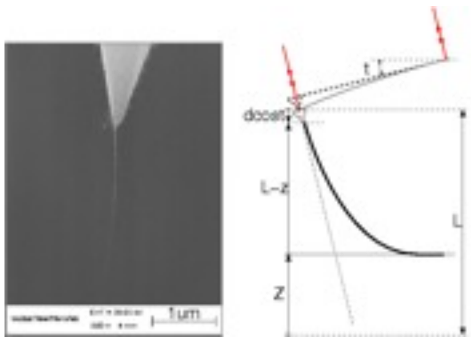
Outline

- Motivation for experiments.
- Fluctuations of injected and dissipated power in an harmonic oscillator.
- Fluctuation Theorems for work, heat and total entropy.
- Injected power in the stochastic resonance.
- Conclusions

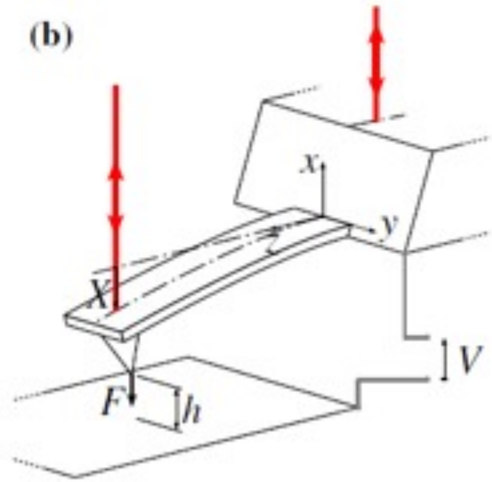
http://perso.ens-lyon.fr/sergio.ciliberto/Teaching/Cours_Phys_Stat/

S.Ciliberto, S. Joubaud, A. Petrosyan, JSTAT (2010) P12003 , arXiv:1009.3362

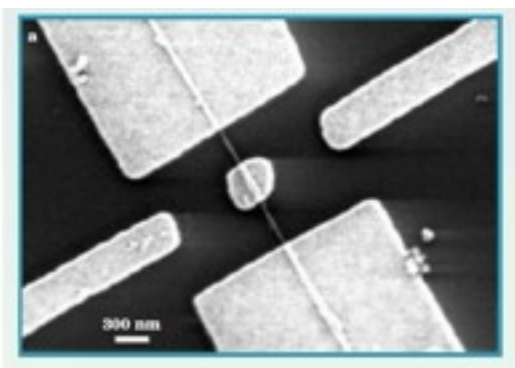
Fluctuations of injected and dissipated power in a harmonic oscillator.



Mechanical properties of nanotubes



Dynamics of AFM tips

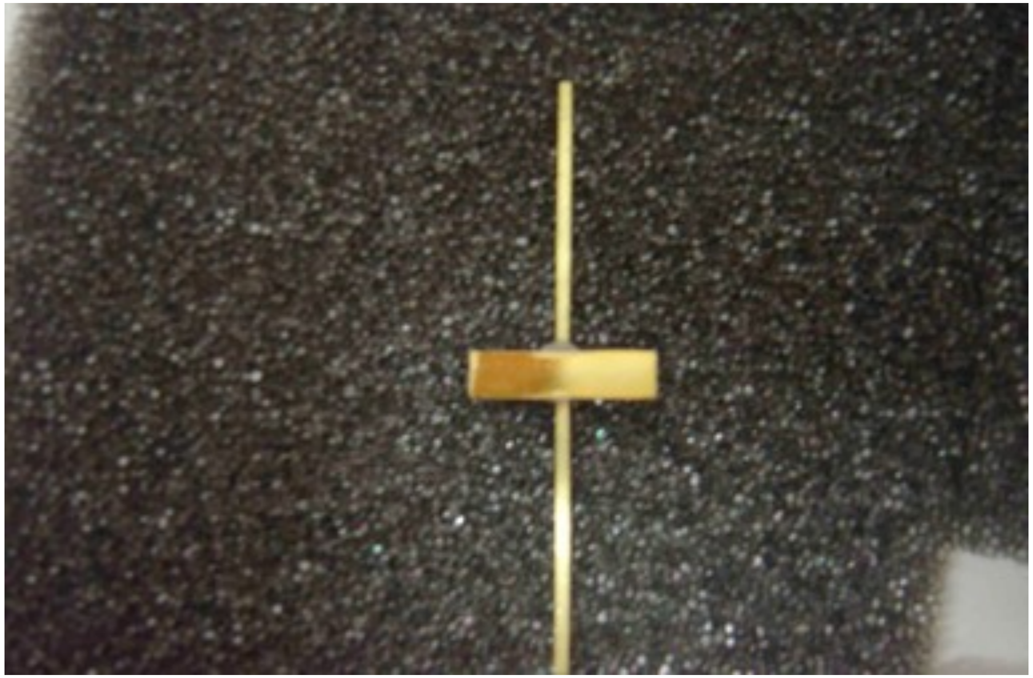


Micro Electro Mechanical Devices

Thermal rheometer

The system of interest

Torsion pendulum



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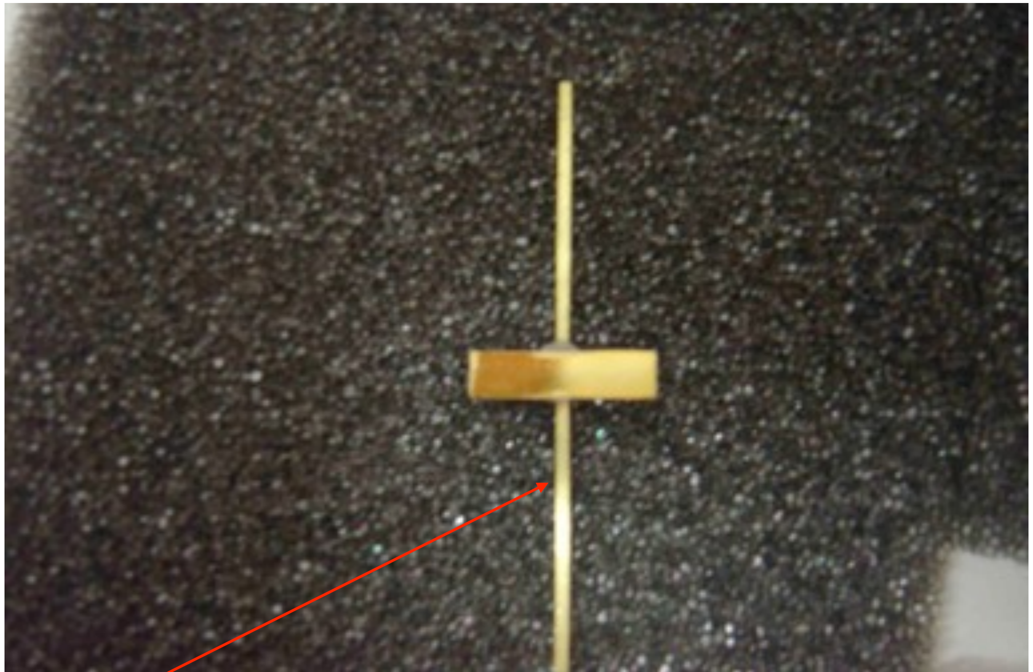
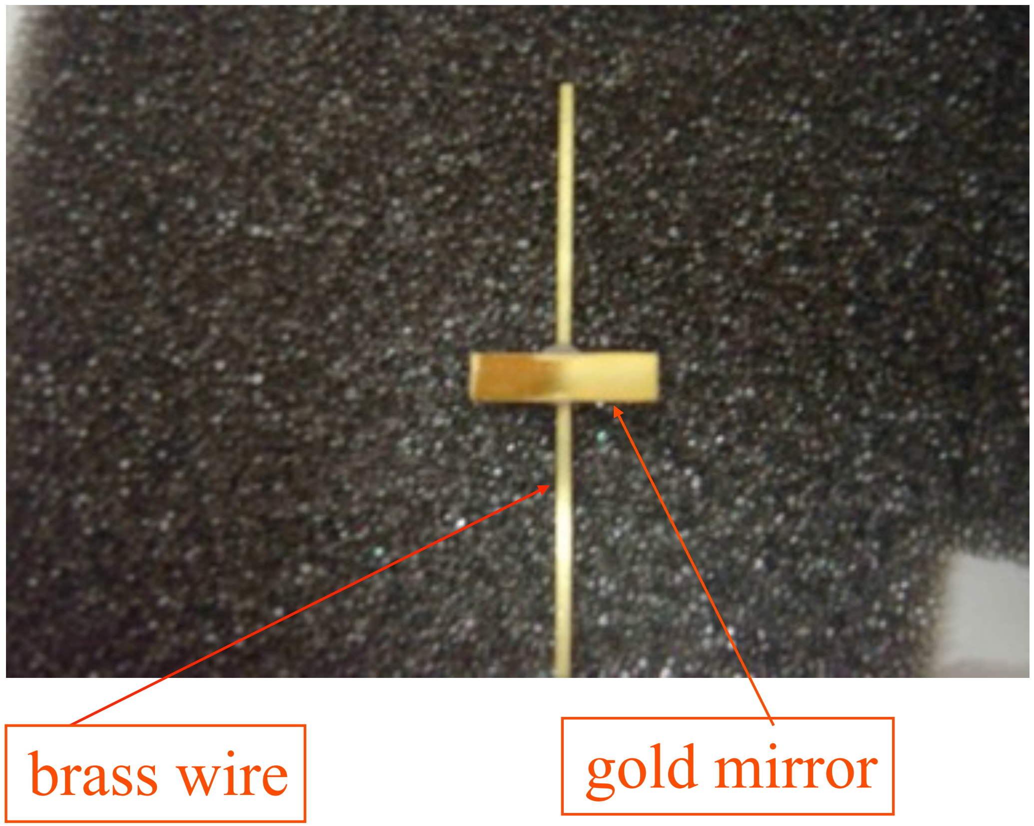


brass wire

The system of interest

Torsion pendulum



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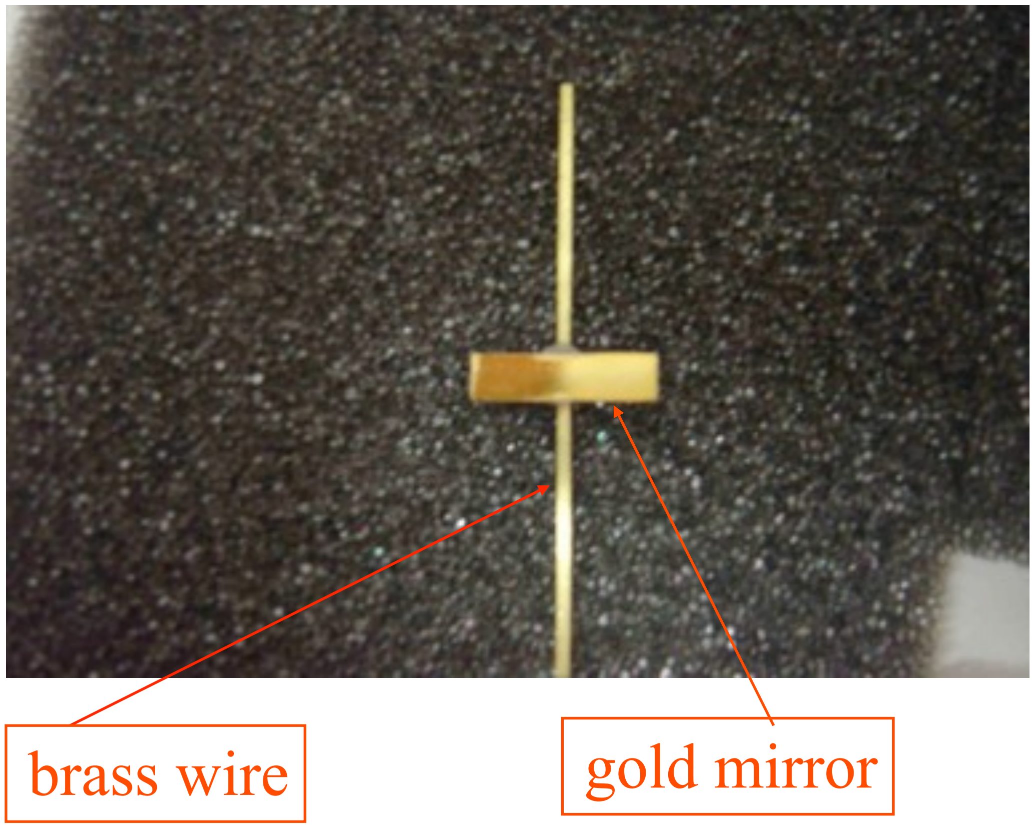
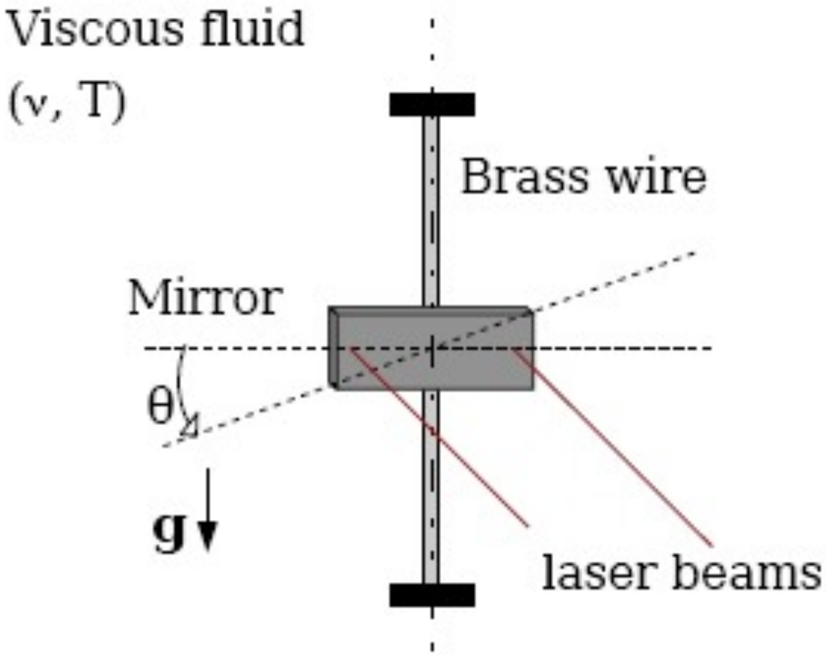
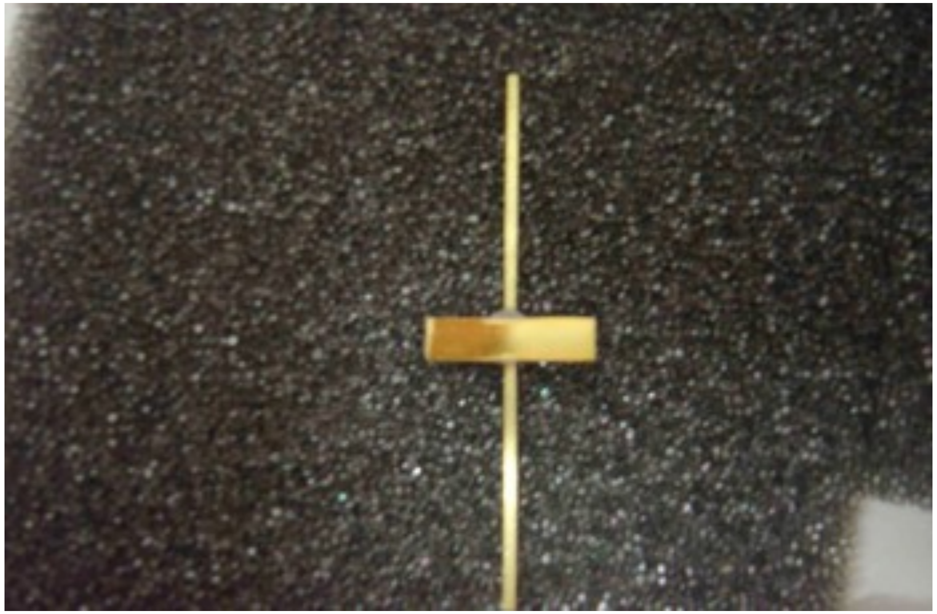
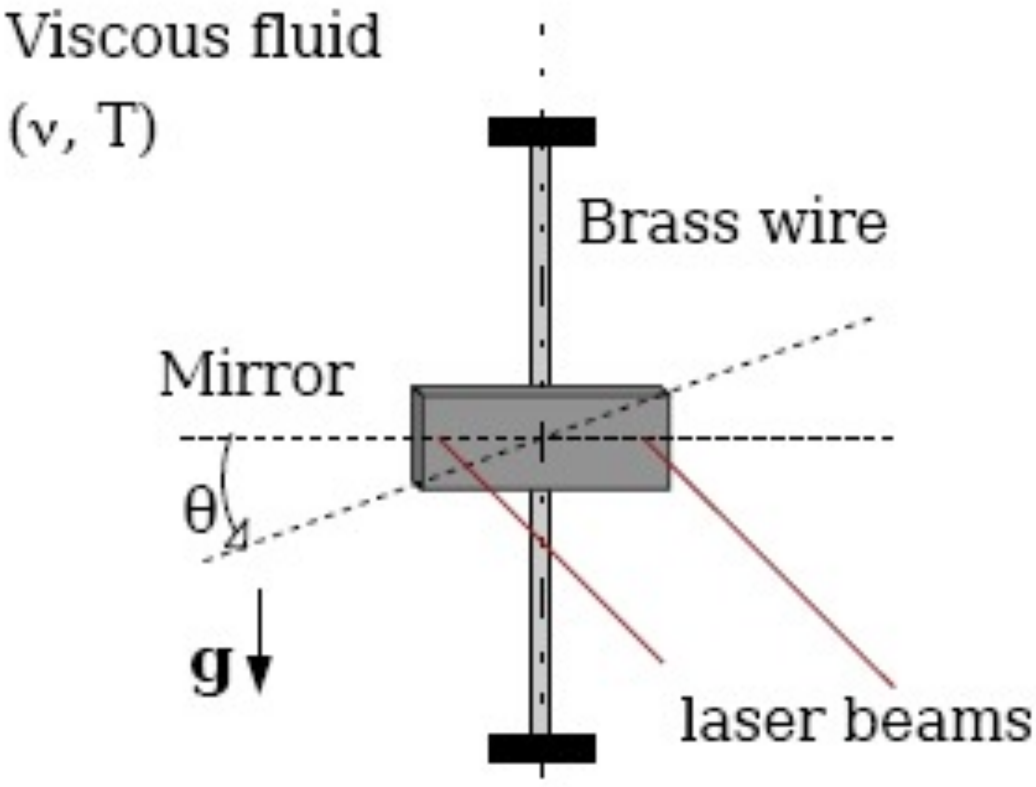






- mirror $2mm \times 8mm \times 1mm$
- whire dimensions : $10mm \times 0.5mm \times 50\mu m$
- stiffness $C = 4.7\ 10^{-4}$ Nm/rad

The torsion pendulum

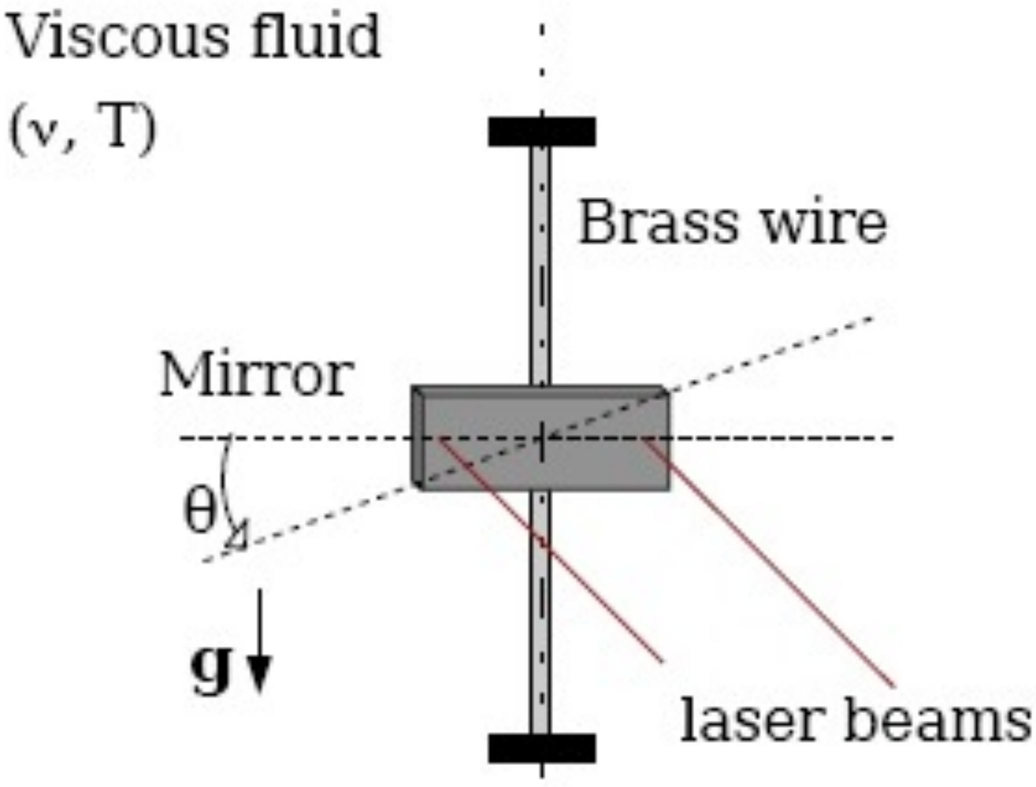


Elastic torque
$M_e = C\ \theta$

Variance
$< \theta^2 >= \frac{k_B T}{C}$

- stiffness $C = 4.7\ 10^{-4}$ Nm/rad
- typical displacement : $\sqrt{< \theta^2 >} = \sqrt{\frac{K_B\ T}{C}} \simeq 3$nrad
- A differential interferometer is used to measure θ
- Measurement noise $\simeq 25$ prad. Signal to noise ratio $\simeq 100$.

The torsion pendulum



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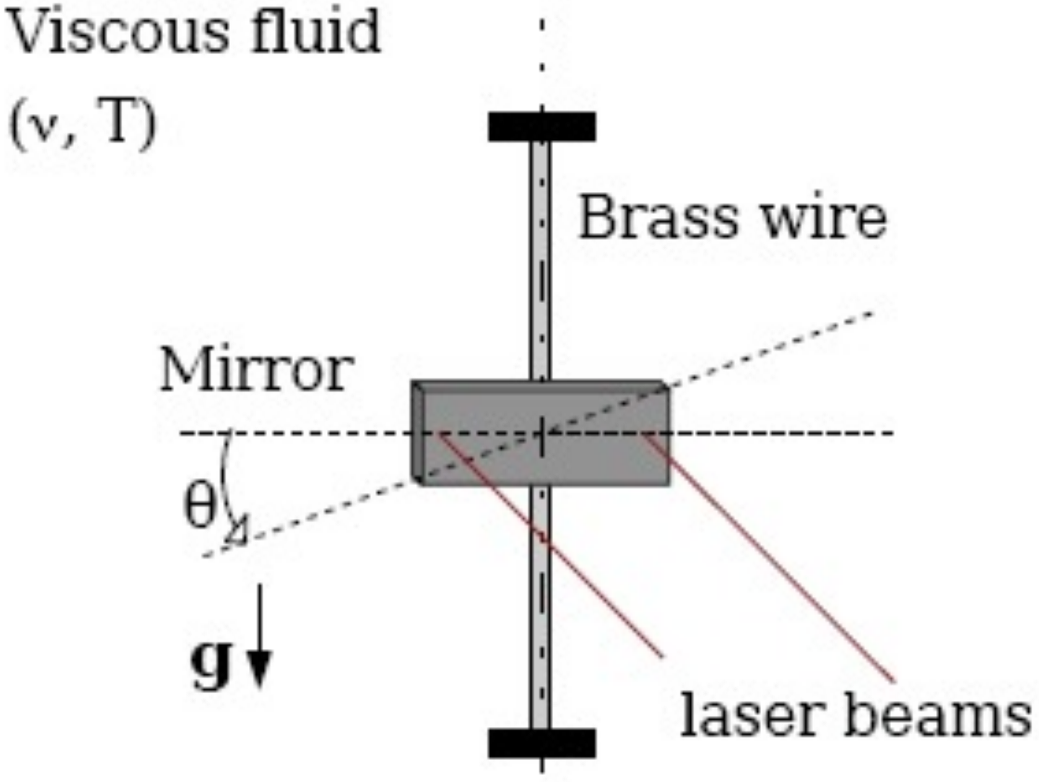

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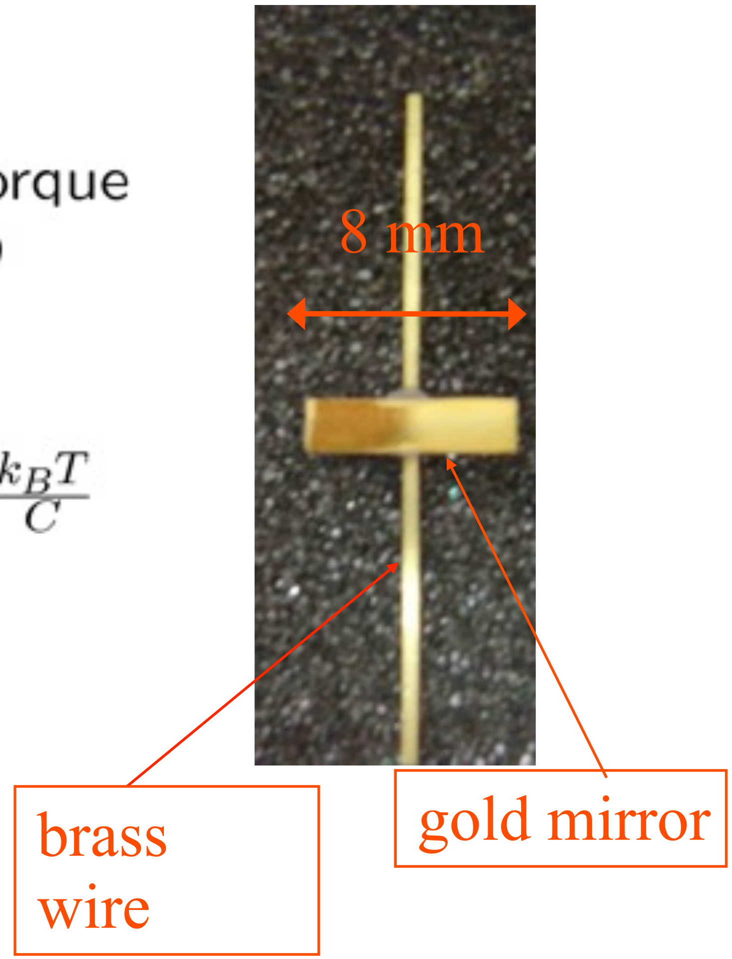

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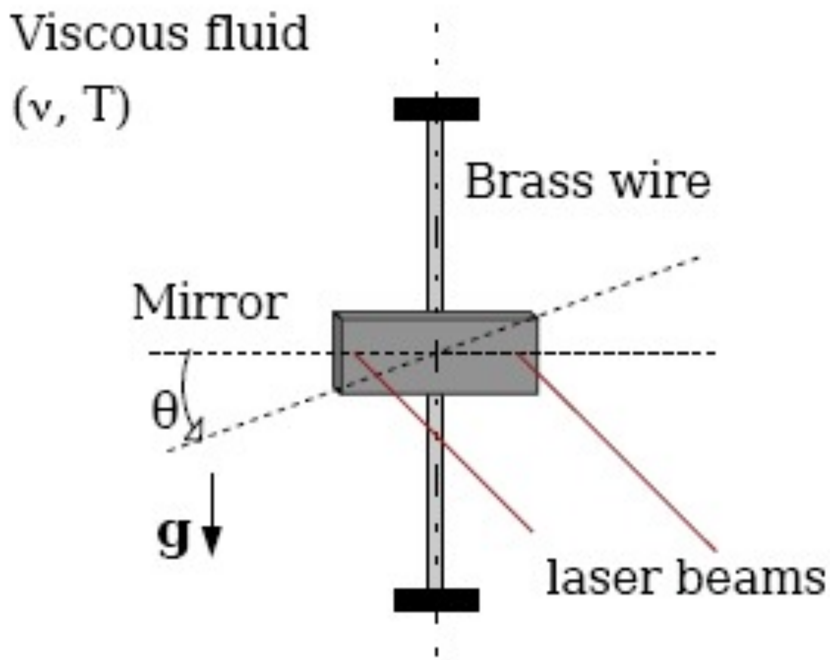
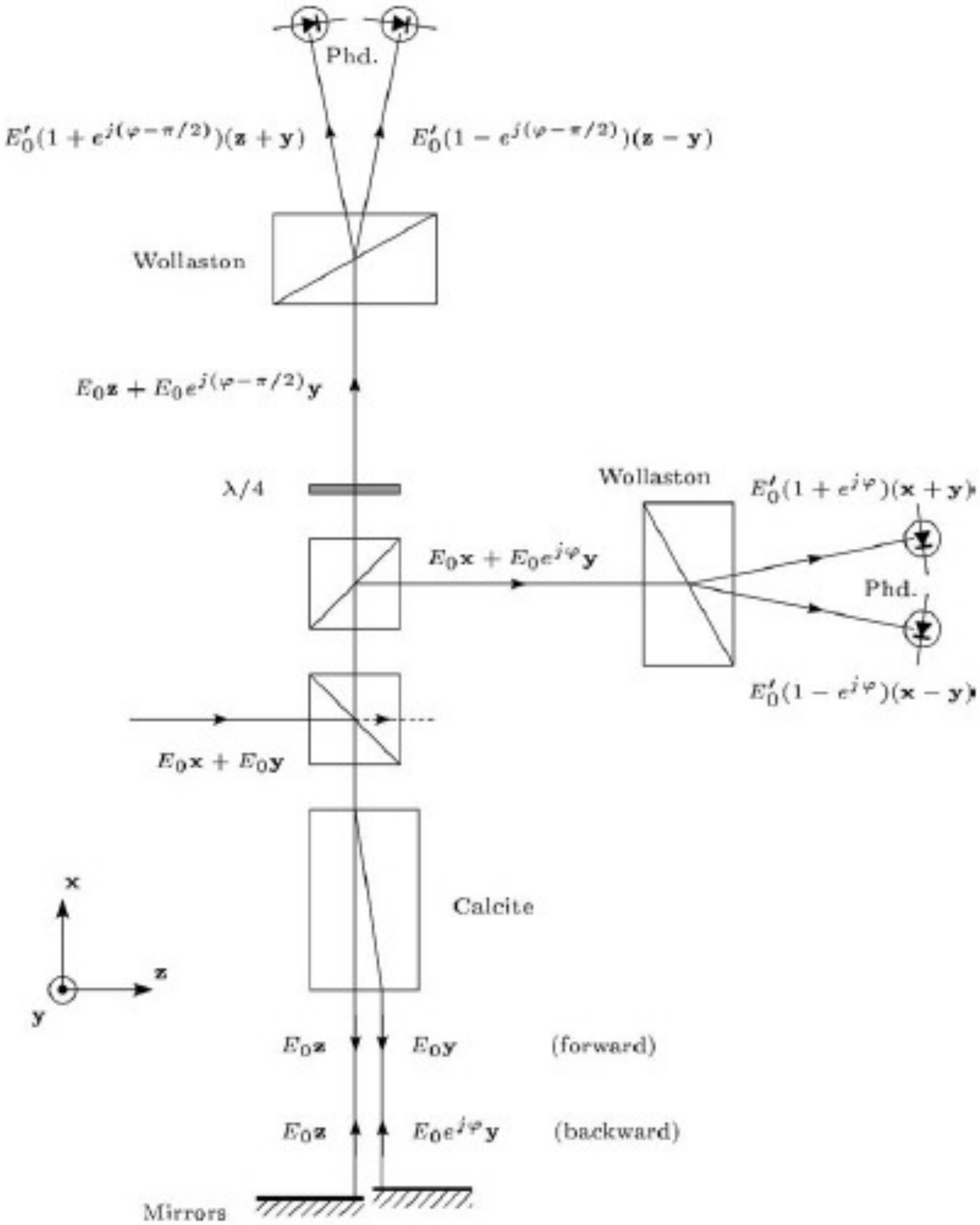
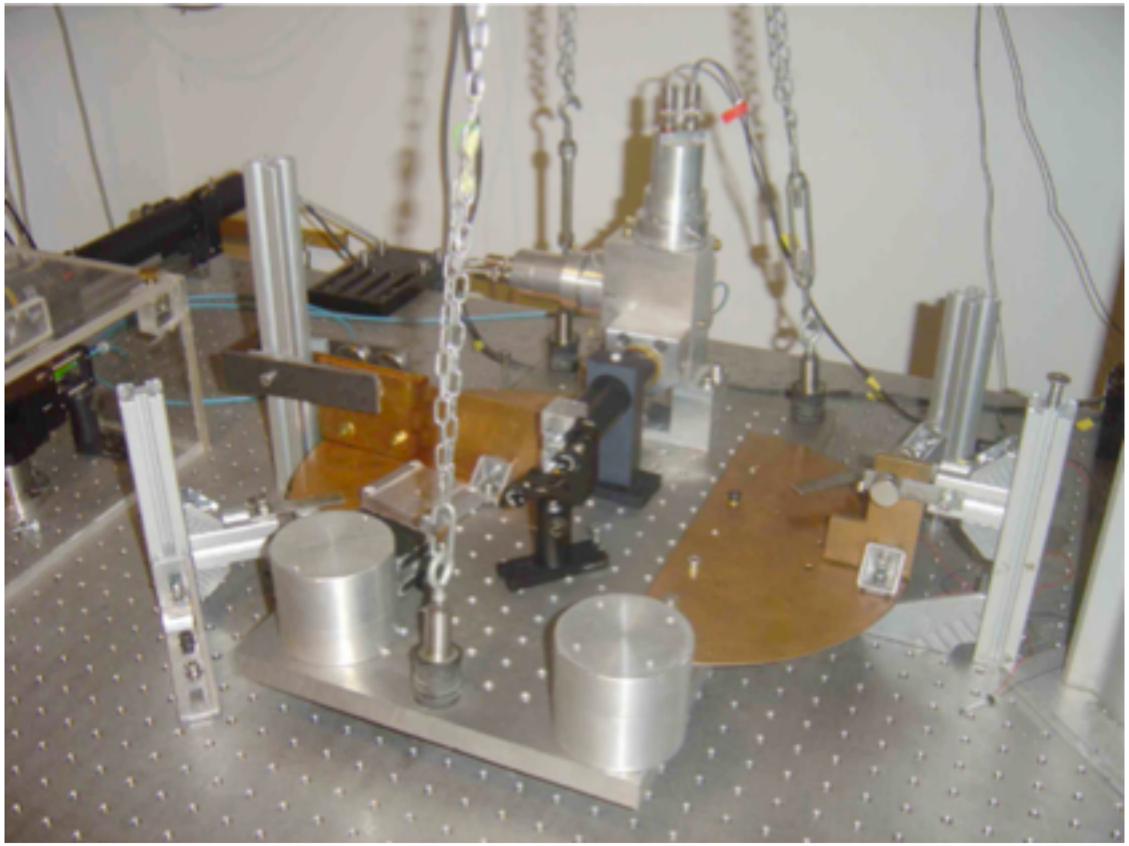


- typical displacement : $rms = \sqrt{<\theta^2>} = \sqrt{\frac{K_B\ T}{C}} \simeq 3nrad$ (i.e. 24 10^{-12} m)
- angular measurement is done using a differential interferometer
- measurement noise $\sqrt{6}.25\ 10^{-12}\text{rad}/\sqrt{Hz}$

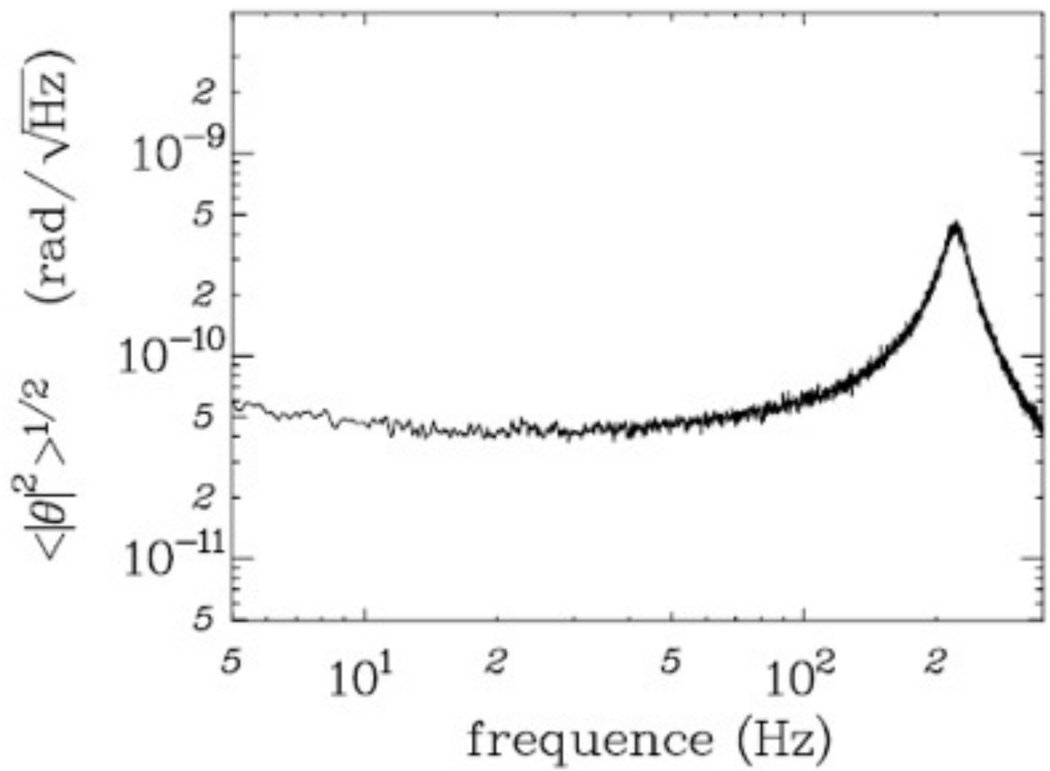
Polarisation interferometer



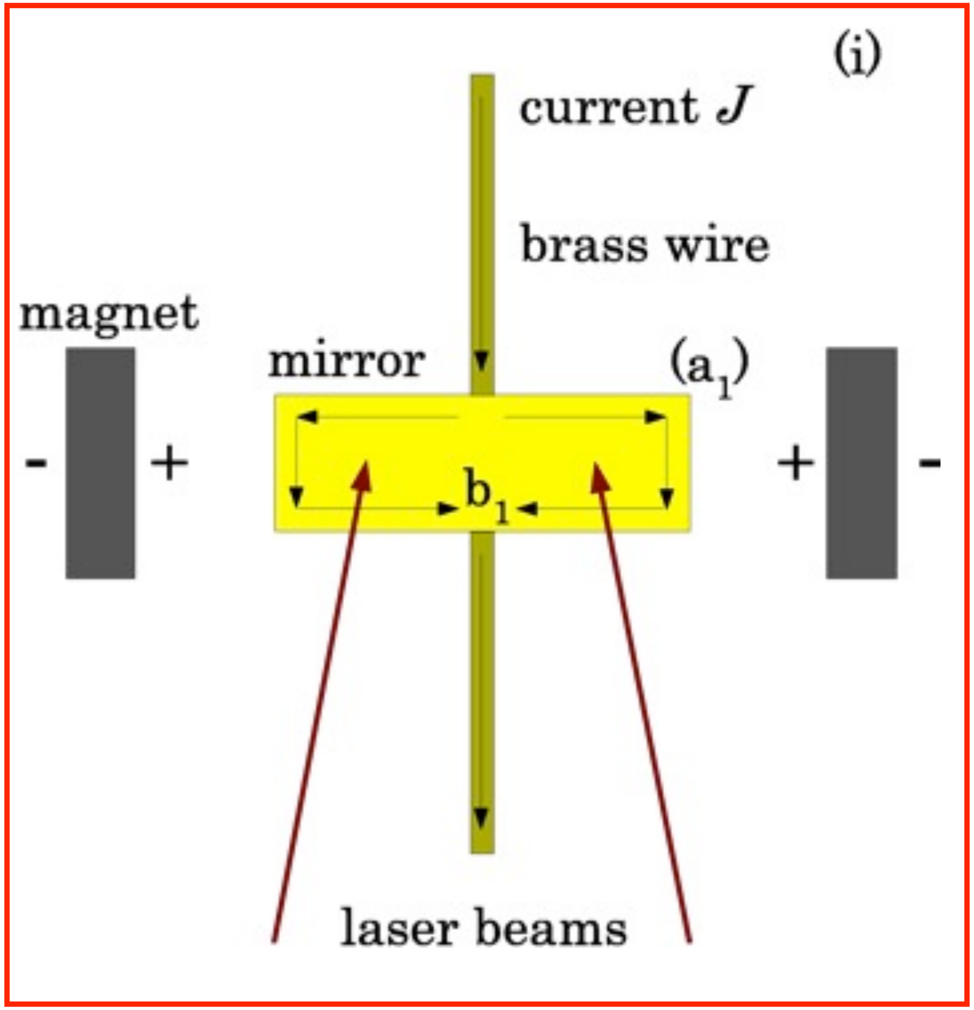
Experimental set up and the interferometer



Typical fluctuation spectrum



External Forcing



The applied torque $M \propto J$

Typical applied torque < 50pN m

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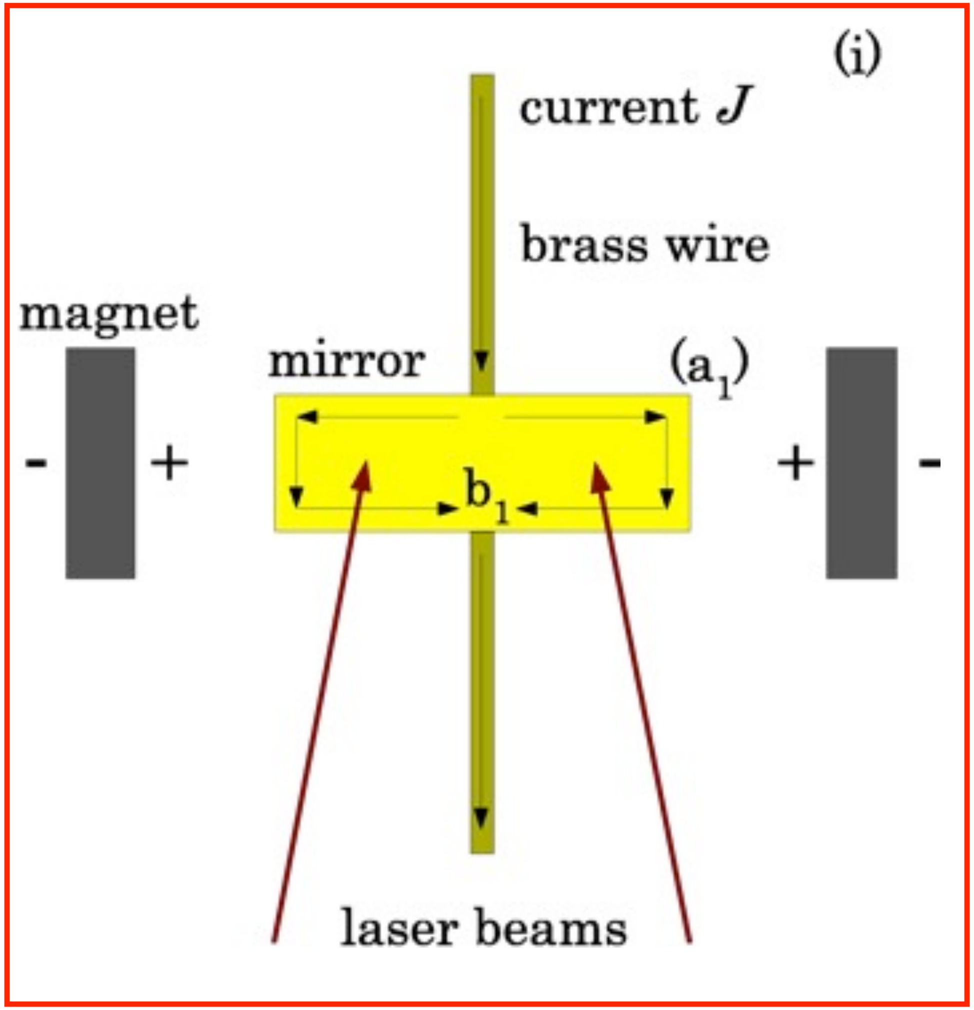
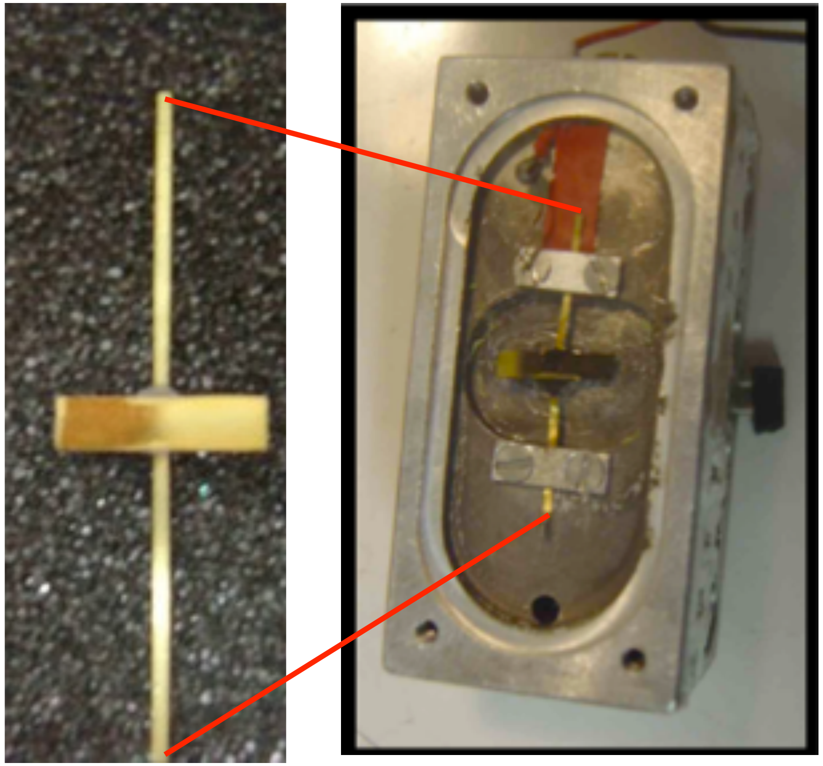




The applied torque $M \propto J$

Typical applied torque < 50pN m

Equation of motion

$$I_{\text{eff}}\,\ddot{\theta} + \int_{-\infty}^{t} G(t-t')\,\dot{\theta}(t')\;dt' + C\theta = M + \eta,$$

In Fourier space

$$[-I_{\text{eff}}\,\omega^2 + \widehat{C}]\,\widehat{\theta} = \widehat{M},$$

where $\widehat{C} = C + i[C_1'' + \omega\nu]$ is the complex frequency-dependent elastic stiffness of the system.

The response funtion is $\widehat{\chi} = \frac{\widehat{\theta}}{\widehat{M}}$

The thermal fluctuation power spectral density is given by FDT

$$\langle|\widehat{\theta}|^2\rangle = \frac{4k_BT}{\omega}\,\mathrm{Im}\,\widehat{\chi} = \frac{4k_BT}{\omega}\,\frac{C_1'' + \omega\,\nu''}{[-I_{\text{eff}}\,\omega^2 + C]^2 + [C_1'' + \omega\,\nu]^2}.$$

Typical Fluctuation spectra

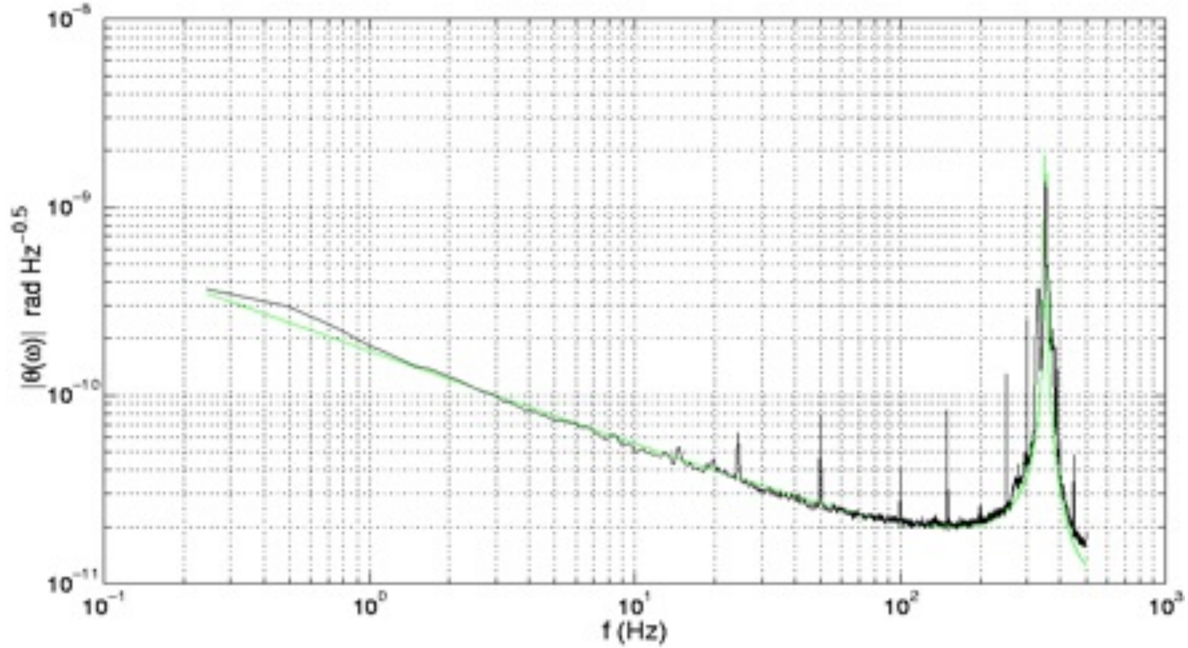
Spectrum of the torsion pendulum made by a brass wire and a mirror

resonance $f_o = 352Hz$

Moment of inertia is $I = 8.4\ 10^{-11} Kg\ m^2$

Stiffness $C' = 4.13\ 10^{-4} N\ mrad^{-1}$

$\frac{C''}{C'} \simeq 5\ 10^{-3}$

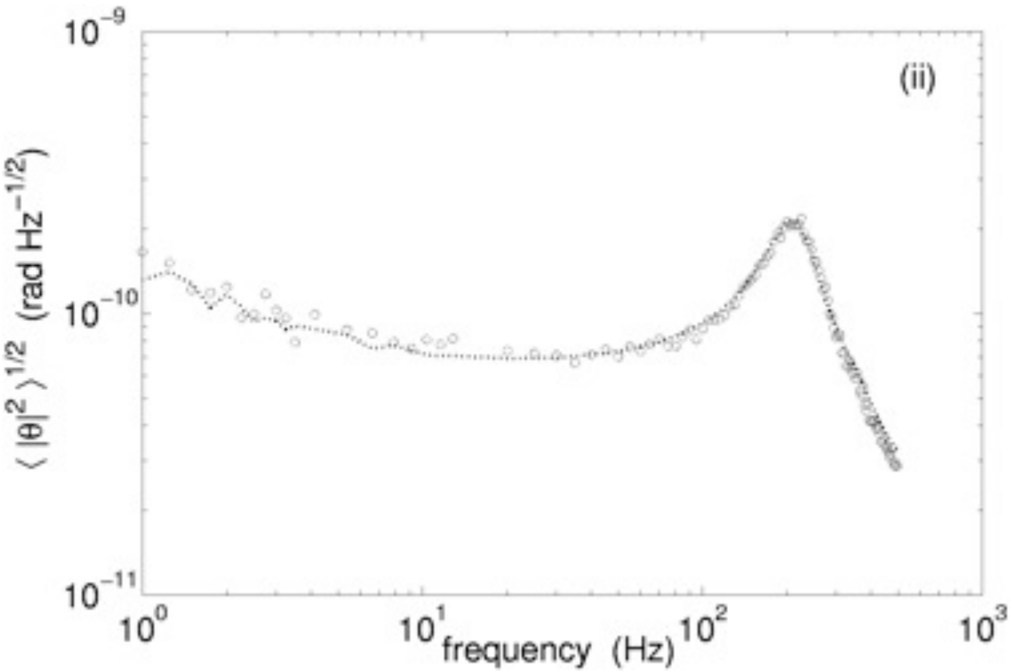


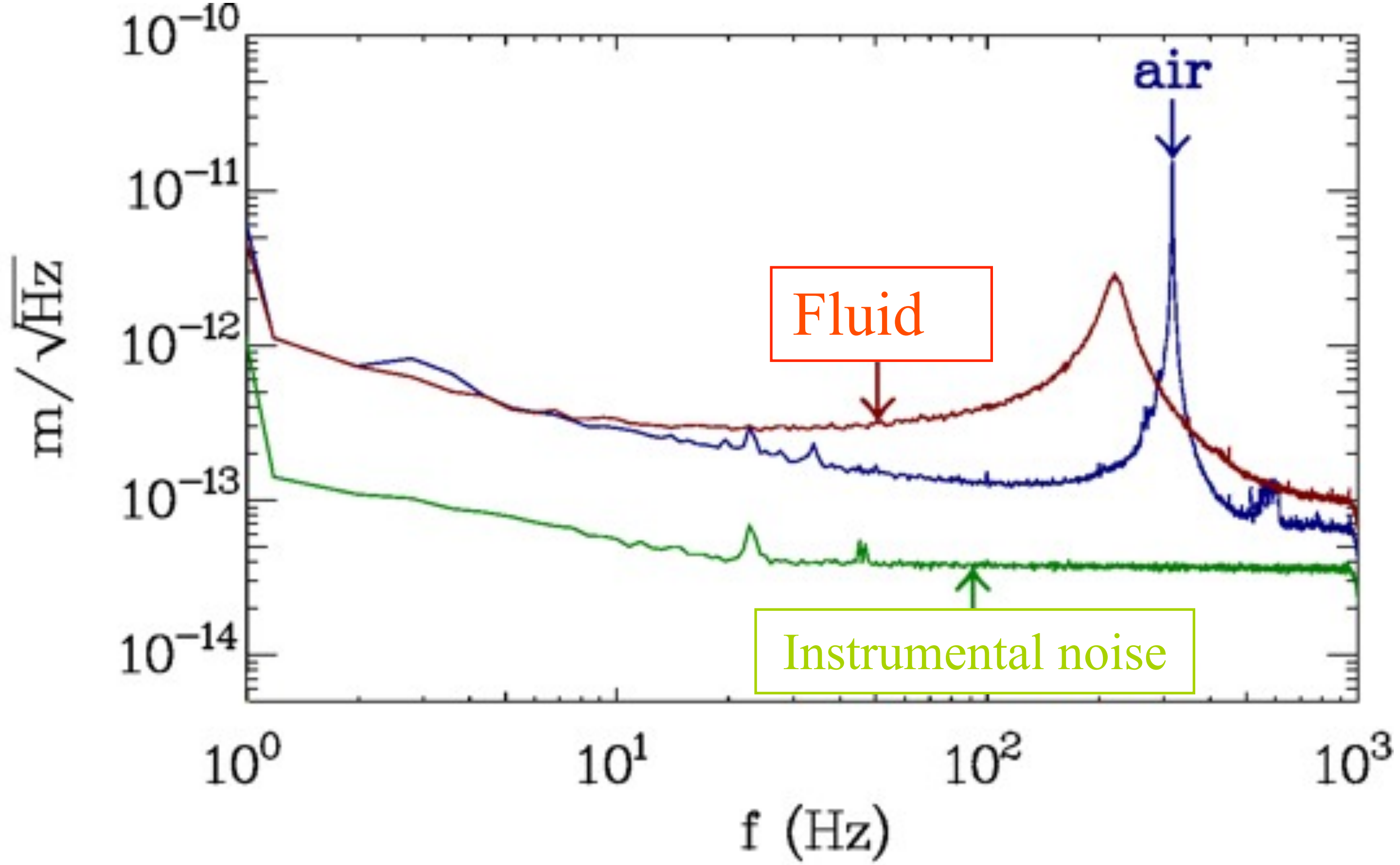
Spectrum of the torsion pendulum inside a viscous oil

$$f_o = \sqrt{C/I_{\text{eff}}}/(2\pi) = 217\text{Hz}$$

relaxation time

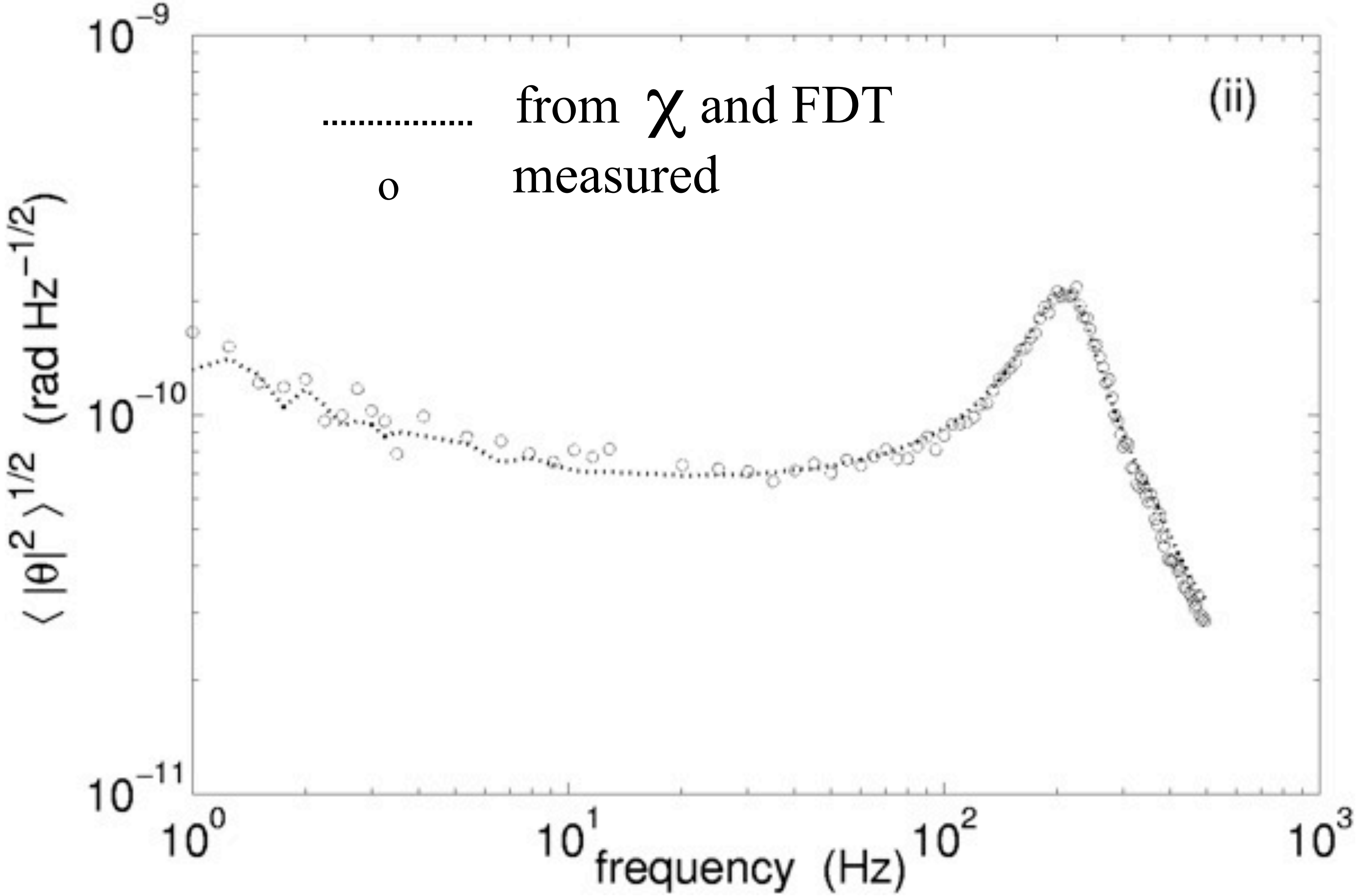
$\tau_\alpha^{-1} = 2 I_{\text{eff}}/\nu = 9.5\text{ms}.$





air
Fluid
Instrumental noise
m/√Hz
f (Hz)
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{0}
10^{1}
10^{2}
10^{3}

Fluctuation Spectrum



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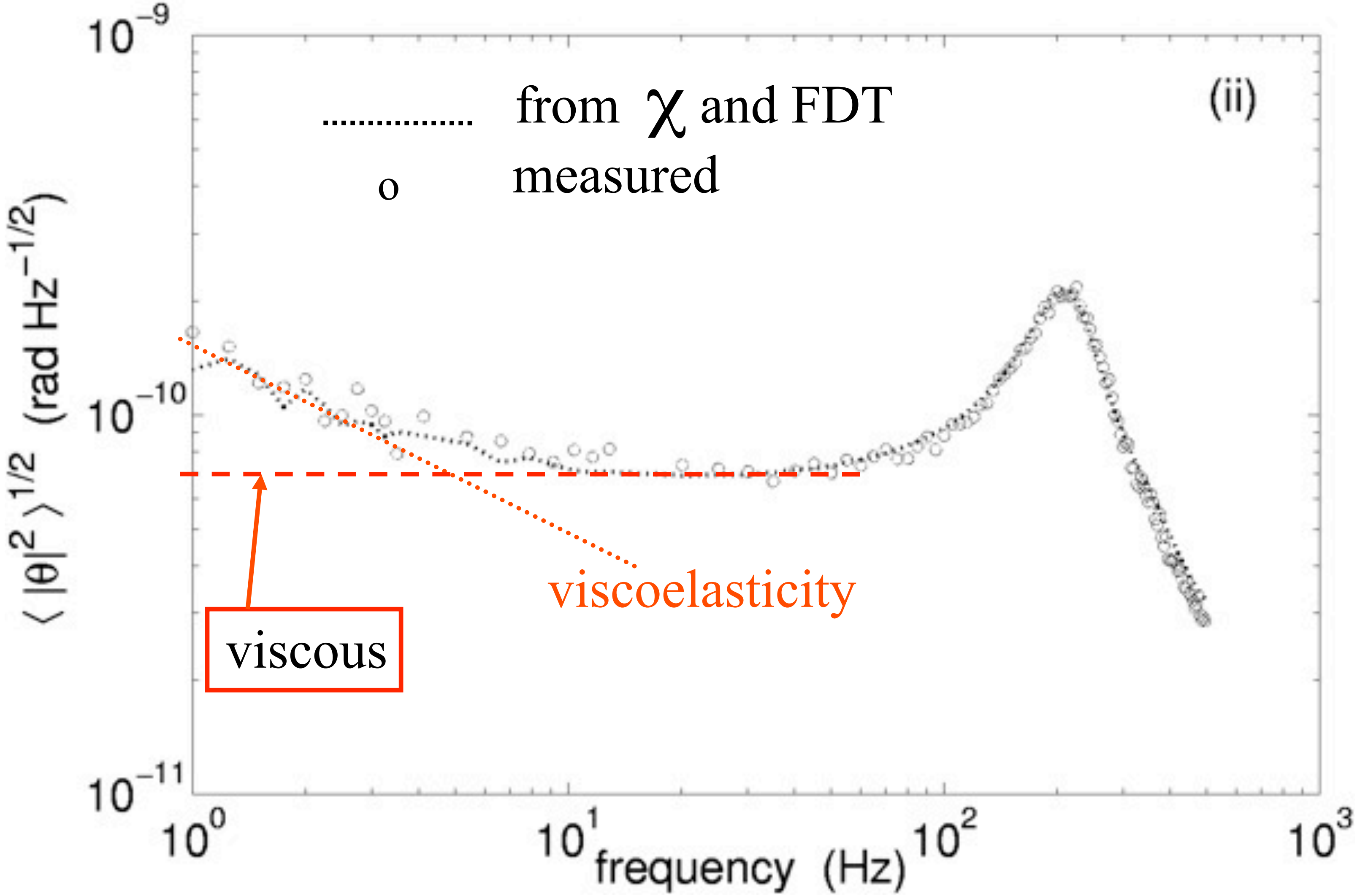
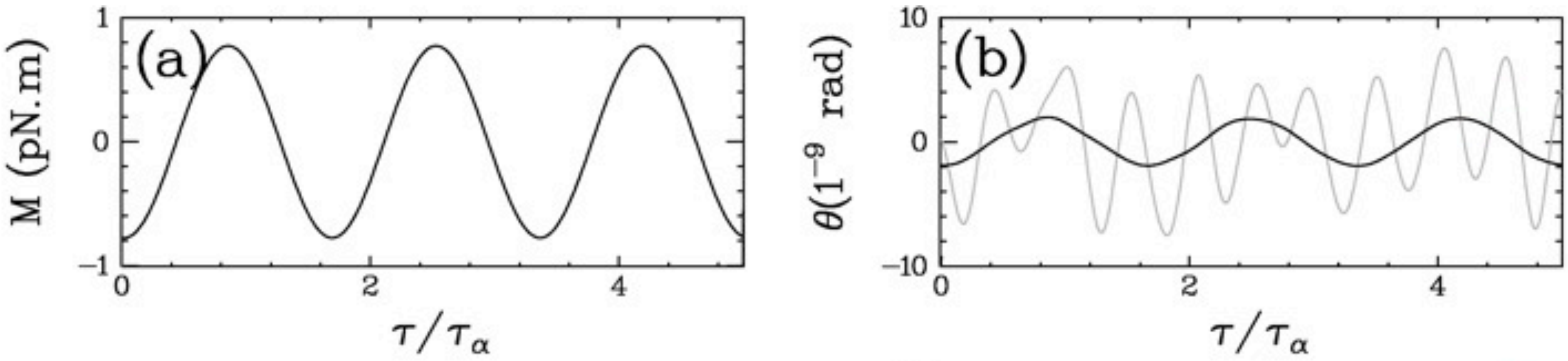
Fluctuation Spectrum



$$f_o = \sqrt{C/I_{\text{eff}}}/(2\pi) = 217\text{Hz}$$

relaxation time $\tau_\alpha = 2I_{\text{eff}}/\nu = 9.5\text{ms.}$

Work during periodic forcing



$$M(t) = M_o \sin \omega_d t$$

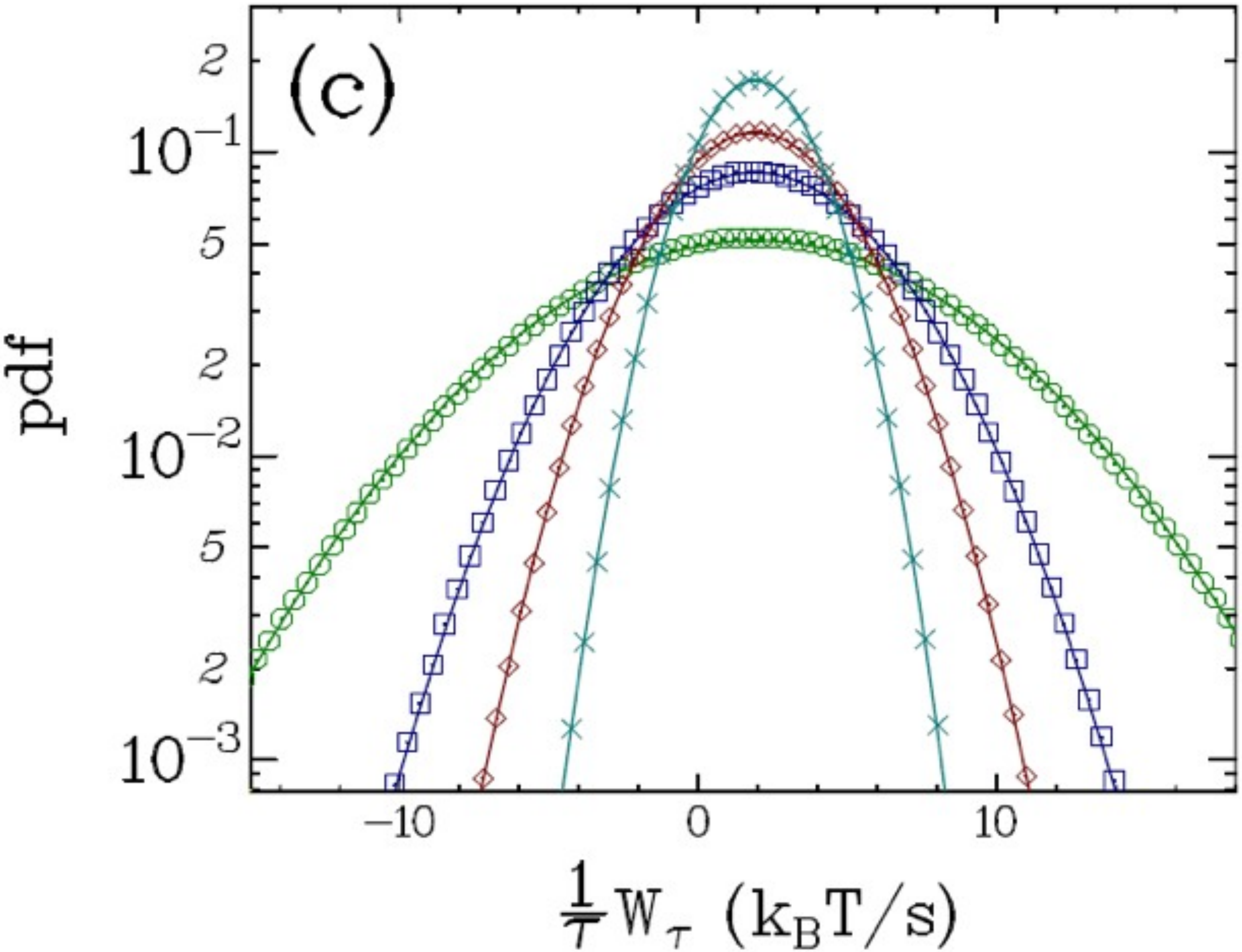
$$W_n = W_{\tau=\tau_n} = \frac{1}{k_B\ T} \int_{t_i}^{t_i+\tau_n} M(t) \frac{d\theta}{dt} dt\,,$$

with $\tau_n = n2\pi/\omega_d$

W_τ is a fluctuating quantity

PDF of the work

$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).



Energy Balance (I)

Sekimoto K, Progress of Theoretical Phys. supplement (130), 17 (1998).

$$I_{\rm eff}\,\frac{{\rm d}^2\theta}{{\rm d}t^2}+\nu\,\frac{{\rm d}\theta}{{\rm d}t}+C\,\theta=M+\sqrt{2k_BT\nu}\,\eta,$$

- We multiply this equation by $\dot{\theta}$ and we get : $\frac{dU(t)}{dt} = P_{inj}(t) - P_{dis}(t)$
- The injected power : $P_{inj}(t) = \frac{1}{k_BT} M(t)\frac{{\rm d}\theta(t)}{{\rm d}t}$
- The dissipated power : $P_{diss}(t) = \frac{1}{k_B\ T}\nu\left[\frac{{\rm d}\theta(t)}{{\rm d}t}\right]^2 - \frac{\sqrt{2k_BT\nu}}{k_B\ T}\eta(t)\frac{{\rm d}\theta(t)}{{\rm d}t}.$
- The internal energy : $U(t) = \frac{1}{k_BT}\left\{\frac{1}{2}I_{\rm eff}\left[\frac{{\rm d}\theta(t)}{{\rm d}t}\right]^2+\frac{1}{2}C\theta(t)^2\right\}.$

Energy Balance (II)

Sekimoto K, Progress of Theoretical Phys. supplement (130), 17 (1998).

$$\frac{dU(t)}{dt} = P_{inj}(t) - P_{dis}(t)$$

- We integrate over a time τ starting at a time t_i. We get:

$$\Delta U_\tau = U(t_i + \tau) - U(t_i) = Q_\tau + W_\tau$$

- W_τ is the work done on the system over a time τ :

$$W_\tau = \frac{1}{k_B T} \int_{t_i}^{t_i+\tau} M(t') \frac{\mathrm{d}\theta}{\mathrm{d}t}(t') \mathrm{d}t'$$

- $Q_\tau = \Delta U_\tau - W_\tau$ is the heat given to the system.

$$Q_\tau = -\frac{1}{k_B\ T} \int_{t_i}^{t_i+\tau} \nu \left[\frac{\mathrm{d}\theta}{\mathrm{d}t}(t')\right]^2 \mathrm{d}t' + \frac{\sqrt{2 k_B T \nu}}{k_B\ T} \int_{t_i}^{t_i+\tau} \eta(t') \frac{\mathrm{d}\theta}{\mathrm{d}t}(t') \mathrm{d}t'.$$

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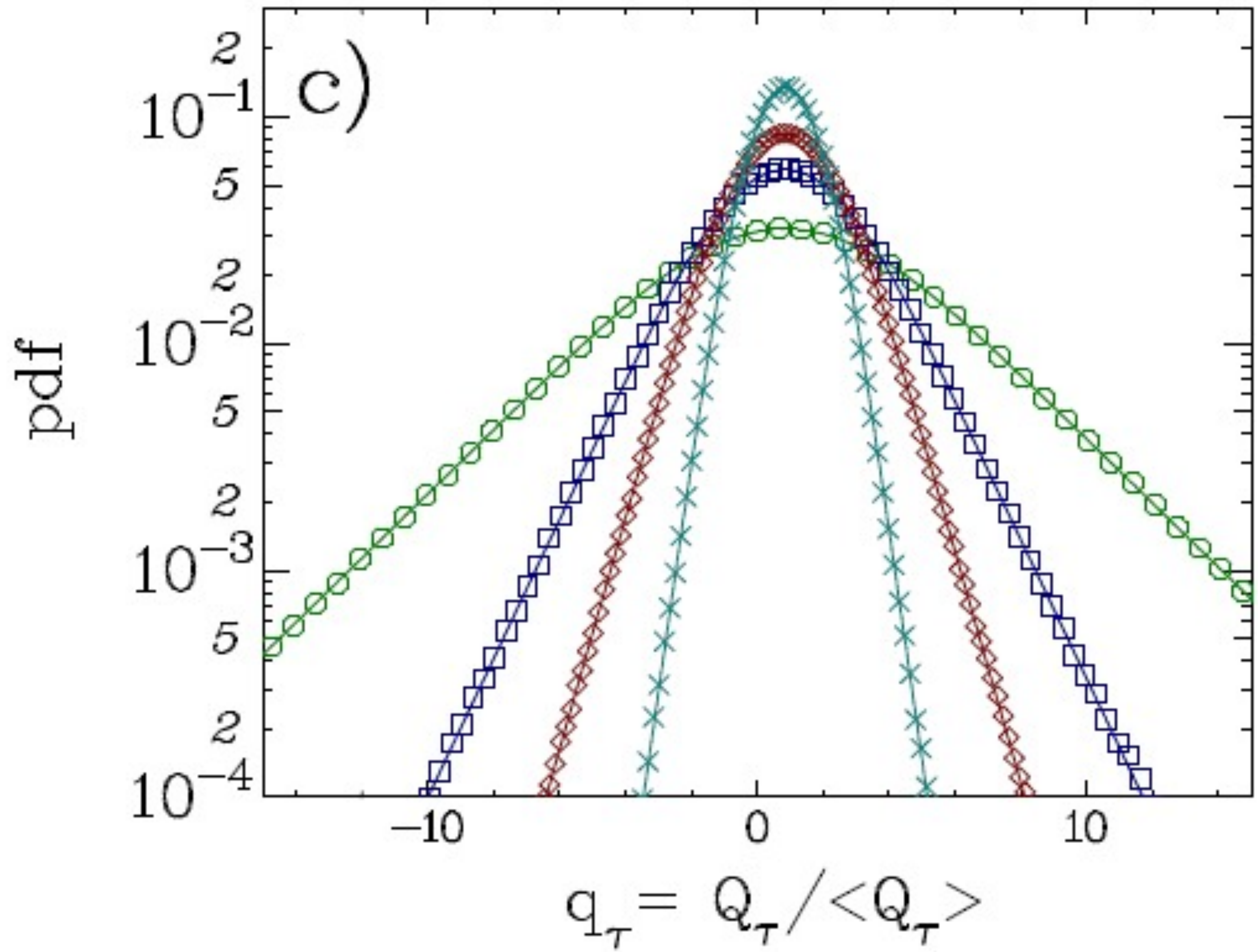
- $Q_\tau = \Delta U_\tau - W_\tau$ is the heat given to the system.

We study the fluctuations of W_τ, Q_τ and the Fluctuation Theorem for these two quantities.

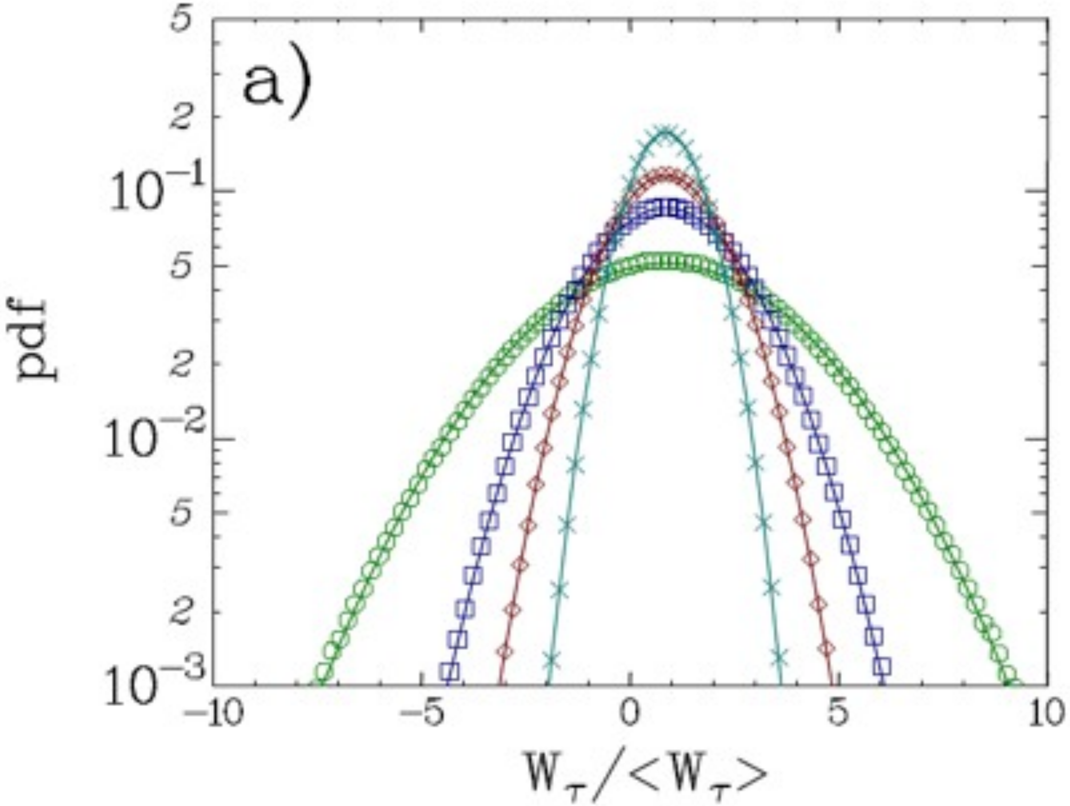
PDF of heat

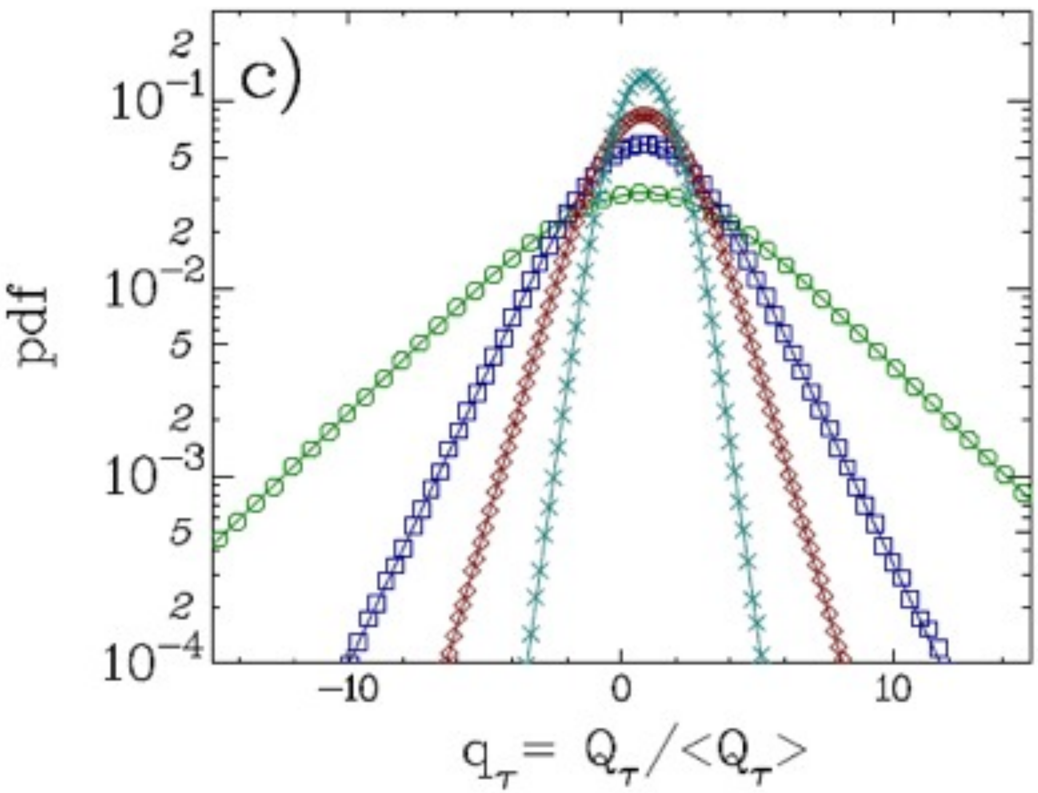
$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).



PDF of the work and of the heat

$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).





$$< W_\tau > = < Q_\tau > \simeq 0.04 \; n \; (k_B T)$$

Stationary State Fluctuation Theorem (SSFT)

(stochastic systems)

$$\log \frac{P(X_\tau)}{P(-X_\tau)} = \frac{X_\tau}{k_B T} \Sigma(\tau)$$

where $\Sigma(\tau) \to 1$ for $\tau \to \infty$

X_τ stands either for Q_τ or for W_τ

The Fluctuation Theorem fixes the symmetry of P(X) around zero

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Transient Fluctuation Theorem (TFT)

At $\tau = 0$ the system is in equilibrium

$$\Sigma(\tau) = 1 \qquad \forall \tau$$

The Fluctuation Theorem (FT)

- 1993 First numercial evidence of fluctuations relations
  D. Evans, E.D.G. Cohen and G. P. Morris.

- 1994 Proof of the transient fluctuation theorem (TFT)
  D. Evans and D.J.Searles

- 1995 Proof of the Stationary State Fluctuation Theorem (SSFT) for dynamical systems. G. Gallavotti and E.D.G. Cohen.

- 1997 Later proofs of FT for systems with stochastic dynamics were given by J. Kurchan, J. Lebowitz and E. Spohn, J. Farago.

- 2003 R. van Zon and E.G.D. Cohen extended the results to the heat fluctuations in stochastic systems

- New kinds of relations for suitably defined entropies have been proposed for stochastic system.

Short comment on FT for Gaussian P(Xτ)

FT imposes that:

$$\log \frac{P(X_\tau)}{P(-X_\tau)} = \frac{X_\tau}{k_B T} \Sigma(\tau)$$

if $$P(X_\tau) = A \ \exp[-\frac{(X_\tau - <X_\tau>)^2}{2\delta_\tau^2}]$$

then from FT $$\delta_\tau^2 = 2 \ k_B \ T \ <X_\tau>$$

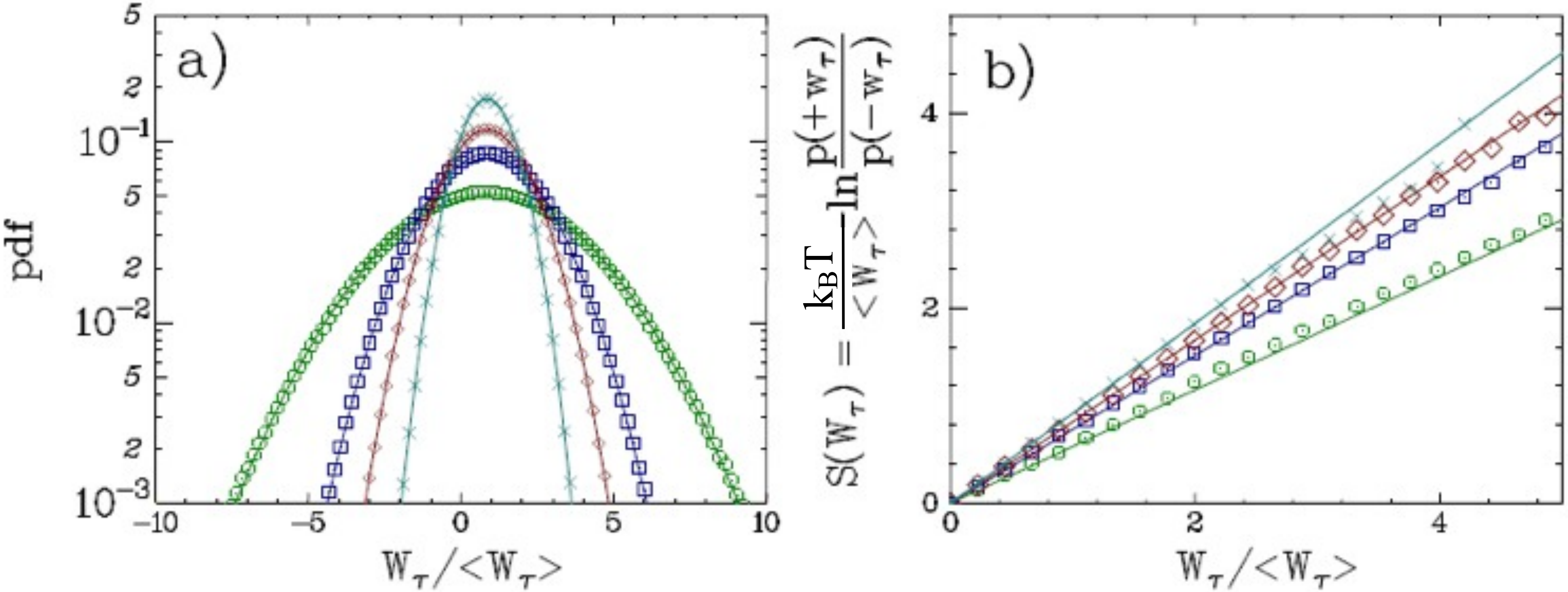
and $$\frac{\delta_\tau}{<X_\tau>} = \sqrt{\frac{2 \ k_B \ T}{<X_\tau>}}$$

SSFT periodic forcing: W

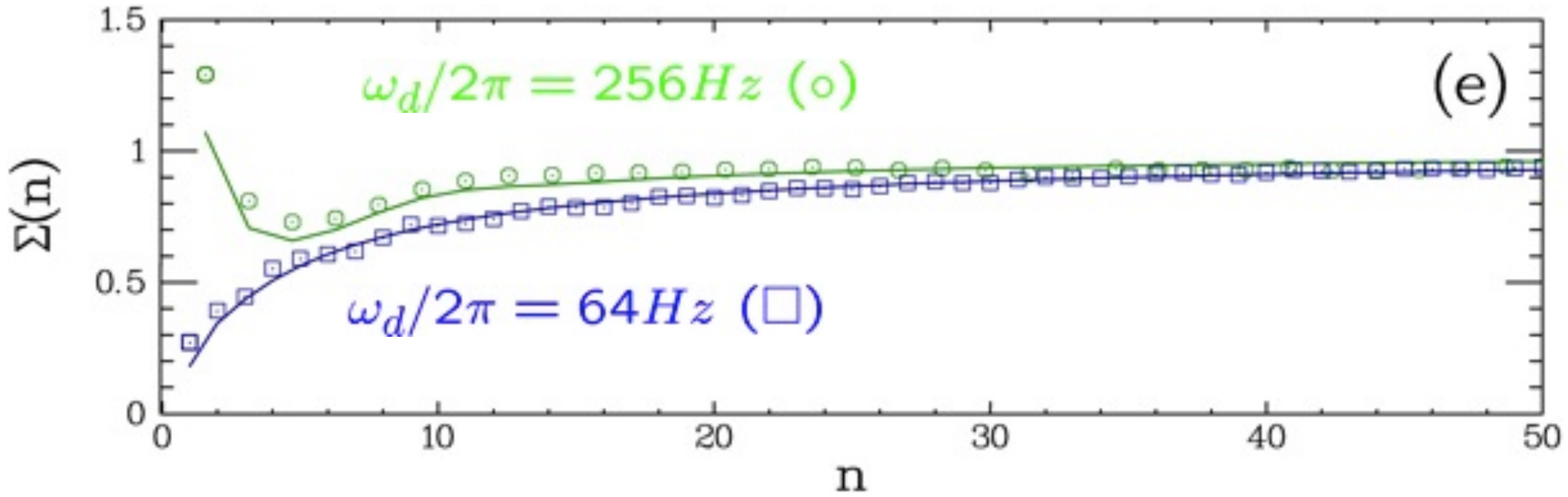
$$\frac{k_B\,T}{<W_\tau>}\log\frac{P(W_\tau)}{P(-W_\tau)} = \frac{W_\tau}{<W_\tau>}\,\Sigma(\tau)$$

$$\omega_d/2\pi = 64\text{Hz} < \omega_o/2\pi$$

$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).

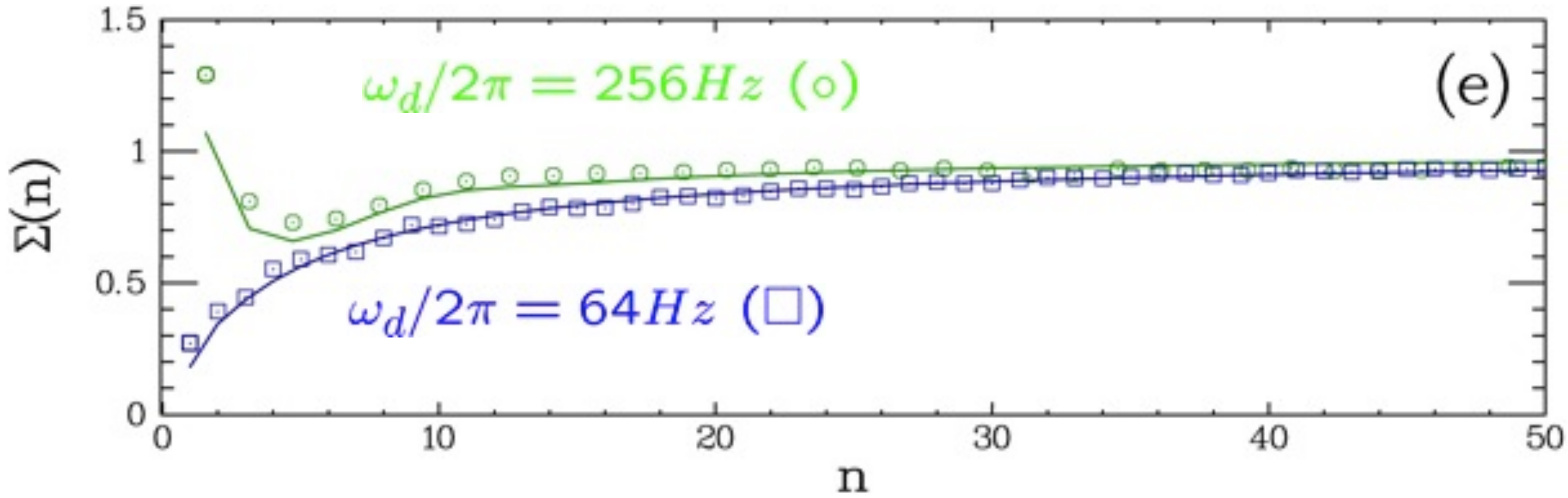


SSFT periodic forcing: Σ for W



$$\frac{k_B\, T}{< W_\tau >} \log \frac{P(W_\tau)}{P(-W_\tau)} = \frac{W_\tau}{< W_\tau >}\, \Sigma(\tau)$$

SSFT periodic forcing: Σ for W



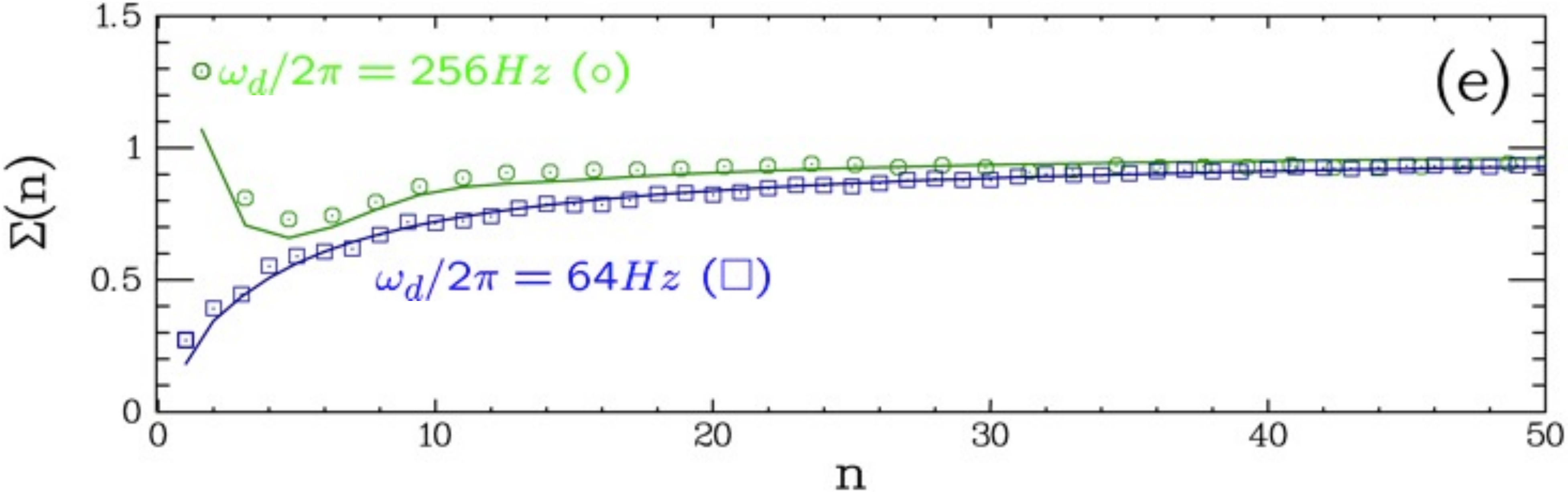
$$\frac{k_B\,T}{< W_\tau >} \log \frac{P(W_\tau)}{P(-W_\tau)} = \frac{W_\tau}{< W_\tau >}\,\Sigma(\tau)$$

Analytically computed from the Langevin equation using two experimental observations

- The statistical properties of the bath are not modified by the driving
- The fluctuations of the work are Gaussian

S. Joubaud, N. B. Garnier, S. Ciliberto, J. Stat. Mech., P09018 (2007)

SSFT periodic forcing: Σ



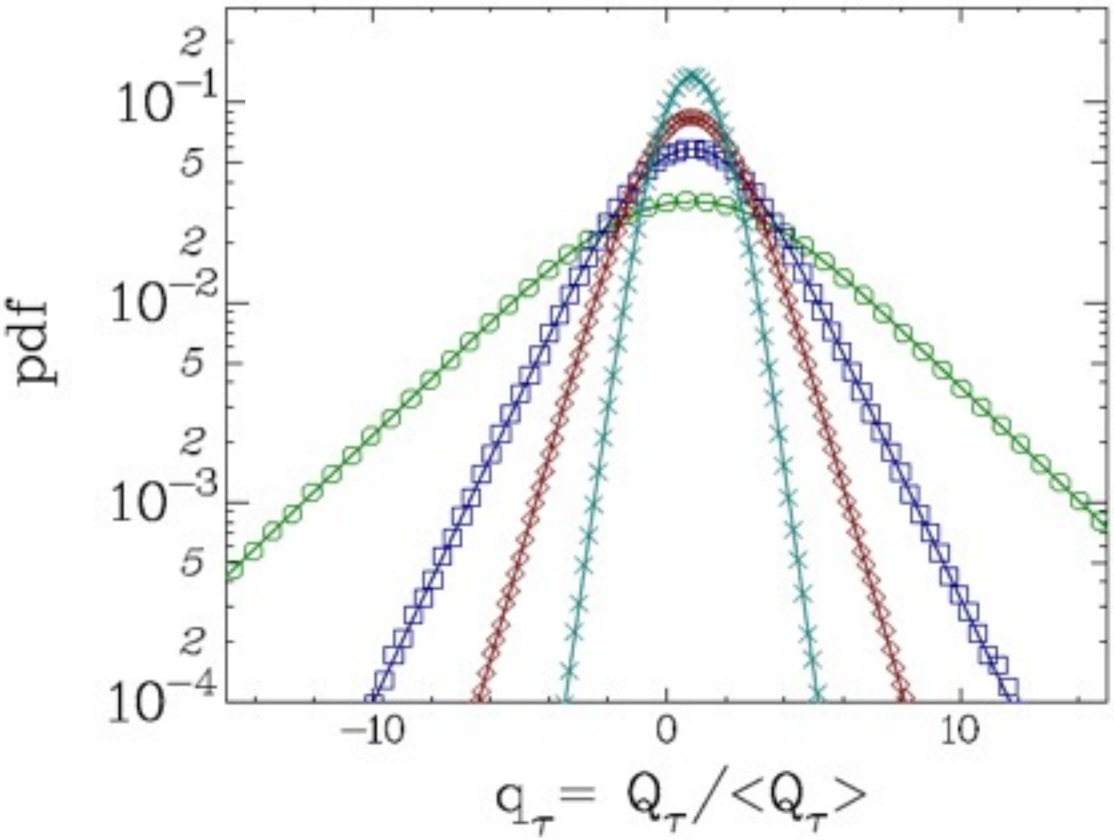
$$\Sigma(\tau) = \frac{1}{\left(1 - \epsilon(\tau)\right)}$$

$$\epsilon(\tau_n) \;=\; -\frac{\cos 2\gamma}{2\alpha\tau_n}\,\frac{\omega_0^2 + \omega_d^2}{\omega_d^2} + \frac{1}{\tau_n}\mathcal{O}\left(\mathrm{e}^{-\alpha\tau_n}\right)$$

where $\tan(\gamma) = -2\alpha\omega_d/(\omega_0^2 - \omega_d^2)$

SSFT periodic forcing: Q

$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).



Energy disipated in a time τ

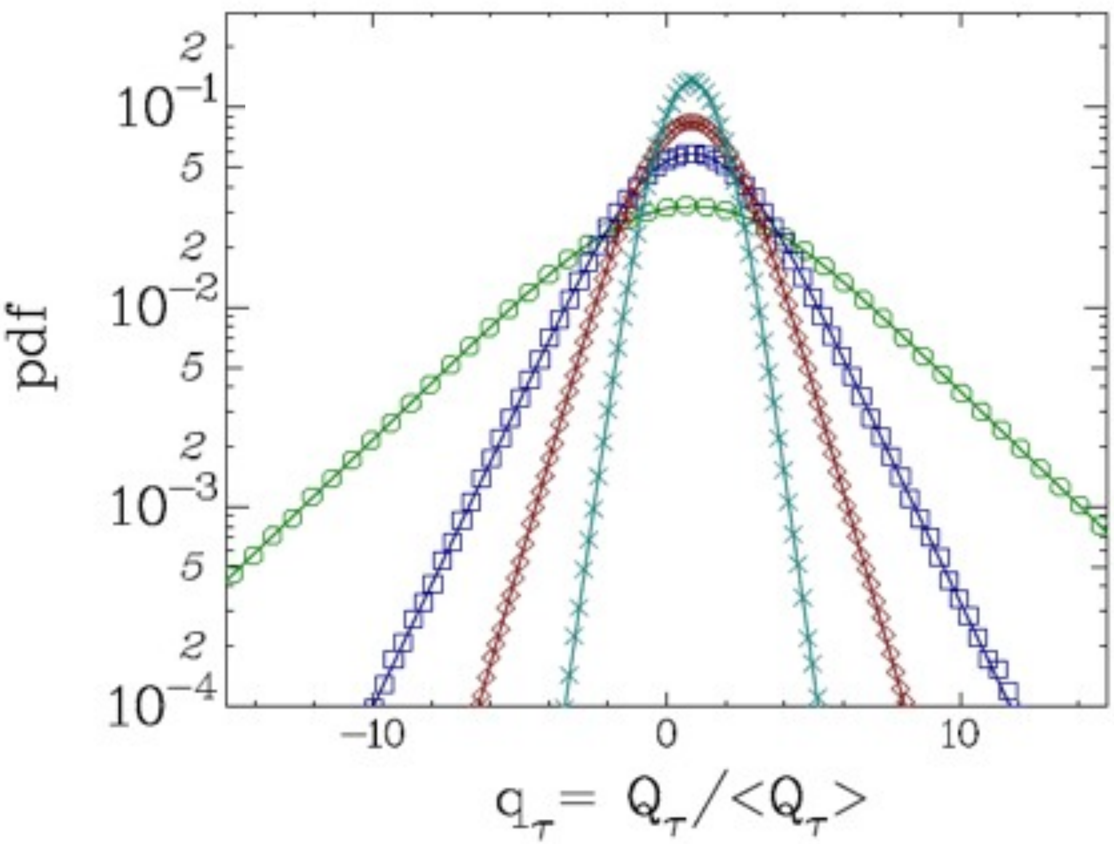
$$Q_\tau = W_\tau - \Delta U_\tau$$

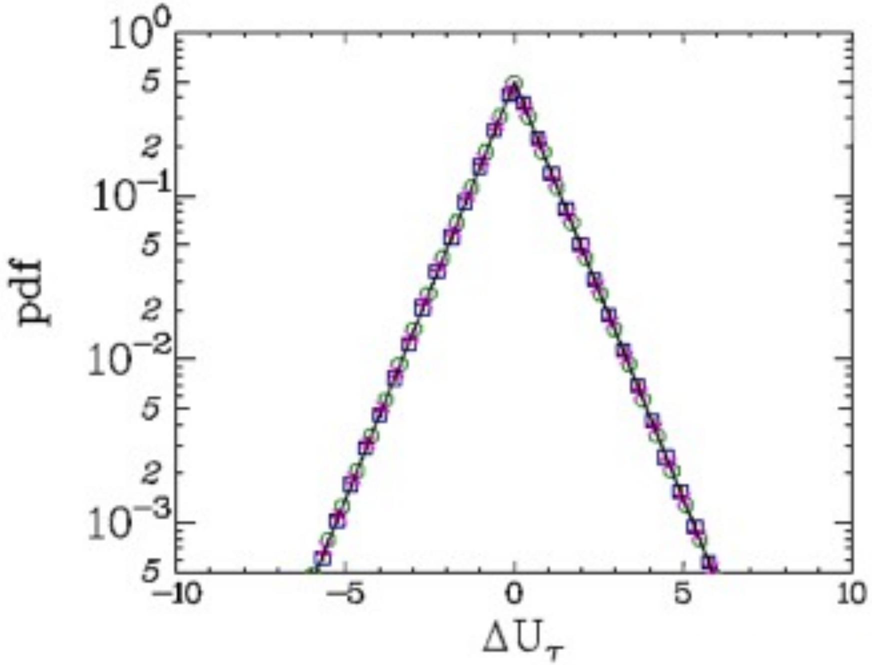
$$P(q) = \frac{\exp\left(\frac{\sigma^2}{2}\right)}{4}\left(\exp(q-\bar{q})\left[erfc\left(\frac{q-\bar{q}+\sigma_W^2}{\sqrt{2\sigma_W^2}}\right)\right] + \exp(-(q-\bar{q}))\left[erfc\left(\frac{-q+\bar{q}+\sigma_W^2}{\sqrt{2\sigma_W^2}}\right)\right]\right)$$

S. Joubaud, N. B. Garnier, S. Ciliberto, J. Stat. Mech., P09018 (2007)

SSFT periodic forcing: Q

$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).





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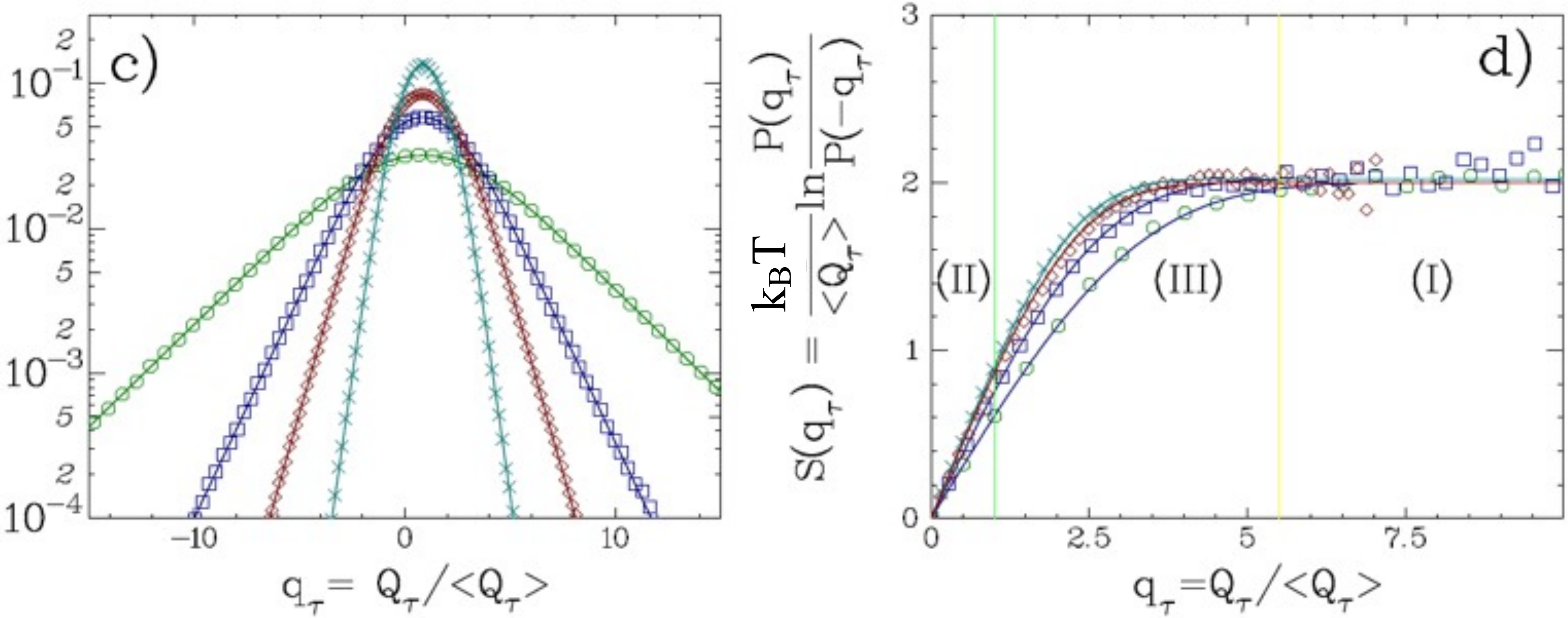
SSFT periodic forcing: Σ for Q

$n = 7$ (○), $n = 15$ (□), $n = 25$ (◇) and $n = 50$ (×).



3 regions :

(I) Large fluctuations are exponential: $S(q_\tau) = 2$ for $q_\tau > 3$

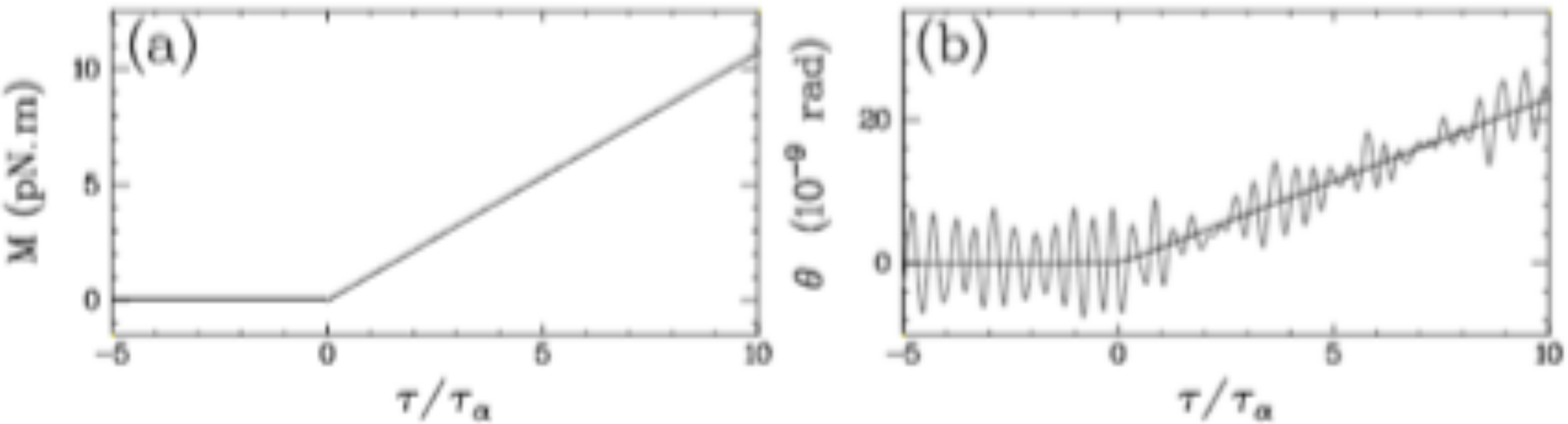
(II) for $q_\tau < 2$, $S(q_\tau) = \Sigma(n)\, q_\tau$ with $\Sigma(n) \to 1$ for $n \to \infty$

(III) Smooth connection .

Linear forcing

- start from an equilibrium state
- linear forcing

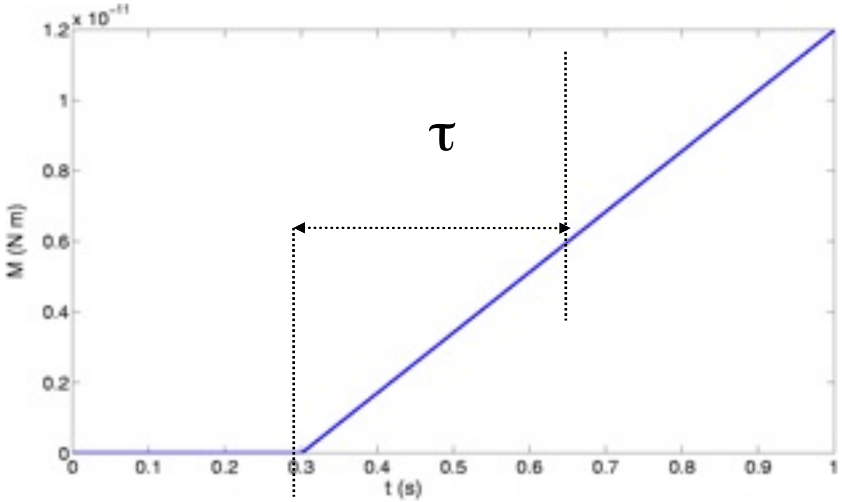
$M(t) = M_o \frac{t}{\tau_r}$ ($M_o = 11.28\, pN.m$ and $\tau_r = 0.1\, s = 10.52\tau_\alpha$)



Transient and Steady State Fluctuation Theorem

$$\log \frac{P(+W_\tau)}{P(-W_\tau)} = W_\tau \; \Sigma(\tau)$$

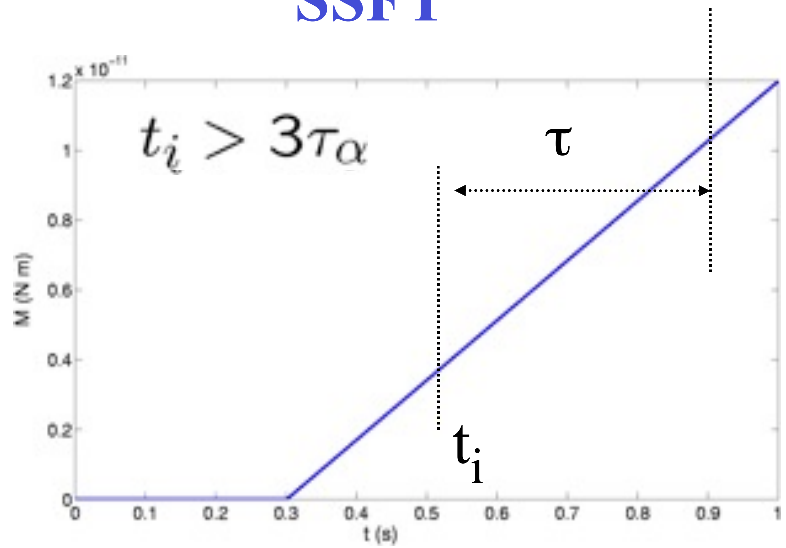
TFT



$$W_\tau = \beta \int_0^\tau M \dot{\theta} \; dt$$

$$\Sigma = 1, \; \forall \; \tau$$

SSFT

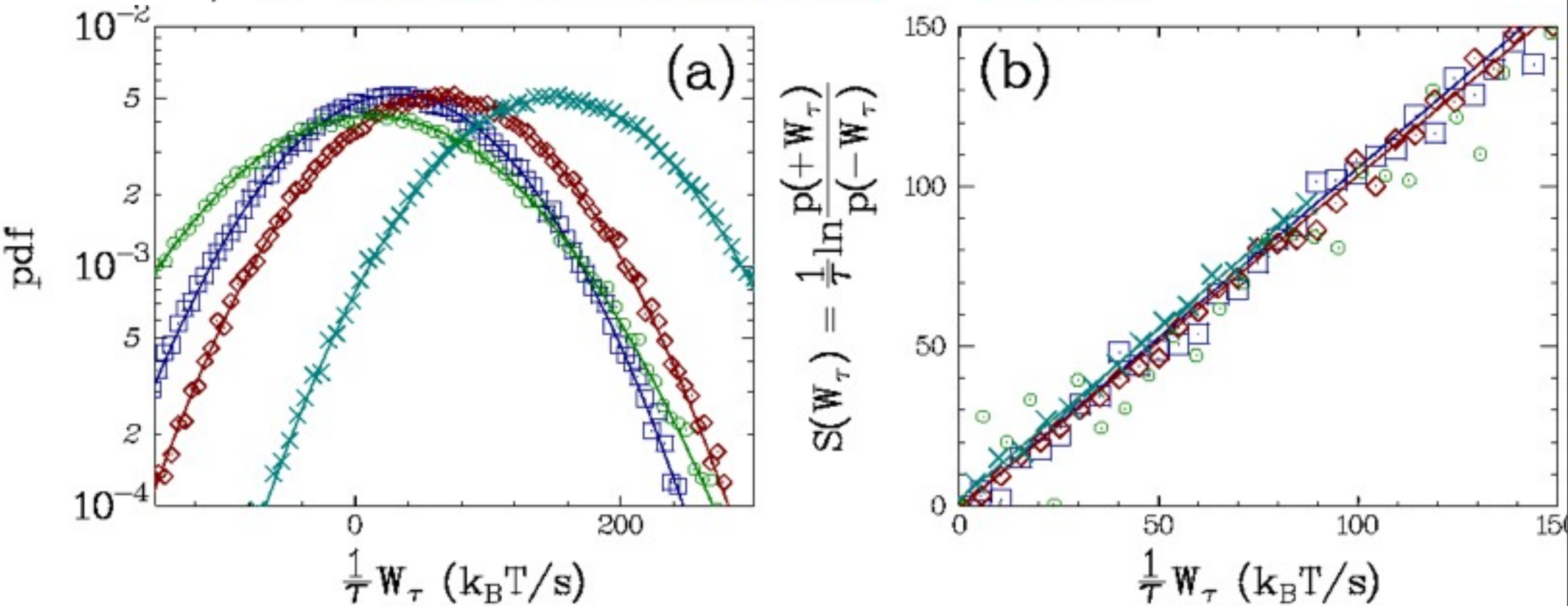


$$W_\tau = \beta \int_{t_i}^{t_i+\tau} (M(t) - M(t_i)) \; \dot{\theta} \; dt$$

$$\Sigma \rightarrow 1 \quad \text{for} \quad \tau \rightarrow \infty$$

TFT

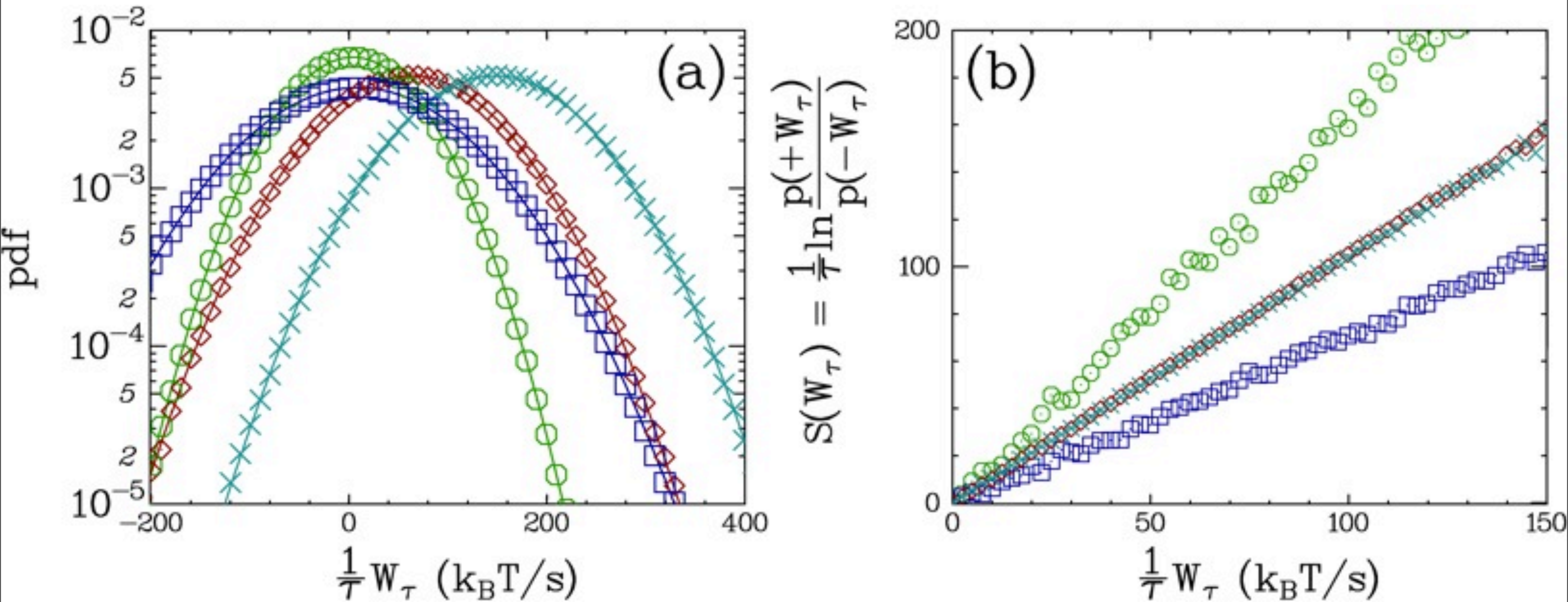
τ/τ_α: 0.31 (○), 1.015 (□), 2.09 (◇) and 4.97 (×)



$$S_\tau = \frac{1}{\tau} \log \frac{P(W_\tau)}{P(-W_\tau)} = \frac{W_\tau}{\tau}$$

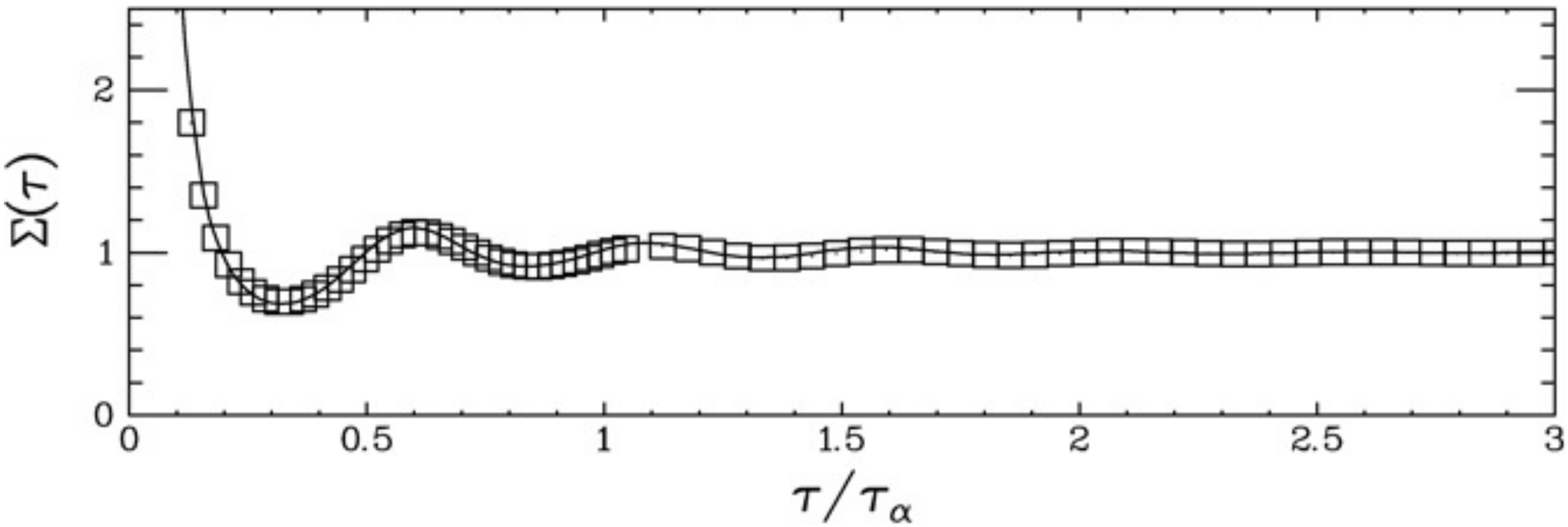
SSFT

τ/τ_α: 0.019 (○), 0.31 (□), 2.09 (◇) and 4.97 (×)



$$S_\tau = \frac{1}{\tau}\log\frac{P(W_\tau)}{P(-W_\tau)} = \frac{W_\tau}{\tau}\,\Sigma(\tau)$$

Σ(τ) for the SSFT



$$\Sigma(\tau) = \frac{1}{\big(1 - \epsilon(\tau)\big)}$$

$$\epsilon(\tau) = \frac{2}{\psi\tau}\left\{\frac{\sin 3\varphi}{\omega_0\tau} - \exp(-\alpha\tau) \times \left(\sin(2\varphi + \psi\tau) + \frac{\sin(3\varphi + \psi\tau)}{\omega_0\tau}\right)\right\}.$$

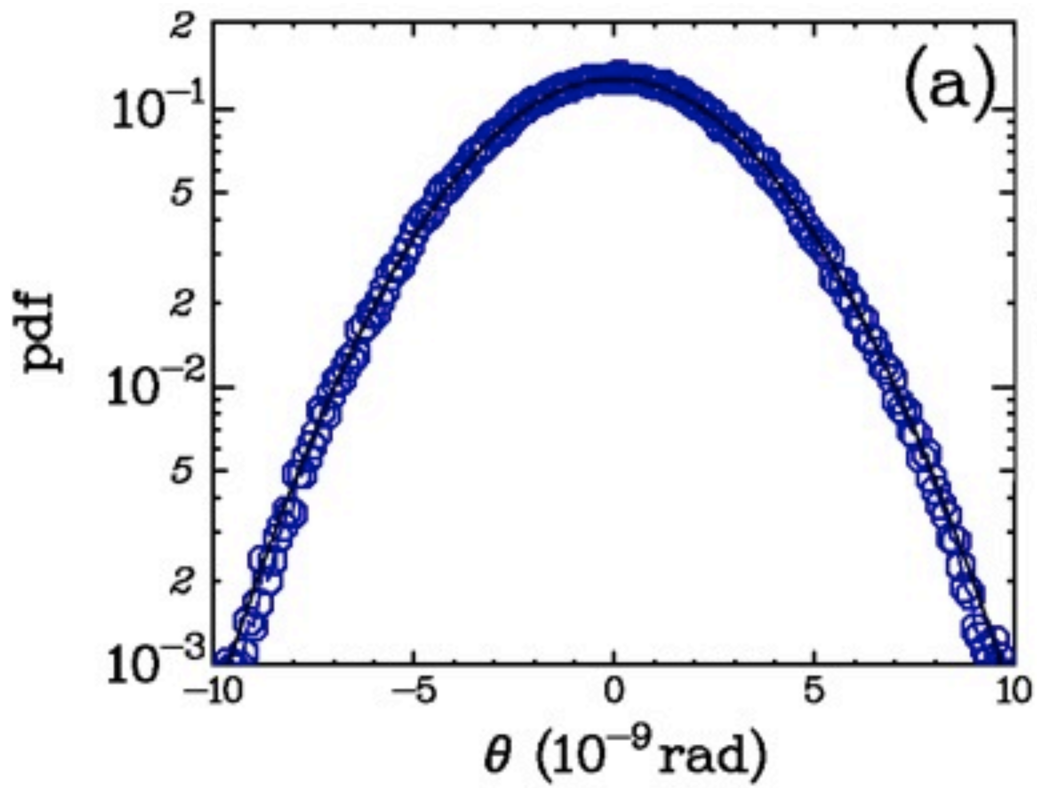
where $\alpha = 1/\tau_\alpha$, $\alpha^2 + \psi^2 = \omega_0^2 = C/I_{\text{eff}}$ and $\sin\varphi = \psi/\omega_0$.

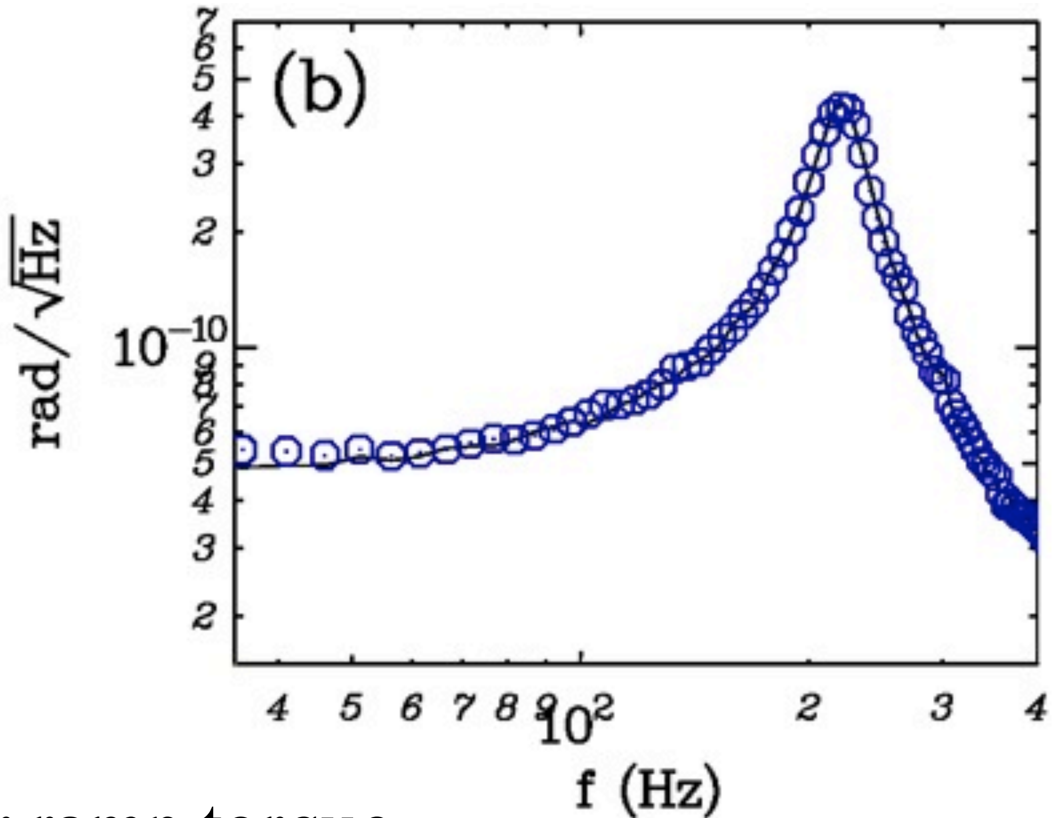
Theoretical description

What are the fluctuations of Θ when the system is out of equilibrium ?

The statistical properties of the thermal fluctuations $\delta\theta$ are not modified by the driving.

$$\theta(t) = \bar{\theta}(t) + \delta\theta(t)$$





Linear ramp torque

Theoretical description

Langevin Equation

Our experiment is well described by:

$$I_{\text{eff}}\,\ddot{\theta} + \int_{-\infty}^{t} G(t-t')\,\dot{\theta}(t')\d t' + C\theta = M,$$

where G is the memory kernel.

In the case of viscous damping:

$$I_{\text{eff}}\,\ddot{\theta} + \nu\,\dot{\theta} + C\,\theta = M(t) + \eta,$$

where η is the thermal noise amplitude.

Using the experimental evidence that $\theta = \overline{\theta} + \delta\theta$. the work is:

$$W = \overline{W}_{\tau}(t_i) + \delta W_{\tau}(t_i) = \left[\int_{t_i}^{t_i+\tau} M\dot{\overline{\theta}}\ dt + \int_{0}^{\tau} M\delta\dot{\theta}(t)\ dt\right]$$

which has a Gaussian statistics.

T. Speck and U. Seifert *Eur. Phys. J. B*, **43** 521

Theoretical description: Fluctuation Theorem for W

When $P(+W_\tau)$ is Gaussian

$$\log \frac{P(+W_\tau)}{P(-W_\tau)} = \frac{2 < W_\tau >}{< \delta {W_\tau}^2 >} W_\tau = W_\tau \ \Sigma(\tau)$$

We compute $\bar{\theta}$, $< \delta\theta(\tau)\delta\theta(0) >$ and $< \delta\dot{\theta}(\tau)\delta\dot{\theta}(0) >$
and we obtain analytic expressions for $< W_\tau >$ and $< \delta {W_\tau}^2 >$

$$R_{\delta\theta}(\tau) = \langle \delta\theta(t+\tau)\delta\theta(t)\rangle = \frac{k_B T}{C\,\sin(\varphi)}\,\exp\left(-\frac{|\tau|}{\tau_\alpha}\right)\sin(\psi|\tau| + \varphi) \qquad (1)$$

where $\psi^2 \equiv (\omega_0)^2 - (1/\tau_\alpha)^2$ and φ is defined by $\cos(\varphi) = 1/(\omega_0\tau_\alpha)$ and $\sin(\varphi) = \psi/\omega_0$.

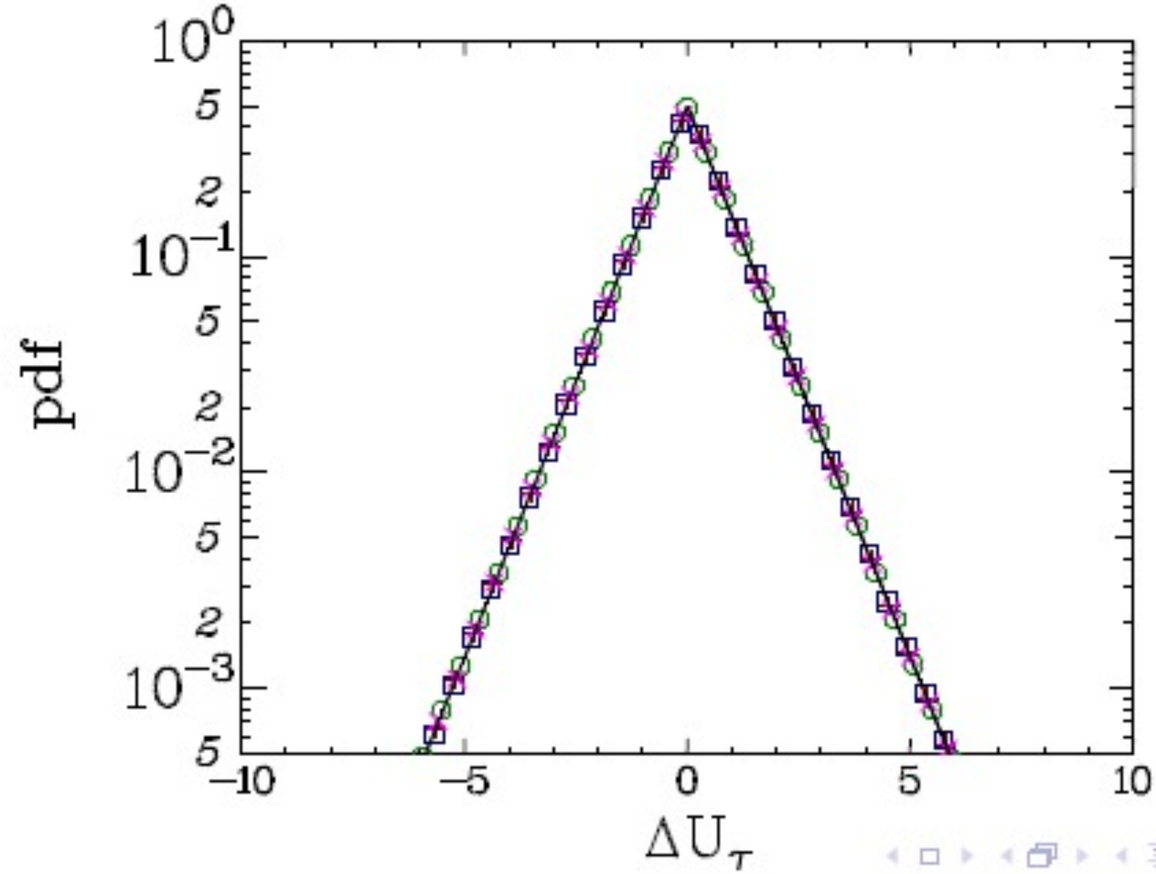
$$\sigma^2_{W_\tau} = \frac{1}{(k_B T)^2}\int_{t_i}^{t_i+\tau}\int_{t_i}^{t_i+\tau} \tilde{M}(t_1).\tilde{M}(t_2)\langle \delta\dot{\theta}(t_2)\delta\dot{\theta}(t_1)\rangle \mathrm{d}t_1\mathrm{d}t_2. \qquad (2)$$

This expression involves the autocorrelation function of the angular speed $\delta\dot{\theta}$, $(\langle \delta\dot{\theta}(t_2)\delta\dot{\theta}(t_1)\rangle)$.

$$\langle \delta\dot{\theta}(t_1)\delta\dot{\theta}(t_2)\rangle = -\frac{k_B T}{I_{\text{eff}}\,\sin(\varphi)}\exp\left(-\frac{|t_2 - t_1|}{\tau_\alpha}\right)\sin(\psi|t_2 - t_1| - \varphi). \qquad (3)$$

Theoretical description: Fluctuation Theorem for Q

- We suppose $\tau_n \gg \tau_\alpha$
- PDFs of ΔU_τ are exponential and independant of n :
  $P(\Delta U_\tau) = \frac{1}{2}\exp(-|\Delta U_\tau|)$



Theoretical description: Fluctuation Theorem for Q

$$Q_\tau = W_\tau - \Delta U_\tau$$

- We suppose $\tau_n \gg \tau_\alpha$
- PDFs of ΔU_τ are exponential and independant of n :
  $P(\Delta U_\tau) = \frac{1}{2}\exp(-|\Delta U_\tau|)$
- θ, $\frac{d\theta}{dt}$ at t_i and $t_i + \tau$ and W_τ are uncorrelated
  - ΔU_τ and W_τ are independant
  - PDF of Q_τ is the convolution between a Gaussian PDF and an exponential PDF

$$P(q) = \frac{\exp\left(\frac{\sigma^2}{2}\right)}{4}\left(\exp(q-\bar{q})\left[erfc\left(\frac{q-\bar{q}+\sigma_W^2}{\sqrt{2\sigma_W^2}}\right)\right] + \exp(-(q-\bar{q}))\left[erfc\left(\frac{-q+\bar{q}+\sigma_W^2}{\sqrt{2\sigma_W^2}}\right)\right]\right)$$

where $q = \frac{Q_\tau}{<Q>}$

- *Ref: Journal Stat. Mech.: Theory and experiment P09018*

Trajectory dependent entropy

- U. Seifert, Phys. Rev. Lett., 95, 040602, (2005), for Langevin dynamics
- A. Puglisi et al.
  J. Stat. Mech.: Theory and Experiment, P08010,(2006) for Markov process

Heat dissipated by the system towards the heat bath:

$$Q_\tau = W_\tau - \Delta U_\tau \, .$$

we define the entropy variation in the system during a time τ as :

$$\Delta s_{\mathrm{m},\tau} = \frac{1}{T} Q_\tau$$

For thermostated systems, entropy change in medium behaves like the dissipated heat. The non-equilibrium Gibbs entropy is :

$$\langle s(t) \rangle = -k_B \int \, d\vec{x} \; p(\vec{x}(t), t, \lambda_t) \ln p(\vec{x}(t), t, \lambda_t)$$

Trajectory dependent entropy

$s(t) \equiv -k_B \ln p(\vec{x}(t), t, \lambda_t)$ " trajectory dependent entropy "

The total entropy $s_{\text{tot}}(t) = s_{\text{m}}(t) + s(t)$

The variation $\Delta s_{\text{tot},\tau}$ of $s_{\text{tot}}(t)$:

$$\Delta s_{\text{tot},\tau} \equiv s_{\text{tot}}(t+\tau) - s_{\text{tot}}(t) = \Delta s_{\text{m},\tau} + \Delta s_\tau$$

We are interested in studying the fluctuations of $\Delta s_{\text{tot},\tau}$.

Trajectory dependent entropy

For the torsion pendulum the "trajectory-dependent" entropy is :

$$\Delta s_{\tau_n} = -k_B \ln \left(\frac{p(\theta(t_i+\tau_n),\varphi).p(\dot\theta(t_i+\tau_n),\varphi)}{p(\theta(t_i),\varphi).p(\dot\theta(t_i),\varphi)} \right)$$

with starting phase $\varphi = t_i \omega_d$ and $\tau_n = n\ 2\pi/\omega_d$

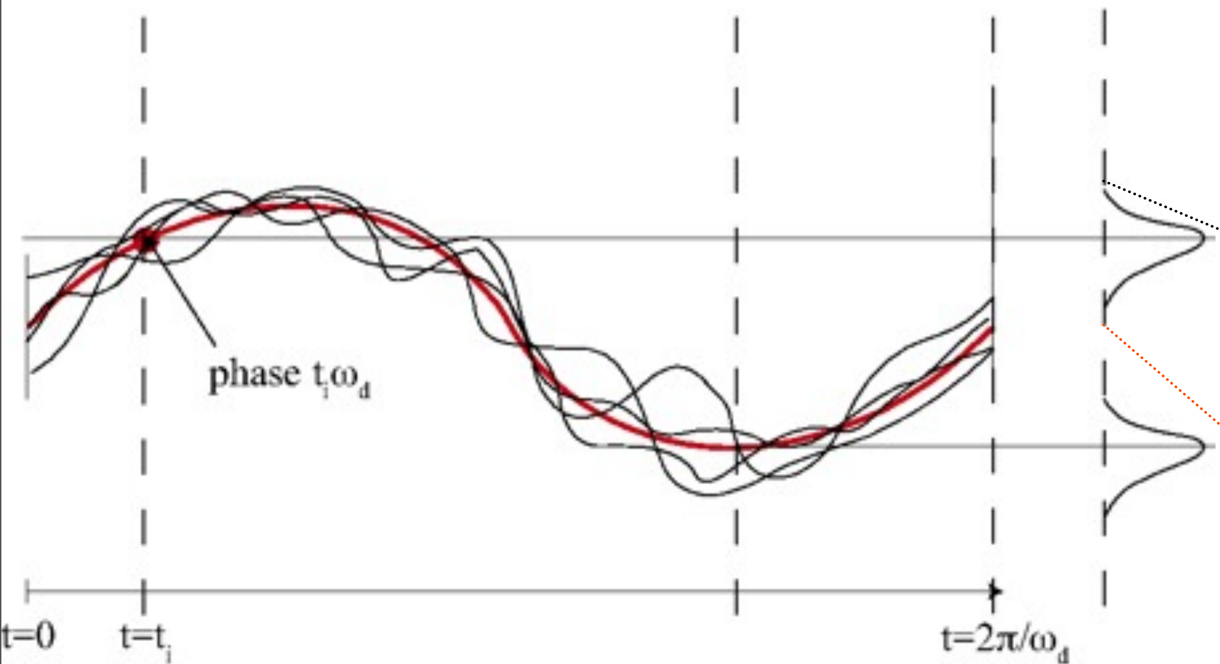
Computing the total entropy

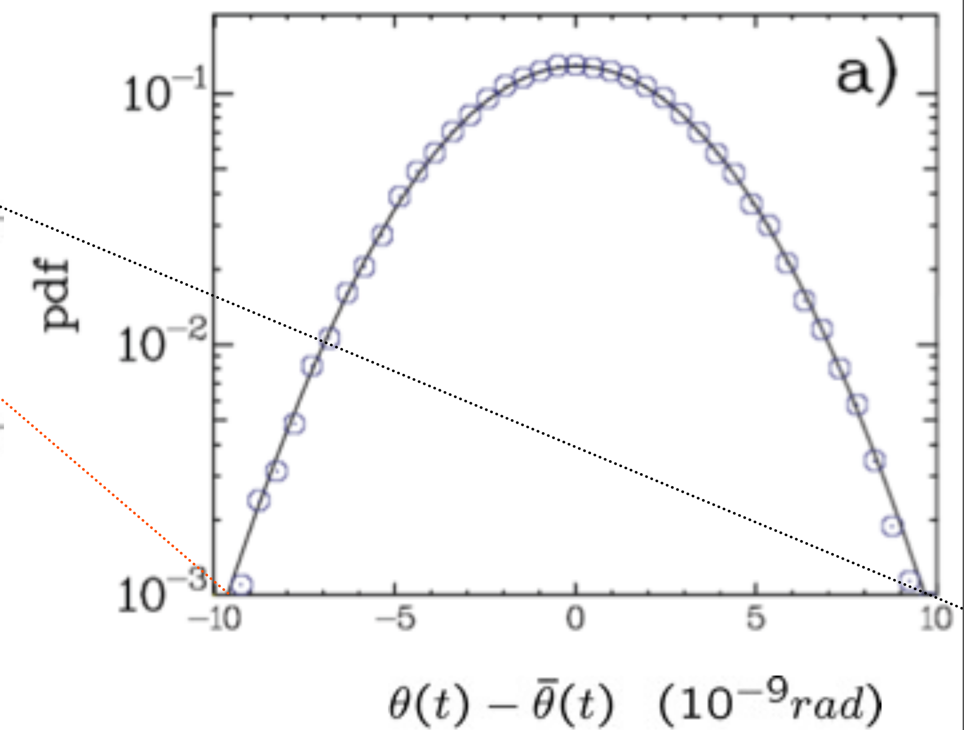
- Compute $p(\theta(t_i),\varphi)$ and $p(\dot\theta(t_i),\varphi)$ for each initial phase φ.
- Compute the "trajectory-dependent" entropy.
- As fluctuations of θ and $\dot\theta$ are independent of φ. Average Δs_{τ_n} over φ.

Tajectoires and averages

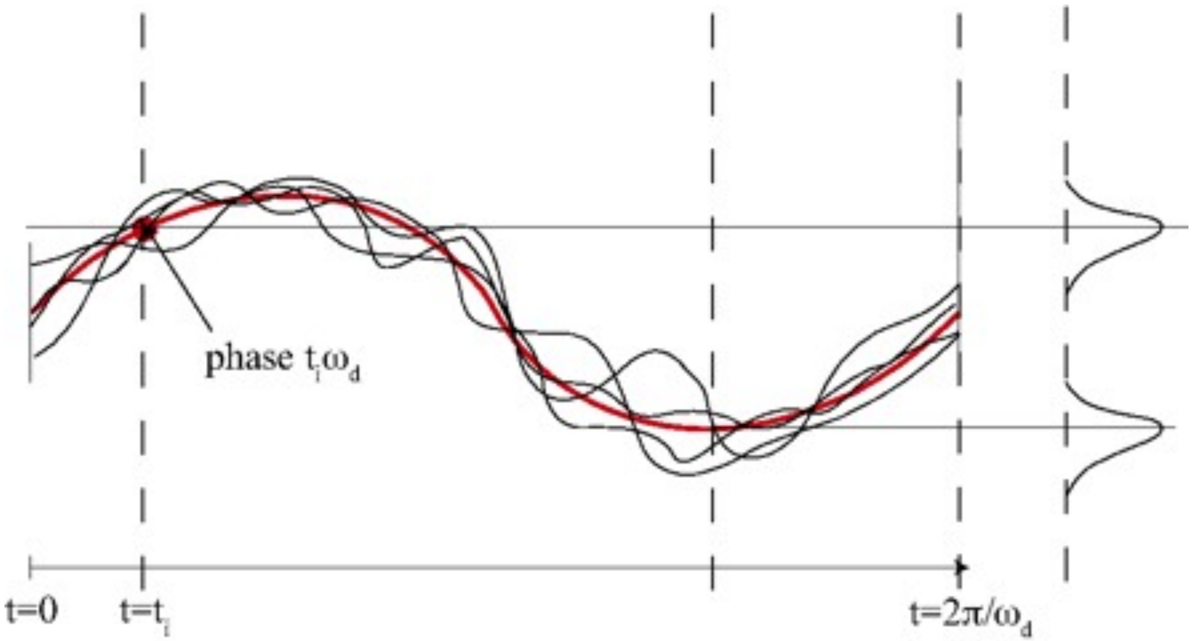
Computing the total entropy

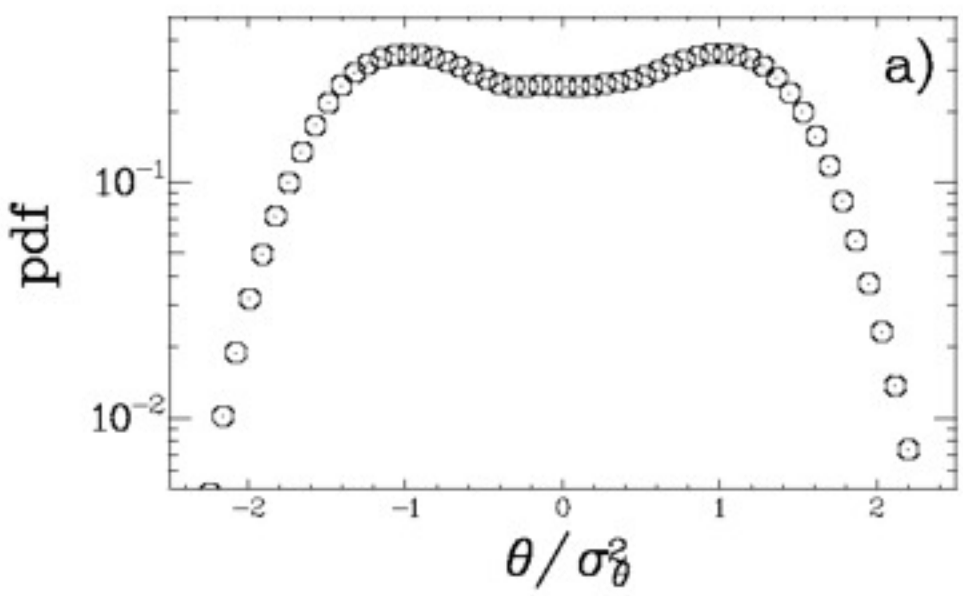
- Compute $p(\theta(t_i),\varphi)$ and $p(\dot{\theta}(t_i),\varphi)$ for each initial phase φ.
- Compute the "trajectory-dependent" entropy.
- As fluctuations of θ and $\dot{\theta}$ are independent of φ. Average Δs_{τ_n} over φ.

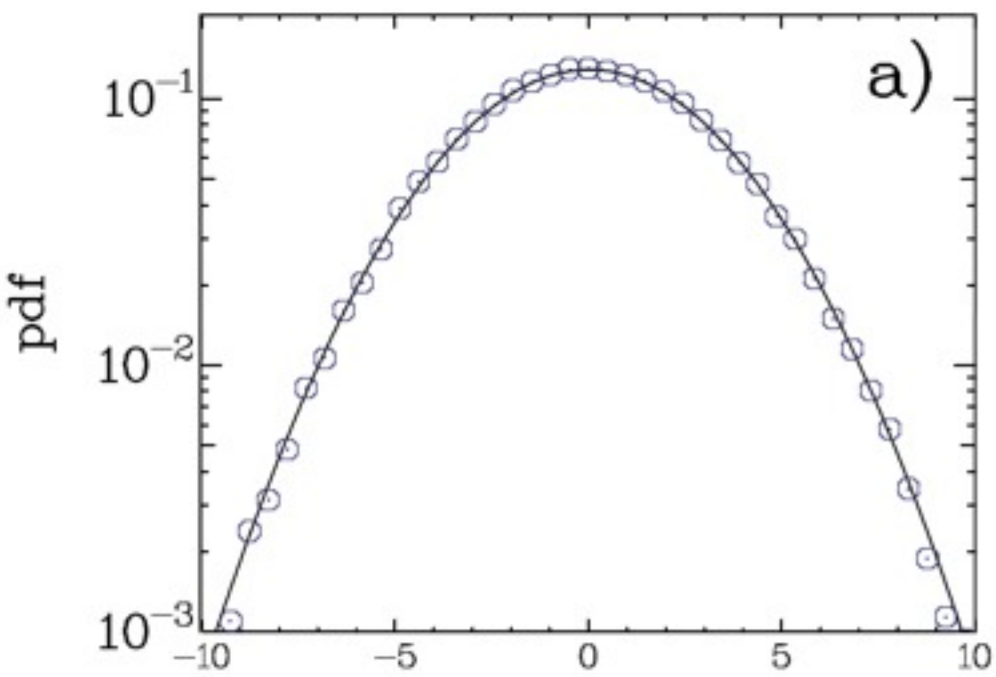




Tajectoires and averages

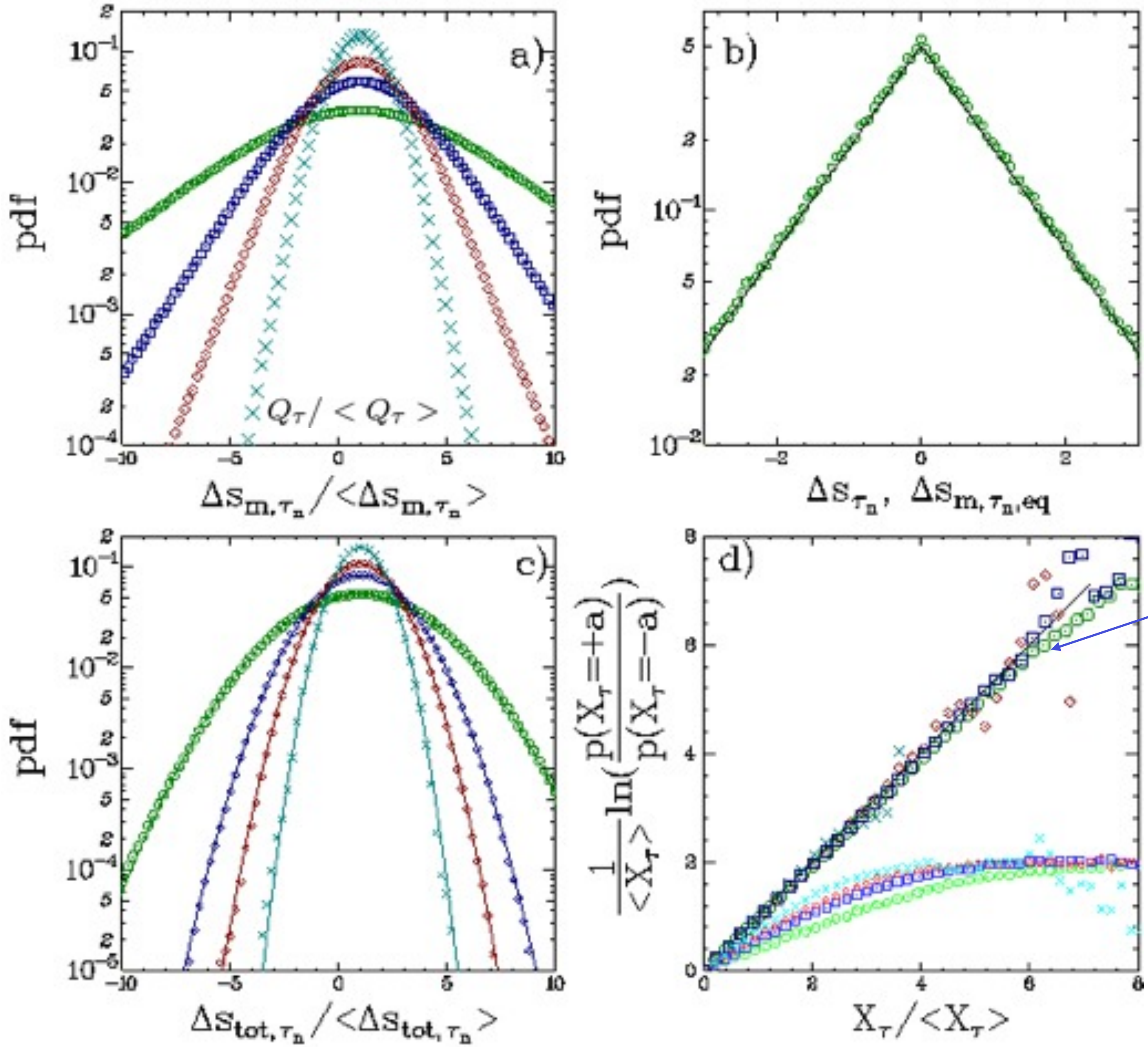






Fluctuations of the total entropy

n=7 (○), n=15 (□), n=25 (◊), n=20 (×)



$\Delta s_{m,\tau_n,eq} = \frac{\Delta U_\tau}{T}$

at $M = 0$

○ Δs_{τ_n}

$X_\tau = \Delta S_{tot}$

$X_\tau = \Delta S_{m,\tau_n}$

FT for total entropy

$$\ln\left(\frac{P(\Delta s_{\text{tot},\tau_n})}{P(-\Delta s_{\text{tot},\tau_n})}\right) = \frac{\Delta s_{\text{tot},\tau_n}}{k_B} \quad \forall\ \tau_n$$

FT for total entropy

$$T.\Delta s_{\text{tot},\tau_n} = Q_\tau + T.\Delta s_{\tau_n} = W_{\tau_n} - \Delta U_{\tau_n} + T.\Delta s_{\tau_n}$$

The data show that : $T\ \Delta s_{\tau_n} = (\Delta U_{\tau_n})_{\text{equilibrium}}$

Out of equilibrium :

$$T.\Delta s_{\text{tot},\tau_n} = Q_\tau + T.\Delta s_{\tau_n} = W_{\tau_n} - (\Delta U_{\tau_n})_{\text{out\_equilibrium}} + (\Delta U_{\tau_n})_{\text{equilibrium}}$$

In equilibrium :

$W_{\tau_n} = 0,\qquad Q_\tau = -(\Delta U_{\tau_n})$ and $T.\Delta s_{\text{tot},\tau_n} = 0$

Conclusions harmonic oscillator

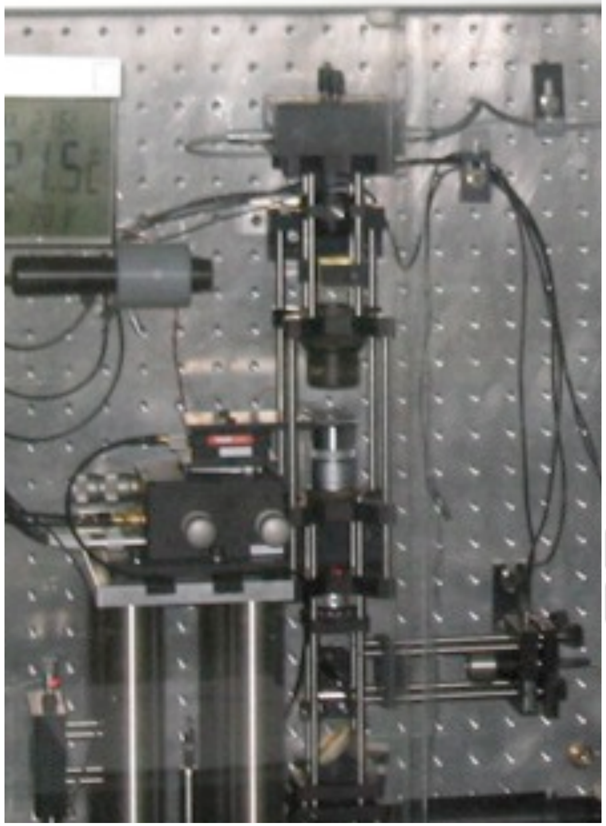
- We have experimentally perturbed an harmonic oscillator very close to equilibrium.
- We have computed and measured the finite time corrections for SSFT and TFT.
- The ‘’ trajectory dependent entropy ‘’ has been computed
- We have checked that for the total entropy SSFT is verified for all times.
- We have shown that in this specific example the ‘’total entropy” takes into account only the entropy produced by the external driving and does not take into account the entropy fluctuations at equilibrium.

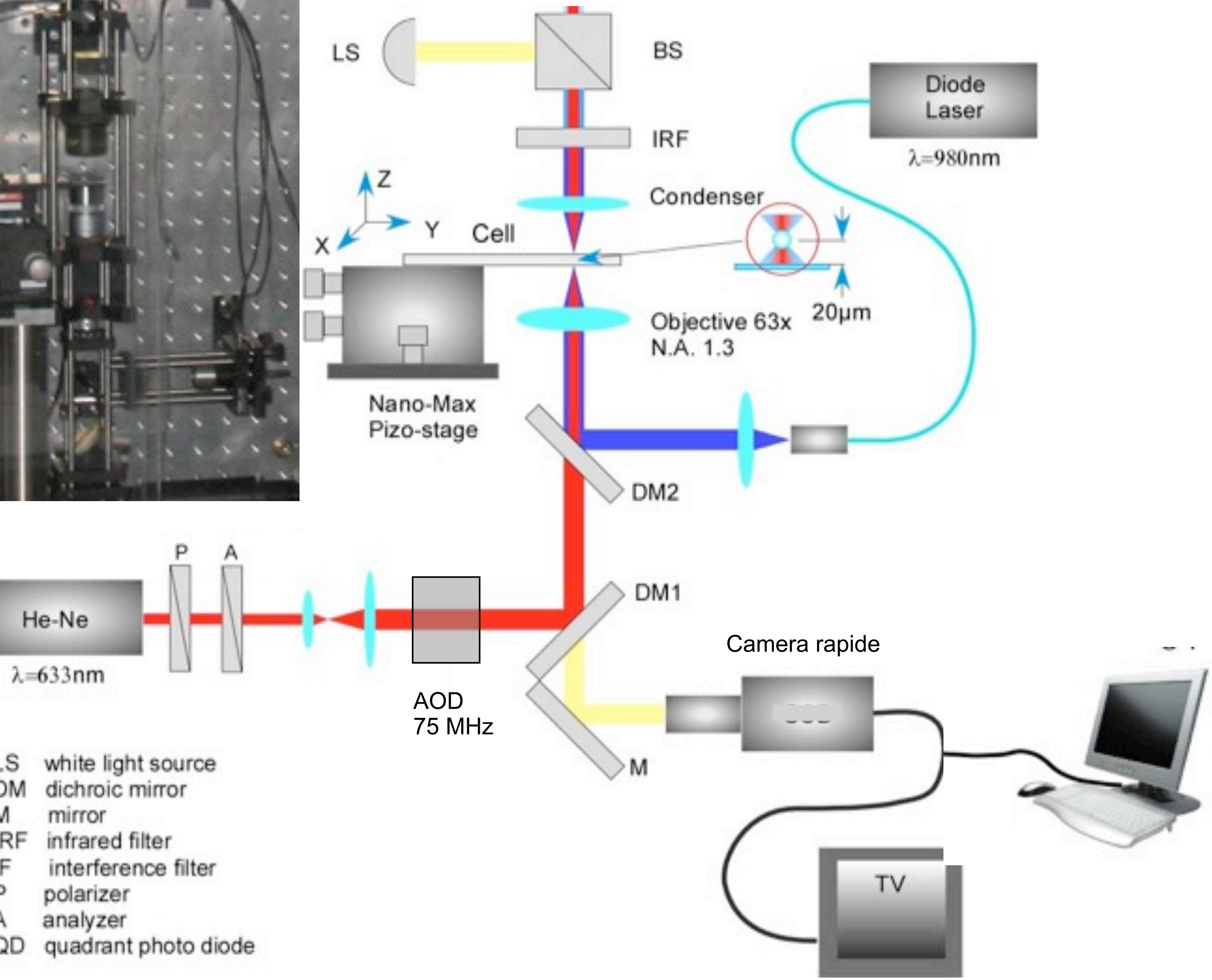
The stochastic resonance and Fluctuation Theorem

P.Jop. A. Petrosian, S. C.

Eur. Phys. Lett. **81,** 5 (2008) 50005

Optical traps





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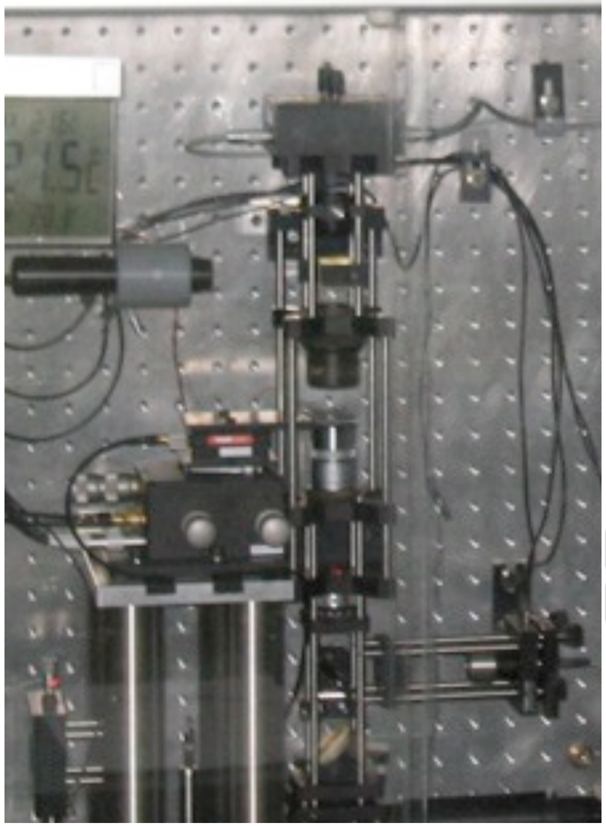
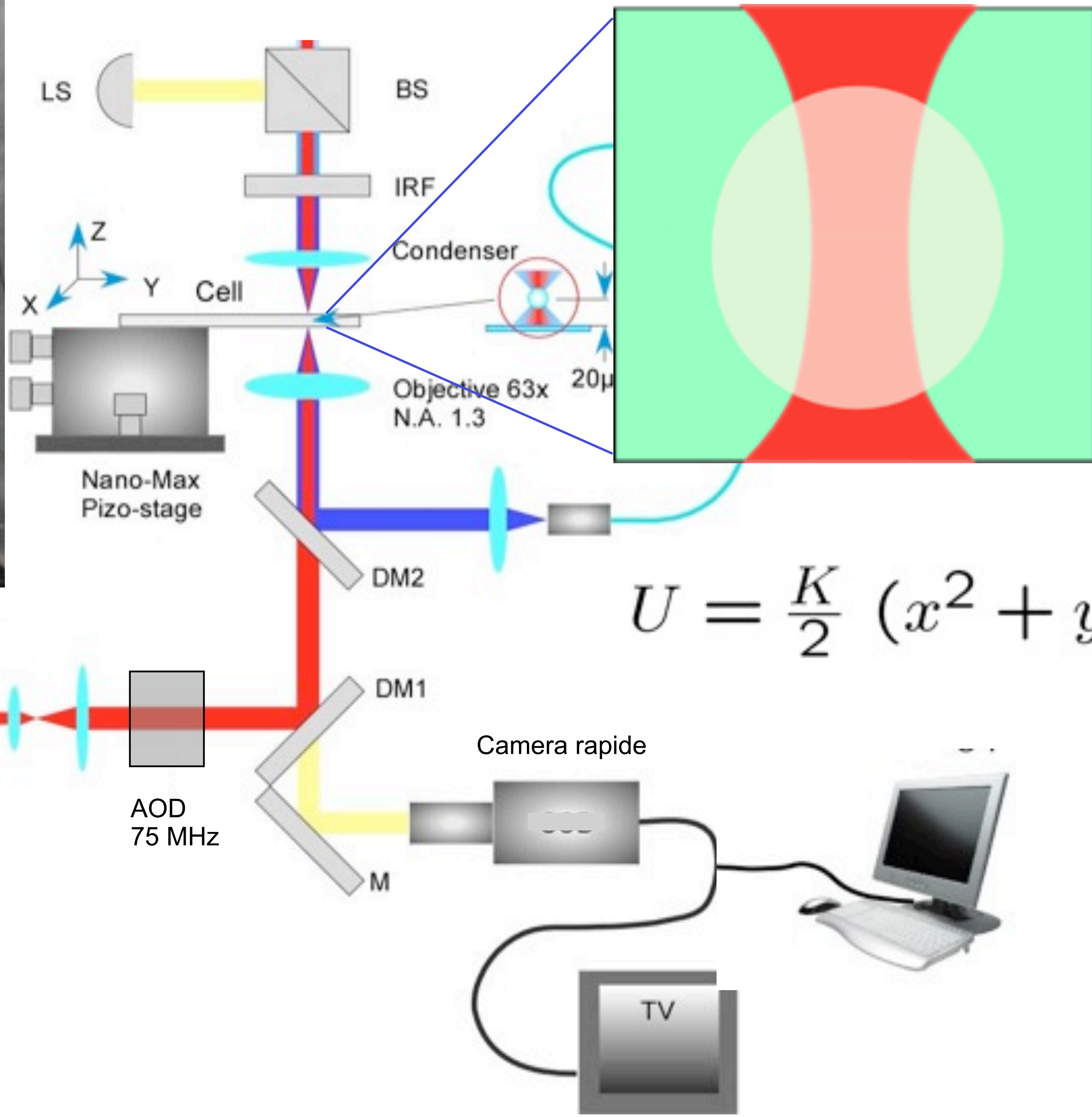
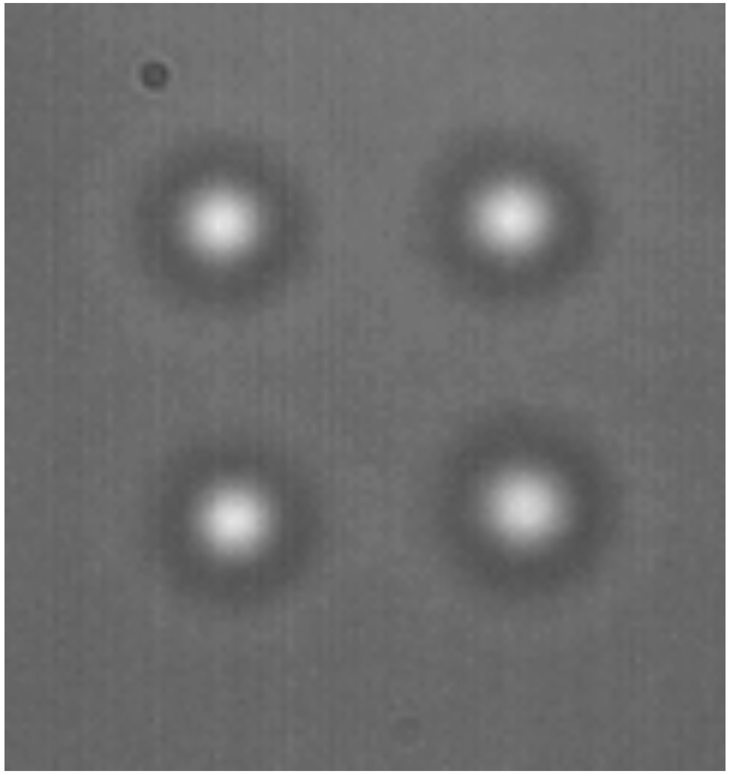
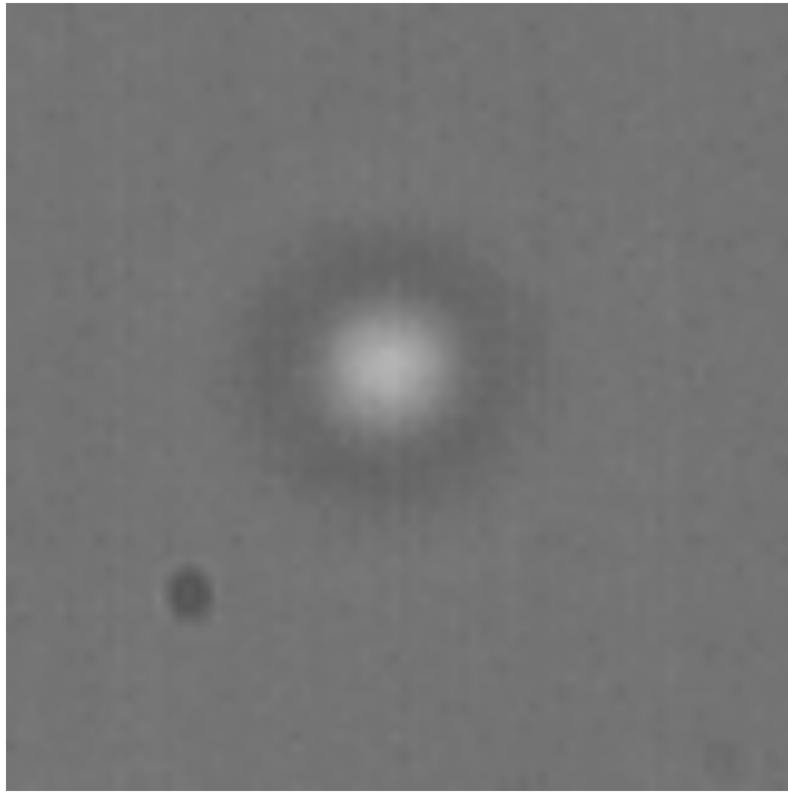


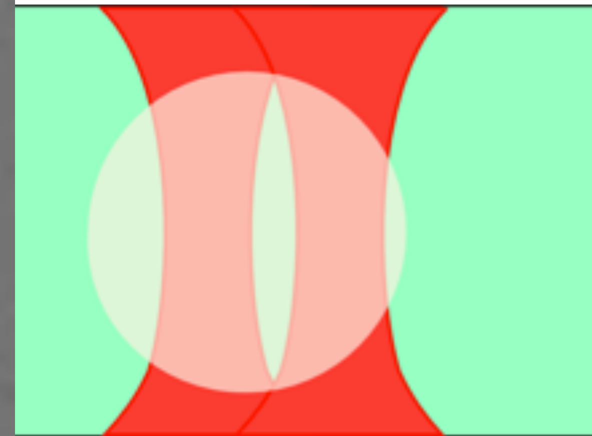


$$U = \frac{K}{2}\left(x^2 + y^2\right)$$

Examples of traps







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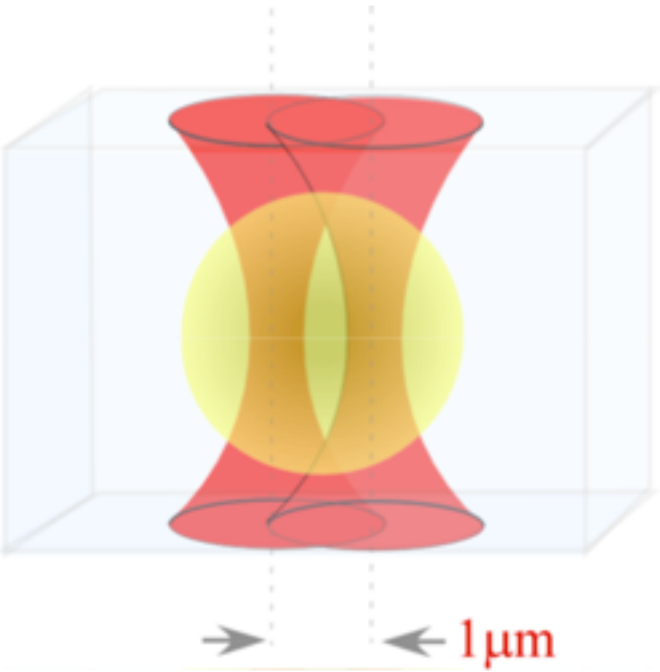
Brownian particle trapped by two laser beams



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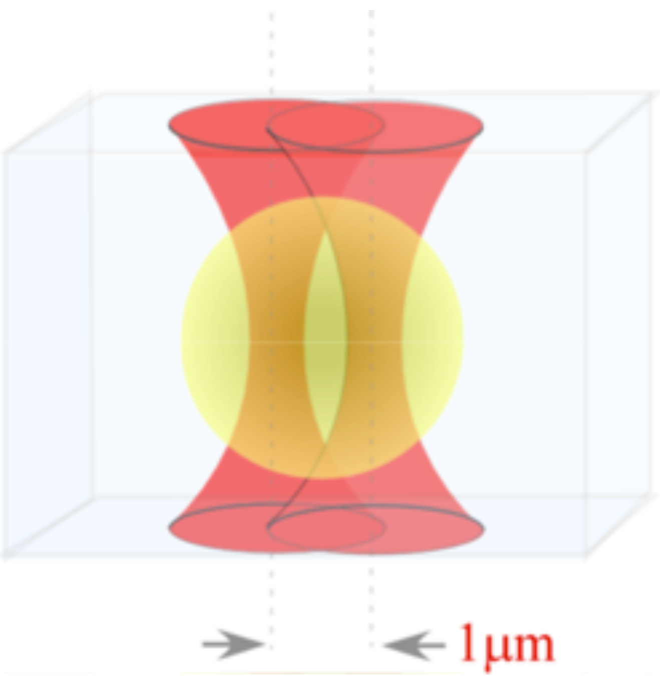

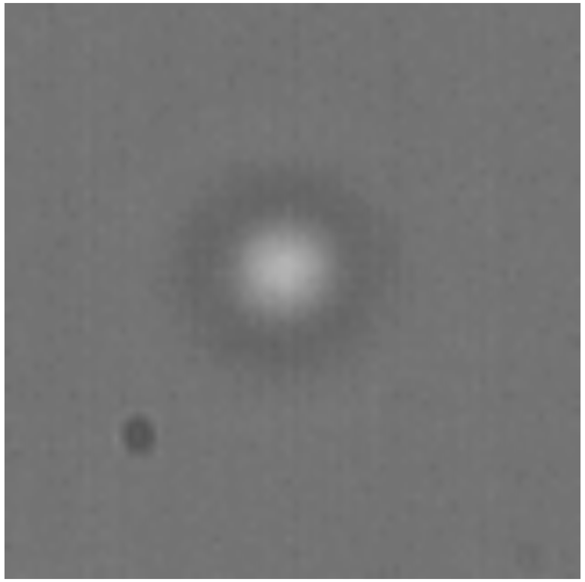

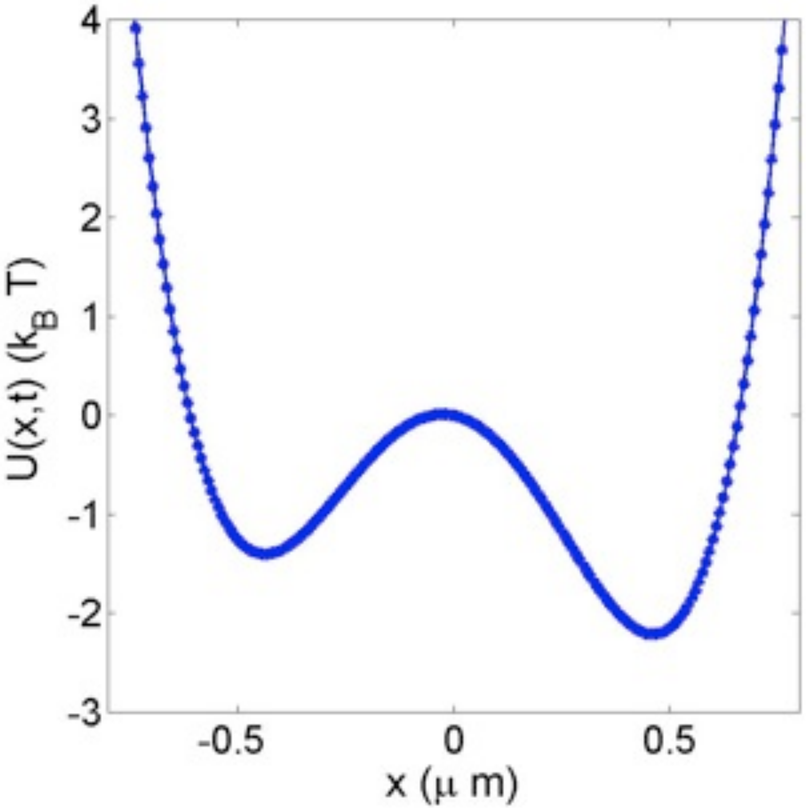

$$U_0(x) = ax^4 - bx^2 - dx$$

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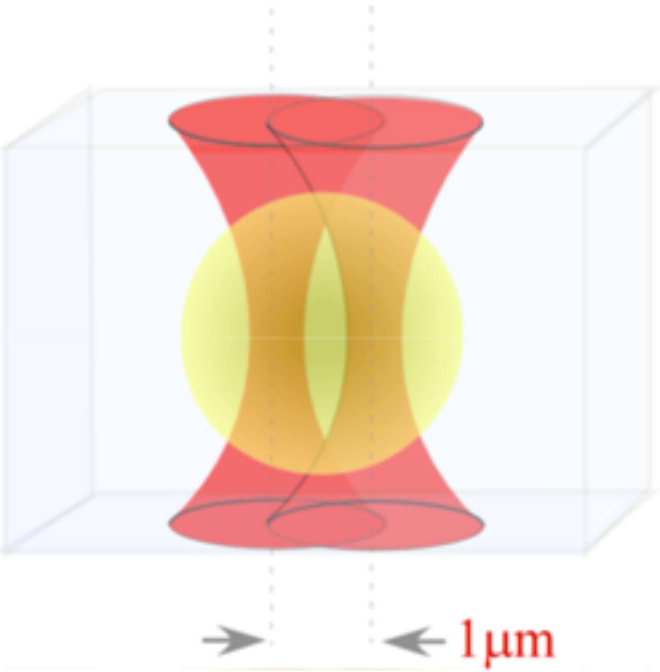

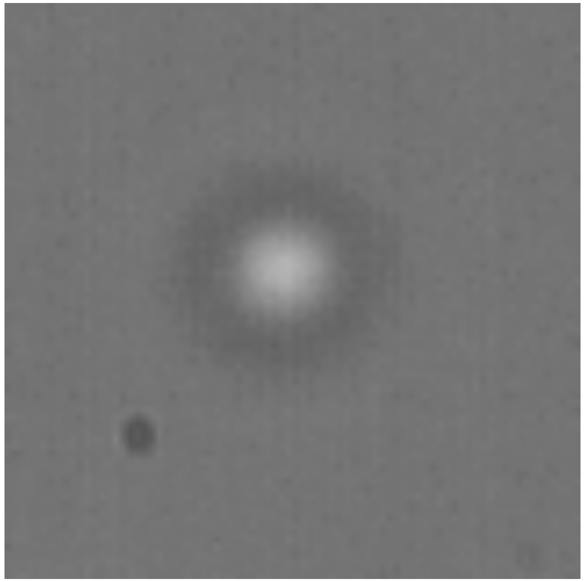

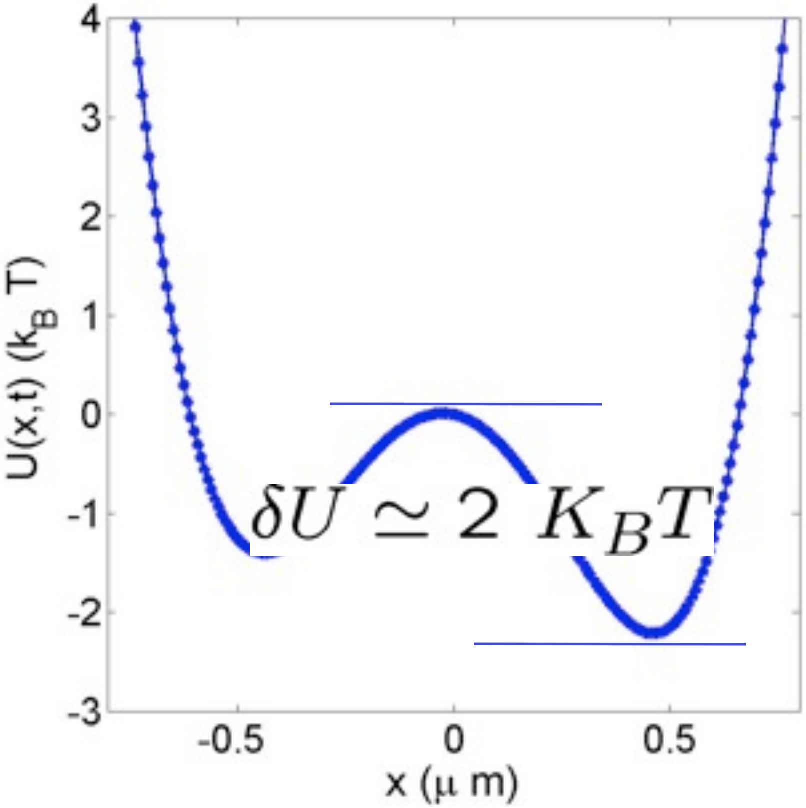

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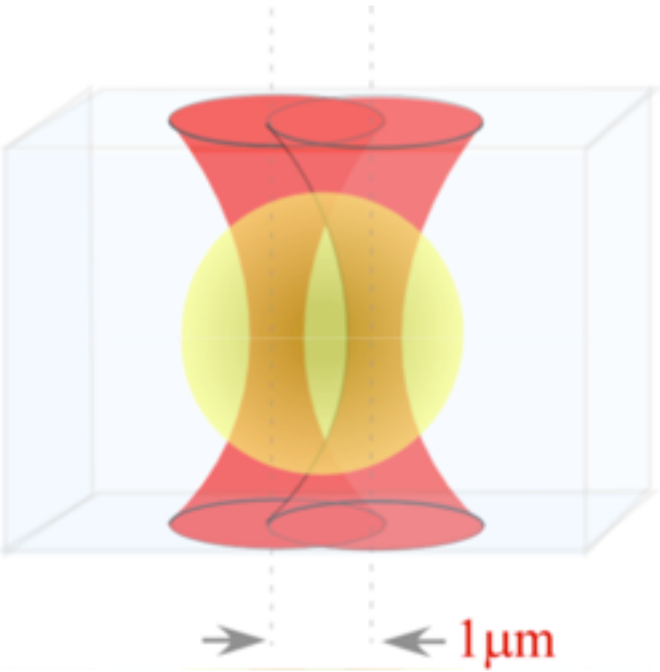

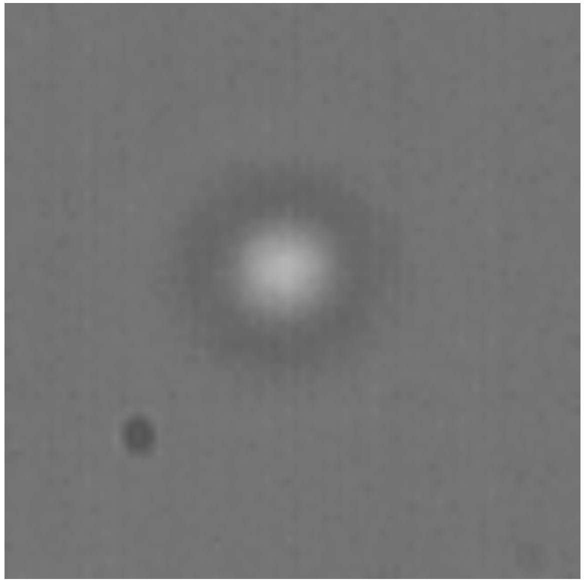

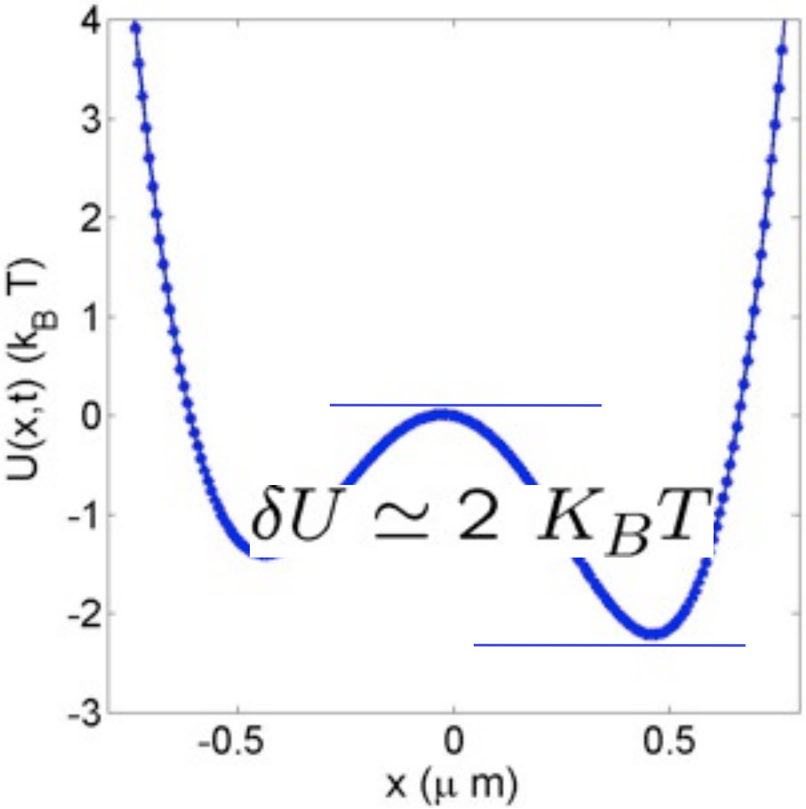

The Kramer rate is

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

$$U_0(x) = ax^4 - bx^2 - dx$$

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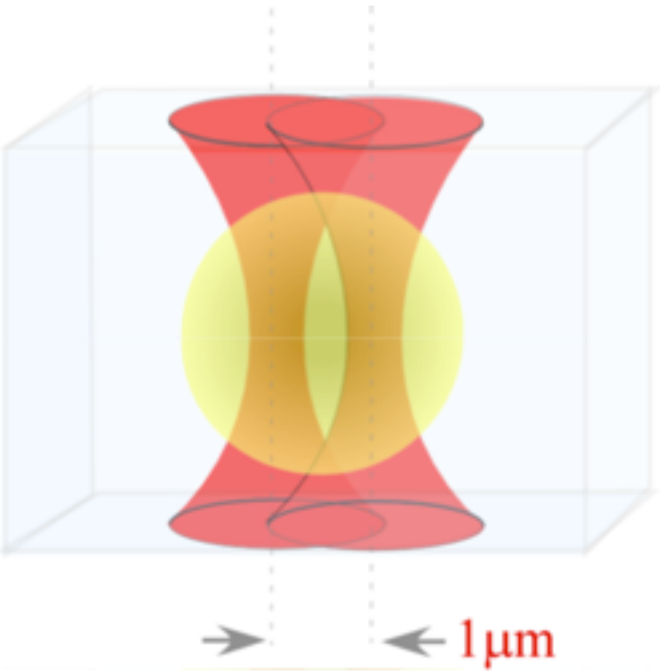

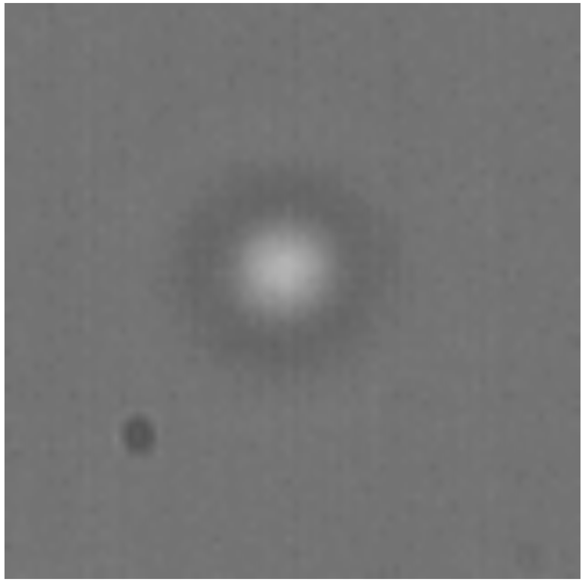

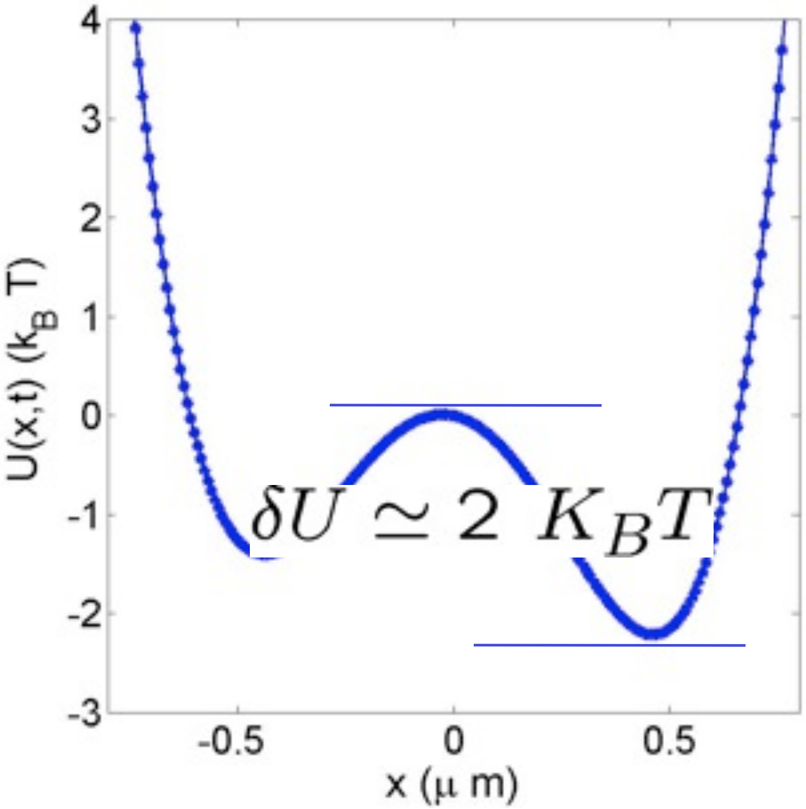

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$$r_k = \tau_o^{-1} \exp(-\frac{\delta U}{k_B T})$$

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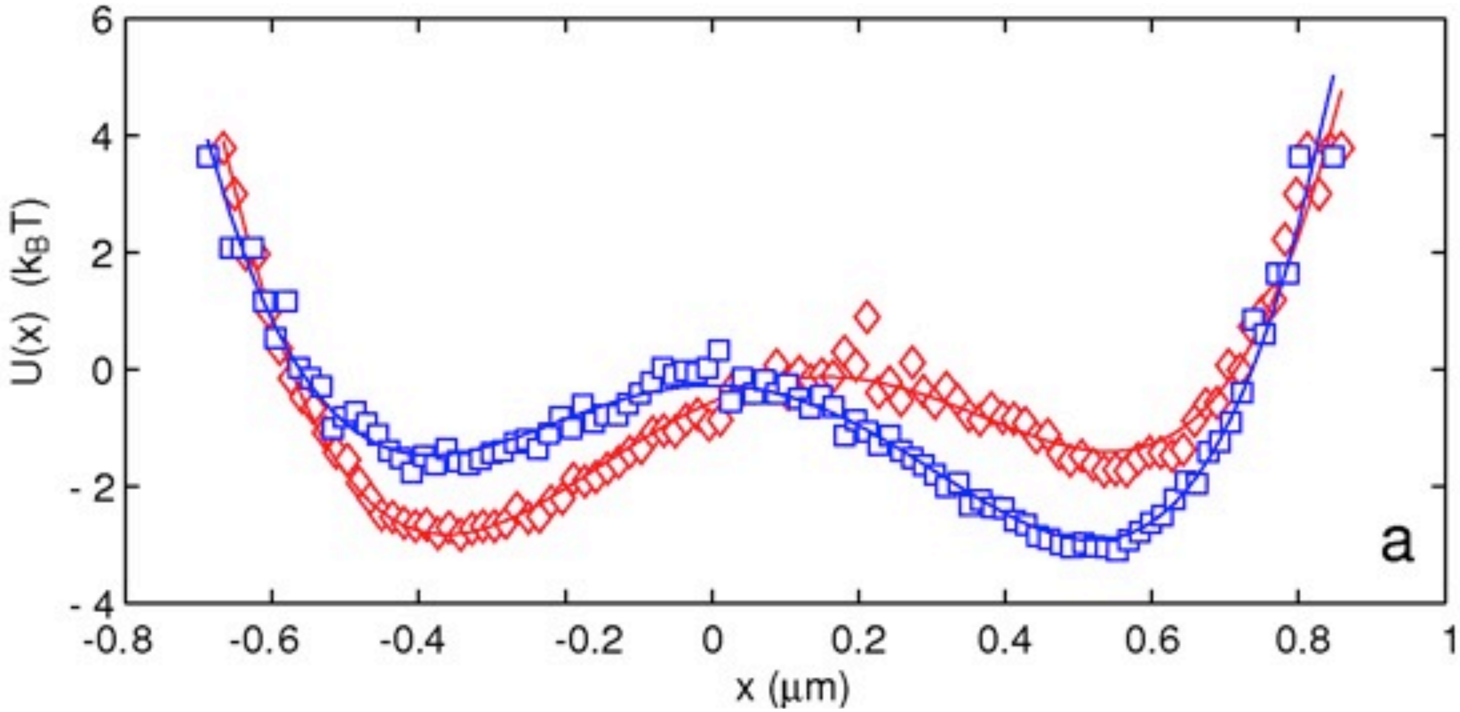
The non linear potential



Kramer rate

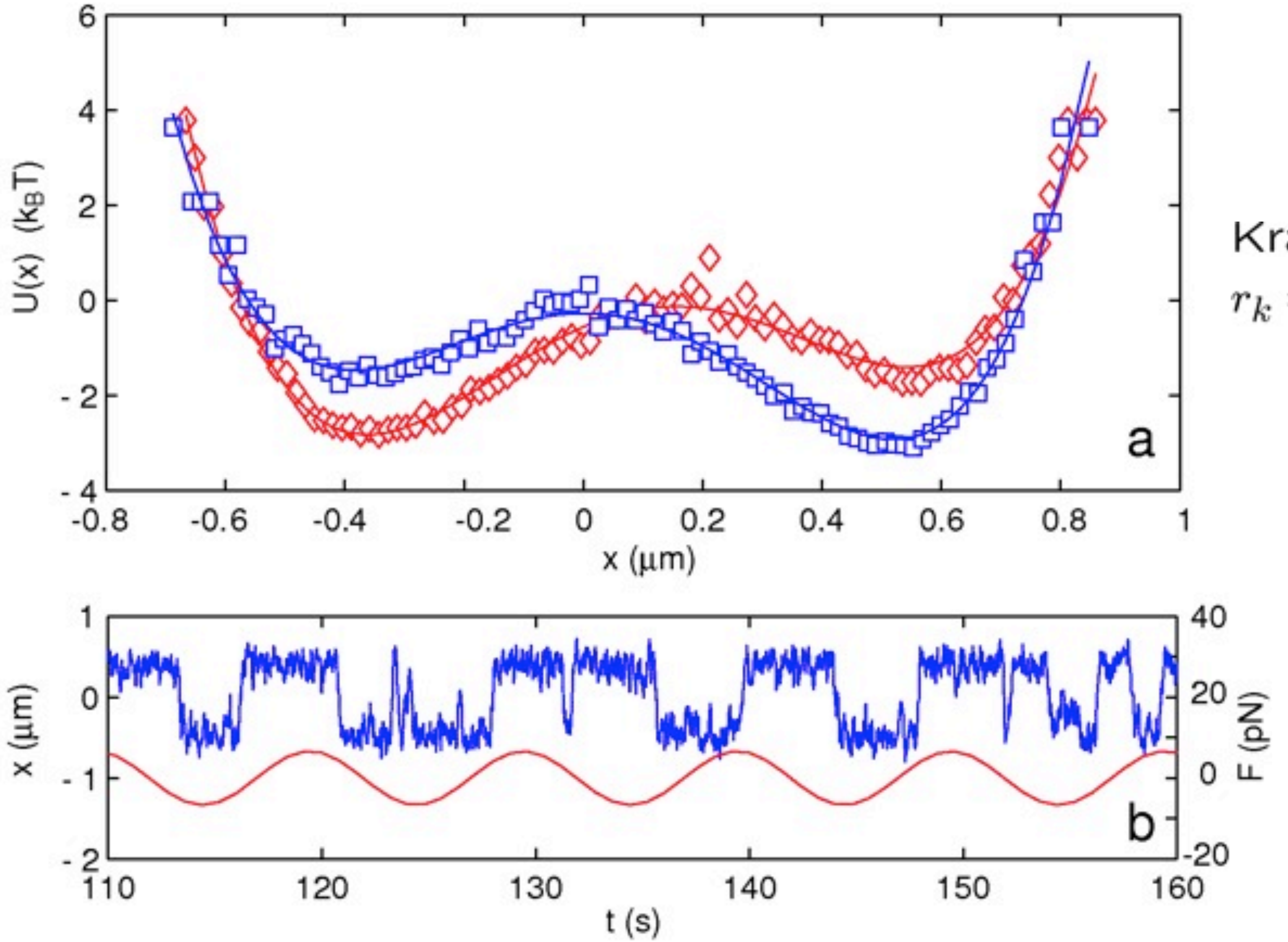
$r_k = \tau_o^{-1} \exp(-\frac{\delta U}{k_B T})$

$$U_0(x) = ax^4 - bx^2 - dx$$

$$U(x,t) = U_0(x) + U_p(x,t) = U_0 + c\ x\ \sin(2\pi f t),$$

with $ax_{min}^4 = 1.8\ k_B T$, $bx_{min}^2 = 3.6\ k_B T$, $d|x_{min}| = 0.44\ k_B T$, $c|x_{min}| = 0.81\ k_B T$ and $x_{min} = \pm 0.45 \mu m$

The non linear potential



Kramer rate

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

f=0.1Hz

At $f \simeq r_k$ the hops of the particle synchronise with the external forcing

Stochastic Resonance

At $f \simeq r_k$ the hops of the particle synchronise with the external forcing

Stochastic Resonance

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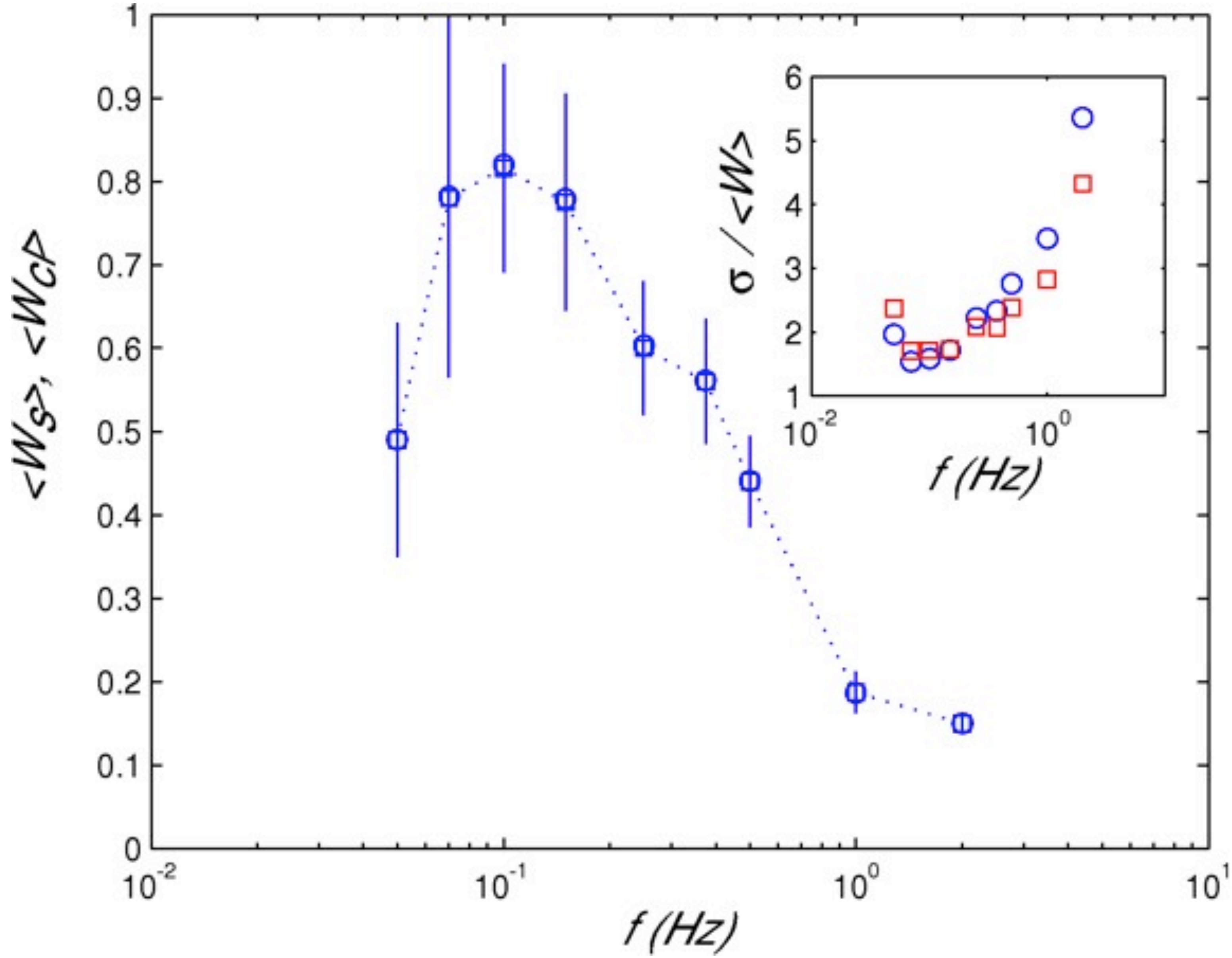


Fluctuations of W and Q at Stochastic Resonance

$$W_s[x(t)] = \int_{t_0}^{t_0+t_f} dt \frac{\partial U(x,t)}{\partial t}$$

- Stochastic work

$$W_{cl}[x(t)] = -\int_{t_o}^{t_o+t_f} dt\dot{x}\frac{\partial U_p(x,t)}{\partial x}$$

- Classical work

$$Q[x(t)] = -\int_{t_0}^{t_o+t_f} dx \frac{\partial U(x,t)}{\partial x}$$

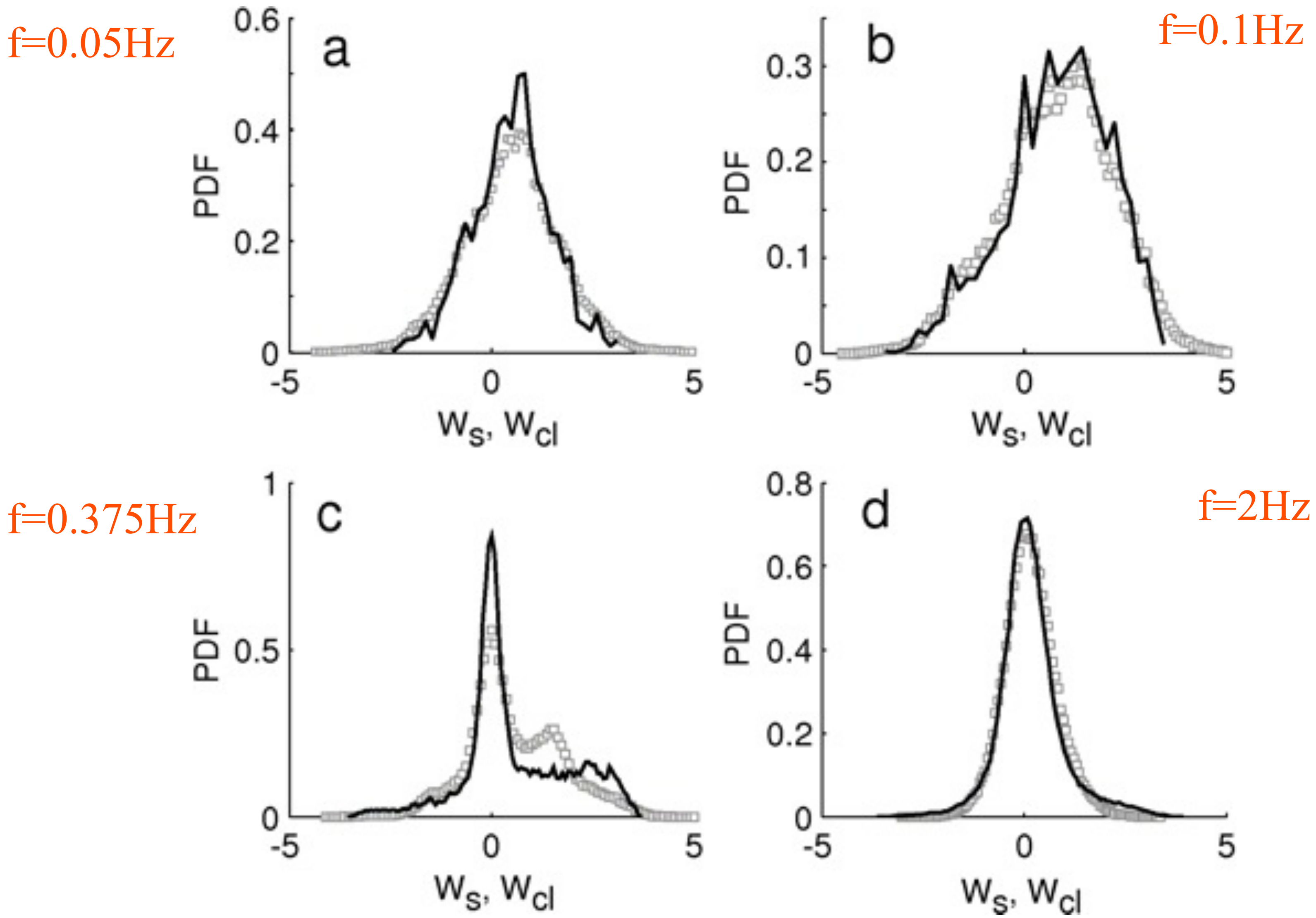
- Heat

$$Q = -\Delta U_0 + W_{cl} = -\Delta U + W_s$$

$$\frac{\Delta U}{T} = -k_B \ln\left(\frac{p(\theta(t_0+\tau),\lambda)}{p(\theta(t_0),\lambda)}\right)$$

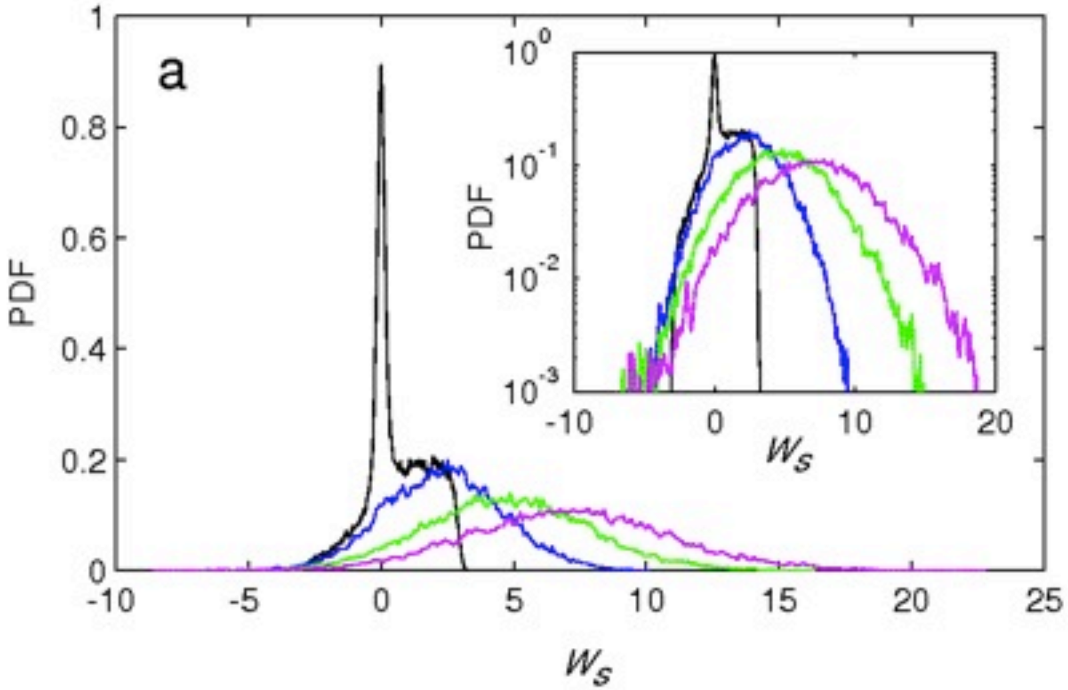
and $\frac{W_s}{T}$ is the total entropy.

PDF of the Work at various frequencies

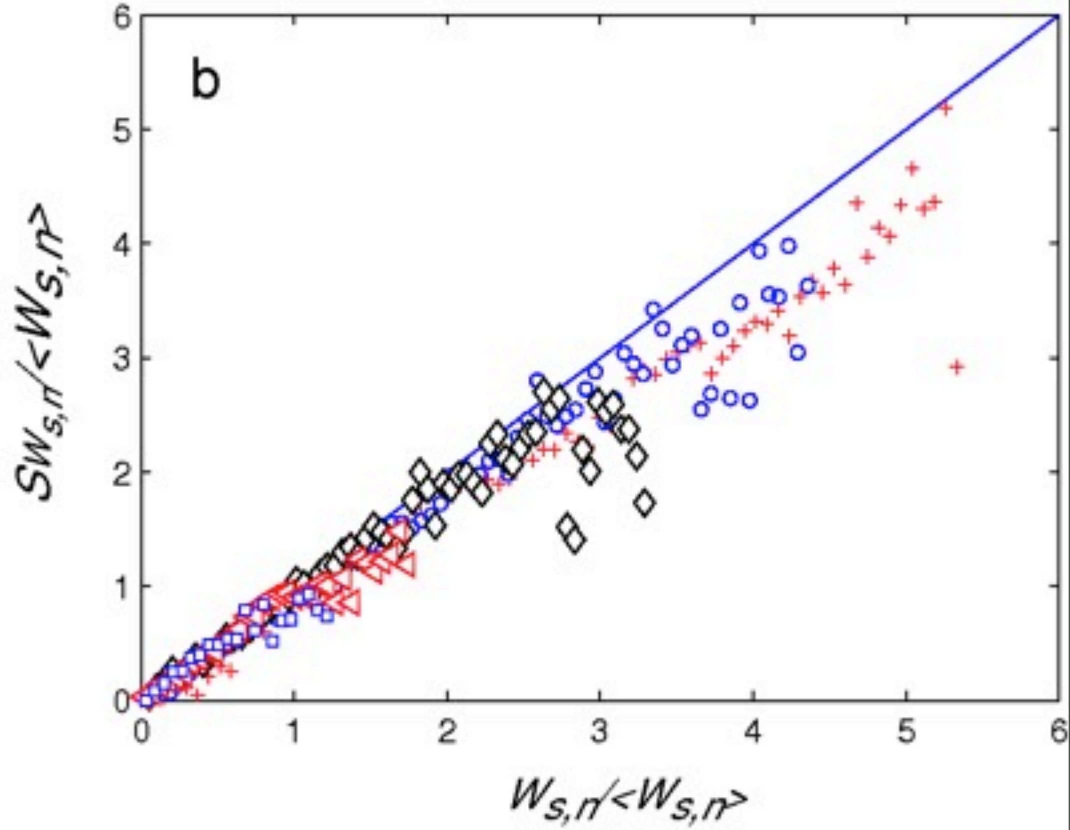


Fluctuation Theorem for Ws

f=0.25Hz

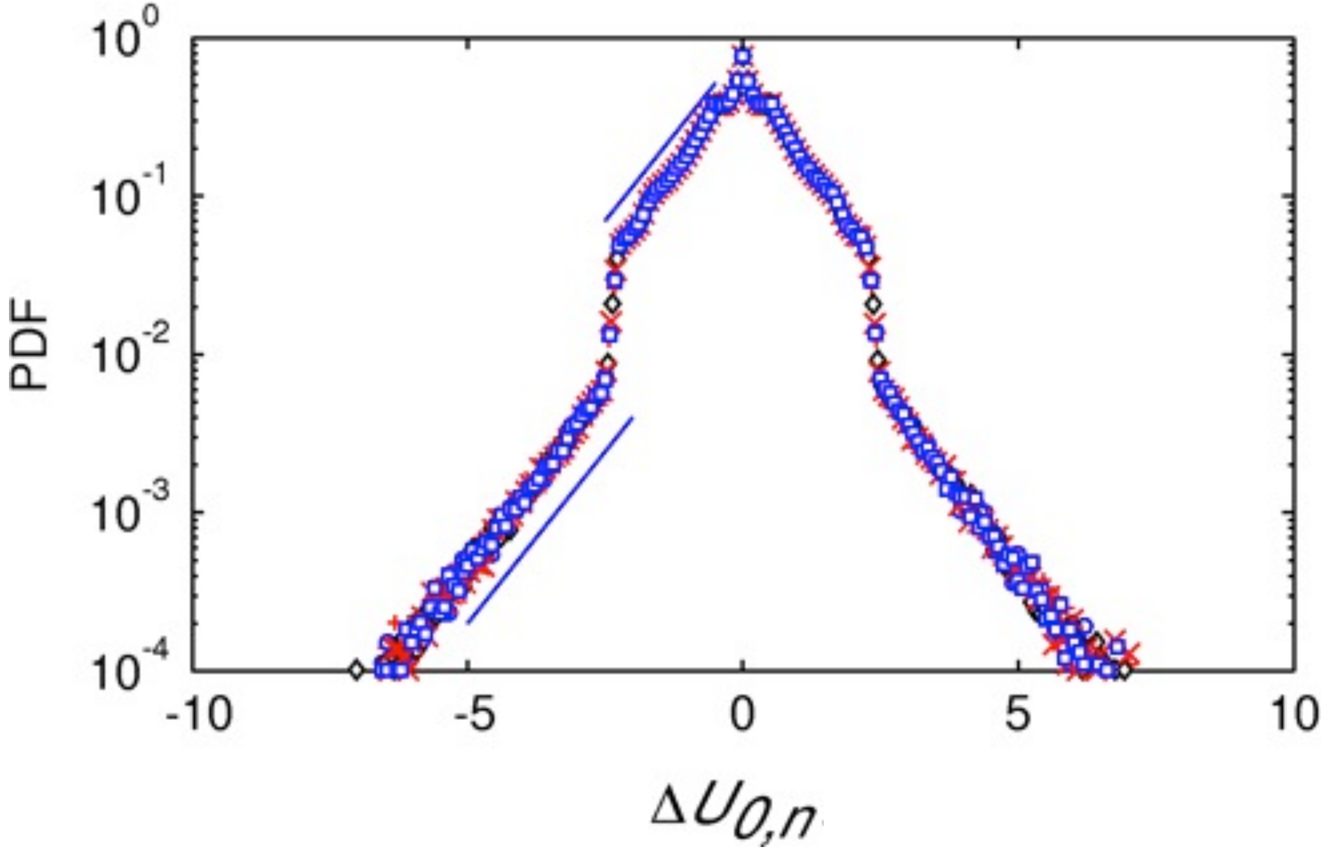


$n = 1,\ 4,\ 8$ and 12



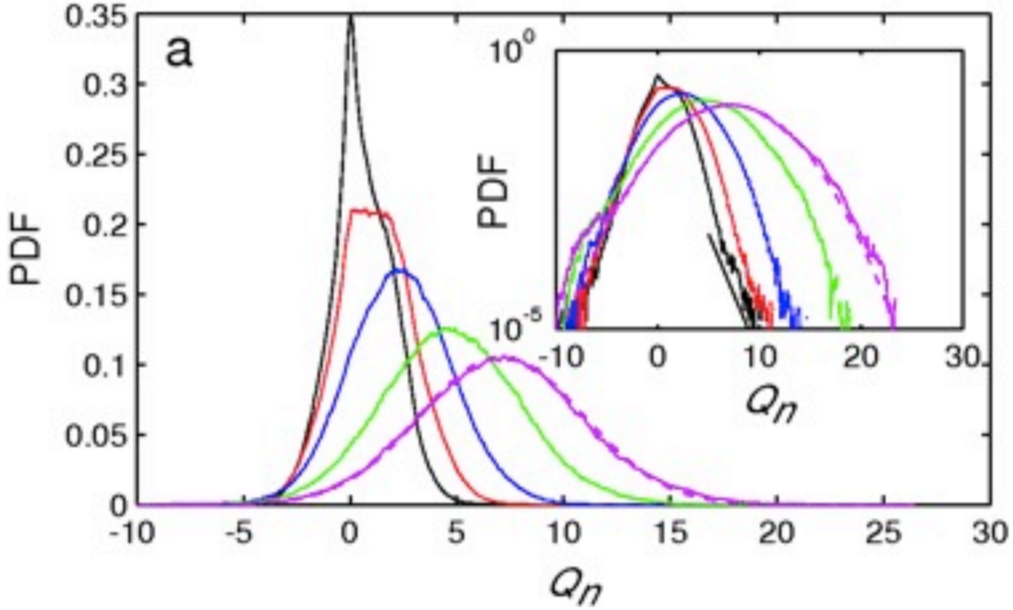
$n = 1\ (+),\ 2\ (\circ),\ 4\ (\diamond),\ 8\ (\triangle),\ 12\ (\square)$

PDF of ΔU

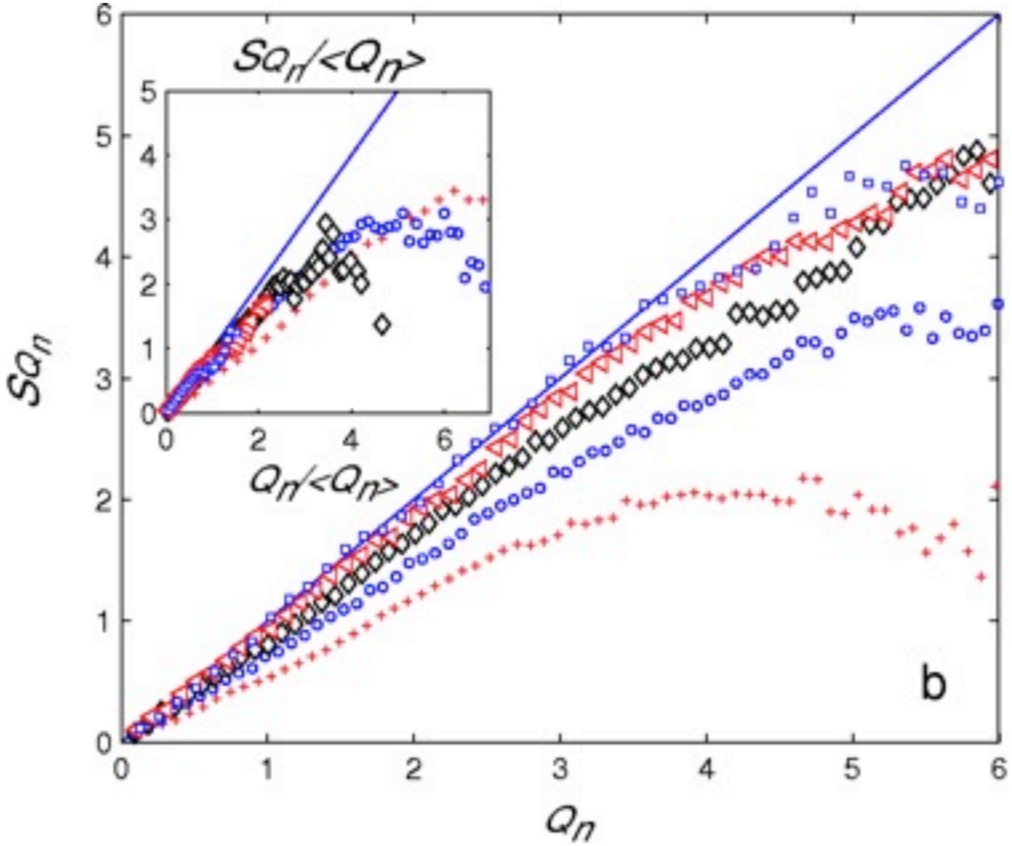


Fluctuation Theorem for Q

$$Q = \quad -\Delta U + W_s$$

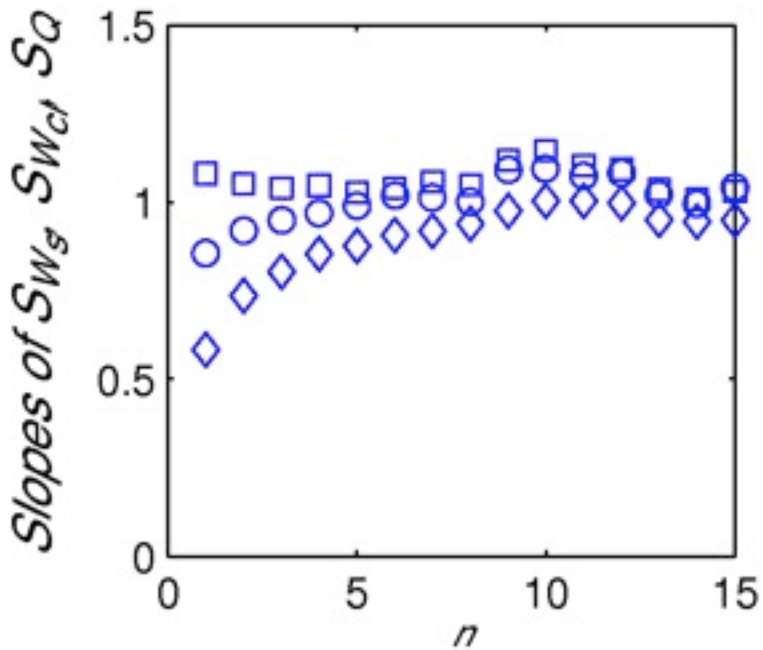


$n = 1,\ 4,\ 8$ and 12



$n = 1\ (+),\ 2\ (\circ),\ 4\ (\diamond),$
$8\ (\triangle),\ 12\ (\square)$

Slope at the origin



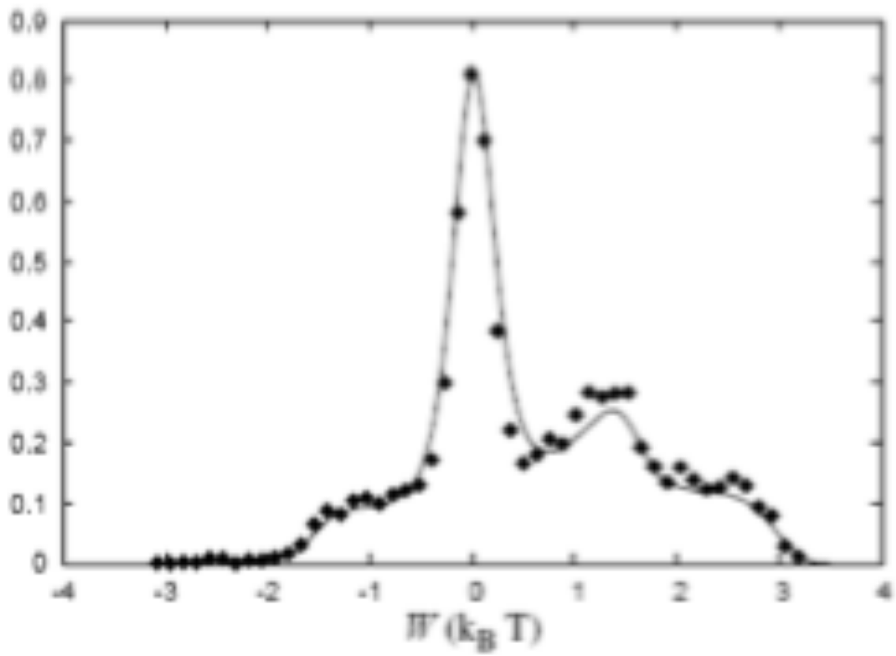
Slope at the origin of the symmetry functions of W_{sn} ($\circ$) ,W_{cln} ($\square$) and Q_n ($\diamond$) as function of n ($f = 0.25$ Hz).

Theoretical comparison I

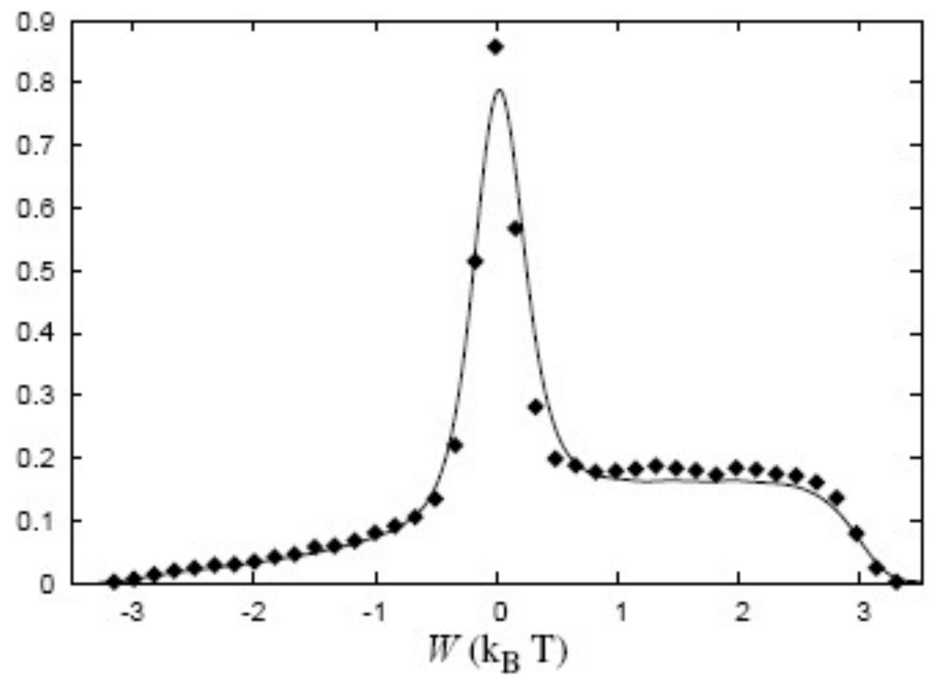
A. Imparato, P. Jop, A. Petrosyan and S. Ciliberto, J. Stat. Mech. (2008) P10017

PDF of the work computed on a single period :

(initial phase=0)



(averaged over different initial phases)

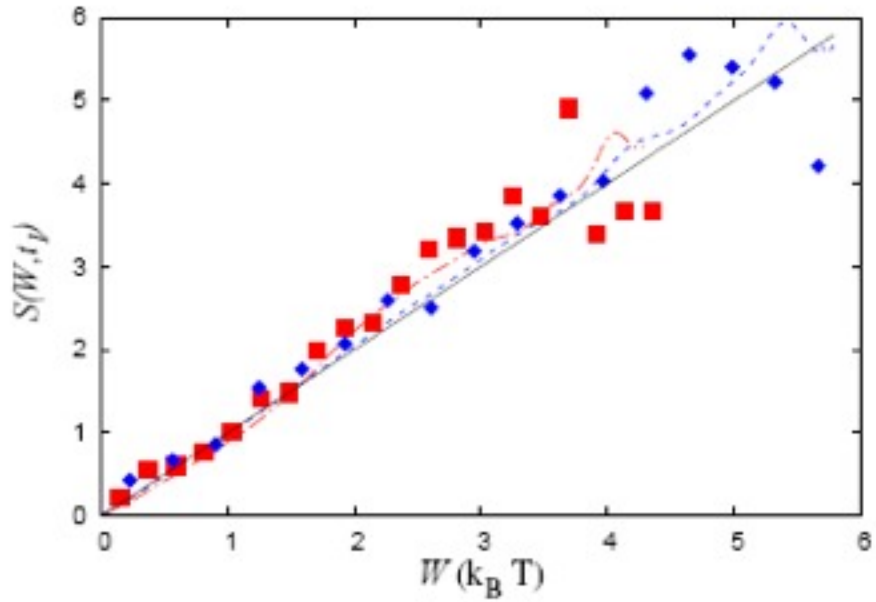


Experimental data

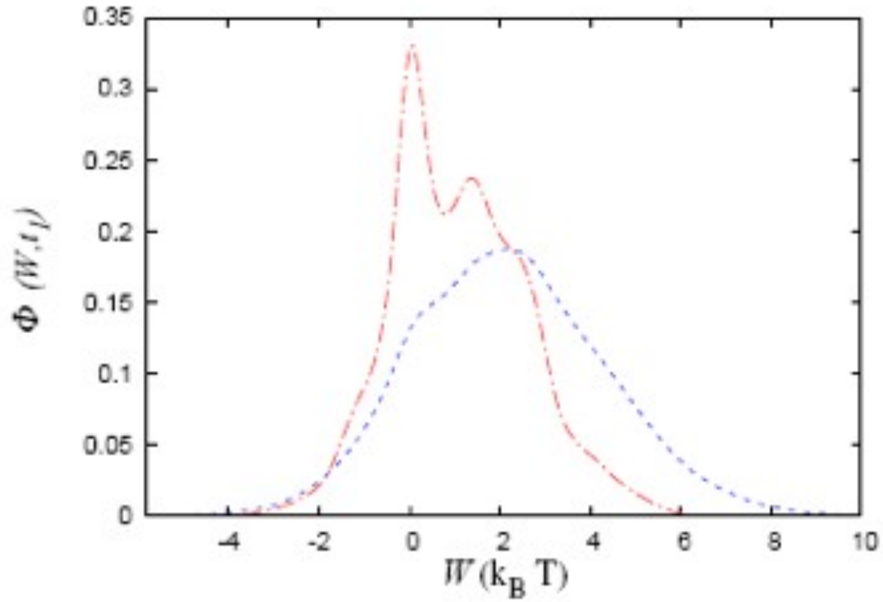
Theoretical prediction based on Fokker-Planck equation

Theoretical comparison II

Symmetry function for the work



PDF of the work



Symbols correspond to experimental data.

Lines to the numerical solution of Fokker-Planck equation.

□ , — · — $\tau = 2/f$

◊ , — · — $\tau = 4/f$

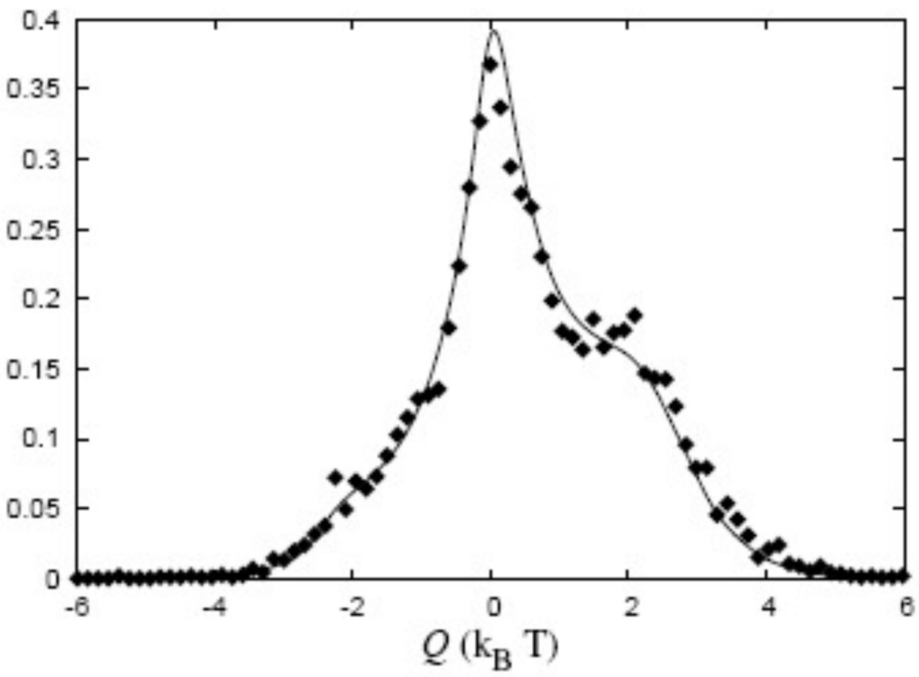
The full line corresponds to the expected behaviour S(W; t1) = W.

Theoretical comparison III

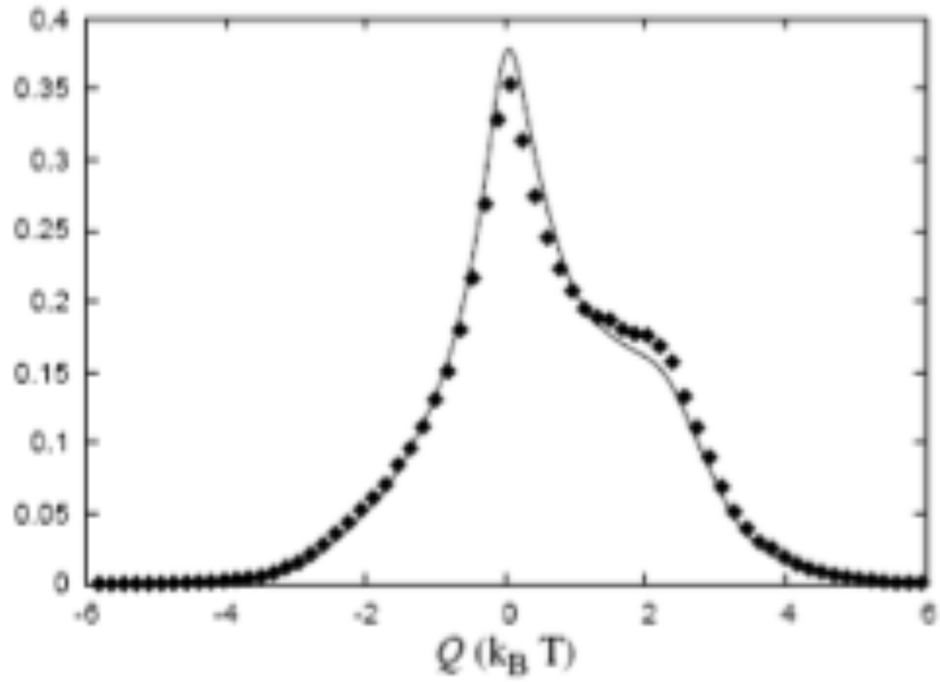
A. Imparato, P. Jop, A. Petrosyan and S. Ciliberto, J. Stat. Mech. (2008) P10017

PDF of the heat computed on a single period :

(initial phase=0)



(averaged over different initial phases)



♦ Experimental data

—— Theoretical prediction based on Fokker-Planck equation

Conclusions

•We have experimentally investigated the power injected in a bistable colloidal system by an external oscillating force.

•We find that the injected power presents a maximum when the frequency of the driving force corresponds to half of the Kramers' rate. (stochastic resonance)

•SSFT is valid for a non-linear potential.

•We have shown that FT rapidly converge to the asymptotic value for rather small n.

•The fact that for the total entropy FT is not satisfied exactly for small n is due to statistical and numerical inaccuracy.

• A theoretical description based on Fokker-Planck equation is in perfect agreeement with the experimental results

What is FT useful for ?

- Several interesting consequences of FT such as the Jarzinsky and Crooks equalities are useful to compute the free energy difference bewteen two equilibrium states using any kind of transformation

- Hatano-Sasa relation and the fluctuation dissipation theorem for non equilibrium steady states(NESS). These are useful to compute the response function of NESS

- FT allows the measure of tiny amount of heat exchange bewteen the system and its heat bath. (example: application to aging and biological systems)

- Measure of the offset of a variable

- Measure of the mean injected power.

Jarzynski equality

Consider a system whose energy is: $H(\Gamma, \lambda)$
Here $\lambda(t)$ is an externally controlled parameter.
We consider a transformation from an initial equilibrium state, $\lambda = A$ to another equlibrium state $\lambda = B$. Thus we have

$$H(\Gamma_r, B) - H(\Gamma_0, A) = W^J$$

where

$$W^J = \int_0^\tau dt \, \frac{d\lambda}{dt} \frac{\partial H}{\partial \lambda}$$

If ΔF is the free energy difference between the two equilibrium states A and B then the **Jarzynski Equality** (JE) states that:

$$< \exp(-\beta \, W^J) > = \exp(-\beta \Delta F)$$

If W^J has a Gaussian PDF then the JE takes a simple form:

$$\Delta F = < W^J > - \frac{\sigma_W^2}{2 \, K_B \, T}$$

Crooks identity

Crooks considered the forward (F) and reverse processes (R). During the F processes λ goes from A to B. During the R the inverse path is done.

Crooks derived the following identity:

$$\frac{P_F(W^J)}{P_R(-W^J)} = \exp(\frac{W^J - \Delta F}{K_B T}) = \exp(\frac{W_{dis}}{K_B T})$$

simple manipulation of this ratio and integration gives:

$$\int_{-\infty}^{\infty} P_F(W^J)\ \exp(-\frac{W^J}{K_B T})\ dW^j = \exp(-\frac{\Delta F}{K_B T})$$

which is the Jarzynski equality:

$$<\ \exp(-\beta\ W^J)\ > = \exp(-\beta \Delta F)$$

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$$< \ \exp(-\beta\ W^J)\ > = \exp(-\beta \Delta F)$$

The derivation has been argued by Cohen and Mauzerall cond-mat/0406128

The Jarzynski work

$$W^J = \int_0^\tau dt\, \frac{d\lambda}{dt}\, \frac{\partial H}{\partial \lambda}$$

$$W^J = -\int_0^\tau dt\, \frac{dx}{dt}\, F = -W^{cl}$$

$$W^J = -\int_0^\tau dt\, \frac{dF}{dt}\, x = -\Big[F\; x\Big]_0^{t_s} + W^{cl}$$

The Jarzynski work

$$W^J = \int_0^\tau dt\, \frac{d\lambda}{dt} \frac{\partial H}{\partial \lambda}$$

- What is the meaning of λ in a real experiment ?

$$W^J = -\int_0^\tau dt\, \frac{dx}{dt} F = -W^{cl}$$

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The Jarzynski work

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- What is the meaning of λ in a real experiment ?

Connections between the macroscopic variables and the microscopic ones

$$W^J = -\int_0^\tau dt \, \frac{dx}{dt} F = -W^{cl}$$

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- What is the quantity wich is controlled in an experiment ?

$$W^J = -\int_0^\tau dt \, \frac{dx}{dt} F = -W^{cl}$$

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$$W^J = \int_0^\tau dt \, \frac{d\lambda}{dt} \frac{\partial H}{\partial \lambda}$$

- What is the meaning of λ in a real experiment ?

Connections between the macroscopic variables and the microscopic ones

- What is the quantity wich is controlled in an experiment ?

If λ is a displacement x then:

$$W^J = -\int_0^\tau dt \, \frac{dx}{dt} \, F = -W^{cl}$$

If λ is a

$$W^J = -\int_0^\tau dt \, \frac{dF}{dt} \, x = -\Big[F \, x\Big]_0^{t_s} + W^{cl}$$

The classical work

$$W^J = -\int_0^{t_s} \dot{M}\theta \; dt = -\Big[M\theta\Big]_0^{t_s} + W^{\text{cl}},$$

where

$$W^{\text{cl}} = \int_0^{t_s} M\dot{\theta} \; dt$$

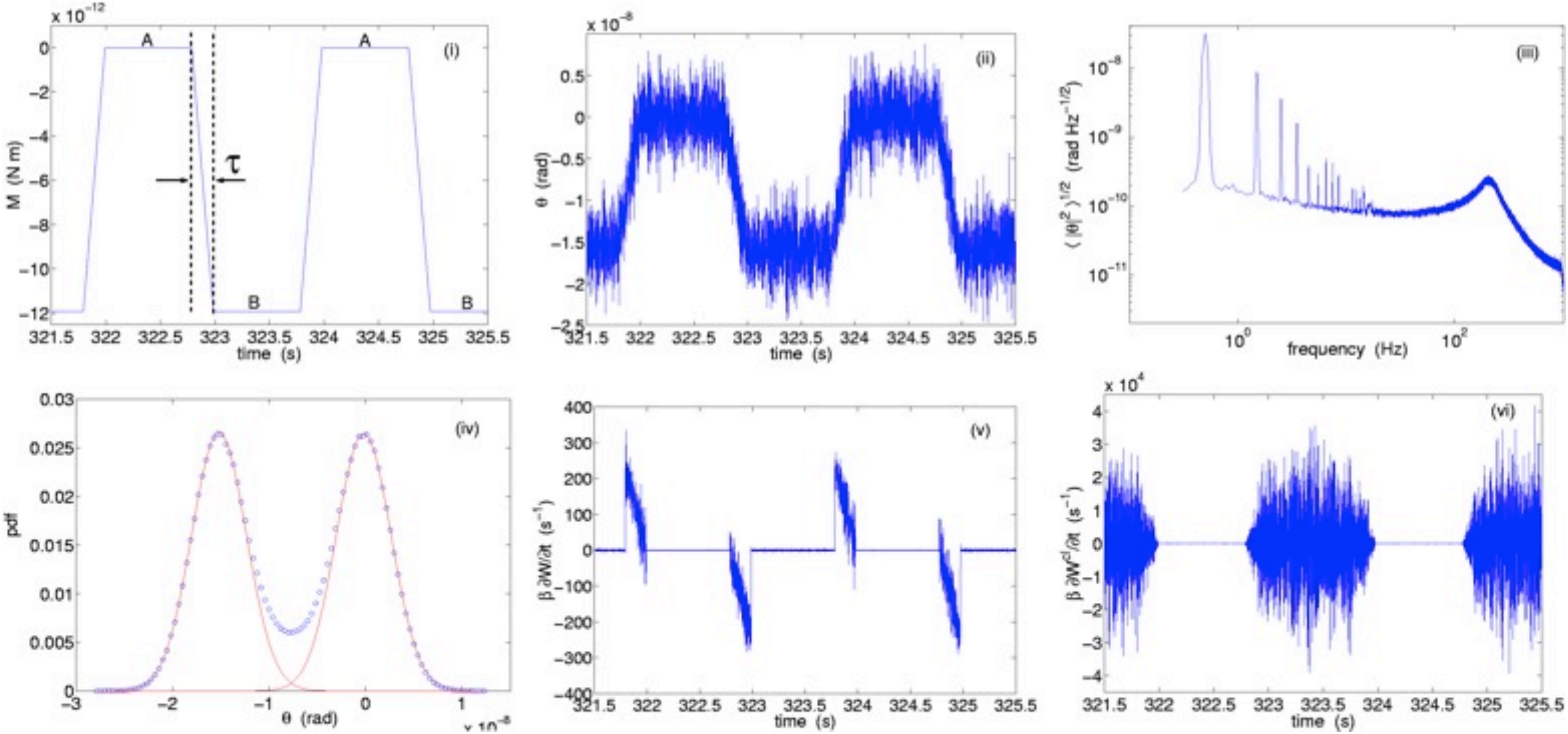
is the classical work

The ΔF computed by the JE in the case of a driven system, composed by the system Ξ plus the external driving, is the total free energy difference

$$\Delta F = \Delta F_0 - \Big[M\theta\Big]_A^B = \Delta F_0 - \Phi,$$

where ΔF_0 is the free energy of Ξ and $\Phi = \Big[M\theta\Big]_A^B$

Typical driving



Oscillator immersed in oil [case (a)]: (i) Applied external torque, (ii) Induced angular displacement, (iii) its psd, (iv) its pdf, (v) Injected power computed from the Jarzynski definition $\dot{W} = -\dot{M}\theta$, (vi) Injected power computed from the standard definition $\dot{W}^{\mathrm{cl}} = M\dot{\theta}$

The Free Energy for the torsion pendulum

The free energy difference of the oscillator alone is

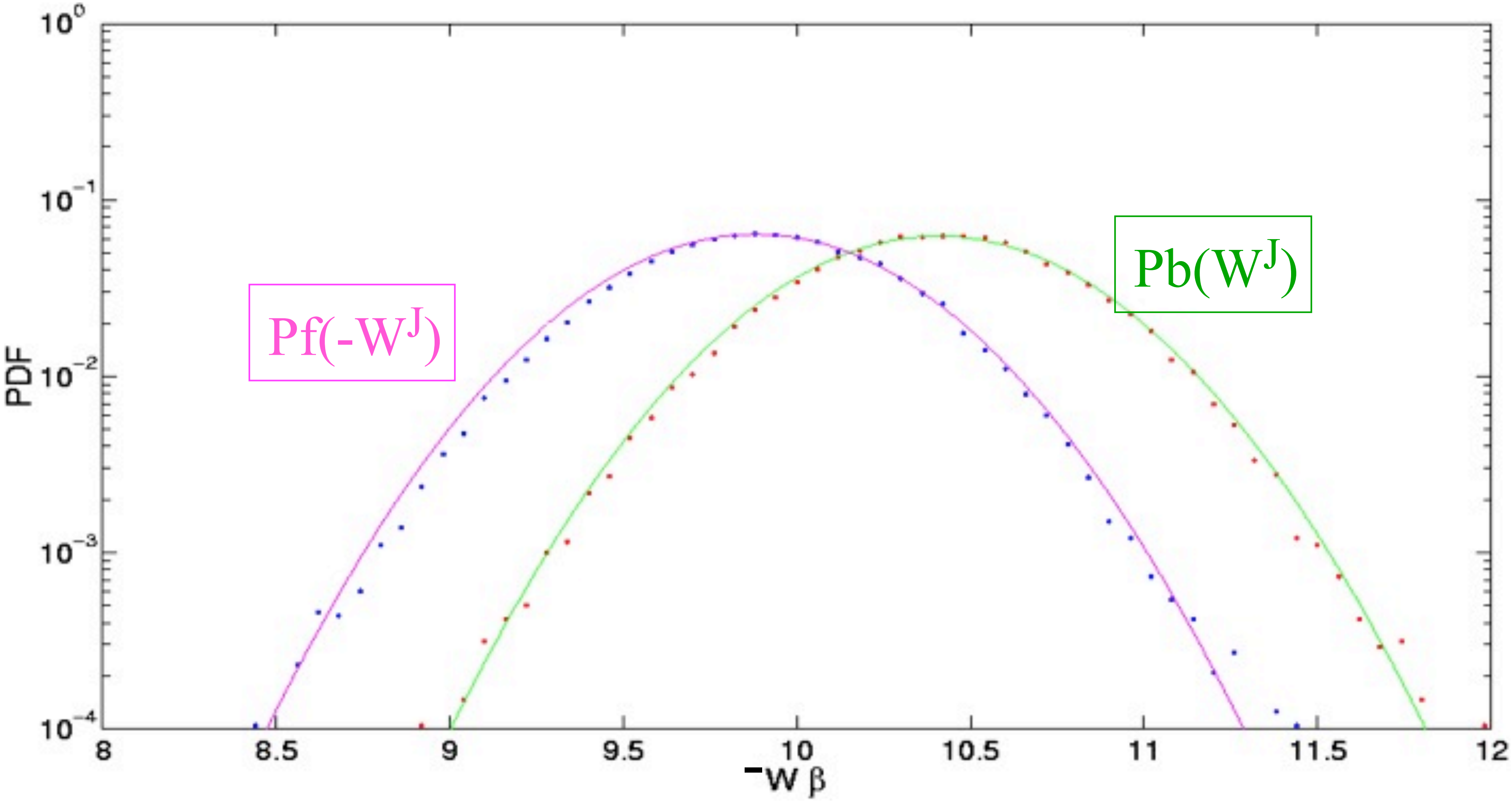
$$\Delta F_0 = \Delta U = \left[\frac{1}{2}C\theta^2\right]_A^B = \left[\frac{M^2}{2C}\right]_A^B,$$

whereas

$$\Delta F = \Delta F_0 - \left[\frac{M^2}{C}\right]_A^B,$$

i.e. for an harmonic potential $\Delta F = -\Delta F_0$.

Jarzynski Work PDF

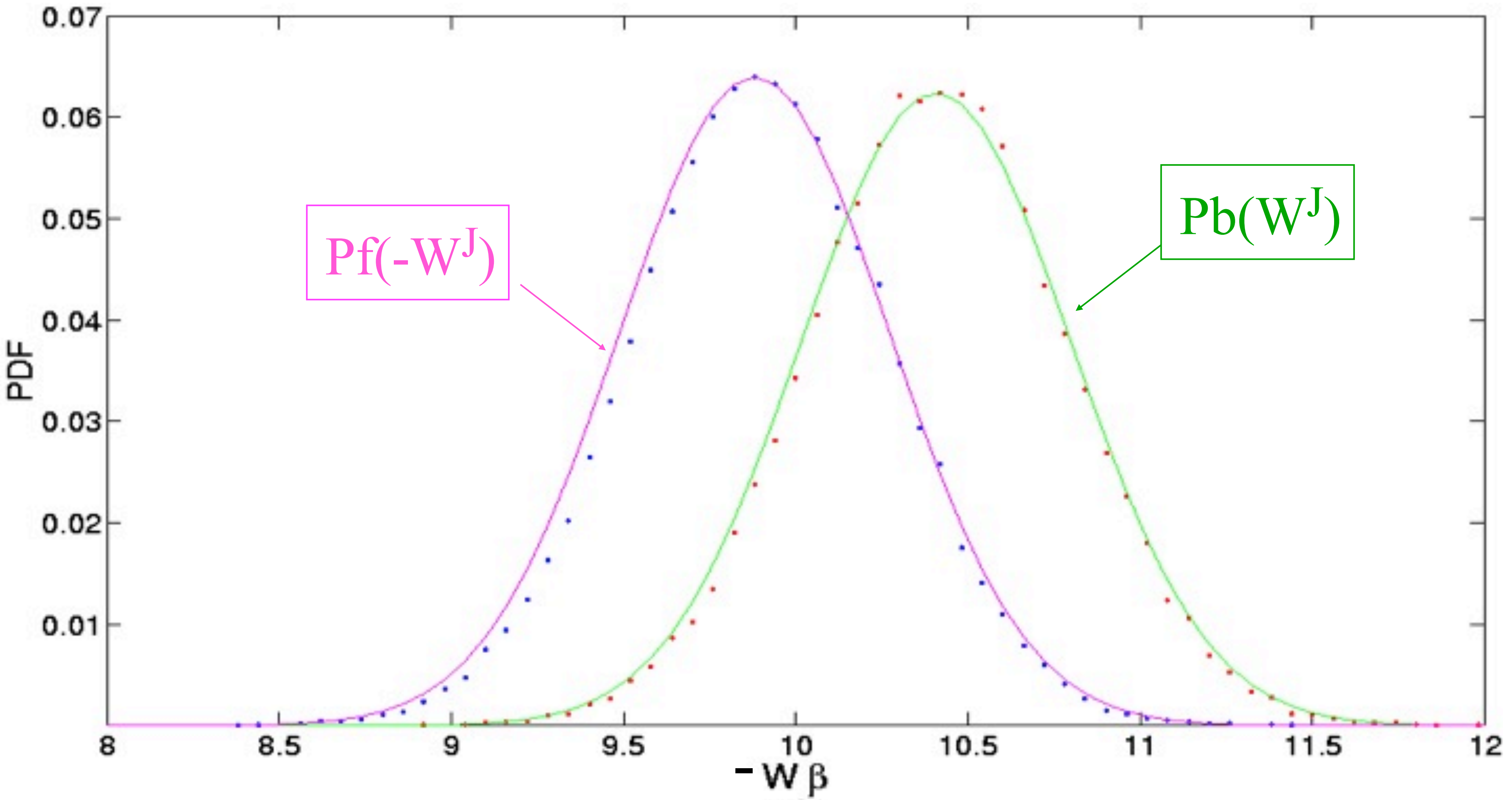


$\overline{W_f^J} = -9.88\ K_BT$, $\overline{W_b^J} = 10.40\ K_BT$, $\sigma_{W^J} = 0.45\ K_BT$

From the crossing point is $\Delta F = -10.15\ K_BT$

From JF $\Delta F \simeq -10.3\ K_BT$ and $\Delta F \simeq -10\ K_BT$

Jarzynski Work PDF

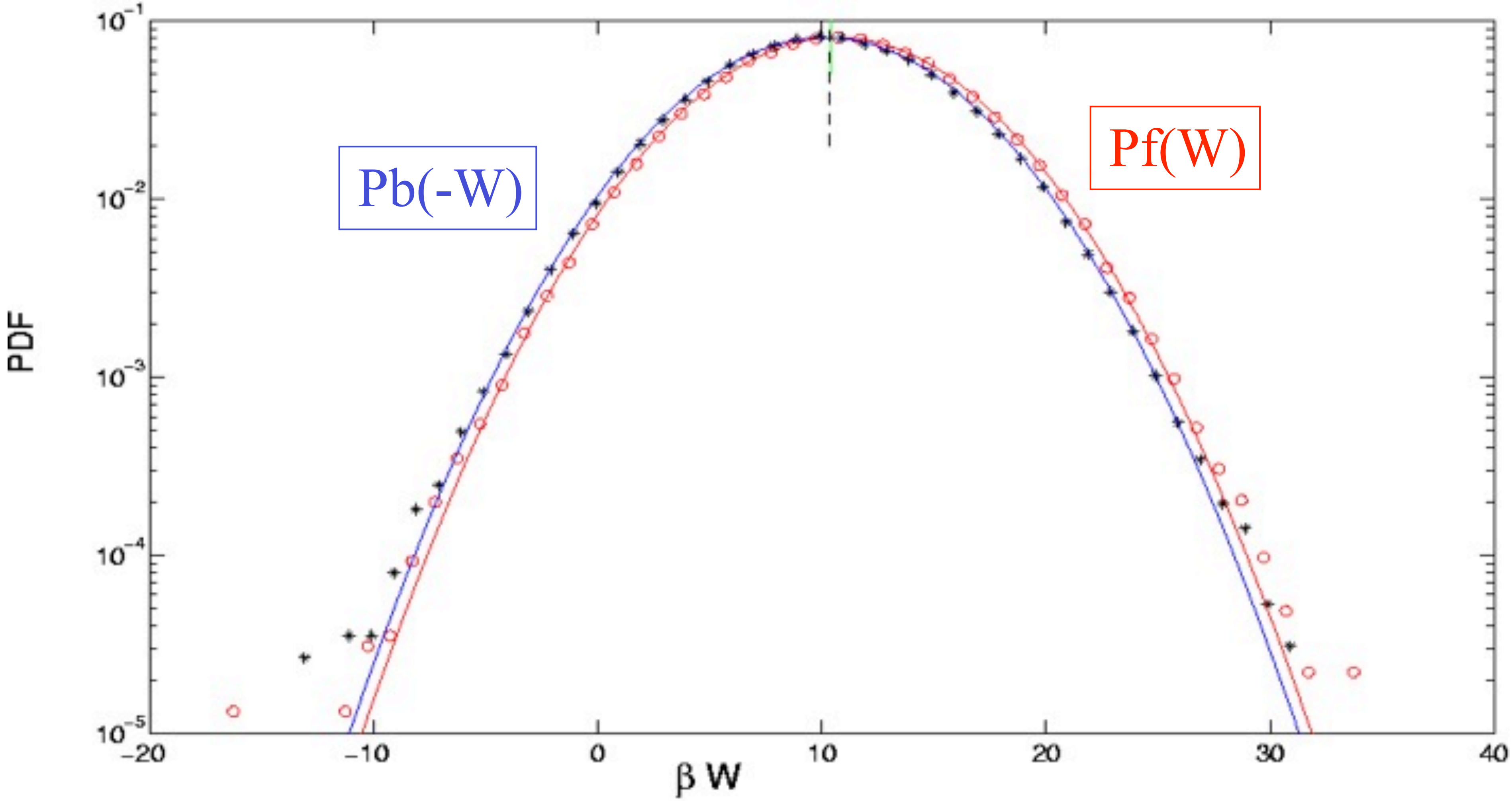


$\overline{W_f^J} = -9.88\ K_B T$, $\overline{W_b^J} = 10.40\ K_B T$, $\sigma_{W^J} = 0.45\ K_B T$

From the crossing point is $\Delta F = -10.15\ K_B T$

From JF $\Delta F \simeq -10.3\ K_B T$ and $\Delta F \simeq -10\ K_B T$

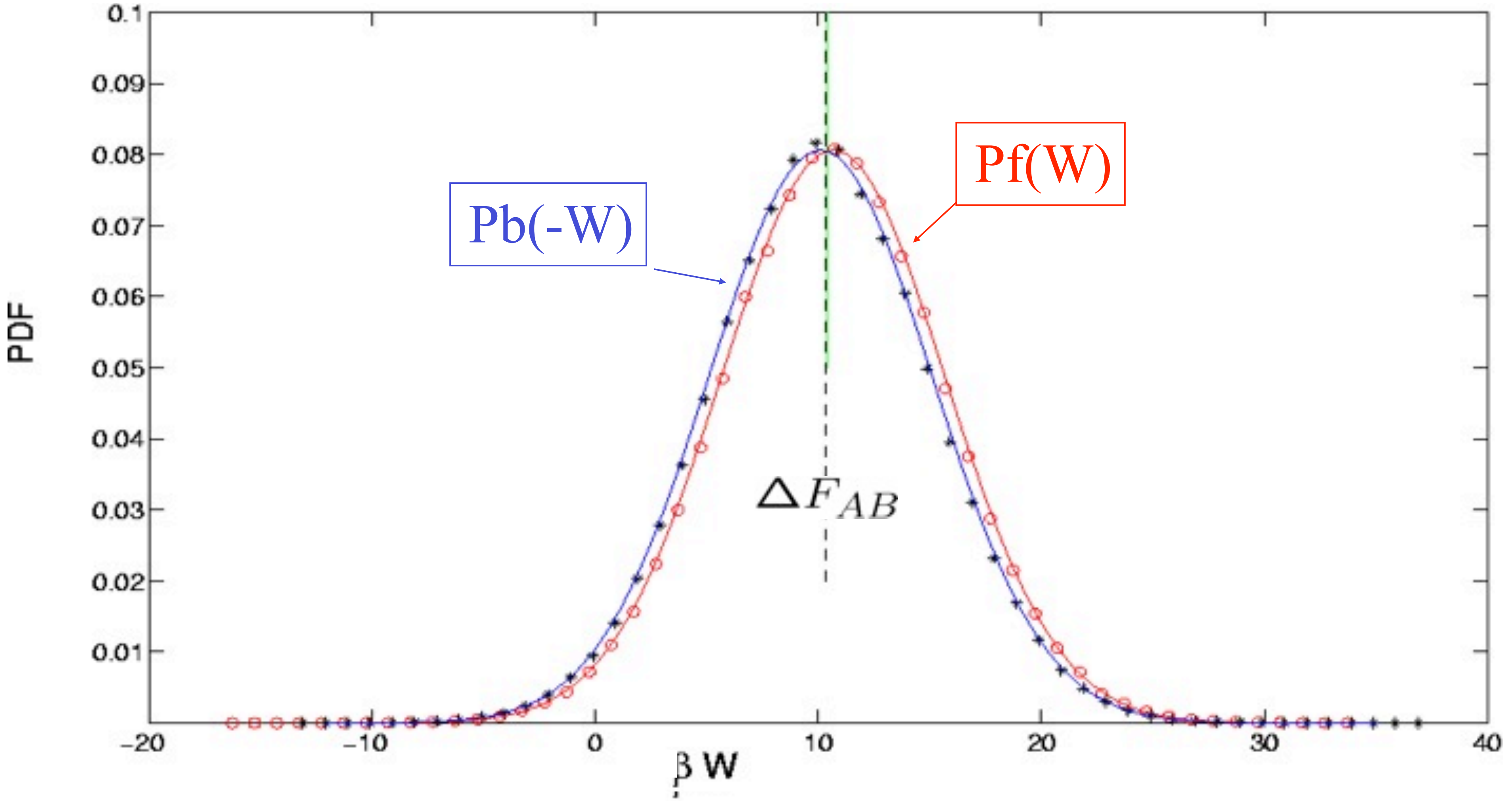
Classical Work PDF



$$\overline{W_f} = 10.67\ K_BT\ ,\ \overline{W_b} = -10.1\ K_BT,\ \sigma_W = 5\ K_BT$$

The crossing point of the PDF is the reversible work ΔF_{AB}

Classical Work PDF



$$\overline{W_f} = 10.67\ K_B T\ ,\ \overline{W_b} = -10.1\ K_B T,\ \sigma_W = 5\ K_B T$$

The crossing point of the PDF is the reversible work ΔF_{AB}

Crossing point of work Gaussian PDF

$$P_f(W) = A \ \exp\,[-\frac{(W - \overline{W_f})^2}{2\sigma^2}] \qquad (1)$$

$$P_b(-W) = A \ \exp\,[-\frac{(-W - \overline{W_b})^2}{2\sigma^2}] \qquad (2)$$

where $\overline{W_f} = \Delta F + \overline{W_{diss}}$ and $\overline{W_b} = -\Delta F + \overline{W_{diss}}$.

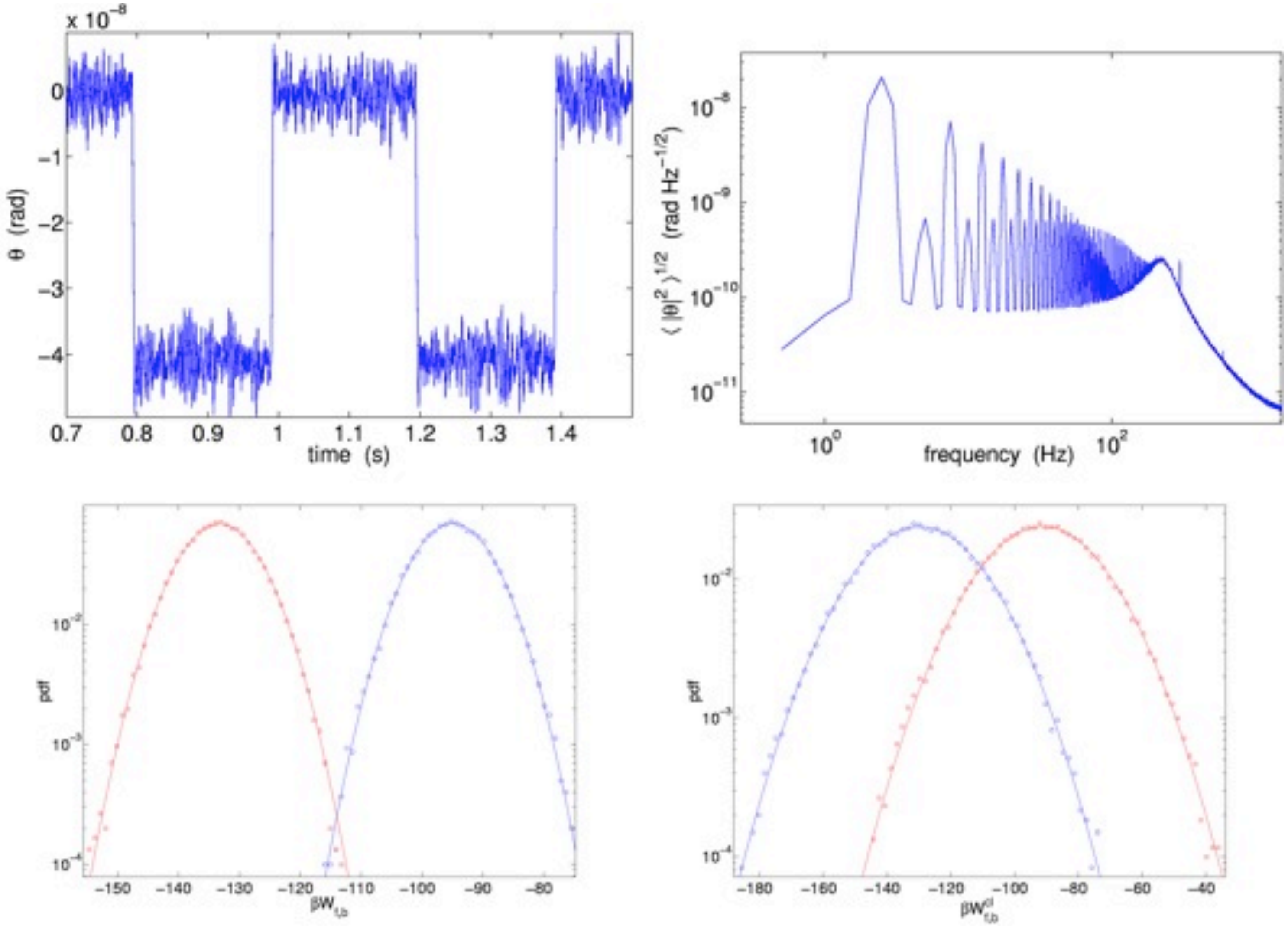
Let us now consider the ratio $P_f(W)/P_b(-W)$. From equations (1) and (2) we get:

$$\frac{P_f(W)}{P_b(-W)} = \exp\,[(\overline{W_f} + \overline{W_b})\ \frac{2\ W \ \ - (\overline{W_f} - \overline{W_b})}{2\sigma^2}] \qquad (3)$$

Thus the point W_o where $P_f(W_o) = P_b(-W_o)$ is:

$$W_o = \frac{(\overline{W_f} - \overline{W_b})}{2} = \Delta F$$

Large driving amplitude



(i) Time evolution of θ, (ii) Its psd $\sqrt{\langle|\widehat{\theta}|^2\rangle}$, (iii) $\mathrm{P_f}(W)$ and $\mathrm{P_b}(-W)$, (iv) $\mathrm{P_f}(W^{\mathrm{cl}})$ and $\mathrm{P_b}(-W^{\mathrm{cl}})$ (experimental forward and backward pdfs are represented by $\circ$ and $\square$ respectively, whereas the continuous lines are Gaussian fits)

τ/τ_{relax}	M_m	$-\beta[\Delta F_{\text{f}} + \Phi]$	$\beta[\Delta F_{\text{b}} + \Phi]$	$-\beta[\Delta F_{\times} + \Phi]$	$\beta W_{\times}^{\text{cl}}$	$\beta \Delta U$	$\lvert\beta \Delta F_{\circlearrowleft}\rvert$
8.5 a)	11.9	23.5	23.1	23.5	23.4	23.8	1.0
0.85 b)	6.1	6.6	6.1	6.0	6.6	6.1	1.0
3.5 c)	6.1	6.1	5.9	6.5	6.1	6.1	0.4
2.8 d)	4.2	2.8	2.6	3.2	2.9	2.7	0.3
4.2 e)	1.2	0.21	0.20	0.22	0.21	0.22	0.04
0.11 f)	11.8	33	30.8	32.54	31.15	31.4	3.6
0.11 g)	22.1	117.6	110.5	114	110.1	111	15.1
0.07 h)	5.9	10.3	10.0	10.1	10.1	10.3	0.4
0.07 i)	9.4	67.4	65.5	66.8	66.4	67.5	2.4

Values of the free energies for various times and driving amplitudes (the values of M_m are in pN m). $\Delta U = \frac{M_m^2}{2C}$ is the computed expected value. Notice that $C = 7.5\times10^{-4}$ N m rad^{-1} for cases a)-e), $C = 5.5\times10^{-4}$ N m rad^{-1} for cases f)-g) and $C = 1.6 \times 10^{-4}$ N m rad^{-1} for cases h)-i)

Conclusions

- We have experimentally perturbed an harmonic oscillator very close to equilibrium.

- We have computed and measured the finite time corrections for SSFT and TFT.

- Different methods to measure the reversible part of the work done by an external force has been checked.

- The Jarzynski equality gives reliable results within experimental errors in the case when work fluctuations are Gaussian and FDT is still valid.

- The crossing point of the 'classical work PDF' gives the best estimation of ΔF when the W^{cl} PDF are Gaussian.

JE and Langevin dynamics

If one considers the experimental observations that:
The thermal noise amplitude and statistics are not modified by the presence of the large forcing
Then it is easy to show that:

- For the Langevin equation the JE is always satisfied independently of driving torque amplitude and rising time.

- The relative width $|\sigma_W/\langle W\rangle|$ of P(W) decreases as $1/M_m$.

From a practical point of view, this means that when $\Delta F \gg k_B T$ the pdfs will never cross, for reasonable values of the work PDF.

TFT and JE

$$< \exp(-\beta \Delta F) >= < \exp(-\beta\ W) >= \int_{-\infty}^{\infty} \exp(-\beta\ W) P(W) dW$$

TFT and JE

$$< \exp(-\beta \Delta F) >= < \exp(-\beta\ W) >= \int_{-\infty}^{\infty} \exp(-\beta\ W) P(W) dW$$

If $P(W)$ satisfies TFT then

$$\int_{-\infty}^{\infty} \exp(-\beta\ W)\ P(W)\ dW = \int_{-\infty}^{\infty} \exp(-\beta\ W)\ P(-W)\ \exp(\beta W)\ dW = 1$$

TFT and JE

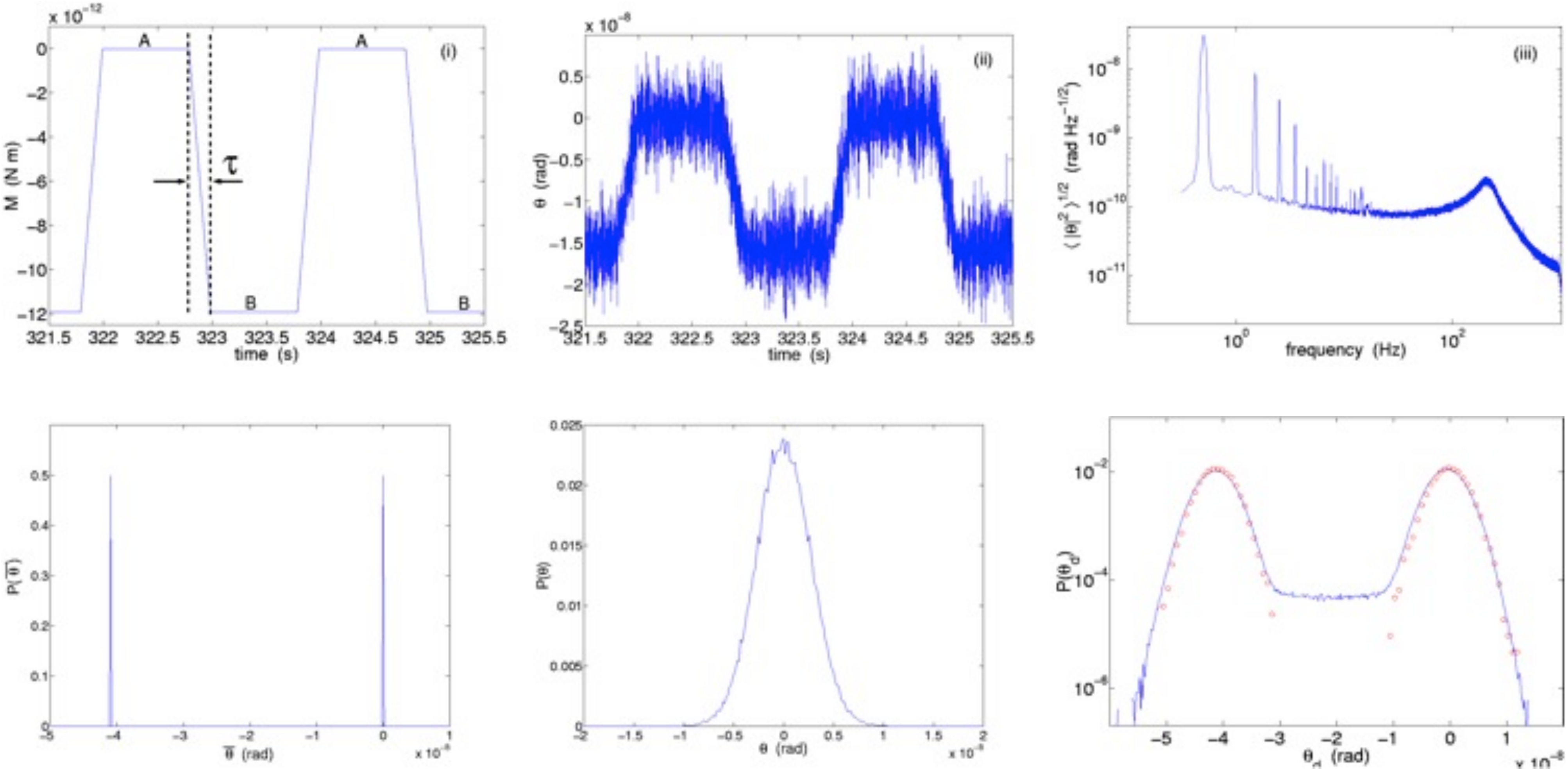
$$< \exp(-\beta \Delta F) > = < \exp(-\beta\ W) > = \int_{-\infty}^{\infty} \exp(-\beta\ W) P(W) dW$$

If $P(W)$ satisfies TFT then

$$\int_{-\infty}^{\infty} \exp(-\beta\ W)\ P(W)\ dW = \int_{-\infty}^{\infty} \exp(-\beta\ W)\ P(-W)\ \exp(\beta W)\ dW = 1$$

If W satisfies TFT then it does not satisfy JE.

PDF of θ with and without driving



In the experiment the statistical properties of the thermal fluctuations $\delta\theta$ are not modified by the driving. Therefore

$$\theta = \overline{\theta} + \delta\theta \qquad \text{and} \qquad W = \overline{W} + \delta W$$

Langevin Equation for the mechanical experiment

Our experiment is well described by:

$$I_{\text{eff}}\,\ddot{\theta} + \int_{-\infty}^{t} G(t-t')\,\dot{\theta}(t')\mathrm{d}t' + C\theta = M,$$

where G is the memory kernel.

In the case of viscous damping:

$$I_{\text{eff}}\,\ddot{\theta} + \nu\,\dot{\theta} + C\,\theta = M(t) + \eta,$$

where η is the thermal noise amplitude.

For $M(t)$ we consider the kind of waveform used in the experiments:

$$M(t) = \begin{cases} \frac{M_m\,t}{\tau_r} & \text{for } 0 < t < \tau, \\ M_m & \text{for } t > \tau_r. \end{cases}$$

The statistical properties of the thermal fluctuations $\delta\theta$ are not modified by the driving.

$$\theta = \overline{\theta} + \delta\theta \qquad and \qquad W_\tau = \overline{W_\tau} + \delta W_\tau$$

with

$$\overline{W}_\tau = \frac{1}{k_B T} \int_{t_i}^{t_i+\tau} \left[M(t) - aM(t_i)\right] \frac{d\overline{\theta}}{dt} dt \,,$$

$$\delta W_\tau = \frac{1}{k_B T} \int_{t_i}^{t_i+\tau} [M(t) - aM(t_i)] \frac{d\delta\theta}{dt} dt$$

with $a = 1$ for the ramp forcing or $a = 0$ for sinusoidal driving.

As the PDF of W is Gaussian then we need only $\langle W \rangle$ and σ_W^2

$$\langle W \rangle = \overline{W}$$

and

$$\sigma^2 \;=\; \frac{1}{(k_B T)^2} \frac{M_0^2}{\tau_r^2} \left[\tau^2 \langle \delta\theta^2(\tau) \rangle + \langle \left(\int_0^\tau \delta\theta(t) dt \right)^2 \rangle - 2\tau \int_0^\tau \langle \delta\theta(\tau) \delta\theta(t) \rangle dt \right].$$

The overdamped case

$$U(\theta) = \frac{1}{2} C\ \theta^2 - \ M\ \theta$$

$$\dot{\theta} + \tau_0^{-1}\,\theta = (C\,\tau_0)^{-1}(M + \eta), \qquad (1)$$

where $\tau_0 = \nu / C$. If η is a white noise of variance $2k_B T$, then when $M = 0$ the correlation function of the thermal fluctuations can be computed from FDT:

$$R_\theta(\delta\tau) = \frac{k_B T}{C} \exp\left(-\frac{|\delta\tau|}{\tau_0}\right).$$

The pdf of θ is Gaussian.

The Jarzynski work to drive the system from $A(M = 0)$ to $B\ (M = M_m)$ is

$$W = -\frac{M_m}{\tau}\int_0^\tau \theta\ dt$$

Thus to compute W we need only the solution of Eq.1 for $0 < t < \tau$. If we neglect the noise, then the mean solution is

$$\bar{\theta} = \frac{M_m}{\tau\, C}\left[t + \tau_0\ \exp\left(-\frac{t}{\tau_0}\right) - \tau_0\right] \qquad \text{for} \qquad 0 < t < \tau$$

We now consider that in the experiment the statistical properties of the thermal fluctuations $\delta\theta$ are not modified by the driving. Therefore

$$\theta = \overline{\theta} + \delta\theta.$$

and

$$W = \overline{W} + \delta W = -\frac{M_m}{\tau}\left[\int_0^\tau \overline{\theta}\ dt + \int_0^\tau \delta\theta\ dt\right].$$

As the PDF of W is Gaussian then to compute ΔF we need only $\langle W \rangle$ and σ_W^2

$$\langle W \rangle = \overline{W} = -\frac{M_m}{\tau}\int_0^\tau \overline{\theta}\ dt = -\frac{1}{C}\left(\frac{M_m}{\tau}\right)^2\left[\frac{(\tau-\tau_0)^2}{2} - \tau_0^2 \exp\left(-\frac{\tau}{\tau_0}\right) + \frac{{\tau_0}^2}{2}\right].$$

and

$$\sigma_W^2 = \langle (\delta W)^2 \rangle = (M_m/\tau)^2 \langle y^2(\tau) \rangle \quad \text{where}$$

$$y(\tau) = \int_0^\tau \delta\theta\ dt.$$

The variance of y can be computed taking into account that

$$\langle y^2(\tau)\rangle = \int_0^\tau \int_0^\tau R_\theta(t_1 - t_2)\ dt_1\ dt_2.$$

Using this equation we get

$$\sigma_W^2 = \left(\frac{M_m}{\tau}\right)^2 \langle y^2(\tau)\rangle = \frac{2k_B T\tau_0}{C}\left(\frac{M_m}{\tau}\right)^2 \left[\tau - \tau_0 + \tau_0 \exp\left(-\frac{\tau}{\tau_0}\right)\right].$$

Taking into account that fluctuations of W are Gaussian

$$\Delta F = \langle W\rangle - \frac{\sigma_W^2}{2k_B T} = -\frac{M_m^2}{2C},$$

that is the expected value.

The variance of y can be computed taking into account that

$$\langle y^2(\tau)\rangle = \int_0^\tau \int_0^\tau R_\theta(t_1 - t_2)\; dt_1\; dt_2.$$

Using this equation we get

$$\sigma_W^2 = \left(\frac{M_m}{\tau}\right)^2 \langle y^2(\tau)\rangle = \frac{2k_BT\tau_0}{C}\left(\frac{M_m}{\tau}\right)^2 \left[\tau - \tau_0 + \tau_0 \exp\left(-\frac{\tau}{\tau_0}\right)\right].$$

Taking into account that fluctuations of W are Gaussian

$$\Delta F = \langle W\rangle - \frac{\sigma_W^2}{2k_BT} = -\frac{M_m^2}{2C},$$

that is the expected value.

The same result is obtained when the inertial term is not negligible

Biological systems

Bustamante-Ritort

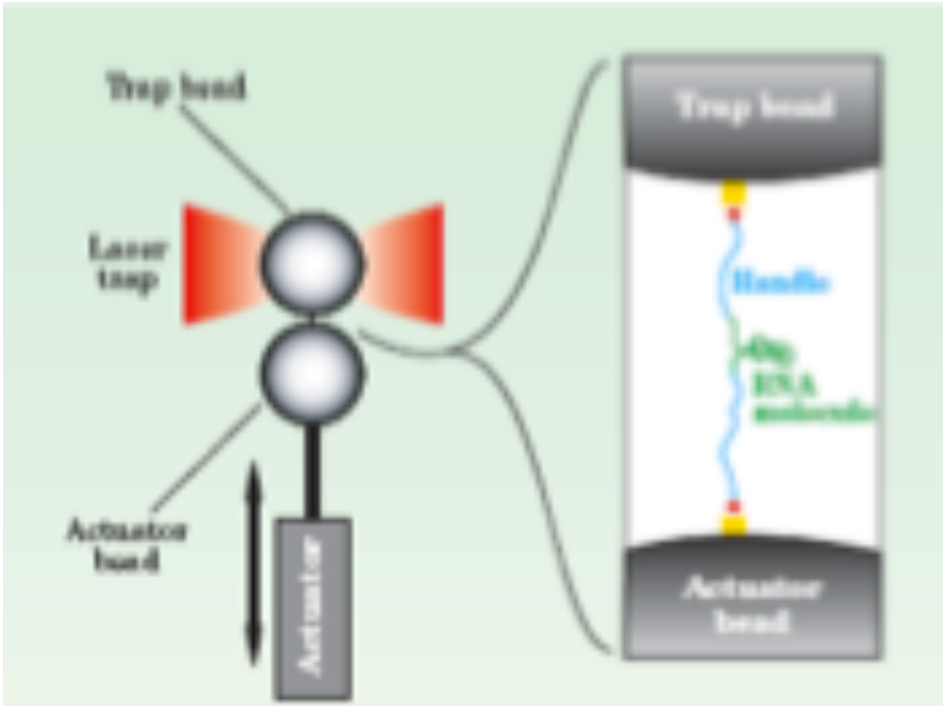
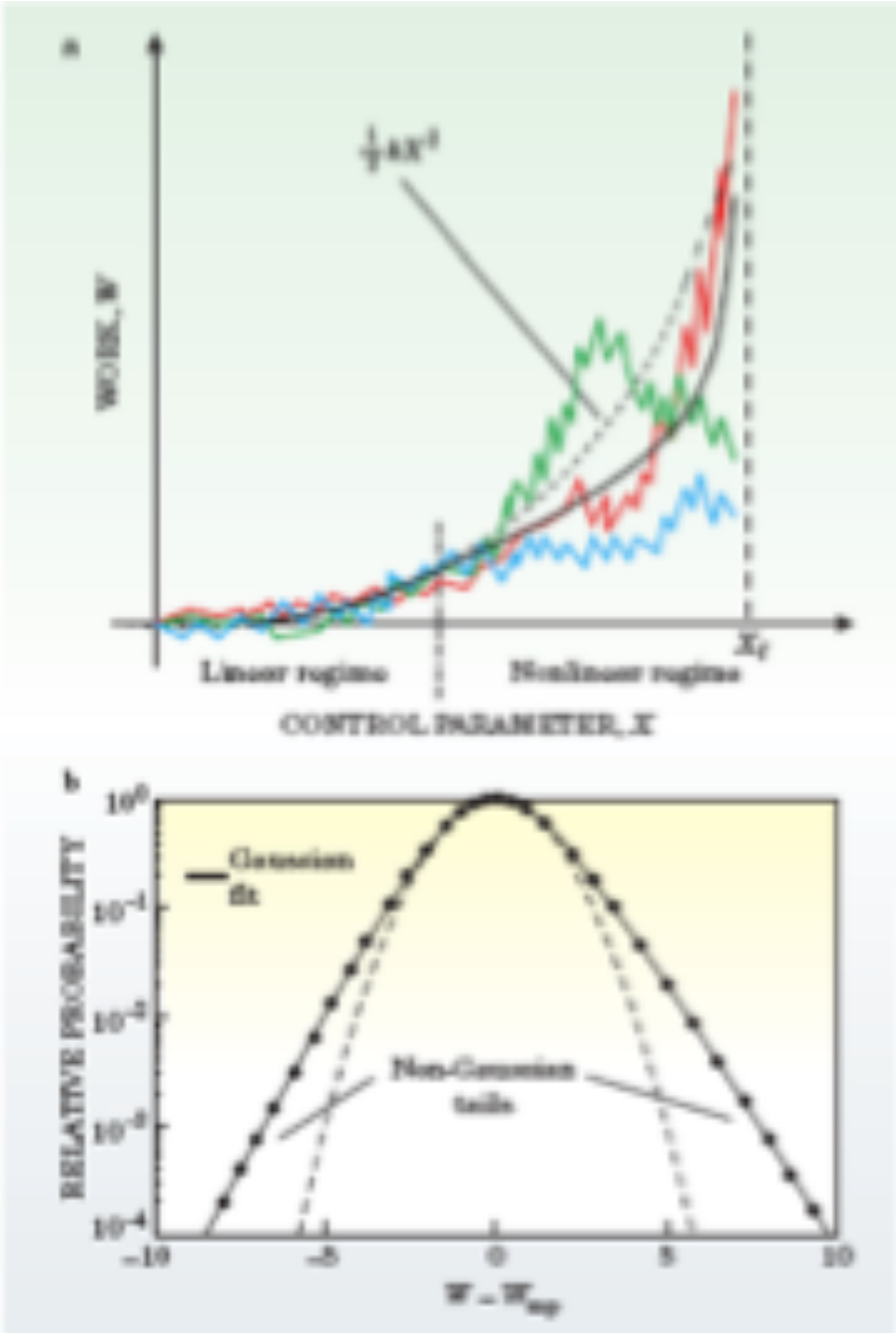
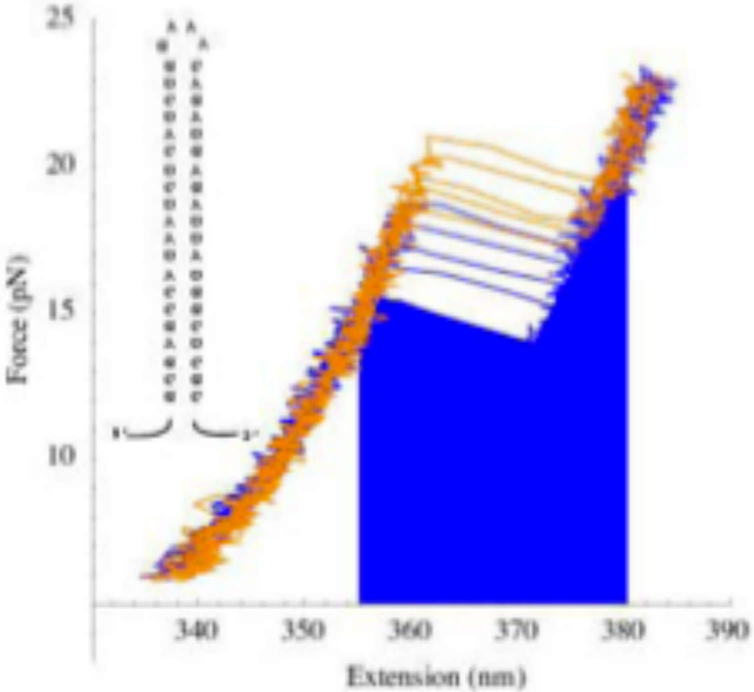
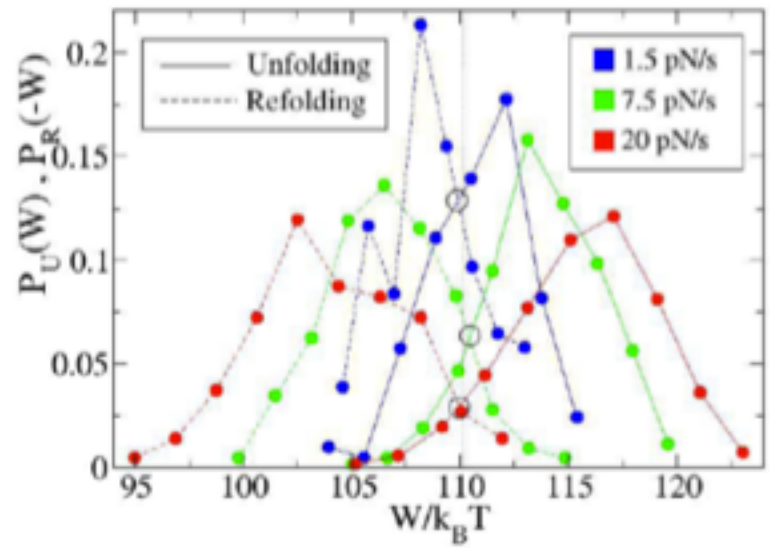
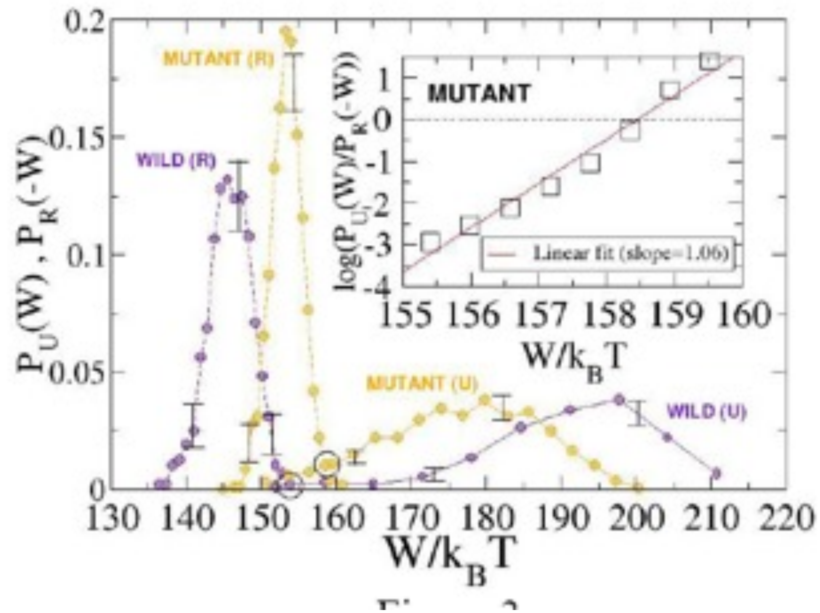


Figure 4. Testing the Jarzynski equality. A molecule of RNA is attached to two beads and subjected to reversible and irreversible cycles of folding and unfolding. A piezoelectric actuator controls the position of the bottom bead, which, when moved, stretches the RNA. An optical trap formed by two opposing lasers captures the top bead, and the change in momentum of light that exits the two-beam trap determines the force exerted on the molecule connecting the two beads. The difference in positions of the bottom and top beads gives the end-to-end length of the molecule. The blowup shows how the RNA molecule (green) is coupled with the two beads via molecular handles (blue). The handles end in chemical groups (red) that can be stuck to complementary groups (yellow) on the bead. The blowup is not to scale: The diameter of the beads is around 3000 nm, much greater than the 20-nm length of the RNA.


a
WORK, W
Linear regime
Nonlinear regime
CONTROL PARAMETER, X
b
RELATIVE PROBABILITY
Gaussian fit
Non-Gaussian tails







mardi 11 février 2014

Kramer Kroening

$$S_j(\omega) = \frac{4\ k_B T}{\omega} \chi_j''(\omega)$$

$$\tilde{\chi}_j'(\omega) = \frac{2}{\pi} P \int_0^\infty \frac{\xi \tilde{\chi}_j''(\xi)}{\xi^2 - \omega^2} d\xi = \frac{1}{2\pi k_B T} P \int_0^\infty \frac{\xi^2 S_j(\xi)}{\xi^2 - \omega^2} d\xi$$

i.e. $\tilde{\chi}_j''(\xi, t_w) = \omega S_j(\omega, t_w)/(4k_B T)$.

To compute $\tilde{\chi}_j'$ we use a Fourier transform algorithm that is:

$$\tilde{\chi}_j'(\omega) = \frac{1}{2\pi k_B T} \int_0^{1/\omega_{min}} \cos(\omega\ t)\ dt\ \int_0^{\omega_{max}} \xi^2 S_j(\xi)\ \sin(\xi\ t) d\xi,$$

where ω_{min}, ω_{max} are the minimum and maximum of the spectrum.