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Detailed Jarzynski Equality applied on a Logically Irreversible Procedure

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A single bit memory system is made with a brownian particle held by an optical tweezer in a double-well potential. For a memory erasure procedure, which is a logically irreversible operation, a detailed Jarzynski Equality is verified, retrieving the Landauer limit independently of the work done on the system. For the two separated subprocesses, i.e. the transition from state 1 to state 0 and the transition from state 0 to state 0, the Jarzynski equality does not hold but the generalized version links the work done on the system to the probability that the it returns to its initial state under the time-reversed procedure.

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The connection between thermodynamics and information is nowadays a widely studied problem [1–5]. The main questions concern the amount of energy necessary in order to perform a logical operation in a given time and how the information entropy is related to the free energy difference between the initial and final state of this logical operation. In this context the Landauer's principle [6] is very important as it states that for any irreversible logical operation the minimum amount of entropy production associated is $-k_B \ln(2)$ per bit computed by the logical operation, with k_B the Boltzmann constant. Specifically a logically irreversible operation is an operation for which the knowledge of the output does not allow to retrieve the initial state, examples are logical AND, OR and erasure. In a recent paper [8] we have experimentally shown that indeed the minimum amount of work necessary to erase a bit is actually associated with this Landauer's bound which can be asymptotically reached for adiabatic transformations. The question that arise naturally is whether this work corresponds to the free energy difference between the initial and final state of the system. To answer to this question it seems natural to use the Jarzynski equality [7] which allows one to compute the free energy difference between two states of a system, in contact with a heat bath at temperature T . When such a system is driven from an equilibrium state A to a state B through any continuous procedure, the Jarzynski equality links the stochastic work W_{st} received by the system during the procedure to the free energy difference $\Delta F = F_B - F_A$ between the two states:

$$\langle e^{-\beta W_{st}} \rangle = e^{-\beta \Delta F} \quad (1)$$

Where $\langle . \rangle$ denotes the ensemble average over all possible trajectories, and $\beta = \frac{1}{k_B T}$ (see eq. 2 for the precise definition of the work W_{st}).

In this letter we analyze the question of the application of eq.1 for estimating the ΔF corresponding to the erasure operation in our experiment, in which a colloidal particle confined in a double well potential is used as a single bit memory. We will show that a detailed Jarzynski

Equality is verified, retrieving the Landauer limit independently of the work done on the system.

The setup has already been described in a previous article [8] and we recall here only the main features.

A custom-built vertical optical tweezers is used to realize a two-state system: a silica bead (radius $R = 1\mu m$) is trapped at the focus of a laser beam (wavelength $1024nm$) which is rapidly switched (at a rate of $10kHz$) between two positions (separated by $1.45\mu m$) using an acousto-optic deflector. A disk-shaped cell ($18mm$ in diameter, $1mm$ in depth) is filled with a solution of beads dispersed in bidistilled water at low concentration. The bead used for the experiment is trapped by the laser and moved into the center of the cell (with gap $\sim 80\mu m$) to avoid all interactions with other beads. The trapped bead feels a double-well potential with a central barrier varying from $2k_B T$ to more than $8k_B T$ depending on the power of the laser (see figure 1, a and b). The left well is called "0" and the right well "1". The position of the bead is tracked using a fast camera with a resolution of $108nm$ per pixel, which after treatment gives the position with a precision greater than $10nm$. The trajectories of the bead are sampled at $502Hz$.

The logical operation performed by our experiment is the erasure procedure. This procedure brings the system initially in one random state (0 or 1 with same probability) in one chosen state (e.g. 0). It is done experimentally in the following way.

At the beginning the laser power is high ($48mW$) so that the central barrier is more than $8k_B T$ and the characteristic jumping time (Kramers Time) is about $3000s$, which is long compared to the time of the experiment, and the bead is trapped in one well-defined state (0 or 1). The laser power is first lowered (in a time $T_{lowering} = 1s$) to $15mW$ so that the barrier is about $2.2k_B T$ and the jumping time falls to $10s$. A viscous drag force linear in time is induced by displacing the cell with respect to the laser using a closed-loop 3-axis NanoMax stage. The force is given by $f = -\gamma v$ where $\gamma = 6\pi R\eta$ (η is the viscosity

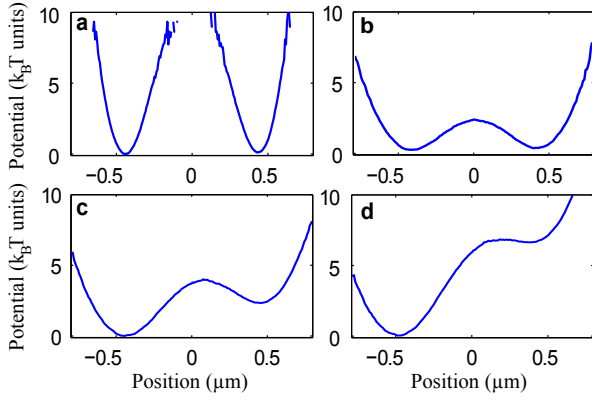


FIG. 1: Measurement of the potential in which the silica bead is confined, with no external force for two different laser powers (a: 48 mW and b: 15 mW), and extrapolation for low power with two different values of the force (c: $1 \times 10^{-14} N$ and d: $3 \times 10^{-14} N$). The potential is computed from the equilibrium probability density function of the bead's position.

of water) and v the speed of displacement. It tilts the double-well potential so that the bead ends always in the same well (e.g. state 0 if the force pushes the bead to the left) independently of where it started. At the end, the force is stopped and the central barrier is raised again to its maximal value (in a time $T_{rising} = 1 s$). Between two successive procedures the system is equilibrating for 4 s. The experimental procedure is sketched figure 2. A procedure is fully characterized by its duration τ and the maximal value of the force applied f_{max} . Its efficiency is characterized by the “proportion of success” which is the proportion of trajectories where the bead ends in the chosen well (e.g. 0), independently of where it started.

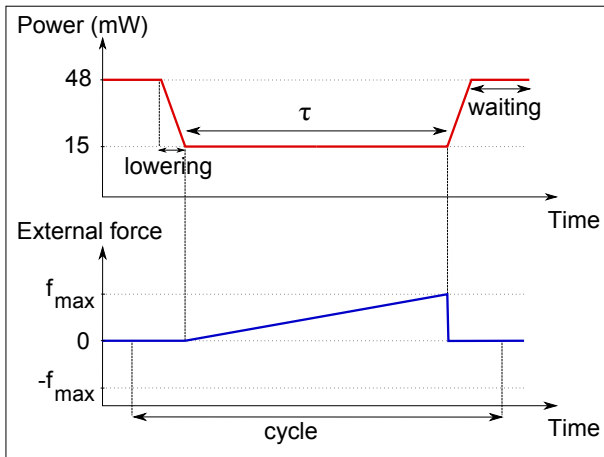


FIG. 2: Schematic representation of the erasure procedure.

The ideal erasure procedure is a logically irreversible operation because the final state gives no information

about the initial state. For one bit of memory [6], it corresponds to a change in the entropy of the system $\Delta S = -k_B \ln(2)$. The procedure can arbitrarily be decomposed in two kinds of sub-procedures: one where the bead starts in one well and ends in the other (e.g. $1 \rightarrow 0$) and one where the bead is initially in the well where it should be at the end of the erasure procedure (e.g. $0 \rightarrow 0$).

The two accessible quantities are $x(t)$, which is measured, and $f(t)$ which is imposed by the displacement of the cell. The derivatives are estimated using the discretization $\dot{x}(t + \Delta t/2) \approx [x(t + \Delta t) - x(t)]/\Delta t$. Starting from these quantities it is possible to measure the stochastic work W_{st} done during the erasure procedure.

For a colloidal particle confined to one spatial dimension and submitted to a conservative potential $V(x, \lambda)$, where $\lambda = \lambda(t)$ is a time-dependent external parameter, one can define the stochastic work received by the system along a single trajectory [5]:

$$W_{st}[x(t')] = \int_0^{t'} \frac{\partial V}{\partial \lambda} \dot{\lambda} dt \quad (2)$$

Here the potential is $V(x, t) = U_0(x, I(t)) - x \times f(t)$, where U_0 is due to the optical trapping and $I(t)$ is the intensity of the laser (see figure 1). If the bead does not jump from one well to the other during the modulation of the height of the barrier this part of the procedure does not contribute to the work received by the bead. Then the work can be computed only when the external force is applied (between $t = 0$ and $t = \tau$). This force is directly the control parameter, and considering that $f(t = 0) = 0 = f(t = \tau)$, it follows that the stochastic work is equal to the classical work W :

$$W_{st}[x(\tau)] = \int_0^\tau -x \dot{f} dt = \int_0^\tau f \dot{x} dt = W[x(\tau)] \quad (3)$$

The two integrals have been calculated for all the trajectories of all the procedures tested. Amongst all of them, the maximal difference $|W_{st} - W|$ observed, was of $0.06 k_B T$, which is negligible.

We now analyse the results of our experiments. For every chosen duration τ , the maximal force f_{max} was set to different values (typically between 1 and $6 \times 10^{-14} N$). For each set of parameters (τ, f_{max}) , the procedure was repeated several hundreds of times to be able to compute statistical values. For each τ , the value of f_{max} is optimized in order to be as small as possible and give a proportion of success $> 90\%$.

The mean of the work received $\langle W \rangle$ and the logarithm of the mean of its exponential $\Delta F_{eff} = -\ln(\langle e^{-\beta W} \rangle)$ were calculated on the trajectories where the information is erased (i.e. the ones where the bead ends where it was supposed to be). For the mean of the exponential, the error bars are estimated by computing the mean on the

data set with 10% of the points randomly excluded, and taking the maximal difference in the mean value observed by repeating this operation 1000 times. The results are shown figure 3. The mean work $\langle W \rangle$ decreases when the duration of the procedure increases. For the optimized values of the force, it follows a law $\langle W(\tau) \rangle = k_B T \ln(2) + B/\tau$ where B is a constant, which is the behavior for the theoretical optimal procedure [9]. A least mean square fit gives $B = 8.45 k_B T.s$. The effective free energy difference ΔF_{eff} is always close to the Landauer limit $k_B T \ln(2)$, independently of the value of the maximal force or the procedure duration.

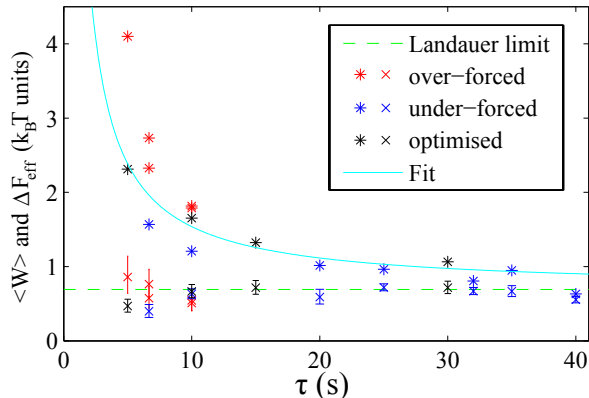


FIG. 3: Mean of the work (*) and effective free energy difference (x) for different procedures. The over-forced procedures (red) have a proportion of success $\sim 95\%$, the optimised procedures (black) have a proportion of success $> 91\%$, the under-forced procedures have a proportion of success $> 83\%$ (except the last point, that has a proportion of success $\approx 75\%$). The fit (blue line) is: $\langle W(\tau) \rangle = k_B T \ln(2) + B/\tau$ with B a constant.

The mean of the exponential can be computed on the sub-procedures by sorting trajectories in function of the initial position of the bead. Specifically $\langle e^{-\beta W} \rangle = (M_{10} + M_{00})/2$, where $M_{10} = \langle e^{-\beta W} \rangle_{1 \rightarrow 0}$ and $M_{00} = \langle e^{-\beta W} \rangle_{0 \rightarrow 0}$. The values M_{10} and M_{00} are plotted figure 4. The sum $M_{10} + M_{00}$ is always close to 1, which corresponds to the fact that ΔF_{eff} is close to $k_B T \ln(2)$, but M_{00} decreases with τ whereas M_{10} increases consequently.

These results can be understood in the following way: Since the memory erasure procedure is made in a cyclic way and $\Delta S = -k_B \ln(2)$ it is natural to await $\Delta F = k_B T \ln(2)$. But the ΔF that appears in the Jarzynski equality is the difference between the free energy of the system in the initial state (which is at equilibrium) and the equilibrium state corresponding to the final value of the control parameter: $F(\lambda(\tau)) - F(\lambda(0))$. Since the height of the barrier is always finite there is no change in the equilibrium free energy of the system between the

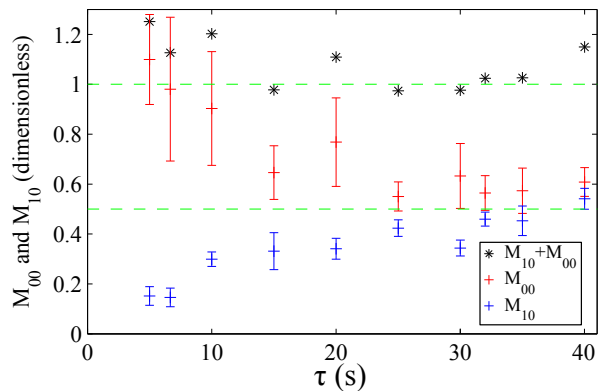


FIG. 4: Mean of the exponential of the work, for the sub-procedures $1 \rightarrow 0$ (blue) and $0 \rightarrow 0$ (red). For readability questions, only one value is shown for each τ : it corresponds to the procedure with the highest proportion of success.

beginning and the end of the procedure. Then $\Delta F = 0$, which implies $\langle e^{-\beta W_{st}} \rangle = 1$. Nevertheless Jarzynski and co-workers [10] have shown that when there is a difference between the actual state of the system (described by the phase-space density ρ_t), and the equilibrium state (described by ρ_t^{eq}), the Jarzynski equality should be modified:

$$\langle e^{-\beta W_{st}(t)} \rangle_{(x,t)} = \frac{\rho^{eq}(x, \lambda(t))}{\rho(x, t)} e^{-\beta \Delta F(t)} \quad (4)$$

Where $\langle \cdot \rangle_{(x,t)}$ is an average over all the trajectories that pass through x at t .

Here, selecting the trajectories where the information is actually erased means taking x corresponding to the final well (e.g. state 0) and $t = \tau$. It follows that $\rho(0, \tau)$ is directly the proportion of success of the procedure, which is made close to 1, and $\rho^{eq}(0, \lambda(\tau)) = 1/2$. Then:

$$\langle e^{-\beta W_{st}(\tau)} \rangle_{(0,\tau)} \approx \frac{1}{2} \quad (5)$$

In the ideal case where the proportion of success goes to 100%, all the trajectories end in state 0 at time τ and finally:

$$\langle e^{-\beta W_{st}} \rangle = 1/2 = e^{-\beta \Delta F_{eff}} \quad (6)$$

Considering the subprocedures $1 \rightarrow 0$ and $0 \rightarrow 0$ separately, the Jarzynski equality does not hold because the initial conditions are not correctly tested (selecting trajectories by their initial condition introduce a bias in the initial equilibrium distribution). But Van den Broeck and coworkers [11] have shown that for a partition of the phase-space into non-overlapping subsets χ_j ($j = 1, \dots, K$) there is a detailed Jarzynski Equality:

$$\langle e^{-\beta W} \rangle_j = \frac{\tilde{\rho}_j}{\rho_j} e^{-\beta \Delta F} \quad (7)$$

With:

$$\rho_j = \int_{\chi_j} \rho(t_a) dx dp \quad \text{and} \quad \tilde{\rho}_j = \int_{\tilde{\chi}_j} \tilde{\rho}(t_a) dx dp \quad (8)$$

Where $\rho(t_a)$ and $\tilde{\rho}(t_a)$ are the phase-space densities of the system measured at the same intermediate but otherwise arbitrary point in time, in the forward and backward protocol, respectively. Here, the two subsets are χ_{10} and χ_{00} , defined by the state where the particle is at the beginning of the procedure. By taking $t_a = 0$ the starting point of the procedure, $\rho_j = 1/2$ and $\tilde{\rho}_j$ identifies with the probability that the systems returns into its initial state for the time-reversed procedure. Since $e^{-\beta\Delta F_{eff}} = 1/2$, it follows that:

$$\langle e^{-\beta W} \rangle_{1 \rightarrow 0} = \tilde{P}_{01} \quad (9)$$

$$\langle e^{-\beta W} \rangle_{0 \rightarrow 0} = \tilde{P}_{00} \quad (10)$$

Where \tilde{P}_{01} (resp. \tilde{P}_{00}) is the probability that the particle ends the time-reversed procedure (which always starts in the state 0) in the state 1 (resp. in the state 0). This result is similar to the one reported by Ueda and coworkers [12, 13] for procedures with feedback. It should be noticed that here $\tilde{P}_{01} + \tilde{P}_{00} = 1$. And it is reasonable to think that for time-reversed procedure the probability of returning to state 1 is lower when the duration of the procedure is lower, which explains qualitatively the behavior observed experimentally. Unfortunately the time-reversed procedure cannot be realized experimentally, because it starts with a very fast rising of the force, which cannot be reached in our experiment.

Therefore in order to analyze this problem we performed a numerical simulation. Our experimental system can be described by the over-damped Langevin equation:

$$\gamma \dot{x} = -\frac{\partial V}{\partial x} + \xi \quad (11)$$

where ξ is a gaussian white noise with zero mean and correlation $\langle \xi(t)\xi(t') \rangle = 2\gamma k_B T \delta(t - t')$.

Simple numerical simulations were made by integrating this equation with Euler method, for a procedure as close as possible to the experimental one. For such a numerical procedure, it is possible to realize the corresponding time-reversed procedure and so to verify that for the sub-procedures the mean of the exponential of the work gives the probability to return in the initial state under the time-reversed procedure. Some results are showed in the following table:

τ (s)	f_{max} ($10^{-14}N$)	M_{10}	\tilde{P}_{01}	M_{00}	\tilde{P}_{00}	success (%)
5	3.77	0.16	0.16	0.84	0.84	96
10	2.83	0.30	0.28	0.73	0.72	94
20	1.89	0.41	0.43	0.60	0.57	90
30	1.89	0.42	0.44	0.57	0.56	93

The agreement is quantitative. It was also verified that for proportions of success $< 100\%$, if one takes all the trajectories, and not only the ones where the bead ends in the state 0, the classical Jarzynski equality is verified: $\langle e^{-\beta W_{st}} \rangle = 1$ (for these specific simulations, $T_{lowering}$ and T_{rising} were taken equal to 0.1s to avoid problems when the bead jumps during this phase of the procedure). This result means that the small fraction of trajectories (sometimes $< 1\%$) where the bead ends the erasure procedure where it shouldn't is enough to retrieve the fact that $\Delta F = 0$.

As a conclusion, it has been experimentally shown that for a memory erasure procedure of a one bit system, which is a logically irreversible operation, a detailed Jarzynski Equality is verified, retrieving the Landauer limit independently of the work done on the system. Furthermore the arbitrary division of the procedure into two sub-procedures allows us to link the work done on the system to the probability that it returns to its initial state under the time-reversed procedure.

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