

Grenoble 29/09-01/10/2014 Workshop hbar kB



Jarzynski Equality and the Landauer's bound: an experimental approach

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Nature 483, 187-189 (2012)

2013 *EPL* **103** 60002 ; arXiv:1302.4417 ; Detailed Jarzynski Equality applied on a Logically Irreversible Procedure





A few notes on stochastic thermodynamics from theory to experiment

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





Applications of FT

Creating

Heat flux between two crcuits kept at different temperature



The Mechanical equivalent



- Trapped Brownian particles
- Molecular motor
- Single molecule experiments



Micro Electro Mechanical Devices

Thermal rheometer





Typical applied torque < 50pN m



Equation of motion



$$\begin{split} I_{\text{eff}} \ddot{\theta} + \int_{-\infty}^{t} G(t - t') \dot{\theta}(t') dt' + C\theta &= M + \eta, \\ \text{In Fourier space} \\ \left[-I_{\text{eff}} \omega^2 + \hat{C} \right] \hat{\theta} &= \hat{M}, \\ \text{where} \quad \hat{C} &= C + i [C_1'' + \omega \nu] \quad \text{is the} \\ \text{complex frequency-dependent elastic} \\ \text{stiffness} \\ \text{The response function is } \hat{\chi} &= \frac{\hat{\theta}}{\hat{M}} \\ \text{The thermal fluctuation power spectral density is given by} \\ \langle |\hat{\theta}|^2 \rangle &= \frac{4k_BT}{\omega} \text{Im } \hat{\chi} &= \frac{4k_BT}{\omega} \frac{C_1'' + \omega \nu''}{\left[-I_{\text{eff}} \omega^2 + C \right]^2 + \left[C_1'' + \omega \nu \right]^2}. \end{split}$$







Energy Balance (I)

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



$$I_{\text{eff}} \frac{\mathrm{d}^2\theta}{\mathrm{d}t^2} + \nu \frac{\mathrm{d}\theta}{\mathrm{d}t} + C \,\theta = M + \sqrt{2k_B T \nu} \,\eta,$$

• We multiply this equation by $\dot{ heta}$ and we get :

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

• The injected power :
$$P_{inj}(t) = M(t) \frac{\mathrm{d}\theta(t)}{\mathrm{d}t}$$

• The dissipated power :
$$P_{diss}(t) =
u \left[rac{\mathrm{d} heta(t)}{\mathrm{d}t}
ight]^2 - \sqrt{2k_BT\nu} \eta(t) \; rac{\mathrm{d} heta(t)}{\mathrm{d}t}$$

• The internal energy :
$$U(t) = \left\{ \frac{1}{2} I_{\text{eff}} \left[\frac{\mathrm{d}\theta(t)}{\mathrm{d}t} \right]^2 + C \ \theta(t)^2 \right\}.$$

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:

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

• $W_{ au}$ is the work done on the system over a time au :

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

• $Q_{\tau} = W_{\tau} - \Delta U_{\tau}$ is the heat dissipated by the system.

We study the fluctuations of W_{τ} , Q_{τ} and the Fluctuation Theorem for these two quantities



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





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

where
$$\Sigma(au)
ightarrow 1$$
 for $au
ightarrow \infty$

 $X_{\mathcal{T}}$ stands either for $Q_{\mathcal{T}}$ or for $W_{\mathcal{T}}$

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

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

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

The Fluctuation Theorem (FT)

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

ENS DE LYON

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.













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



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 .



Trajectory dependent entropy



- U. Seifert, Phys. Rev. Lett., 95, 040602, (2005),
- A. Puglisi, L. Rondoni, A. Vulpiani,
 J. Stat. Mech.: Theory and Experiment, P08010,(2006)

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 :

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

for Langevin dynamics

for Markov process















What is FT useful for ?



• Several interesting consequences of FT such as the Jarzynski 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.





(drawing not in scale)



Standard method to determine the torque N

$$N = \frac{\langle \dot{\theta} \rangle}{\gamma}$$



Standard method to determine the torque N







Molecular motor and FT





New method based on FT to determine the torque N

$$\gamma \dot{\theta} = N + \eta$$

$$W_{\tau} = N \int_{t}^{t+\tau} \dot{\theta} dt = N \Delta \theta_{\tau}$$
 where $\Delta \theta_{\tau} = (\theta(t+\tau) - \theta(t))$

SSFT for
$$W_{\tau}$$
: $\log\left(\frac{P(\Delta\theta_{\tau})}{P(-\Delta\theta_{\tau})}\right) = \Sigma(\tau) N \frac{\Delta\theta_{\tau}}{k_B T}$

with $\Sigma(au)
ightarrow 1$ for $au
ightarrow \infty$

γ is not needed


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 equilibrium 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:

$$\Delta F = \langle W^J \rangle - \frac{\sigma_W^2}{2 \ K_B \ T}$$

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:

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

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

The Jarzynski work

$$W^{J} = \int_{0}^{\tau} dt \, \frac{d\lambda}{dt} \, \frac{\partial H}{\partial \lambda}$$

• 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

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

The classical work

$$W^{J} = -\int_{0}^{t_{s}} \dot{M}\theta \ dt = -\left[M\theta\right]_{0}^{t_{s}} + W^{\mathsf{CI}},$$

where

$$W^{\mathsf{C}\mathsf{I}} = \int_0^{t_s} M\dot{\theta} \ dt$$

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

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

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



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 $\dot{W}^{Cl} = M\dot{\theta}$

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 $\Delta F = -\Delta F_0$.









INFORMATION AND THERMODYNAMICS

- Landauer's principle
- How to realise it ?
- Experimental set-up
- Data analysis
- Comparison with numerical results
- Landauer's limit and the Jarzynski equality
- Conclusions





Landauer's Principle and The Maxwell's Demon

A



The first explanation came in 1929 by Leó Szilárd, and later by Léon Brillouin



• fast molecules



Β







The Landauer's principle (I)

Any logically irreversible transformation of classical information is necessarily accompanied by the dissipation of at least $k_BT \cdot ln 2$ of heat per lost bit (about $3 \cdot 10^{-21}$ Joules at room temperature)

Typical examples of logically irreversible transformations are Boolean functions such as AND, NAND, OR and NOR They map several input states onto the same output state

The erasure of information, the RESET TO ONE operation, is logically irreversible and leads to an entropy production of $k_B \cdot ln 2$ per erased bit





Landauer's principle II

Landauer's principle is a central result which exorcises the Maxwell's demon

It has been criticised and never tested in a real experiment

Questions

- Can the Landauer's limit be reached in any experiment?
- Does any experimentally feasable procedure allow us to reach the limit ?

Following Bennett we use in our experiment the RESET to ONE operation

Bennett, C. H. The thermodynamics of computation, a review. Int. J. Theor. Phys. 21, 905-940 (1982).





Procedure



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Quasi Static : -T\Delta S=Q
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Energy variation : \Delta U=0
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First principle : \Delta U = -Q + W
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In average : $\langle W \rangle = \langle Q \rangle = -T \Delta S \ge k_B T \ln(2)$

Numerical result : Memory Erasure in Small Systems, R. Dillenschneiderand E. Lutz, Phys. Rev. Lett. 102, 210601 (2009)







The cell for the bead





















The work on the erasure cycle



$$\nu \dot{x} = -\frac{\partial U_o(x,t)}{\partial x} + f(t) + \eta$$

multiplying by $\dot{\mathbf{x}}$ and integrating for a time τ we get :

$$\Delta U_{ au} = W_{ au} - Q_{ au}$$
 Stochastic thermodynamics

$$\Delta U_{\tau} = -\int_{0}^{\tau} \frac{\partial U_{o}}{\partial x} \dot{x} dt \qquad \qquad W_{\tau} = \int_{0}^{\tau} f \dot{x} dt$$

$$Q_{\tau} = \int_0^{\tau} \nu \dot{x}^2 dt - \int_0^{\tau} \eta \dot{x} dt$$

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













Why in the experiment r < 1?

Is this result produced by 3D effects of the trap ?

Is the finite height of the initial barrier responsible of r<1 ?





We use all the experimental parameters and procedure

with two different initial barriers $8k_BT$ and $15k_BT$



The success rate r



Why in the experiment r< 1 ? Is this result produced by 3D effects of the trap ?

Is the finite height of the initial barrier responsible of r<1 ?

$$\nu \dot{x} = -\frac{\partial U_o(x,t)}{\partial x} + \eta$$





Conclusions (partials)



• Our experimental results indicate that the thermodynamic limit to information erasure, the Landauer bound, can be approached in the quasistatic regime, but not exceeded.

- The asymptotic limit is reached in $1/\tau$ for $\tau > 3 \tau_k$
- The fact that r<1 is due to the finite height of the initial barrier
- Thermal fluctuations play an important role to reach the limit

Question: Does Jarzynski equality compute the right ΔF ?


Landauer's limit and the Jarzynski equality



$$< \exp(-W_s) >= \exp(-\Delta F)$$

with $W_s = -\int_o^{\tau_{cycle}} \dot{\lambda} \frac{\partial H(x,\lambda)}{\partial \lambda} dt$

In our case this equality transforms

$$W_{s} = \int_{o}^{\tau} \dot{f} x \, dt = [f \, x]_{o}^{\tau} - \int_{o}^{\tau} f \, \dot{x} \, dt = -W_{f}$$

Since the height of the barrier is always finite there is no change in the *equilibrium* F of the system between the beginning and the end of the procedure.

$$<\exp(-W_s)>=\frac{\rho_{eq}(\tau)}{\rho(\tau)}\exp(-\Delta F)$$

S. Vaikuntanathan and C. Jarzynski, Euro. Phys. Lett. 87, 60005 (2009).

Generalized Jarzynski









Conclusions



• Our experimental results indicate that the thermodynamic limit to information erasure, the Landauer bound, can be approached in the quasistatic regime, but not exceeded.

- The asymptotic limit is reached in $1/\tau$
- The fact that r<1 is due to the finite height of the initial barrier
- Thermal fluctuations play an important role to reach the limit
- Jarzinsky equality computes the Landauer limit independently of the rapidity of the procedure

Question : Does any procedure allows us to reach the Landauer's limit ? Answer : NO. The barrier reduction and tilt must be two separate process See recent paper on optimisation : E. Aurell, et al. J. Stat. Phys.147, 487-505 (2012).



The ramping time of the laser intensity has been changed from 1s to 50s



The work is mainly due to the jump of the particle The Landauer limit can never be reached



Numerical results



1.5

1.5

1.25



0.5

0.75

t/т

-1

0

0.25







Conclusions



• Our experimental results indicate that the thermodynamic limit to information erasure, the Landauer bound, can be approached in the quasistatic regime, but not exceeded.

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