Convex entropy production for fast and weak drivings

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Knowing if an optimal solution is local or global has always been a hard question to answer in more sophisticated situations of optimization problems. In this work, for fast and weak driving processes, we show the existence of a unique global optimal protocol for entropy production. We prove that by showing its convexity as a functional in the control parameter. This property also proves its monotonicity in such context, in contrast with our previous results where the entropy production rate is not necessarily positive for all times. In the end, we exemplify that the analytical technique used in our previous work [Journal of Physics Communications 6, 083001 (2022)] delivers the global optimal protocol, by comparing it with the results of the global optimization technique of genetic programming.

I. INTRODUCTION

In real life, thermodynamics processes always occur in finite time [1], and energy is irreversibly spent in this manner [2]. An important question is naturally posed: is it possible to execute this same process with minimal dissipation? Mathematically this is nothing more than an optimization problem, where a physical quantity will be minimized in a control parameter under certain conditions. A gas contained in a box, where its volume is changed to accomplish some goal, is a typical example of this scenario.

Several tools have been developed to treat problems of optimization: from the basic techniques of calculus of variations and optimal control theory [3, 4] to numerical techniques like algorithms in convex, global and nonlinear optimizations [5–7]. In any of those scenarios, questions involving the global minimum, that is, the least minimum among all possible solutions, are always present. Even though answers are hard to find in general, a simple criterion always used to guarantee their existence is the idea of convexity. It affirms that if a function is convex, any local minimum will be always a global one [5]. Similarly, the existence of a global maximum is guaranteed with the concept of concavity.

Although those concepts seem like pure mathematical ideas, it has important physical consequences. In classical Thermodynamics, for instance, the concavity of the entropy with respect to the energy guarantees the existence of a unique new equilibrium state to where the system converges when the constraints are changed [2]. Also, since a convex function is always monotonic [5], the fact that informational and quantum entropy productions are convex [8, 9] implies the idea that the rate of entropy in time must be always positive [10].

Some years ago, we presented works where we have shown that, for fast and weak driving processes with non-monotonic protocols, the entropy production rate will not be always greater than zero for all times of the process [11, 12]. Inevitably, critics were raised, since the community proclaim a positive entropy production rate as a law of nature [10]. In this work, we try to answer those critics. Indeed, the property of monotonicity resists in our entropy production, but not in the usual sense: we must observe it as a functional in the control parameter and not as a function in time. We prove that showing that our entropy production is a convex functional and, therefore, monotonic in such context [13].

Besides that, the convexity of the entropy production will lead to the existence of the global minima [13], ever since by the Second Law of Thermodynamics this quantity presents a lower bound. Therefore, any method that uses the functional of entropy production to minimize it will return the global optimal protocol. In particular, the analytical method used in Ref. [14] should be in that case. We exemplify that in the same problem of Ref. [14], by using a global optimization technique called genetic programming [6], where the cost function – our entropy production – will be minimized by routines of evolutionary selecting processes [15, 16].

II. LINEAR RESPONSE THEORY

We start defining our framework and notations to develop the main concepts to be used in this work.

A. Entropy production

Consider a classical system with a Hamiltonian $\mathcal{H}(z(z_0, t), \lambda(t))$, where $z(z_0, t)$ is a point in the phase space $\Gamma$ evolved from the initial point $z_0$ until time $t$ and $\lambda(t)$ is a time-dependent external parameter. During a switching time $\tau$, the external parameter is changed from $\lambda_0$ to $\lambda_0 + \delta \lambda$, with the system being in contact with a heat bath of temperature $\beta \equiv (k_B T)^{-1}$, where $k_B$ is Boltzmann’s constant. The average work performed on
the system during this interval of time is

\[ W \equiv \int_0^\tau \langle \partial_\lambda H(t) \rangle \dot{\lambda}(t) dt, \]  

(1)

where \( \partial_\lambda \) is the partial derivative with respect to \( \lambda \) and the superscripted dot is the total time derivative. The generalized force \( \langle \partial_\lambda H \rangle \) is calculated using the averaging \( \langle \cdot \rangle \) over a non-equilibrium ensemble \( \rho(z_0, t) \)

\[ \langle A(t) \rangle = \int_\Gamma A(z_0) \rho(z_0, t) dz_0, \]  

(2)

where \( A(z_0) \) is some observable. The non-equilibrium ensemble \( \rho(z_0, t) \) evolves according to Liouville equation

\[ \dot{\rho} = -\{\rho, H\}, \]  

(3)

where \( \{\cdot, \cdot\} \) is the Poisson bracket and \( \rho(z_0, 0) \) is the initial canonical ensemble. Consider also that the external parameter can be expressed as

\[ \lambda(t) = \lambda_0 + g(t)\delta\lambda, \]  

(4)

where to satisfy the initial conditions of the external parameter, the protocol \( g(t) \) must satisfy the following boundary conditions

\[ g(0) = 0, \quad g(\tau) = 1. \]  

(5)

We consider as well that \( g(t) \equiv g(t/\tau) \), which means that the intervals of time are measured according to the switching time unit.

Linear response theory aims to express average quantities until the first order of some perturbation parameter considering how this perturbation affects the observable to be averaged and the non-equilibrium ensemble [17]. In our case, we consider that the parameter does not considerably changes during the process, \( |g(t)\delta\lambda/\lambda_0| \ll 1 \), for all \( t \in [0, \tau] \). In that manner, using the framework of linear response theory, the generalized force can be approximated until the first-order as

\[ \langle \partial_\lambda H(t) \rangle = \langle \partial_\lambda H \rangle_0 + \delta\lambda \langle \partial_\lambda^2 H \rangle_0 g(t) - \delta\lambda \int_0^t \phi_0(t - t')g(t')dt', \]  

(6)

where \( \langle \cdot \rangle_0 \) is the average over the initial canonical ensemble. The quantity \( \phi_0(t) \) is the so-called response function [17], which can be conveniently expressed as the derivative of the relaxation function \( \Psi_0(t) \) [17]

\[ \phi_0(t) = -\frac{d\Psi_0}{dt}. \]  

(7)

In our particular case, the relaxation function is calculated as

\[ \Psi_0(t) = \beta \langle \partial_\lambda H(0) \partial_\lambda H(t) \rangle_0 - C, \]  

(8)

where the constant \( C \) is calculated to vanish the relaxation function for long times [17]. The generalized force, written in terms of the relaxation function, can be expressed as

\[ \langle \partial_\lambda H(t) \rangle = \langle \partial_\lambda H \rangle_0 - \delta\lambda \tilde{\Psi}_0 g(t) + \delta\lambda \int_0^t \Psi_0(t - t')\dot{g}(t')dt', \]  

(9)

where \( \tilde{\Psi}_0(t) \equiv \Psi_0(0) - \langle \partial_\lambda^2 H \rangle_0 \). Finally, combining Eqs. (1) and (9), the average work performed at the linear response of the generalized force is

\[ W = \delta\lambda \langle \partial_\lambda H \rangle_0 - \frac{\delta\lambda^2}{2} \tilde{\Psi}_0 + \delta\lambda^2 \int_0^\tau \int_0^t \Psi_0(t - t')\dot{g}(t')\dot{g}(t')dt'dt. \]  

(10)

We observe that the double integral on Eq. (10) vanishes for long switching times [11]. Therefore the other terms are part of the contribution of the difference of free energy since this quantity is exactly the average work performed for quasistatic processes in isothermal drivings. Thus, we can split the average work in the difference of free energy \( \Delta F \) and irreversible work \( W_{\text{irr}} \)

\[ \Delta F = \delta\lambda \langle \partial_\lambda H \rangle_0 - \frac{\delta\lambda^2}{2} \tilde{\Psi}_0, \]  

(11)

\[ W_{\text{irr}} = \delta\lambda^2 \int_0^\tau \int_0^t \Psi_0(t - t')\dot{g}(t')\dot{g}(t')dt'dt. \]  

(12)

In particular, the irreversible work can be rewritten using the symmetric property of the relaxation function, that is, \( \Psi(t) = \Psi(-t) \),

\[ W_{\text{irr}} = \frac{\delta\lambda^2}{2} \int_0^\tau \int_0^t \Psi_0(t - t')\dot{g}(t')\dot{g}(t')dt'dt. \]  

(13)

This irreversible work is exactly the part of the entropy which is internally raised along the driving. Therefore, the entropy production of the system, given by \( S_i = W_{\text{irr}}/T \), will be

\[ S_i = \frac{\delta\lambda^2}{2} \int_0^\tau \int_0^t \Psi_0(t - t')\dot{g}(t')\dot{g}(t')dt'dt, \]  

(14)

where we assume without loss of generality that the temperature of the heat bath is \( T = 1 \). Also, the entropy production rate will be

\[ \dot{S}_i = \delta\lambda^2 \ddot{g}(t) \int_0^t \Psi_0(t - t')\dot{g}(t')dt'dt, \]  

(15)

which can be positive or negative, depending on the characteristics of the system and process [11].

B. Diagram of non-equilibrium regions

We establish the regimes where linear response theory can describe thermodynamic driving processes. Those
regimes are determined by the relative strength of the driving with respect to the initial value of the protocol, \( \delta \lambda / \lambda_0 \), and by the ratio between relaxation time of the system for the rate by which the process occurs, \( \tau_R / \tau \). See Fig. 1 for a diagram depicting the regimes. In region 1, the so-called slowly varying processes, the ratio \( \delta \lambda / \lambda_0 \) is arbitrary, while \( \tau_R / \tau \ll 1 \). By contrast, in region 2, the so-called finite-time and weak processes, the ratio \( \delta \lambda / \lambda_0 \ll 1 \), while \( \tau_R / \tau \) is arbitrary. In region 3, the so-called arbitrarily far-from-equilibrium processes, both ratios are arbitrary. Linear response theory is only able to describe regions 1 and 2. In this work, we are going to focus on region 2 only.

C. Overdamped Brownian motion

To be presented in Sec. V A, we describe now the examples of overdamped Brownian motions subjected to time-dependent harmonic traps [14, 18]. Consider a particle of mass \( m = 1 \) and position \( x(t) \), subjected to a heat bath and time-dependent harmonic potentials \( V(x(t), \lambda(t)) \), where \( \lambda(t) \) is the external control parameter. Its dynamics is govem by the Langevin equation

\[
m \ddot{x}(t) + \gamma \dot{x} + \partial_t V(x(t), \lambda(t)) = \eta(t),
\]

where \( \gamma \) is the friction constant and \( \eta(t) \) is a Gaussian white noise, which obeys

\[
\langle \eta(t) \rangle = 0, \quad \langle \eta(t) \eta(t') \rangle \propto \delta(t - t').
\]

We say that the system is subjected to a moving laser trap when

\[
V(x(t), \lambda(t)) = \frac{\omega_0^2}{2} (x(t) - \lambda(t))^2,
\]

where \( \omega_0 \) is the natural frequency of the system. Also, we say that the system is subjected to a stiffening trap when

\[
V(x(t), \lambda(t)) = \frac{\lambda(t)}{2} x(t)^2.
\]

D. Optimization of the entropy production

Consider the entropy production rewritten in terms of the protocols \( g(t), g(t') \) instead of their derivatives

\[
S_t = \frac{\Psi(0)}{2} \delta \lambda^2 + \frac{\delta \lambda^2}{2} \int_0^\tau \dot{\Psi}_0(\tau - t) g(t) dt - \frac{\delta \lambda^2}{2} \int_0^\tau \int_0^\tau \dot{\Psi}(t - t') g(t) g(t') dt dt'.
\]

Using the calculus of variations [3, 4], we can derive the Euler-Lagrange equation that gives the optimal protocol of the system to minimize, in principle, the entropy production locally

\[
\int_0^\tau \dot{\Psi}_0(t - t') g^*(t') dt' = \dot{\Psi}_0(\tau - t).
\]

For applications of the method, see Ref. [14].

At this point, to work with the ideas of global minima and monotonicity of the entropy production, we must look it as a convex functional in the control parameters. In particular, this property is proved by showing that the functional is twice Gâteaux differentiable.

III. GÂTEAUX DIFFERENTIABILITY

In the following sections, the demonstrations of the main results are omitted. We recommend therefore the book [13] for a more detailed discussion.

A. Gâteaux derivative

Consider an inner product space of functions. The Gâteaux differentiability is a generalization of the traditional directional derivative applied to functionals defined in that space. In this manner, the functional \( J \) is Gâteaux differentiable at \( u \), along the direction \( v \), if two things happen: the derivative

\[
J'[u; v] := \left. \frac{d J[u + \epsilon v]}{d \epsilon} \right|_{\epsilon=0}
\]
exists for all \( v \) and

\[
\frac{dJ[u + \epsilon v]}{d\epsilon} \bigg|_{\epsilon=0} = (J'[u], v),
\]

(24)

where \((\cdot, \cdot)\) is the inner product of that space. The quantity \( J'[u] \) is called the Gâteaux derivative of \( J \) in \( u \).

Extensions of that concept to higher derivatives exist as well. For example, we say that \( J \) is twice Gâteaux differentiable at \( u \) in the direction \( v \) and \( w \) if the limit

\[
J''[u; v, w] := \frac{dJ'[u + \epsilon v; w]}{d\epsilon} \bigg|_{\epsilon=0}
\]

(25)

exists for all \( v \) and \( w \), and

\[
\frac{dJ'[u + \epsilon v; w]}{d\epsilon} \bigg|_{\epsilon=0} = (J''[u]v, w),
\]

(26)

being \( J''[u] \) called the second Gâteaux derivative of \( J \) in \( u \).

B. Convexity

In what follows, we present a criterium that connects convexity with twice Gâteaux differentiability. Starting from the beginning, a functional \( J(u) \) is convex if

\[
J((1-\theta)u + \theta v) \leq (1-\theta)J(u) + \theta J(v),
\]

(27)

for all \( \theta \in [0,1] \), \( u \) and \( v \).

In the case where the functional is twice Gâteaux differentiable, it is convex if, and only if,

\[
(J''(u)w, w) \geq 0,
\]

(28)

for all \( u \) and \( w \) [13]. In the following, we briefly present, from convexity, results involving monotonicity and global minimization.

C. Monotonicity of Gâteaux derivative

A functional \( J(u) \) is convex if, and only if, its Gâteaux derivative is monotonic [13]

\[
(J'(u) - J'(v), u - v) \geq 0.
\]

(29)

This property will show that the entropy production preserves the idea of monotonicity [11], but in the sense of a functional depending on the control parameter.

D. Global optimization

If a functional is convex, every local minimum will be a global minimum [13]. Suppose for instance that \( u \) is a local minimum. If it is not a global minimum, it exists a \( v \) such that \( J(u) < J(v) \). By convexity, it holds

\[
J((1-\theta)u + \theta v) < J(u),
\]

(30)

for sufficiently small \( \theta \), \( J(u) \) is not a local minimum, which contradicts the hypothesis.

We apply those concepts presented at the functional of entropy production derived from linear response theory for fast and weak driveings.

IV. MONOTONICITY OF ENTROPY PRODUCTION

We are going to show that the functional of the entropy production \( S_i[\dot{g}(t)] \) is monotonic in \( \dot{g}(t) \) in the sense of functionals. We use the idea of convexity of \( S_i \). First, we observe that Eq. (15) defines a natural inner product of the space of functions

\[
(\dot{g}(t), \dot{h}(t)) = \frac{\delta \lambda^2}{2} \int_0^T \int_0^T \Psi(t - t') \dot{g}(t') \dot{h}(t) dt'dt, \]

(31)

where \( \Psi(t) \) is the relaxation function. In Ref. [11], we have shown that such relaxation function must be a positive kernel, such that the inner product becomes well-defined. The first Gâteaux derivative of \( S_i \) with respect to \( \dot{g}(t) \) is

\[
S_i'[\dot{g}(t)] = \dot{g}(t),
\]

(32)

and the second one

\[
S_i''[\dot{g}(t)] = 1.
\]

(33)

In that manner, since Eq. (33) is a positive number, \( S_i \) is a convex functional. Therefore, \( S_i[\dot{g}(t)] \) must be monotonic

\[
(S_i'[\dot{g}_1(t)] - S_i'[\dot{g}_2(t)], \dot{g}_1(t) - \dot{g}_2(t)) \geq 0.
\]

(34)

Indeed

\[
\int_0^T \int_0^T \Psi(t - t') (\dot{g}_1(t) - \dot{g}_2(t))(\dot{g}_1(t') - \dot{g}_2(t')) dt'dt' \geq 0,
\]

(35)

for all \( \dot{g}_1(t) \) and \( \dot{g}_2(t) \). Therefore, as we have shown in our previous works [11, 12], the entropy production, seen as a function of time, is not a monotonic function. However, if we consider it as a convex functional in the control parameter, \( S_i \) becomes monotonic. This new concept seems more appropriate to be used in our definition of entropy production since the many other definitions used in the literature, like thermodynamic entropy, Shannon entropy, relative entropy and their quantum versions are concave and therefore monotonic [2, 8, 9].
V. GLOBAL MINIMUM FOR ENTROPY PRODUCTION

Another important consequence of $S_t$ being convex is that any local minimum will be the global minimum. Also, since the entropy production has a lower bound accordingly to the Second Law of Thermodynamics, this implies in the existence of a local minimum and, therefore, in the existence of a global one. In this manner, the optimal protocols calculated in Ref. [14] by solving Eq. (22) are indeed global minimum. We verify that comparing the analytical results with a global optimization technique called genetic programming [6, 15, 16].

A. Global minimum with genetic programming

Consider the global optimization method of genetic programming [6, 15, 16]. It consists basically of finding the optimal protocol evaluating, among members of a family of functions, the minimal cost functional using evolutionary selecting routines along generations. Using the MATLAB package MCL2 [16], we develop a code to find the optimal protocol to minimize the entropy production functional of an overdamped Brownian motion subjected to time-dependent harmonic traps [14, 18]. In both cases of moving laser and stiffening traps, the relaxation function is

$$
\Psi(t) \propto e^{-|t|/\tau_R},
$$

where $\tau_R$ is the characteristic relaxation timescale of the problem. The cost function of genetic programming will be Eq. (15). We expect that the code converges to the global optimal protocol unless it presents an error in their algorithm or bad choice of parameters [6]. In this manner, the simulations were repeated several times with different but reasonable initial conditions and parameters [16]. Except for the final solution, no momentary stop in a particular protocol was found within our criterion of convergence in any simulation. This highly suggests the nonexistence of local minima different than that of the global one. Our criterion of convergence was achieved when graphically the protocol does not change significantly for 30 generations.

On the other hand, the analytical optimal protocols of this problem are given by [14, 18]

$$
g^*(t) = \frac{t + \tau}{\tau + 2\tau_R}.
$$

The comparison between genetic programming and analytical results is depicted in Fig. 2. The matching between both results illustrates that the analytical optimal protocol is indeed a global minimum, as predicted by its property of convexity. Other optimization methods using the entropy production functional (15), like the minimization of a finite quadratic form with Lagrange multipliers [19–21], presents as well the same property of having an unique global optimal protocol.

VI. FINAL REMARKS

We have proved that, for fast and weak driving processes, entropy production is a convex functional in the control parameter. Therefore, this quantity presents a global optimal protocol, and it is monotonic. We verify the first consequence by comparing the results of the analytical method presented in Ref. [14] with those of genetic programming presented in Sec. VA. In the second consequence, the entropy production, by contrast with our previous works [11, 12], is monotonic when seen as a functional in an inner product space of functions, being in accord with other entropy productions proposed in the literature that present concavity properties.

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