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Faster than Nature: Engineered Swift Equilibration of a Brownian particle

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A fundamental and intrinsic property of any device or natural system is its relaxation time τ_{relax} , which indicates how long equilibrium recovery takes after a sudden change of a control parameter [1]. Epitomized by the charge of a capacitance or the thermalisation of a material, examples abound from physics to biology, and from engineering to chemistry. The reduction of τ_{relax} , which is frequently desired and necessary, is often obtained by a complex feedback process. To overcome the limitations of such an approach, alternative methods based on an appropriate driving have been recently demonstrated [2, 3], for isolated quantum and classical systems [4–9]. Their extension to open systems in contact with a thermostat is a stumbling block for applications. Here, we design a protocol of Engineered Swift Equilibration (ESE) that shortcuts time-consuming relaxations, and we apply it to a Brownian particle trapped in an optical potential whose properties can be controlled in time. We implement the ESE process experimentally, showing that it allows the system to reach equilibrium 100 times faster than the natural equilibration rate. We also estimate the increase of the dissipated energy needed to get such a time reduction. Beyond its fundamental interest, the ESE method paves the way for applications in micro and nano devices, where the reduction of operation time represents as substantial a challenge as miniaturization [10].

PACS numbers:

The concepts of equilibrium and of transformations from an equilibrium state to another, are cornerstones of thermodynamics. A textbook illustration is provided by the expansion of a gas, starting at equilibrium and expanding to reach a new equilibrium in a larger vessel. This operation can be performed either very slowly by a piston, without dissipating energy into the environment, or alternatively quickly, letting the piston freely move to reach the new volume. In the first case, the transformation takes a long (virtually infinite) time to be completed, while the gas is always in a quasi-equilibrium state. In the second case instead, the transformation is fast but the gas takes its characteristic relaxation time τ_{relax} to reach the new equilibrium state in the larger volume. This is the time required for the exploration of the new vessel. More generally, once a control parameter is suddenly changed, the accessible phase space changes too [1, 11]; the system adjusts and needs a finite time to reach the final equilibrium distribution. This equilibration process plays of course a key role in out of equilibrium thermodynamics.

An important and relevant question related to optimization theory is whether a targeted statistical equilibrium state can be reached in a chosen time, arbitrarily shorter than τ_{relax} . Such strategies are reminiscent of those worked out in the recent field of Shortcut to Adiabaticity [2, 3]; they aim at developing protocols, both in quantum and in classical regimes, allowing the system to move as fast as possible from one equilibrium position to a new one, provided that there exist an adiabatic transformation relating the two [12–14]. So far, proof of principle experiments have been carried out for isolated

systems [4–9] and for photonics circuit design [15–18]. Yet, the problem of open classical systems is untouched. We solve here this question by putting forward an accelerated equilibration protocol for a system in contact with a thermal bath. This is a key step for a number of applications in nano oscillators [19], in the design of nanothermal engines [20], or in monitoring mesoscopic chemical or biological processes [21], for which thermal fluctuations are paramount and an accelerated equilibration desirable for improved efficiency. We dub the method Engineered Swift Equilibration (ESE).

However, an arbitrary reduction of the time to reach equilibrium will have unavoidable consequences from an energetical point of view [22]. The question of the corresponding cost is relevant as such, but also for applications, for example in nano-devices [10] where the goal is the size and execution time reduction of a given process. Here, beyond the theoretical derivation of the procedure, we develop an experimental demonstration of ESE, studying the dynamics of a colloidal particle within an optical potential. The energetics of the system will also be analyzed in depth, shedding light on the inherent consequences of time-scale reduction.

Our experimental system consists of a microsphere immersed in water [23]. The particle is trapped by an optical harmonic potential $U(x, t) = \kappa(t)x^2/2$, where x is the particle position and $\kappa(t)$ is the stiffness of the potential which can be controlled by the power of the trapping laser [20]. The system is affected by thermal fluctuations; its dynamics is overdamped and described by a Langevin equation (see Methods). Our Brownian particle has a relaxation time defined as $\tau_{\text{relax}} = \gamma/\kappa$,

where γ is the fluid viscous coefficient. At equilibrium, the probability density function (pdf) $\rho(x)$ of x is Gaussian $\rho_{\text{eq}}(x) = 1/\sqrt{\pi\sigma_x^2} \exp(-x^2/(2\sigma_x^2))$ with variance $\sigma_x^2 = k_B T/\kappa$ as prescribed by the equipartition theorem. Here k_B is the Boltzmann constant and T the bath temperature. In this system, we consider the compression process sketched in Fig. 1, in which the stiffness is changed from an initial value to a larger one. The evolution of the system during the relaxation towards the new equilibrium state is monitored through the position pdf $\rho(x, t)$, which is Gaussian at all times (see Methods). Thus, the distribution $\rho(x, t)$ is fully characterized by the time evolution of its mean and its standard deviation $\sigma_x(t)$. The main question is now that of finding, provided it exists, a suitable time evolution of the stiffness $\kappa(t)$ (our control parameter), for which the equilibration process is much faster than τ_{relax} . This question can be affirmatively answered using a particular solution of the Fokker-Planck equation (see Methods).

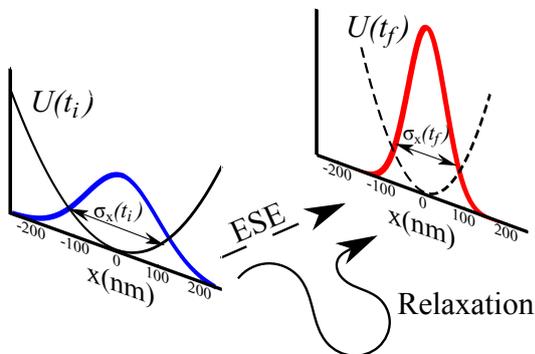


FIG. 1: **Sketch of the process.** At initial time t_i , the particle is at equilibrium, confined in a potential of stiffness κ_i (black line), and $\rho(x)$ (blue histogram) has variance $\sigma_x^2(t_i) = k_B T/\kappa_i$. After a long relaxation where κ is gradually increased, the particle is at time t_f at equilibrium in a stiffer potential (black line). Since $\kappa_f > \kappa_i$, the variance $\sigma_x^2(t_f)$ of position (red histogram) is smaller than its initial counterpart. The goal is to work out a protocol with a suitable dynamics $\kappa(t)$, that would ensure equilibrium at an arbitrary chosen final time t_f , no matter how small.

In this Letter, two methods are compared. On the one hand, at a given instant $t_i = 0$, we suddenly change κ from the initial value κ_i to the final value κ_f . During this protocol, referred to as STEP, the particle mean position does not change while the spread σ_x equilibrates to the new value $\sqrt{k_B T/\kappa_f}$ in about 3 relaxation times $\tau_{\text{relax}} = \gamma/\kappa_f$. On the other hand, following the ESE procedure, $\kappa(t)$ is modulated in such a way that σ_x is fully equilibrated at $t_f \ll \tau_{\text{relax}}$. The protocol which meets our requirements is given by eq. (8) (in Methods). In the experiment, we select $\kappa_i = 0.5$ pN/ μm and $\kappa_f = 1.0$ pN/ μm in such a way that $\tau_{\text{relax}} \simeq 15$ ms. Furthermore, in order to have a well defined separation between time scales, we choose $t_f = 0.5$ ms, which is roughly 100 times

smaller than the thermalization time in the STEP protocol. Both protocols are displayed in Fig. 2a where we can appreciate the rather complex time dependence of the ESE control procedure. This is a necessity to allow for a quick evolution to the new equilibrium state. The faster the evolution (smaller t_f), the stiffer the transient confinement must be, (the maximum stiffness reached in Fig. 2a is $37\kappa_i$). In order to study the evolution of $\rho(x, t)$ for the two protocols, we perform the following cycle. First, the particle is kept at κ_i for 50 ms to ensure proper equilibration. Then, at $t = 0$ ms we apply the protocol (either STEP or ESE) and $x(t)$ is measured for 10 ms in the case of ESE and 100 ms for STEP. Finally, the stiffness is set again to κ_i and this cycle is repeated N times. The evolution of $\sigma_x(t)$ for $t > 0$ is obtained by performing an ensemble average over $N = 2 \cdot 10^4$ cycles.

The results are shown in Fig. 2b, where $\sigma_x(t)$ is plotted as a function of time for the two protocols, from one equilibrium configuration to the other. It appears that the engineered system reaches the target spread precisely at t_f and subsequently does not evolve. On the other hand, the STEP equilibration occurs after a time close to $3\tau_{\text{relax}}$. Figure 2c-d represent the complete STEP and ESE dynamics of $\rho(x)$. The Gaussian feature is confirmed experimentally during ESE, even far from equilibrium, since the kurtosis is $K = (3.00 \pm 0.01)$. The results of Fig. 2 clearly show the efficiency of ESE, driving the system into equilibrium in a time which is 100 times shorter than the nominal equilibration time $3\tau_{\text{relax}}$.

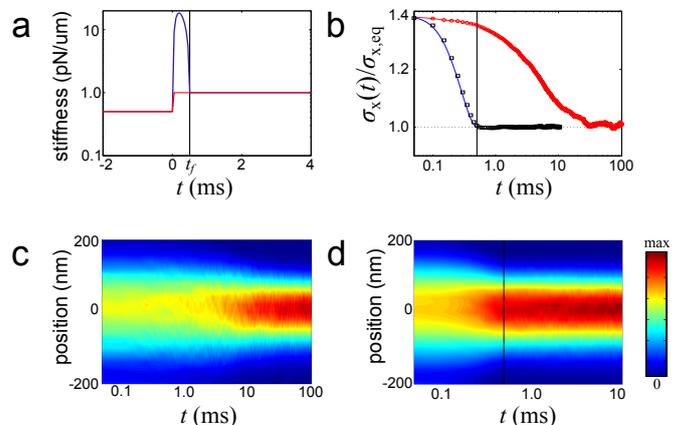


FIG. 2: **Dynamics of the system along the STEP and ESE protocol.** **a-** Experimental protocols: STEP route (red) and ESE route (blue). The system starts with $\kappa_i = 0.5$ pN/ μm at $t = 0$ to finish with $\kappa_f = 1.0$ pN/ μm . In all figures, the vertical solid line at $t = t_f$ indicates the end of the ESE protocol. **b-** Normalized standard deviation $\sigma_x(t)$ of the particle's trajectory along the STEP (red circles) and ESE protocol (black squares). The blue solid line represents the theoretical prediction of the variance evolution, Eq. (7). **c-** Time evolution of the position pdf. The color map of $\rho(x, t)$ is plotted after an instantaneous change of the stiffness at $t = 0$ (STEP). **d-** ESE counterpart of panel c.

We now turn our attention to the energy required for achieving such a large time reduction. Developments in the field of stochastic thermodynamics [24] endow work W and heat Q with a clear mesoscopic meaning, from which a resolution better than $k_B T$ can be achieved experimentally (see Methods for an explicit definition). In Fig. 3, the complete energetics of our system is shown for the ESE and STEP protocols. The evolution of the mean cumulative work $\langle W(t) \rangle$ reveals the physical behavior of the system undergoing ESE. In the first part of the protocol ($t < 0.2$ ms), confinement is increased which provides positive work to the system. In the subsequent evolution ($0.2 < t < 0.5$ ms), work is delivered from the system to the environment through the decrease of the stiffness. In striking contrast with an adiabatic transformation, the value of heat increases monotonically, as the system dissipates heat all over the protocol. In the inset of Fig. 3, $\langle Q \rangle$ and $\langle W \rangle$ are shown for the STEP process. Notice how the work exerted on the system is almost instantaneous, while heat is delivered over a wide interval of time, up to complete equilibration. Quite expectedly, there is a price to pay for ESE. A significant amount of work is required to speed up the evolution and beat the natural time scale of our system [22]. It can be shown that the cost $\langle W(t_f) \rangle$ behaves like τ_{relax}/t_f for $t_f \rightarrow 0$. More precisely, this amounts to a time-energy uncertainty relation: $t_f \langle W(t_f) \rangle \sim 0.106 \tau_{\text{relax}} k_B T$. If instead, one proceeds in a quasi-static fashion ($t_f \gg \tau_{\text{relax}}$), the cost reduces to the free energy difference, $k_B T \log(\kappa_f/\kappa_i)/2$ which is $0.35 k_B T$ when $\kappa_f = 2\kappa_i$. For the ESE experiments shown, we have $\langle W(t_f) \rangle \simeq 3.5 k_B T$, about 10 times larger.

Our results show the feasibility and expediency of accelerated protocols for equilibrating confined Brownian objects. The ESE path allowed to gain two orders of magnitude in the thermalization time, as compared to an abrupt change of control parameter (STEP process). The associated energetic cost has been assessed. Finally, while an over-damped problem has been solved here, generalizing the ESE protocol to non-isothermal regimes for under-damped systems, such as an AFM tip, vacuum optical traps, or to transitions between non-equilibrium steady states, constitutes a timely challenge in this emerging field.

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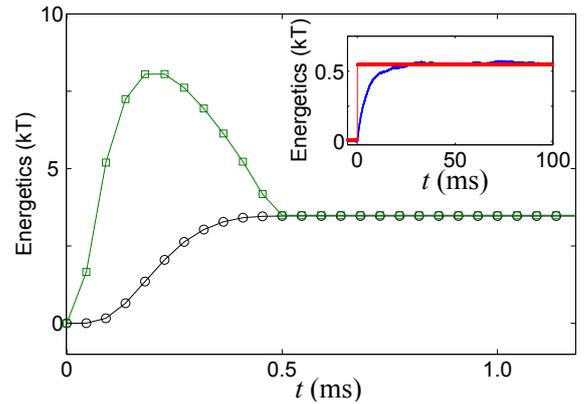


FIG. 3: **Energetics of the ESE protocol.** Average value of the cumulative work W (green squares) and heat Q (black circles) are represented as a function of time. The energy exchange stops within the protocol time $t_f = 0.5$ ms. For $t > t_f$, $\langle W \rangle = \langle Q \rangle$: the system is in an equilibrium steady state, in contact with an isothermal reservoir. **Inset.** Energetics of the STEP protocol. Work (red curve) is exerted onto the system quasi-instantaneously, with an abrupt change of trap stiffness. On the other hand, heat (blue curve) is delivered along the whole equilibration process. Energy-wise, the ESE method appears more costly: this is the price for accelerating the thermalization process.

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Methods

Experimental setup. Silica microspheres of radius $1\mu\text{m}$ were diluted in milliQ water to a final concentration of a few spheres per milliliter. The microspheres were inserted into a fluid chamber, which can be displaced in 3D by a piezoelectric device (Nanomax TS MAX313/M). The trap is realized using a near infrared laser beam (Lumics, $\lambda=980\text{nm}$ with maximum power 500mW) expanded and inserted through an oil-immersed objective (Leica, $63\times$ NA 1.40) into the fluid chamber. The trapping laser power, which determines the trap stiffness, is

modulated by an external voltage V_κ via a Thorlabs ITC 510 laser diode controller with a switching frequency of 200kHz . V_κ is generated by a National Instrument card (NI PXIe-6663) managed by a custom made Labview program. The detection of the particle position is performed using an additional HeNe laser beam ($\lambda=633\text{nm}$), which is expanded and collimated by a telescope and passed through the trapping objective. The forward-scattered detection beam is collected by a condensor (Leica, NA 0.53), and its back focal-plane field distribution projected onto a custom Position Sensitive Detector (PSD from First Sensor with a band pass of 257kHz) whose signal is acquired at a sampling rate of 20kHz with a NI PXIe-4492 acquisition board.

Energetic measurement. From the experimental observables, the stiffness κ and the particle position x , it is possible to infer the energetic evolution of our system within the stochastic energetics framework [24]. The notion of work W is related to the energy exchange stemming from the modification of a given control parameter, here the trap stiffness. Alternatively, heat Q pertains to the energy exchanged with the environment, either by dissipation or by Brownian fluctuations. The work $W(t)$ and dissipated heat $Q(t)$ are expressed as $W(t) = \int_0^t \frac{\partial U}{\partial \kappa} \circ \frac{d\kappa}{dt'} dt'$, $Q(t) = -\int_0^t \frac{\partial U}{\partial x} \circ \frac{dx}{dt'} dt'$ where \circ denotes Stratonovich integral and U is the potential energy. Under this definition, the first law reads as $\Delta U(t) = W(t) - Q(t)$, where $W(t)$, $Q(t)$ and $\Delta U(t)$ are fluctuating quantities. Since T is fixed, both ESE and STEP processes share the same value $\langle \Delta U(t_f) \rangle = 0$ between the initial and the final state. As a consequence, we have $\langle W(t_f) \rangle = \langle Q(t_f) \rangle$.

ESE protocol. The dynamics of the system is ruled by the Langevin equation

$$\dot{x} = -\frac{\kappa(t)}{\gamma}x + \sqrt{D}\xi(t) \quad (1)$$

where a dot denotes time derivative and x is for the position of the Brownian particle. The friction coefficient $\gamma = 6\pi\eta R$ is here constant, η being the the kinetic viscosity coefficient and R the radius of the bead. The diffusion constant then reads as $D = k_B T/\gamma$. The stiffness κ has an explicit dependence on time and $\xi(t)$ is a white Gaussian noise with autocorrelation $\langle \xi(t)\xi(t+t') \rangle = 2\delta(t')$. Eq (1) is over-damped (there is no acceleration term in \ddot{x}), which is fully justified for colloidal objects [25]. The Langevin description (1) can be recast into the following Fokker-Planck equation for the probability density[26]:

$$\partial_t \rho(x, t) = \partial_x \left[\frac{\kappa}{\gamma} x \rho \right] + D \partial_x^2 \rho \quad (2)$$

At initial and final times (t_i and t_f), $\rho(x, t)$ is Gaussian, as required by equilibrium. A remarkable feature of the ESE (non-equilibrium) solution is that for intermediate

times, $\rho(x, t)$ is Gaussian as well, of the form

$$\rho(x, t) = \sqrt{\frac{\alpha(t)}{\pi}} \exp[-\alpha(t)x^2]. \quad (3)$$

We demand that

$$\alpha(0) = \frac{\kappa_i}{2k_B T} \quad \text{and} \quad \alpha(t_f) = \frac{\kappa_f}{2k_B T}. \quad (4)$$

Combining eq. (2) with eq. (3), we obtain

$$\left[\frac{\dot{\alpha}}{2\alpha} - \dot{\alpha}x^2 \right] \rho = \frac{\kappa}{\gamma} (1 - 2\alpha x^2) \rho - 2 \frac{k_B T}{\gamma} \alpha (1 - 2\alpha x^2) \rho. \quad (5)$$

Requiring that the equality holds for any position x , the equation is simplified into:

$$\frac{\dot{\alpha}}{\alpha} = \frac{2\kappa}{\gamma} - \frac{4k_B T \alpha}{\gamma}. \quad (6)$$

We supplement our description with the constraints $\dot{\alpha}(0) = \dot{\alpha}(t_f) = 0$, as a fingerprint of equilibrium for both $t < 0$ and $t > t_f$.

Next, the strategy goes as follows. We choose the time evolution of α , complying with the above boundary conditions. To this end, a simple polynomial dependence of

degree 3 is sufficient. Other more complicated choices are also possible. Introducing the rescaled time $s = t/t_f$, we have

$$\alpha(s) = \frac{1}{2k_B T} [\kappa_i + \Delta\kappa(3s^2 - 2s^3)], \quad (7)$$

where $\Delta\kappa = \kappa_f - \kappa_i$. Finally, eq. (6) has to be satisfied, from which we infer the appropriate evolution $\kappa(t)$ that is then implemented in the experiment:

$$\kappa(t) = \frac{3\gamma\Delta\kappa s(1-s)/t_f}{\kappa_i + \Delta\kappa(3s^2 - 2s^3)} + \kappa_i + \Delta\kappa(3s^2 - 2s^3). \quad (8)$$

The analysis, restricted here to the one dimensional problem, can be easily recast in three dimensions. It is also straightforward to generalize the idea to account for a time-dependent temperature $T(t)$, which can be realized experimentally [20]. In this latter situation, the key relation (6) is unaffected, and therefore indicates how κ should be chosen, for prescribed $\alpha(t)$ and $T(t)$. This highlights the robustness of the ESE protocol.