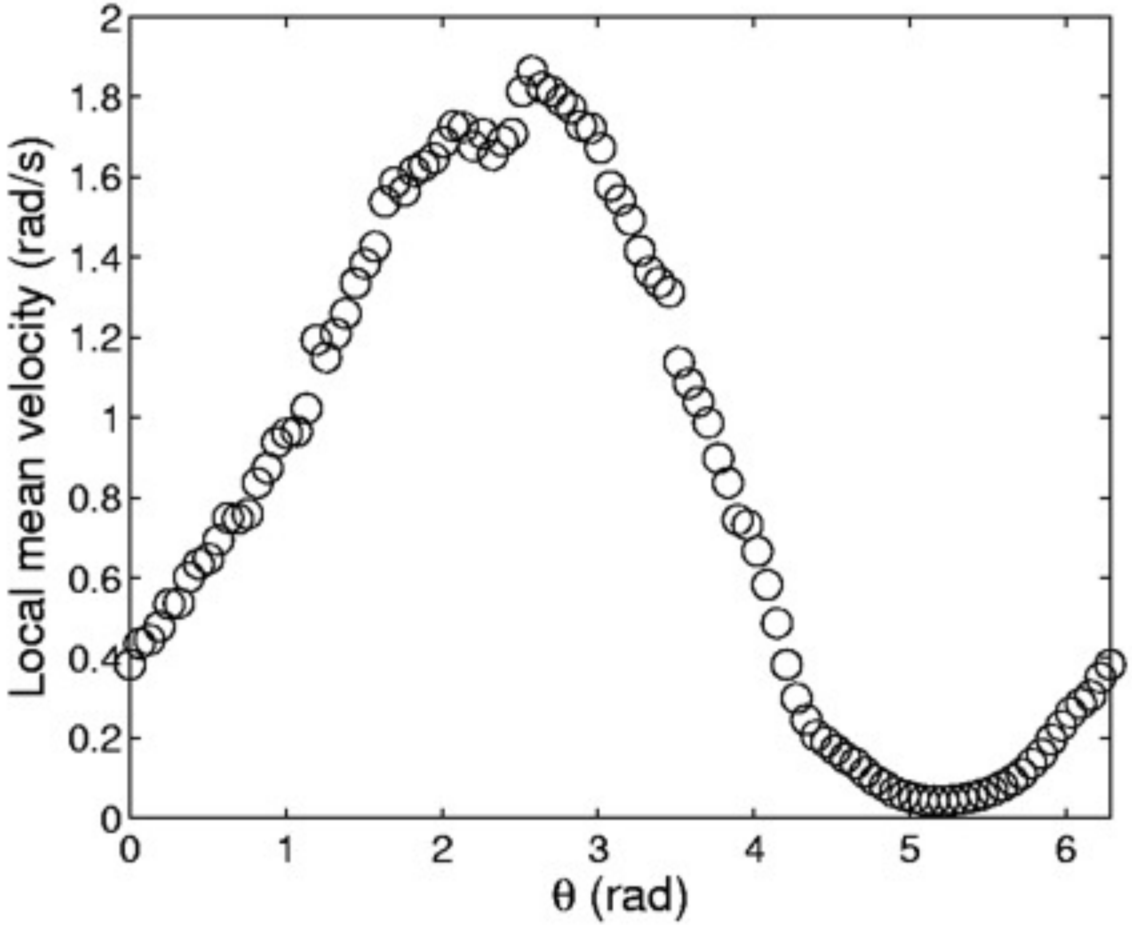
$$j = \text{probability} \quad \text{current} = <\dot{\theta}>_0 /(2\pi)$$

$$\rho(\theta) = \text{probability} \quad \text{density}$$

$$v_0(\theta) = \frac{j}{\rho(\theta)}$$


30
25
20
15
10
5
0
θ (rad)
0
10
20
30
40
50
60
t (s)

Local mean velocity



$j = \text{probability} \quad \text{current} = < \dot{\theta} >_0 / (2\pi)$

$\rho(\theta) = \text{probability} \quad \text{density}$

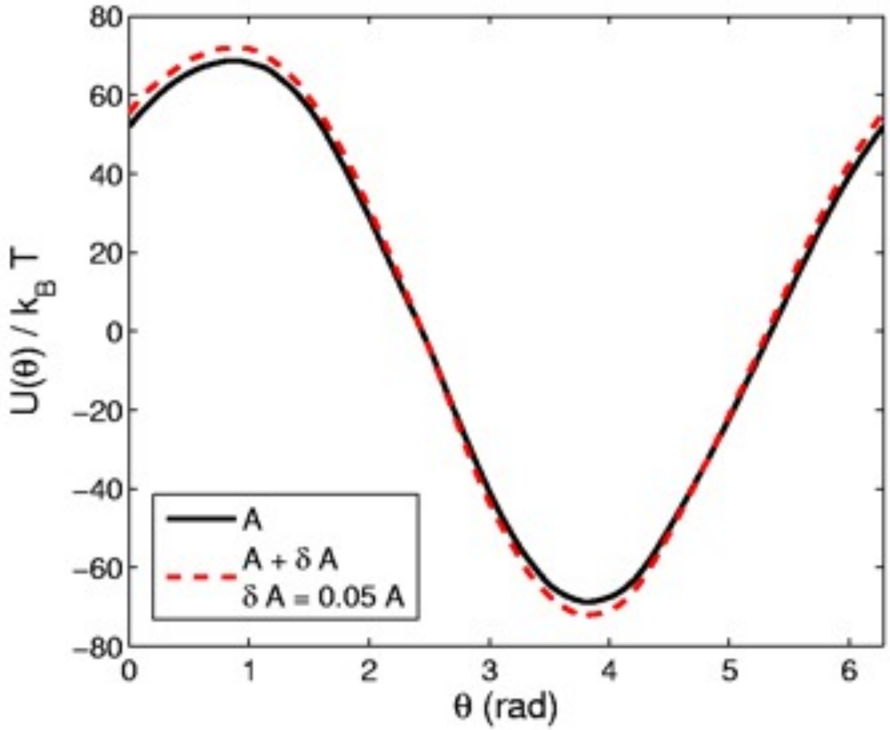
$v_0(\theta) = \frac{j}{\rho(\theta)}$

The observable O(θ)

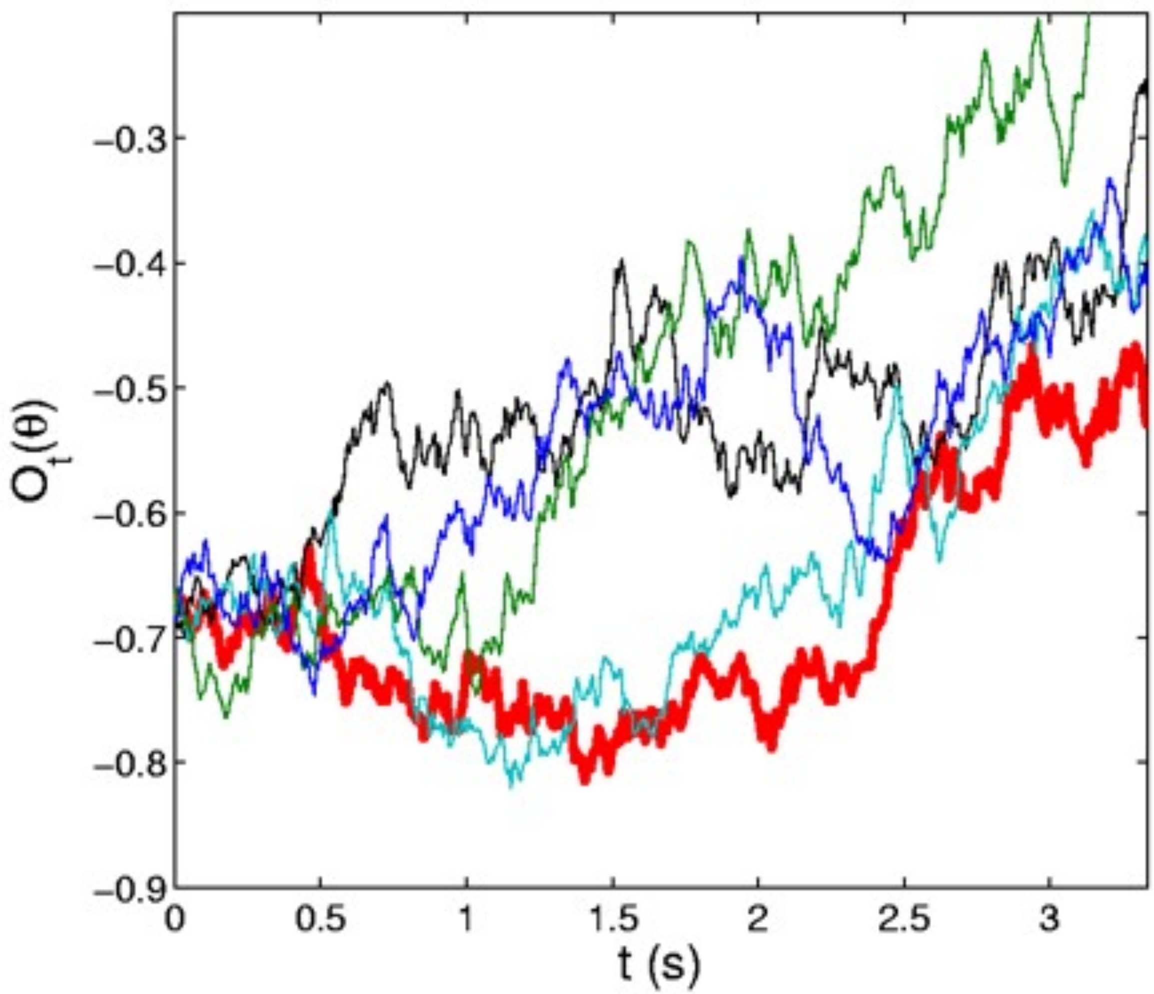
To measure the response, the perturbation is applied in the follwing way:

$$U(\theta) \longrightarrow U(\theta) + \delta A \ \sin(\theta + \varphi)$$

Thus the observable is $O(\theta(t)) = \sin(\theta(t) + \varphi)$



Time evolution of O(t)



MFDT for NESS

The observable is : $O(\theta(t)) = \sin(\theta(t) + \varphi)$

$$\chi(t)\ k_B T = [C(0) - C(t)] - B(t)$$

with

$$B(t) = \int_0^t < O(\theta(t'))v_0(\theta(t'))\partial_\theta O(\theta(0)) > dt'$$

$$C(t) =< O(\theta(t))O(\theta(0)) >$$

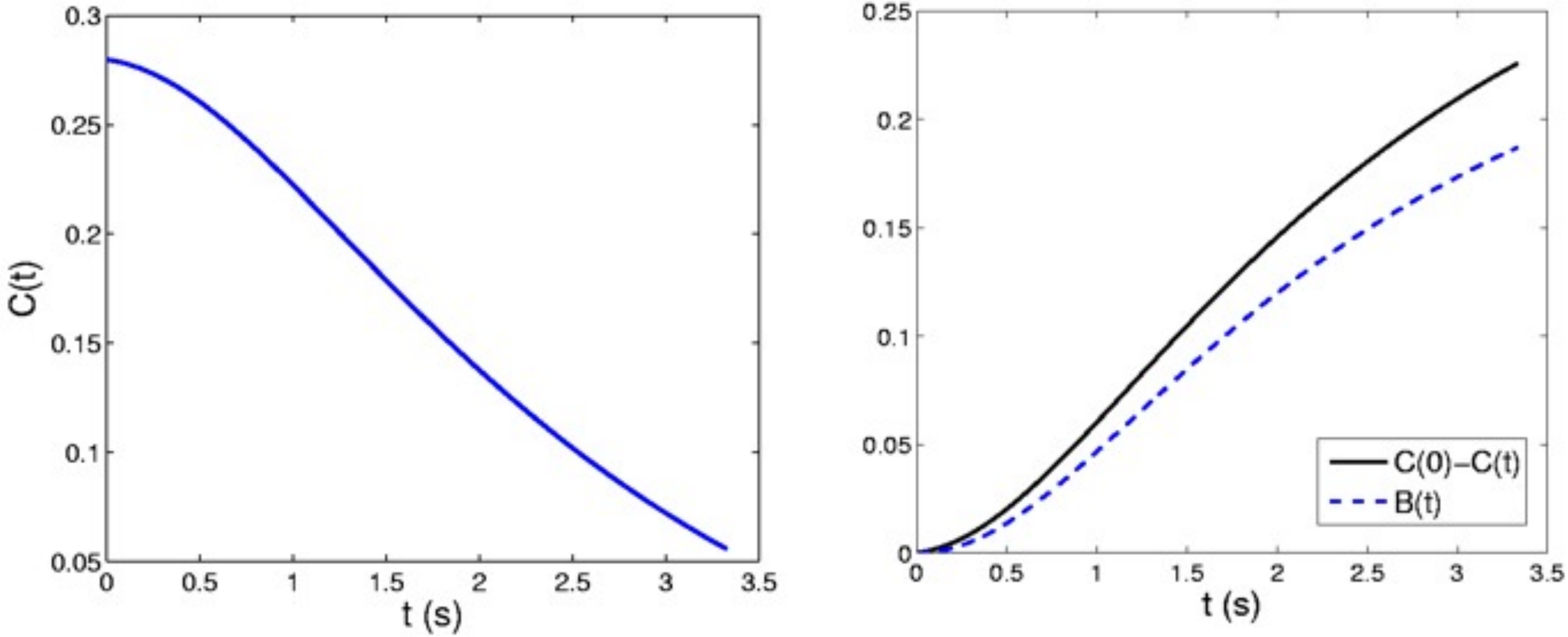
The integrated response $\chi(t)$

to a Heaviside perturbation of A, switched on at $t = 0$, is:

$$\chi(t) = \frac{< O(\theta(t))_{\delta A} - O(\theta(t + t^*))_0 >}{\delta A}$$

such that $O(\theta(0))_{\delta A} = O(\theta(t^*))_0$

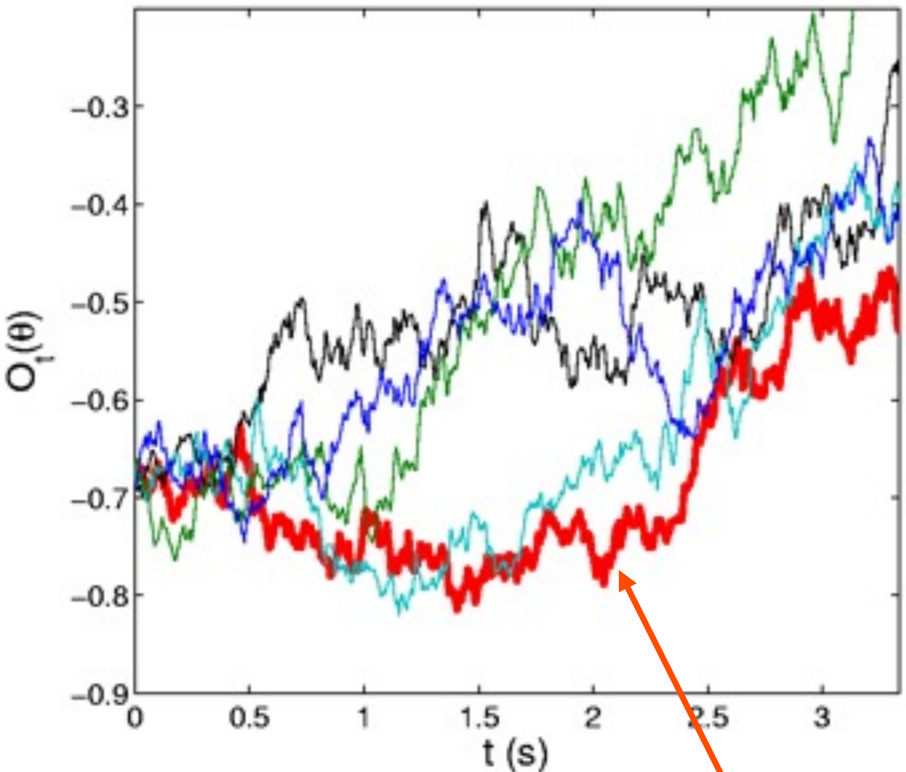
Correlation function and B(t)



The integrated response

to a Heaviside perturbation of A, switched on at $t = 0$, is:

$$\chi(t) = \frac{< O(\theta(t))_{\delta A} - O(\theta(t+t^*))_0 >}{\delta A}, \text{ with } O(\theta(0))_{\delta A} = O(\theta(t^*)_0$$



- Select 200 unperturbed trajectories such that at time t^*

$$O(\theta(0))_{\delta A} = O(\theta(t^*))_0$$

- Compute the mean of $O(\theta(t))_{\delta A} - O(\theta(t+t^*))_0$ on the 200 trajectories

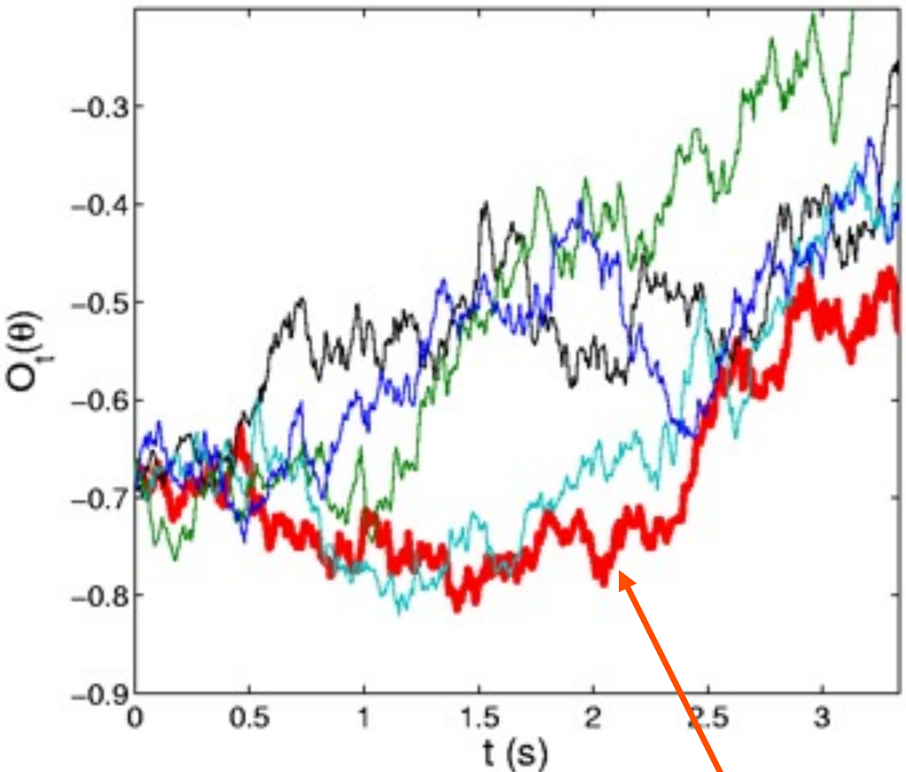
- Repeat the procedure on several perturbations and make the average

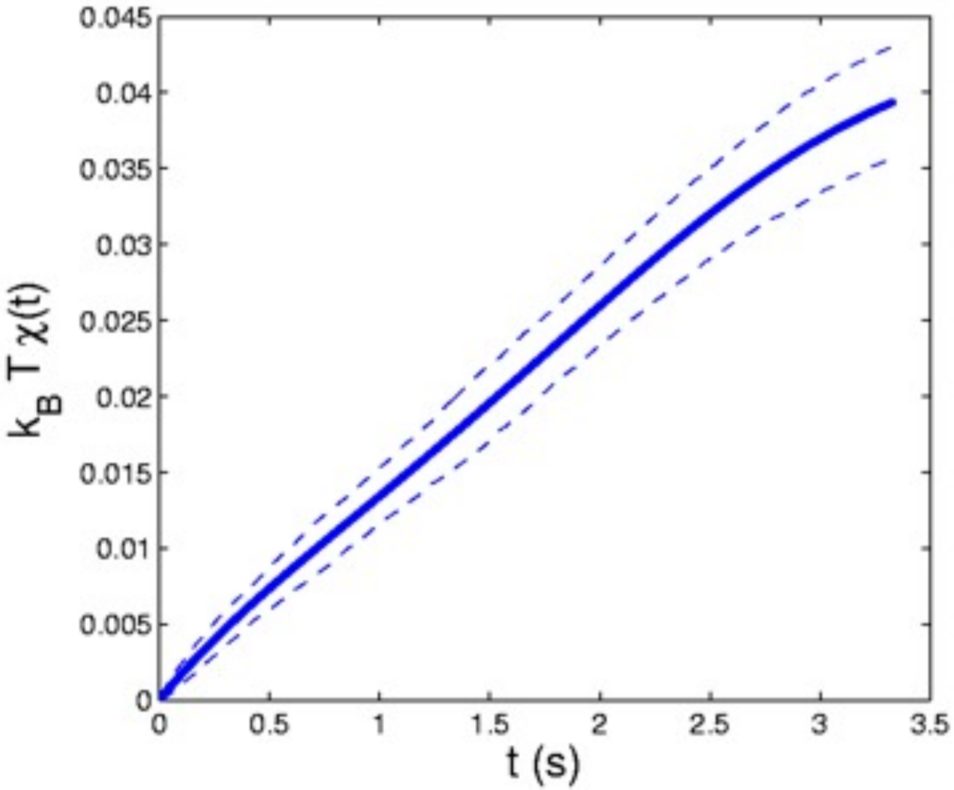
Perturbed trajectory

The integrated response

to a Heaviside perturbation of A, switched on at $t = 0$, is:

$$\chi(t) = \frac{< O(\theta(t))_{\delta A} - O(\theta(t + t^*))_0 >}{\delta A}, \text{ with } O(\theta(0))_{\delta A} = O(\theta(t^*)_0$$

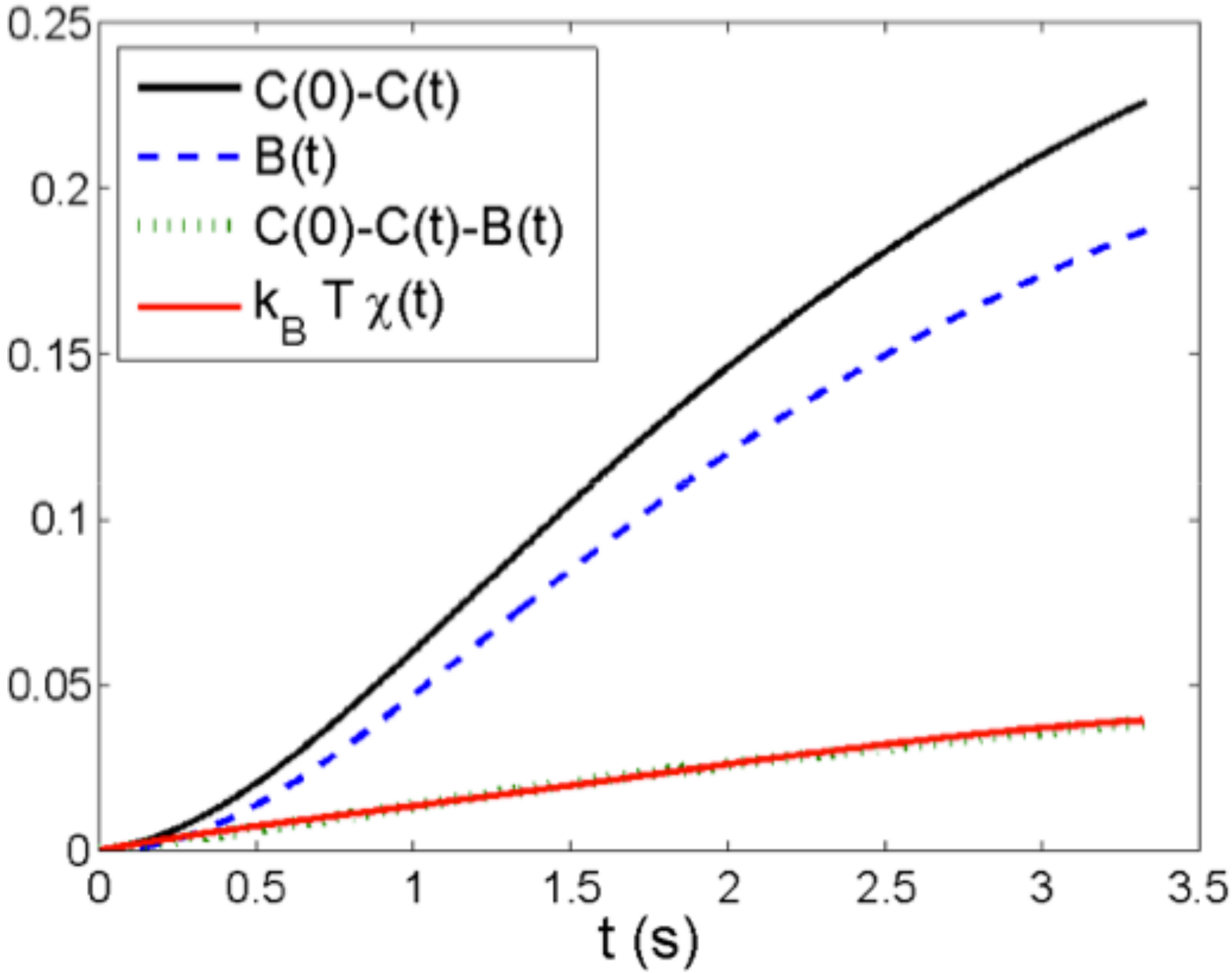




Perturbed trajectory

MFDT

$$\chi(t)\ k_B T = [C(0) - C(t)] - B(t)$$



MFDT

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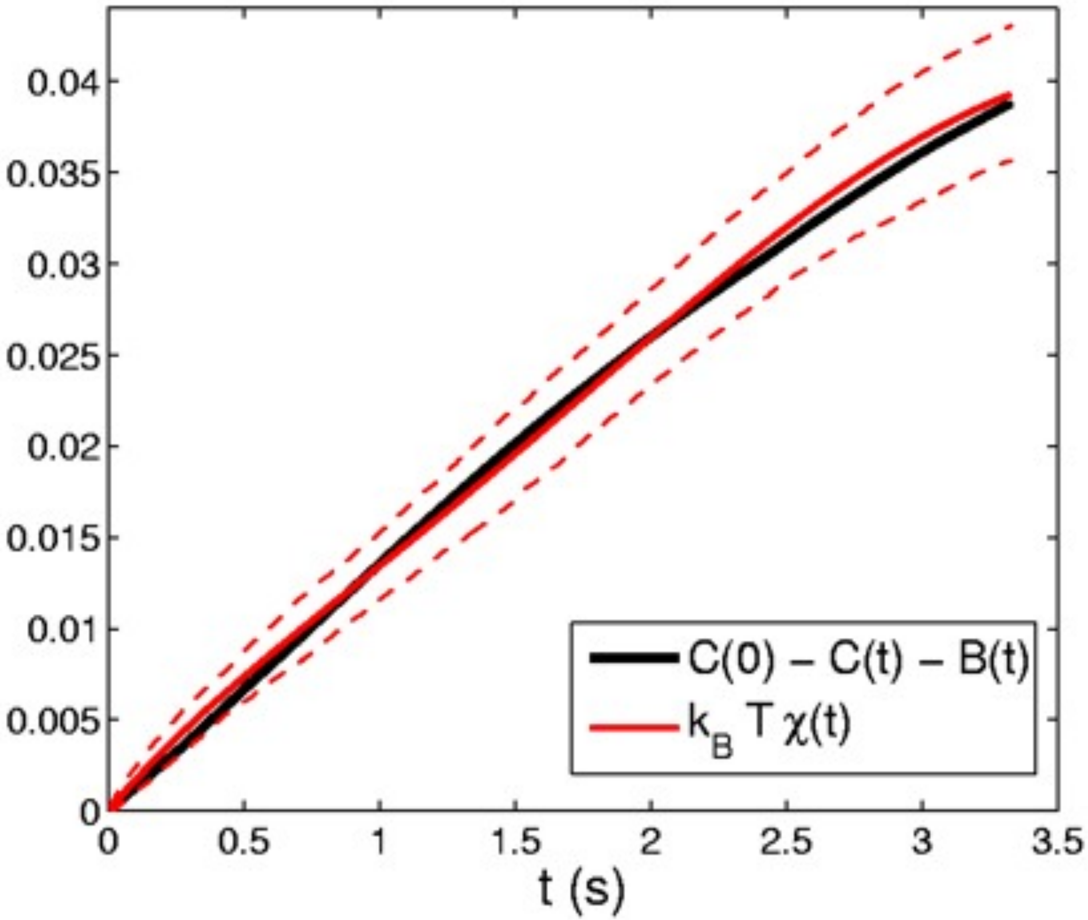


Conclusions on MFDT

based on a Lagrangian formulation

- We have shown that MFDT holds for a bead moving in a toroidal optical trap and submitted to a non conservative force and to a periodic potential.
- The results can be interpreted as an equilibrium like FDT in the Lagrangian frame moving at the velocity determined by the probability current.
- The main drawback of the method is the knowledge of the probability current which is not always obvious to measure.

MFDT based on frenesy

E. Lippiello, F. Corberi, and M. Zannetti, Phys. Rev.E, 71 (036104) 2005.
M. Baiesi, C. Maes and B. Wynants, Phys. Rev. Lett., 103 (010602) 2009.

$$U(q) \to U(q) - h_s V(q)$$

$$\chi_{OV}(t) = \int_0^t R_{OV}(t,s)\,\mathrm{d}s = \frac{\langle O(q_t)\rangle_h - \langle O(q_t)\rangle_0}{h},$$

$$\chi_{QV}(t) = \tfrac{\beta}{2}[C_{OV}(0) - C_{OV}(t) + K(t)],$$

$$C_{OV}(t) = \langle V(q_0)O(q_t)\rangle_0,$$

$$K(t) = -\textstyle\int_0^t \langle LV(q_s)O(q_t)\rangle_0\,\mathrm{d}s,$$

The frenesy $\beta LV(q)$ can be regarded as a generalized escape rate of a trajectory from a given phase-space point q *(Baiesi et al)*.

MFDT based on frenesy

In our experiment

$$\nu \ a^2\dot{\theta} = -A\frac{\partial O(\theta)}{\partial\theta} + F + \eta \ a$$

$U(\theta) = A \ O(\theta)$ with $O(\theta) \simeq \sin(\theta + \varphi)$

and $\quad V(\theta) = U(\theta)$

$$U(\theta) \to U(\theta) - \frac{\delta A}{A} U(\theta)$$

$$\chi_{OV}(t) = \frac{A(\langle O(\theta(t))\rangle_h - \langle O(\theta(t+t^*))\rangle_0)}{\delta A} = A \ \chi(t)$$

with $O(\theta(0))_{\delta A} = O(\theta(t^*))_0$

MFDT based on frenesy

$$\chi_{QV}(t) = \frac{\beta}{2}[C_{OV}(0) - C_{OV}(t) + K(t)],$$

$$K(t) = -\int_0^t \langle LV(q_s)O(q_t)\rangle_0 \, \mathrm{d}s,$$

For the Langevin dynamics of θ the analytical expression of the generator L is

$$L = \frac{1}{\nu \ a^2}\left[(F - AO'(\theta))\partial_\theta + k_B T \partial_\theta^2 .\right]$$

Hence in this case

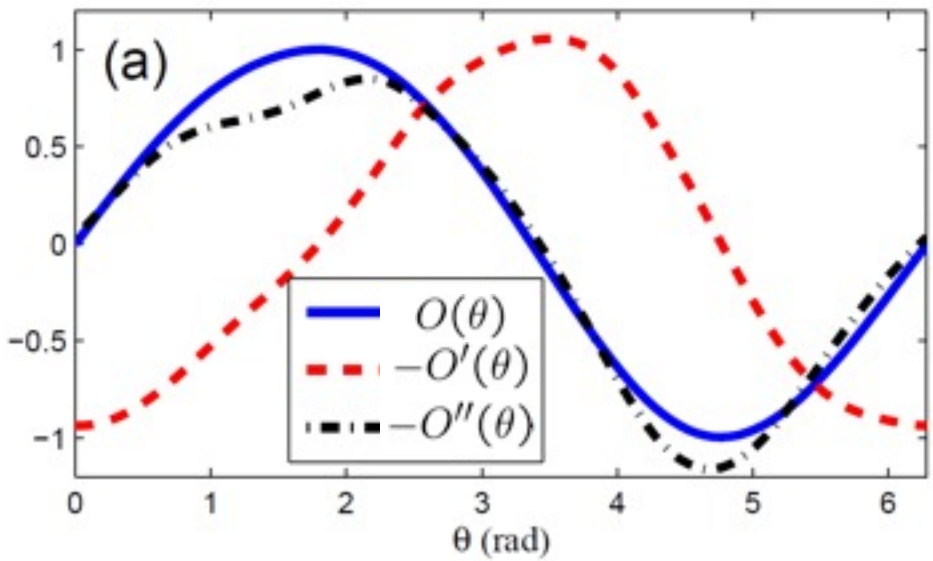
$$k_B T \ \chi(t) = \frac{C(0) - C(t) + \tilde{K}(t)}{2},$$

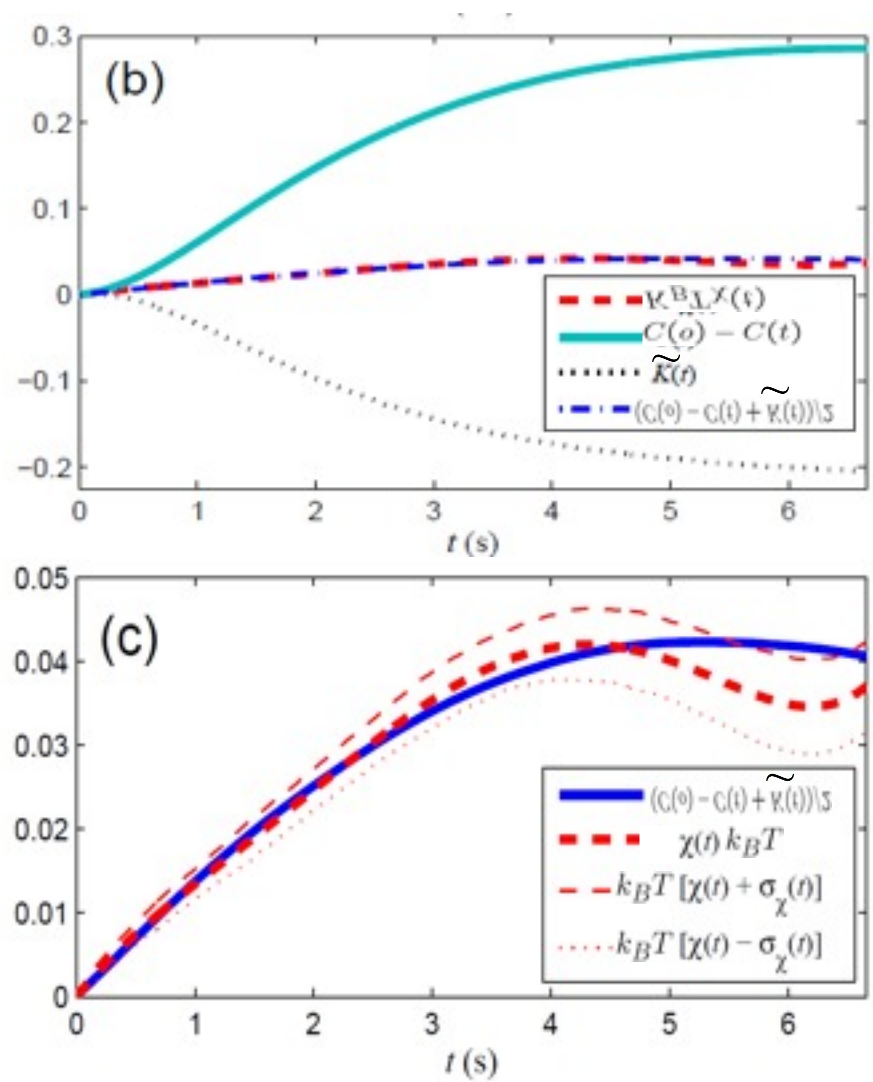
where the entropic and frenetic terms are

$$A \ C(t) = A \ \langle O(\theta_0)O(\theta_t)\rangle_0 = C_{OV}(t)$$

$$K(t) = A\tilde{K}(t) = -\frac{A}{\nu \ a^2}\int_0^t ds \langle [k_B T \ O''(\theta_s) + (F - A \ O'(\theta_s)) \ O'(\theta_s)]O(\theta_t)\rangle_0,$$

Results on the FDT based on frenesy





- The method is sensitive to the values of the experimental derivative of the potential
- Two drawbacks:

a) the knowledge of the generator of the dynamics;

b) The Markofian nature of the system

Generalized FDT

The starting point is the Hatano-Sasa relation for Markofian process

$$\rho_{ss}(c, \lambda^{ss}) = \exp[-\phi(c, \lambda^{ss})].$$

Probability density for a NESS

$$\phi(c; \lambda) = -\log[\rho_{ss}(c; \lambda)]$$

Pseudo-potential

$$\left\langle \exp\left\{-\int_{t_i}^{t_f} dt \dot{\lambda}_\alpha(t) \frac{\partial \phi(c(t); \lambda(t))}{\partial \lambda_\alpha}\right\}\right\rangle = 1,$$

The average is taken over a large number of realizations of a given dynamical process defined by the variation of λ(t)

Generalized FDT

The starting point is the Hatano-Sasa relation for Markofian process

$$\rho_{ss}(c, \lambda^{ss}) = \exp[-\phi(c, \lambda^{ss})].$$

Probability density for a NESS

$$\phi(c;\lambda) = -\log[\rho_{ss}(c;\lambda)]$$

Pseudo-potential

$$\left\langle \exp\left\{-\int_{t_i}^{t_f} dt\,\dot{\lambda}_\alpha(t)\frac{\partial\phi(c(t);\lambda(t))}{\partial\lambda_\alpha}\right\}\right\rangle = 1,$$

Hatano-Sasa

The average is taken over a large number of realizations of a given dynamical process defined by the variation of λ(t)

Generalized FDT

$$\left\langle \exp\left\{-\int_{t_i}^{t_f} dt\,\dot{\lambda}_\alpha(t)\frac{\partial\phi(c(t);\lambda(t))}{\partial\lambda_\alpha}\right\}\right\rangle = 1,$$

Consider small variations of the control parameters around a steady-state value λ^{ss}.

$$\delta\lambda(t) = \lambda(t) - \lambda^{ss} \qquad \text{with} \qquad \delta\lambda(t_i) = 0$$

Expanding to second order in the integrand and taking into account the normalisation conditions one obtains:

J. Prost, J.F. Joanny, J.M. Parrondo, PRL 103, 090601 (2009)

Generalized FDT

$$\left\langle \frac{\partial \phi(c(t); \lambda^{ss})}{\partial \lambda_\alpha} \right\rangle = \int_{t_i}^{t} R_{\alpha\gamma}(t - t')\delta\lambda_\gamma(t')dt',$$

$$R_{\alpha\gamma}(t - t') = \frac{d}{dt} C_{\alpha\gamma}(t - t')$$

$$= \frac{d}{dt} \left\langle \frac{\partial \phi(c(t); \lambda^{ss})}{\partial \lambda_\alpha} \frac{\partial \phi(c(t'); \lambda^{ss})}{\partial \lambda_\gamma} \right\rangle_{ss}.$$

Where now $\langle . \rangle_{ss}$ is computed on the sationary state

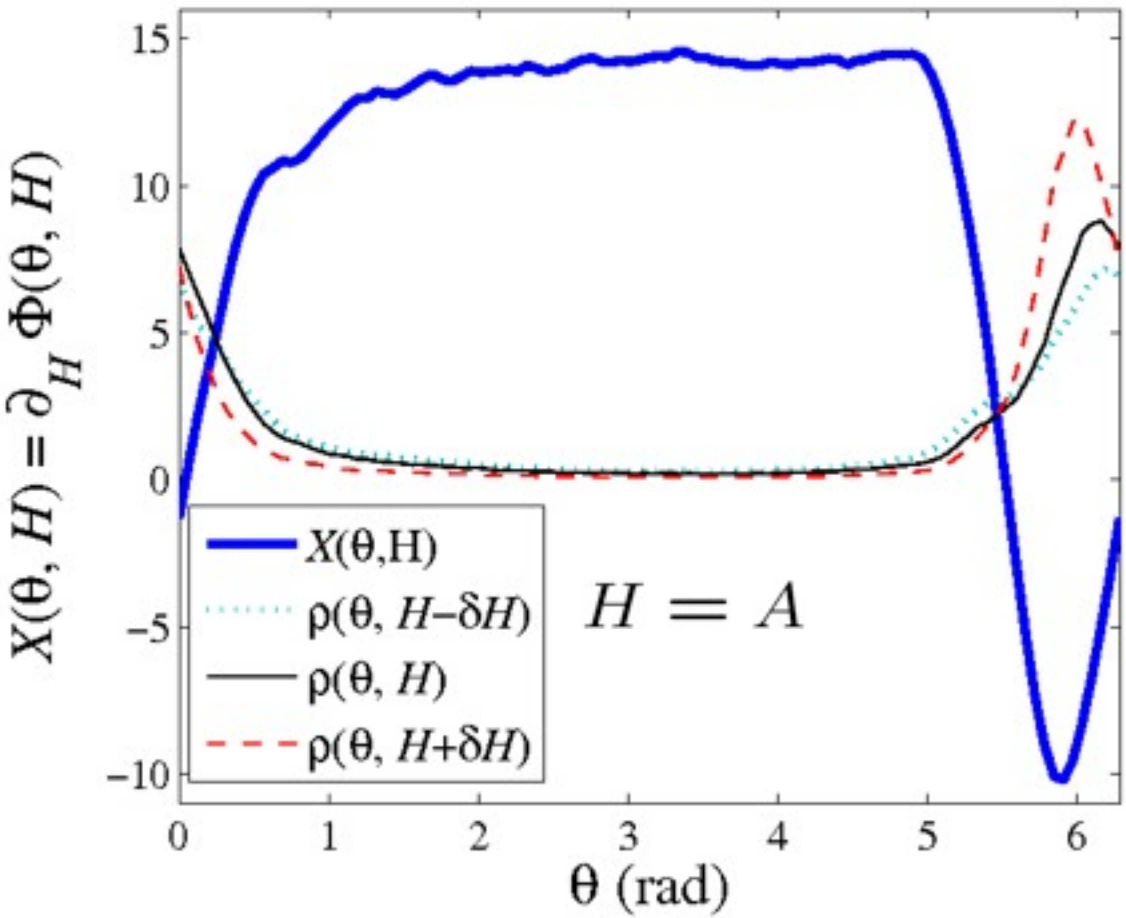
$$X_\alpha(t) = \frac{\partial \phi(t)}{\partial \lambda_\alpha}$$ is the observable

J. Prost, J.F. Joanny, J.M. Parrondo, PRL 103, 090601 (2009)

Generalized FDT

In the experiment

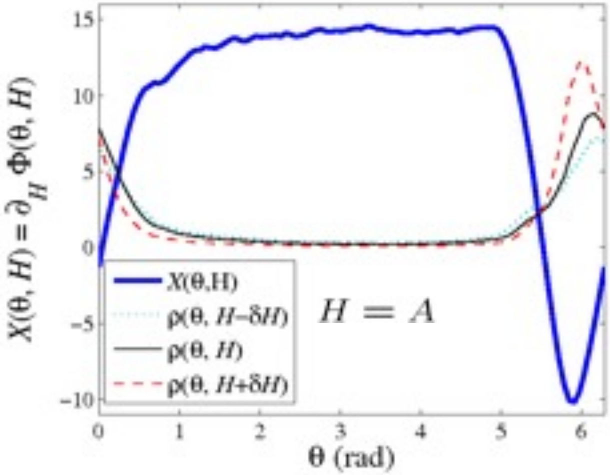
$$X(t) = \frac{\partial \phi(\theta(t), A)}{\partial A}$$



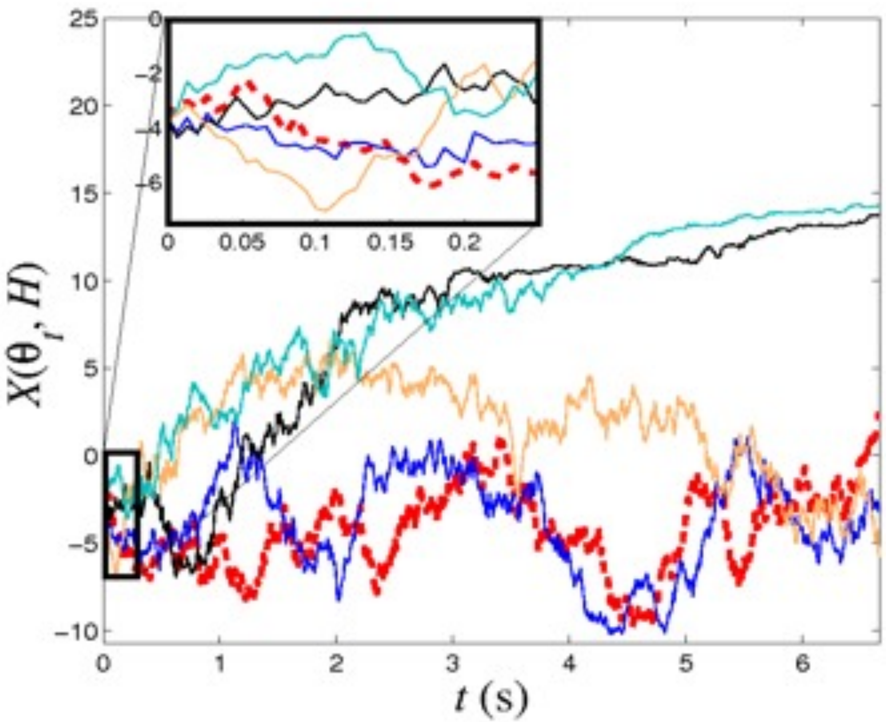
Generalized FDT

In the experiment

$$X(t) = \frac{\partial \phi(\theta(t), A)}{\partial A}$$



Time evolution of X



Generalized FDT

The response function in the experiment

$$\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle = \int_0^t R(t-t')\ \delta A(t')\ dt'$$

If δA is an Heaviside perturbation

$$\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle = (C(0) - C(t))\delta A$$

where $$C(t) = \left\langle \frac{\partial \phi(\theta(t))}{\partial A} \ \frac{\partial \phi(\theta(0))}{\partial A} \right\rangle_{ss}$$

Generalized FDT

The response function in the experiment

$$\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle = \int_0^t R(t-t')\ \delta A(t')\ dt'$$

If δA is an Heaviside perturbation

$$\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle \neq (C(0) - C(t))\delta A$$

where

$$C(t) = \left\langle \frac{\partial \phi(\theta(t))}{\partial A} \ \frac{\partial \phi(\theta(0))}{\partial A} \right\rangle_{ss}$$

Experimentally it does not work

Generalized FDT

The response function in the experiment

$$\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle = \int_0^t R(t-t') \; \delta A(t') \; dt'$$

Generalized FDT

The response function in the experiment

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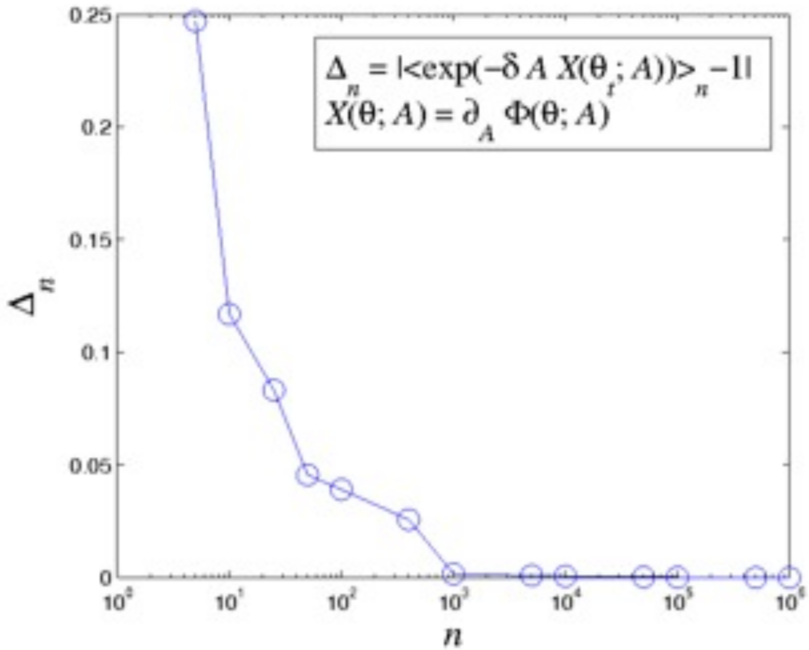
The Hatano-Sasa relation
is not exactly 1

and

$$\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle_{ss} \neq 0$$



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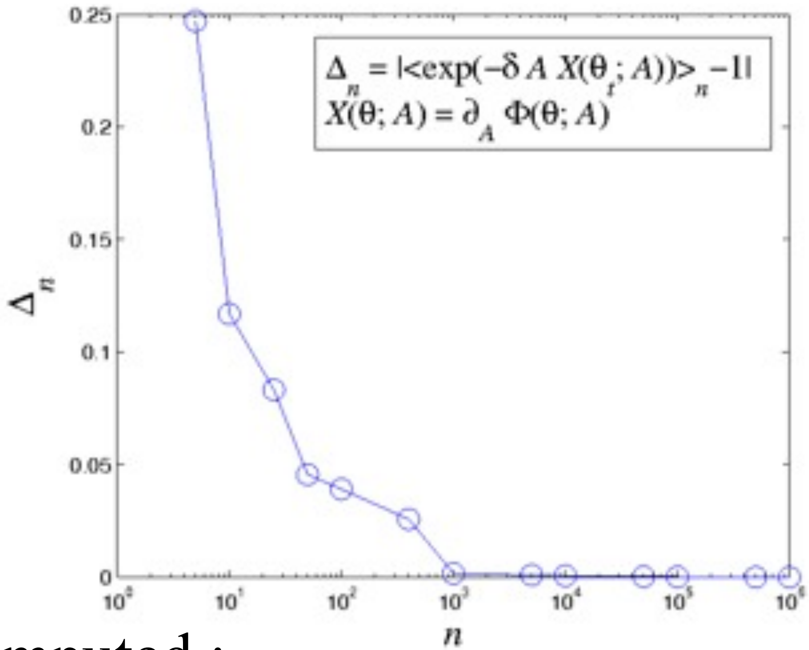

and

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The integrated response must be computed :

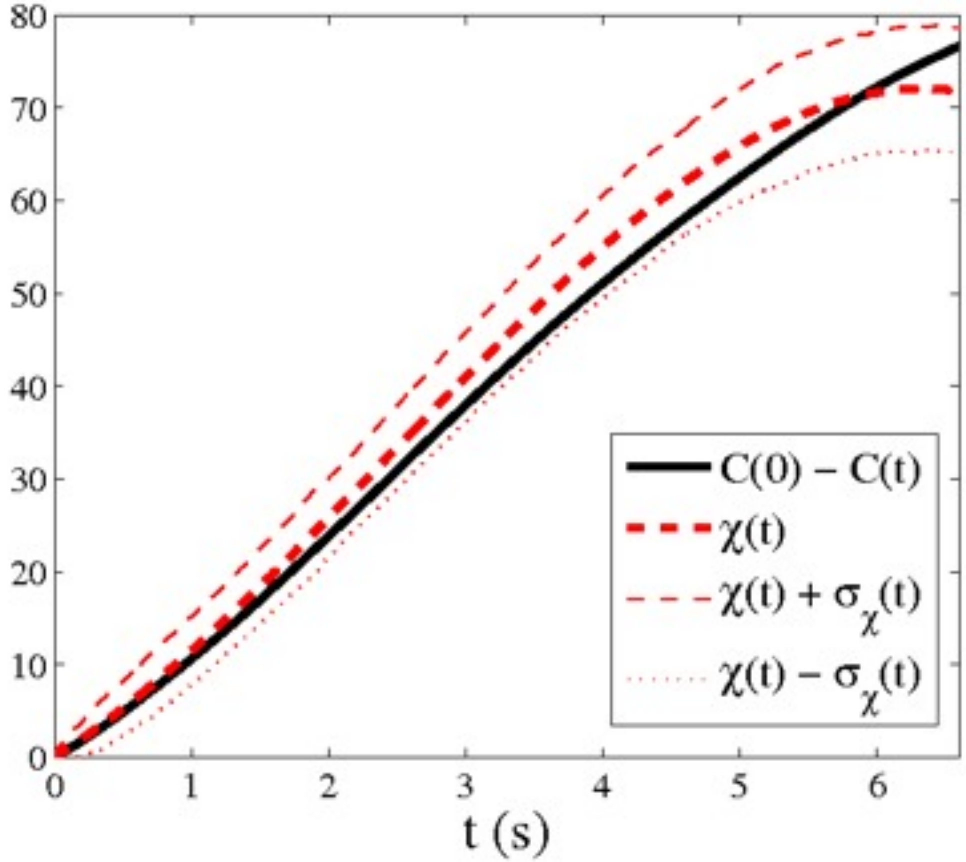
$$\frac{\left\langle \frac{\partial \phi(\theta(t))}{\partial A} \right\rangle - \left\langle \frac{\partial \phi(\theta(t+t^*))}{\partial A} \right\rangle_{ss}}{\delta A} = \chi(t)$$

under the contion $\left\langle \frac{\partial \phi(\theta(0))}{\partial A} \right\rangle = \left\langle \frac{\partial \phi(\theta(t^*))}{\partial A} \right\rangle_{ss}$

Generalized FDT

$$C(t) = \left\langle \frac{\partial \phi(\theta(t))}{\partial A} \quad \frac{\partial \phi(\theta(0))}{\partial A} \right\rangle_{ss}$$

$$\chi(t) = (C(0) - C(t))$$



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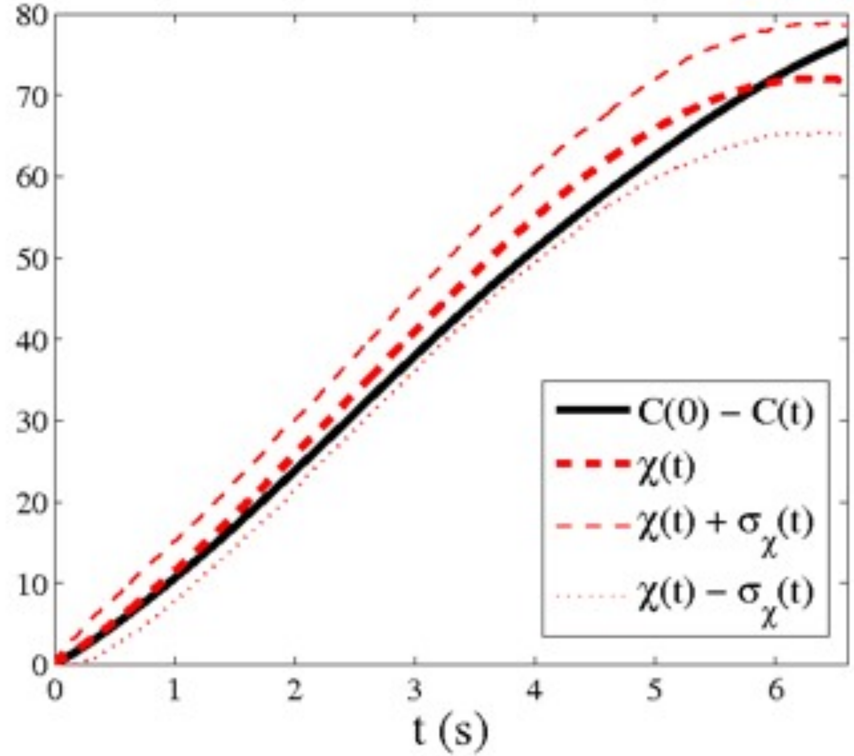

Conclusions

- GFDT as been checked on the experimental data taking into account the finite sampling.
- It is certainly the more general formulation for a Markofian dynamics

Conclusions on FDT on NESS

- We checked three formulations of FDT for NESS
- The Langrangian formulation can be applied to any process but the knowledge of the current is needed
- The frenesy formulation needs the knowledge of the generator of the dynamics, but it can in principle be applied to non-stationary cases. It is limited to Markofian systems
- The formulation based on Hatano-Sasa relation is certainly the most general of the three if the dynamics is Markofian

FR for NESS driven by a random forcing

Motivation :

We consider a Langevin dynamics driven out of equilibrium

$$m\ddot{x} + \gamma\dot{x} = -kx + \zeta_T + f_0.$$

and

$$w_\tau = \frac{1}{k_B T}\int_t^{t+\tau} \dot{x}(t')f_0(t')\,\mathrm{d}t'.$$

if f_0 is deterministic the Fluctuation Theorem holds.

$$\ln\frac{P(W_\tau = W)}{P(W_\tau = -W)} \to \frac{W}{k_B T}, \quad \tau \to \infty$$

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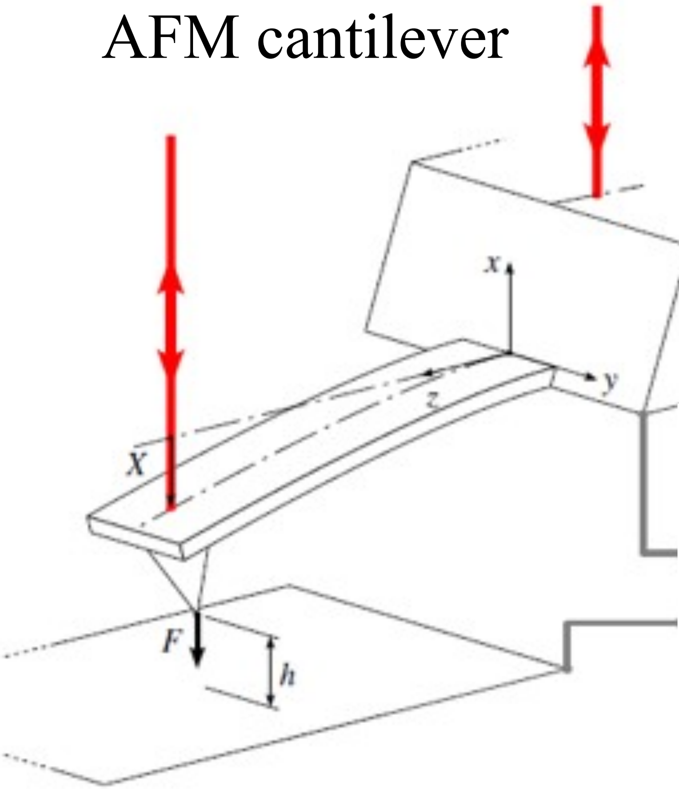
What happens if the external force is random ?

FR for NESS driven by a random forcing

AFM cantilever



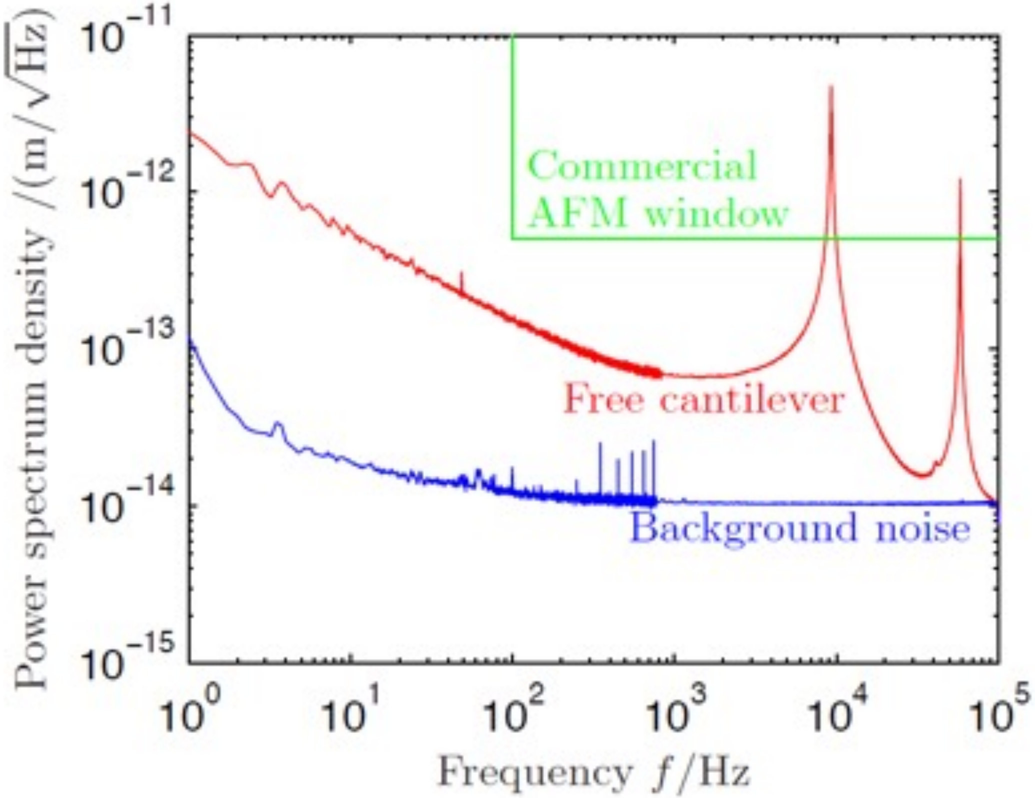
$$E_c = \frac{1}{2} C(X) V^2$$

$$F = -\partial_X E_c = -a V^2$$

a = 15 pN/V^2

The experiment

$$m\ddot{X} + \gamma \dot{X} = -kX + \zeta_T$$



FR for NESS driven by a random forcing

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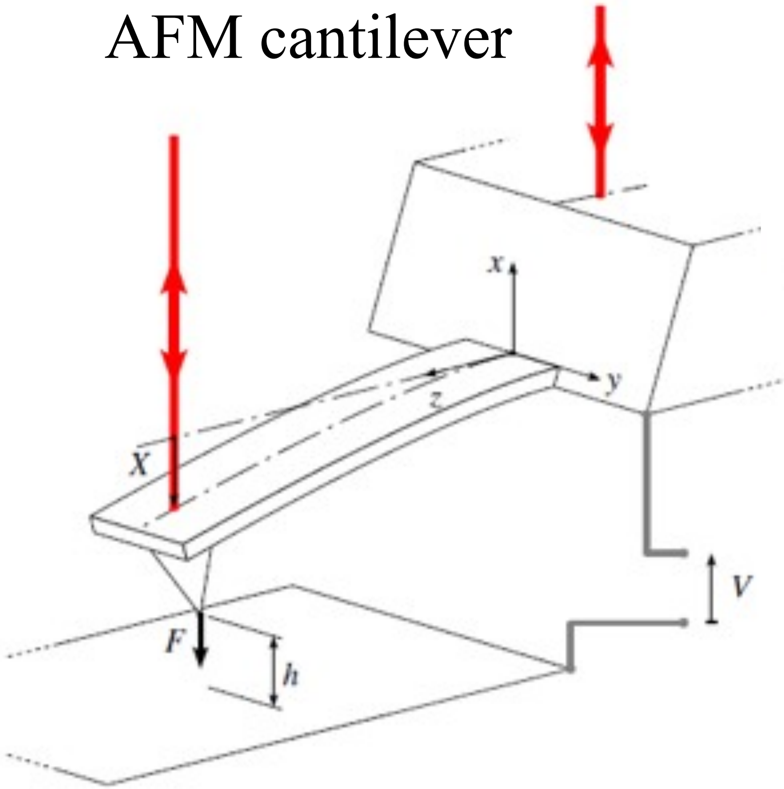


The experiment

$$m\ddot{X} + \gamma\dot{X} = -kX + \zeta_T + F$$

$$F = \overline{F} + f_0$$

$$x = X - \overline{X}$$ with $$\overline{X} = \overline{F}/k$$

$$m\ddot{x} + \gamma\dot{x} = -kx + \zeta_T + f_0.$$

$$E_c = \frac{1}{2}C(X)V^2$$

$$F = -\partial_X E_c = -aV^2$$

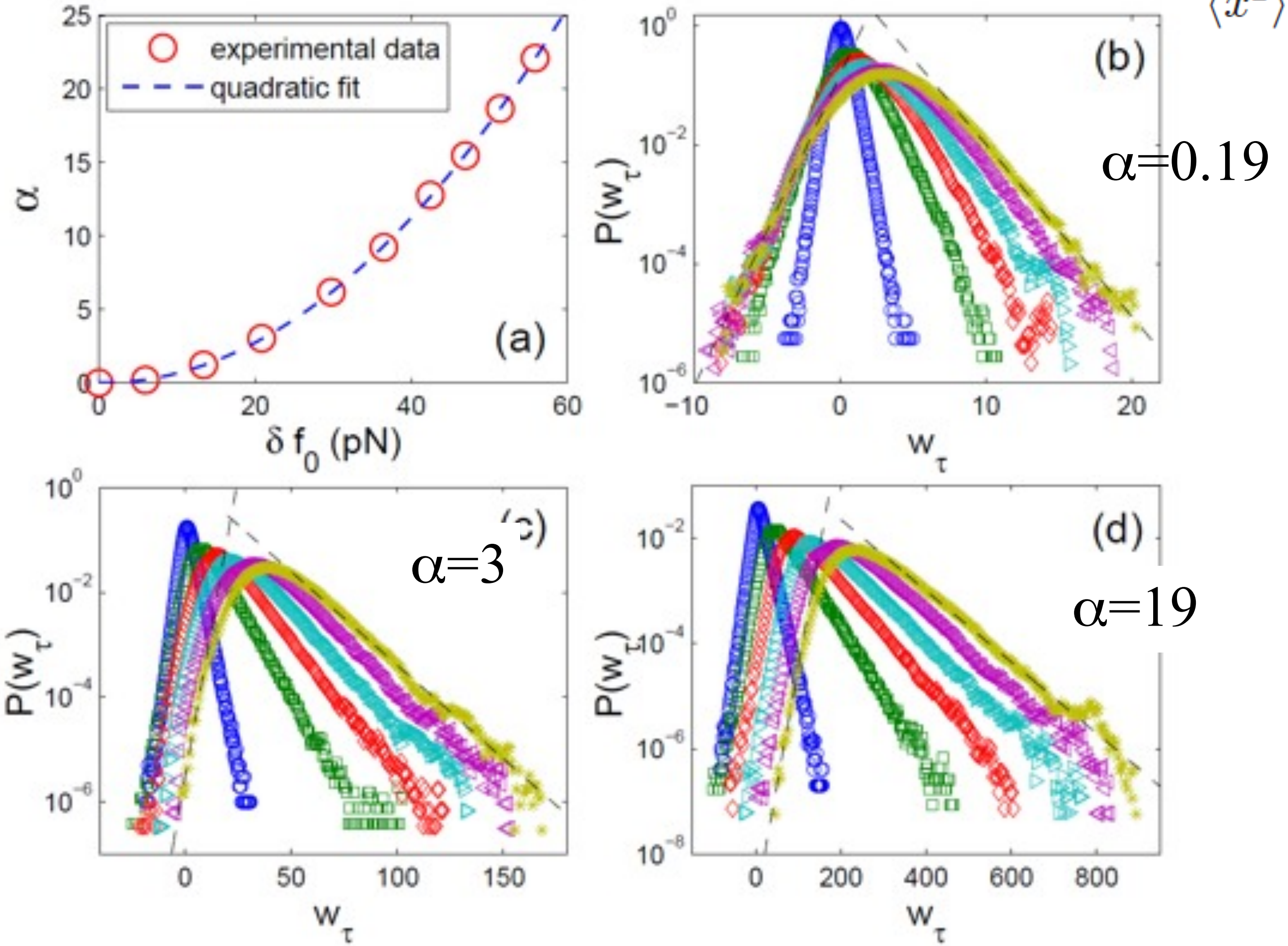
$a = 15$ pN/V^2

fo is random Gaussian force with white spectrum

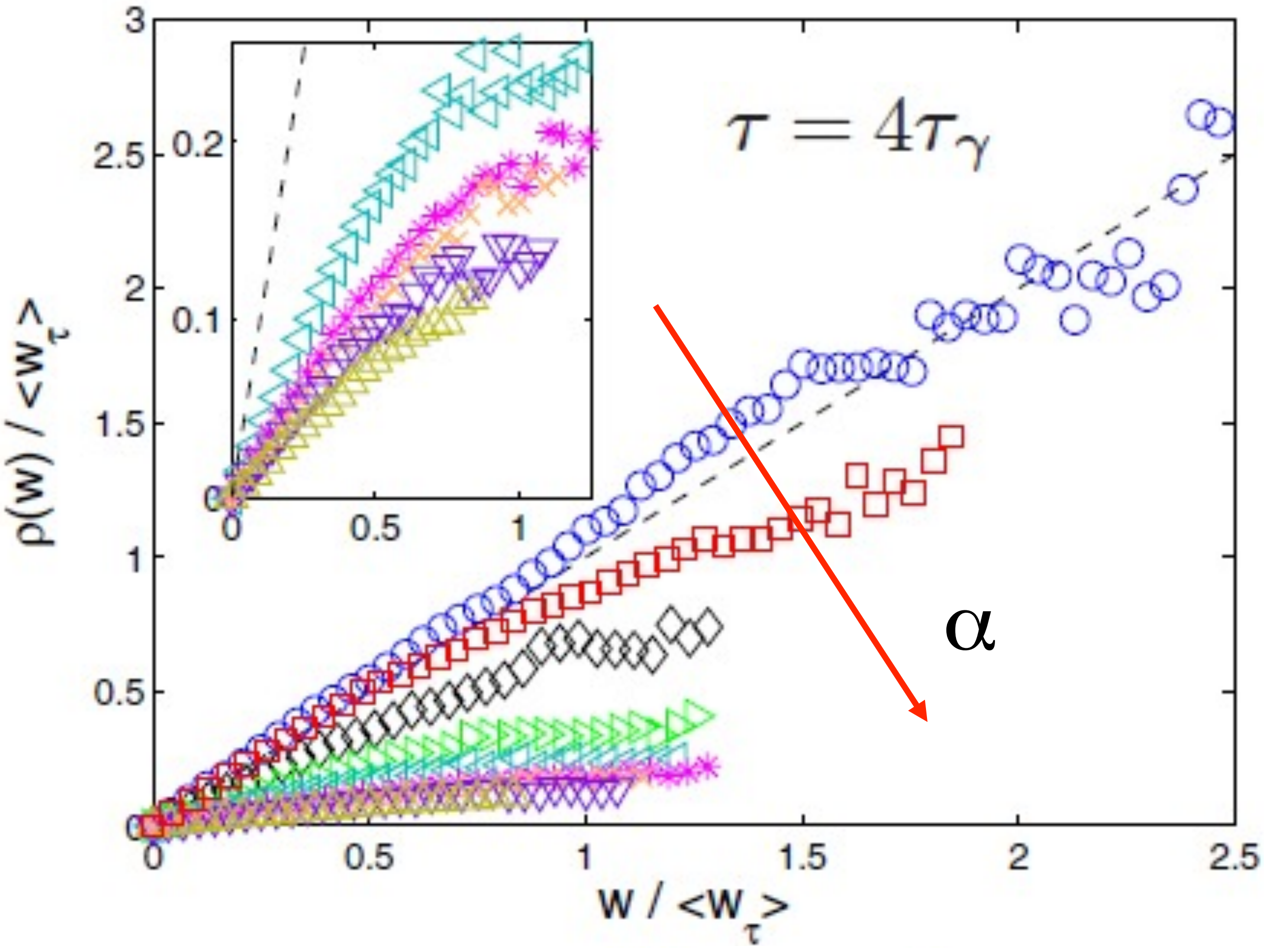
FR for NESS driven by a random forcing

The relevant control parameter is $\alpha = \frac{\langle x^2 \rangle}{\langle x^2 \rangle_{eq}} - 1,$ where

$\langle x^2 \rangle_{eq} = k_B T / k$



FR for NESS driven by a random forcing

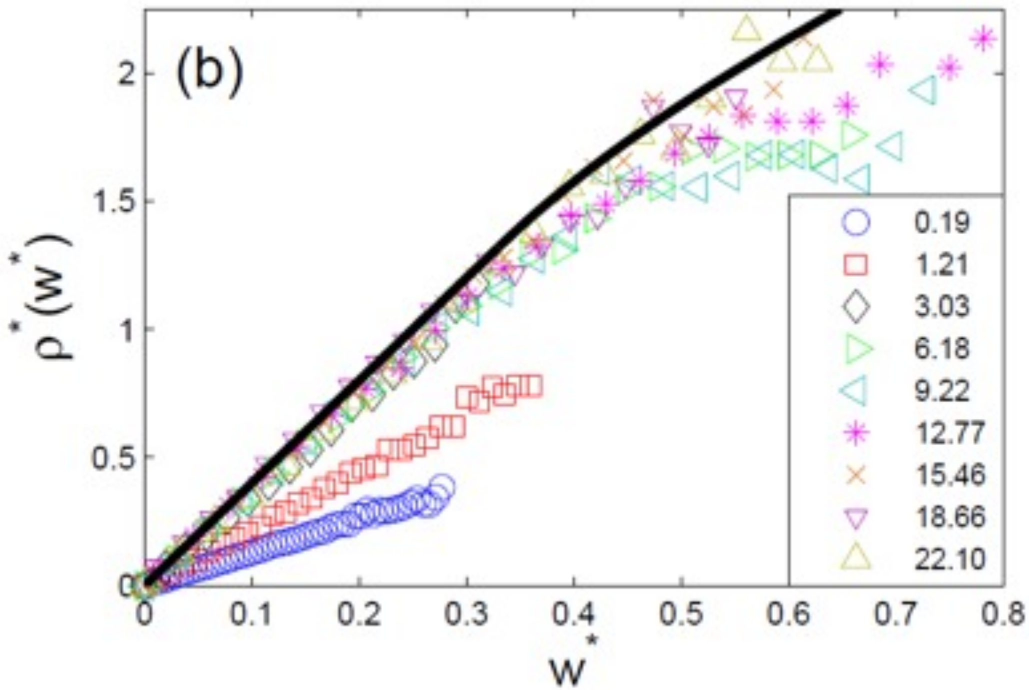


$$\rho(w) = \ln \frac{P(w_\tau = w)}{P(w_\tau = -w)}$$

FR for NESS driven by a random forcing

$$w^*_\tau = \frac{\tau_c}{\tau} \frac{w_\tau}{1+\alpha} \qquad k\langle x^2 \rangle / k_B = (1+\alpha)T \approx \alpha T$$

$$\rho^*(w^*) = \lim_{\tau/\tau_c \to \infty} \frac{\tau_c}{\tau} \ln \frac{P(w^*_\tau = w^*)}{P(w^*_\tau = -w^*)}.$$



FR for NESS driven by a random forcing

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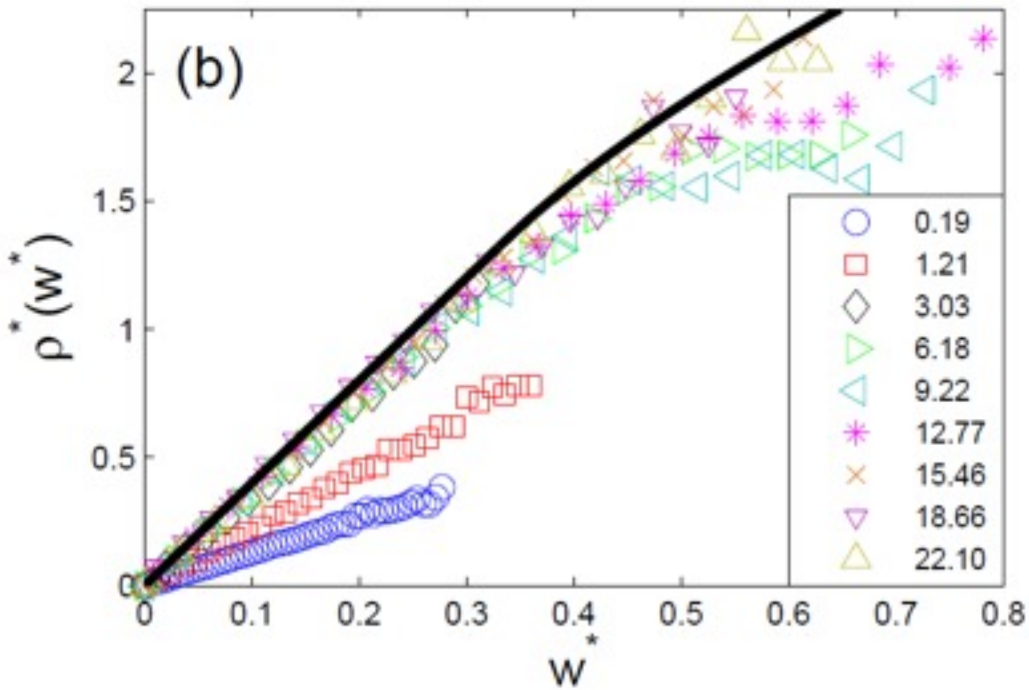
$$\rho^*(w^*) = \begin{cases} 4w^* & w^* < 1/3 \\ \frac{7}{4}w^* + \frac{3}{2} - \frac{1}{4w^*} & w^* \geq 1/3 \end{cases}$$

Farago J., Physica A, 331 (2004) 69.



FR for NESS driven by a random forcing

Conclusions

- We have studied the FT for the work fluctuations in two experimental systems in contact with a thermal bath and driven out of equilibrium by a stochastic force.

- The main result of our study is that the validity of FT is controlled by the parameter . For $\alpha < 1$ we have shown that the validity of the steady-state FT is a very robust result.

- In contrast for $\alpha > 1$, when the randomness of the system becomes dominated by the external stochastic forcing, we have shown that FT is violated.

- For $\alpha >> 1$ the data can be described by a master curve with a suitable effective temperature