Fluctuation theorems for a mechanical work observable

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Of indisputable relevance for non-equilibrium thermodynamics, fluctuations theorems have been generalized to the framework of quantum thermodynamics, with the notion of work playing a key role in such contexts. The typical approach consists of treating work as a stochastic variable and the acting system as an eminently classical device with a deterministic dynamics. Inspired by technological advances in the field of quantum machines, here we look for eventual corrections to work fluctuations theorems when the acting system is allowed to enter the quantum domain. This entails including the acting system in the dynamics and letting it share a nonclassical state with the system acted upon. Moreover, favoring a mechanical perspective to this program, we employ a concept of work observable. For simplicity, we choose as theoretical platform the autonomous dynamics of a two-particle system with an elastic coupling. For some specific processes, we derive several fluctuation theorems within both the quantum and classical statistical arenas. In the quantum results, we find that, along with entanglement and quantum coherence, aspects of inertia also play a significant role since they regulate the route to mechanical equilibrium.

1 Introduction

Going beyond the linear response regime and standing out as insightful relations connecting fluctuating quantities to aspects of thermal equilibrium, fluctuation theorems (FTs) have been extended from the field of stochastic thermodynamics to general quantum scenarios \cite{1–7}. Within the regarded fluctuating quantities, work plays a prominent role for two reasons: (i) it is of key relevance for complete statements of the energy conservation law and (ii) work FTs yield sensible formulations of the second law of thermodynamics in terms of equilibrium free energy.

Paramount for any unambiguous definition of work is the specification of both the “acting system” (from now on referred to as agent), the one that applies the driving force, and the “system acted upon” (hereafter, receiver), the one which the force is applied on. Of course, in light of Newton’s third law, there is no fundamental reason preventing one to assign to a given physical system the role of either agent or receiver—this labeling is done by free choice—but the notion of work and internal energy can only make sense through such a clear definition.

In usual stochastic thermodynamics scenarios, the agent is classical in essence, meaning that it is rigidly controlled by an external observer who assigns to it a pre-determined time dependence. In effect, the agent’s influence over time is entirely encoded in a function \( \lambda(t) \) \cite{3,5,8}, a prescription also adopted in the formalism of statistical physics \cite{9}. As a result, the Hamiltonian describing the receiver’s dynamics is an explicitly time-dependent function usually written in the form \( \mathcal{H}(t) \equiv \mathcal{H}(\lambda_t) = \mathcal{H}_0 + V(\lambda_t) \), where \( \mathcal{H}_0 \) is the so-called bare Hamiltonian and \( V(\lambda) \) is an interaction term \cite{5,10}. Within this perspective, concepts of work and acclaimed work FTs \cite{5,11–13} were proposed, with work depending either implicitly or explicitly on \( \lambda_t \) \cite{10,14}.

Among the results known today, the Jarzynski equality \cite{11} certainly stands out, being suitable for a large set of applications and experimental platforms (see \cite{1,5,15,16} and references therein), with some extensions to more general scenarios \cite{5,17,18}. Departing from the so-called inclusive work \cite{10}, \( \mathcal{W}_{\text{inc}}(t,0) = \int_0^t dt' \frac{\partial \mathcal{H}(t')}{\partial t'} \), Jarzynski
arrived at
\[ \langle e^{-\beta W_{\text{exc}}(t,0)} \rangle = \frac{Z_t}{Z_0}, \]  
(1)

with \( Z_t = \int d\Gamma e^{-\beta H(t)} \) denoting the partition function at the instant \( t \) and \( d\Gamma \) the infinitesimal phase-space volume accessible to the receiver. In another vein, it was only posteriorly acknowledged [5,10,14,19] that a distinct fundamental relation had already been derived by Bochkov and Kuzovlev (BK) in their late 1970s article [12]. BK deduced the equality
\[ \langle e^{-\beta W_{\text{exc}}(t,0)} \rangle = 1 \]  
(2)

under assumptions very similar to those of Jarzynski’s approach, except that an exclusive form of work, \( W_{\text{exc}}(t,0) = \int_0^t dt' \frac{\partial H}{\partial \lambda_t} \), was used instead. The distinction between inclusive and exclusive work led not only to different FTs, as in Eqs. (1) and (2), but also to distinguishable work-energy relations, this being the source of an intense debate [10,14,20–24]. It turns out that the inclusive approach used to deduce the Jarzynski equality is close to a thermodynamical picture of work [25,26], where the interaction energy with external bodies is accounted as part of the internal energy. On the other hand, the exclusive definition has its essential features very closely related to those of a mechanical notion of work, as in the Newtonian description of massive point particles, where the internal energy does not generally encompass external degrees of freedom [20].

When going to a quantum regime, the usual route to describe work and work FTs has been to directly quantize the classical Hamiltonian \( H(t) \) into a time-dependent operator \( H(t) \equiv H(\lambda_t) \) describing the internal energy, with the agent’s influence being encoded in the control parameter \( \lambda_t \). As a consequence, \( \lambda_t \)-dependent work definitions analogous to the classical ones were proposed [25,27–36]. Still in the nonautonomous context, a debate emerged around the fact that some of the work definitions lead to results that deviate from the usual classical FTs [28–30,37,38]. Indeed, it was later shown that work definitions could not simultaneously satisfy two natural requirements, namely, (i) that mean energy variation corresponds to average work and (ii) that work statistics agree with usual classical results for initial states with no coherence in the energy basis [35]. Further definitions of work were then introduced and modified work FTs deduced [5,29,37,39]. In none of these approaches, however, the role of the agent’s configuration was critically assessed, a state of affairs that changed only when autonomous systems came into focus.

With the ever growing interest on thermodynamics phenomena in quantum regime, a generalization of the concept of work as well as FTs for autonomous scenarios started to be pursued. Within this agenda, autonomous machines have been analyzed [40–43], effects of correlations, coherences, degeneracy, thermal fluctuations, and information resources on thermodynamics have been studied [44–48], and batteries (or work reservoirs) have explicitly been considered in the dynamics [49,50]. Alternatively, some constraints (sometimes taken as general quantum FTs) have been obtained for general dynamics [51–53] and other forms of statistically describe work and other thermodynamics properties have been discussed [54–58].

In this paper, we examine how work FTs manifest themselves when we move one step further into the quantum domain. Basically, we pursue a fundamentally mechanical treatment characterized by two key elements. First, we let the agent be submitted, along with the receiver, to a closed energy-conserving autonomous dynamics, upon which no external control \( \lambda_t \) is ever imposed. In particular, we allow the composite system “agent + receiver” to be prepared in nontrivial quantum states, eventually encoding coherence, quantum correlations, and local thermal effects. To the best of our knowledge, these regimes have remained widely unexplored so far. Second, we abandon the usual thermodynamical stochastic essence assigned to work in favor of an operator-based model, which naturally attaches a fundamentally quantum mechanical bias to this concept. In effect, this model treats work as a Heisenberg observable admitting an eigensystem for each given process and genuine quantum fluctuations [59]. Despite some skepticism to treating work as an observable [5,7,30,37], the work observable formalism was shown to be experimentally testable and physically sound, besides being approachable as a two-time element of reality. At last, taking the operator \( W \) as the work done by the agent on the receiver, we compute the average \( \langle e^{-\beta_1 W} \rangle \), with \( \beta_1 \) being an effective inverse temperature underlying the receiver’s initial state. To free the discussion of unnecessary technicalities, our theoretical platform is chosen to be
as simple as possible: we consider a two-particle system, with elastic coupling, evolving over specific time intervals. Our results are then compared with the BK equality (2), which is closer than Jarzynski’s formula (1) to the mechanical paradigm. To highlight the genuinely quantum aspects of our results, we conduct classical studies in parallel employing the usual Newtonian notion of work, with its statistics being raised in accordance with the Liouvillian framework. Although our work FTs are shown to accurately retrieve BK’s equality in some regimes, they manifest themselves rather differently (and somewhat surprisingly) in quantum instances.

2 Classical autonomous scenario

We start by investigating the classical statistical framework, wherein the celebrated FTs have originally been derived. Consider two particles of masses \(m_{1,2}\) interacting via an elastic potential of characteristic constant \(k\). The autonomous dynamics is governed by the Hamiltonian function

\[
\mathcal{H} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{k}{2}(x_2 - x_1)^2, \tag{3}
\]

where \(x_i (p_i)\) is the position (momentum) of the \(i\)-th particle. Henceforth, particle 1 (2) will assume the role of receiver (agent). Within a mechanical perspective, the work \(W(t_2, t_1)\) done by particle 2 on particle 1 during the time interval \([t_1, t_2]\), is defined as

\[
W(t_2, t_1) := \int_{t_1}^{t_2} dt \ m_1 \dot{x}_1 \dot{x}_1 = \Delta \mathcal{K}, \tag{4}
\]

where \(\Delta \mathcal{K} = \mathcal{K}_1(t_2) - \mathcal{K}_1(t_1)\), with \(\mathcal{K}_1(t) = \frac{m_1 x_1^2(t)}{2}\) being the kinetic energy of particle 1 (receiver’s internal energy). Thus, equation (4) is the usual statement of the energy-work theorem [60].

Aiming at computing the statistics underlying \(W(t_2, t_1)\), we explicitly solve the Hamilton equations in terms of the initial phase space point \(\Gamma_0 = (x_1^0, p_1^0, x_2^0, p_2^0) \equiv (x_1(0), p_1(0), x_2(0), p_2(0))\). The procedure is facilitated by the use of the center-of-mass and relative coordinates

\[
\begin{align*}
x_{cm} &= \frac{(m_1 x_1 + m_2 x_2)}{M},
x_r &= x_2 - x_1, 
p_{cm} &= p_1 + p_2, 
p_r &= \mu (p_2/m_2 - p_1/m_1),
\end{align*}
\]

with \(\mu = m_1 m_2/M\) and \(M = m_1 + m_2\). In the transformed Hamiltonian, \(\mathcal{H} = p_{cm}^2/2M + p_r^2/2\mu + k x_r^2/2\), the new degrees of freedom decouple and the trajectories are trivially derived:

\[
\begin{align*}
x_{cm}^i &= x_{cm}^0 + p_{cm}^0 t/M, 
\dot{x}_r^i &= x_r^0 \cos (\omega t) + (p_r^0/\mu \omega) \sin (\omega t), 
\dot{p}_{cm}^i &= p_{cm}^0, 
\dot{p}_r^i &= p_r^0 \cos (\omega t) - \mu \omega x_r^0 \sin (\omega t),
\end{align*}
\]

with \(\omega = \sqrt{k/\mu}\). Returning to the original variables, we can write an expression for the momentum of particle 1 at a generic time \(t\),

\[
\begin{align*}
p_1^t (\Gamma_0) &= a(t) p_1^0 + b(t) p_2^0 + c(t) (x_2^0 - x_1^0), 
&\begin{cases}
a(t) = [m_1 + m_2 \cos (\omega t)]/M, 
b(t) = [1 - \cos (\omega t)] m_1/M, 
c(t) = \mu \omega \sin (\omega t).
\end{cases}
\end{align*}
\]

As a result, we are able to write the kinetic energy \(\mathcal{K}_1(t)\) and the work \(W(t_2, t_1)\) as explicit functions of the initial phase point \(\Gamma_0\). For simplicity, hereafter we restrict our analysis to processes occurring within the time intervals \([t_1, t_2] = [0, v \tau]\), with \(v\) an odd integer and \(\tau = \pi/\omega\). With the notation \(W(\Gamma_0) \equiv W(v \tau, 0)\), the resulting work can be written as

\[
W(\Gamma_0) = \frac{2}{M^2} (m_1 p_2^0 - m_2 p_1^0)(p_1^0 + p_2^0). \tag{9}
\]

To raise the work statistics, we consider an initial distribution \(\varrho(\Gamma_0)\), so that the mean value of a well-behaved function \(f(W(\Gamma_0))\) is given by

\[
\langle f(W) \rangle_\varrho = \int_{\Gamma_0} d\Gamma_0 \ f(W(\Gamma_0)) \ \varrho(\Gamma_0). \tag{10}
\]

2.1 Case studies

Focusing on scenarios associated with the BK equality, we consider, as our first case study, the initial thermal-Gaussian (TG) distribution

\[
\varrho_{TG}(\Gamma_0) = T_{\Delta,1}(x_1^0, p_1^0) \ G_{\sigma_2, \sigma_2}(x_2^0, p_2^0), \tag{11}
\]

which assigns to the receiver the thermal distribution

\[
T_\Delta(x, p) := \frac{\exp \left(- \frac{\Delta^2}{2\sigma^2} \right)}{\sqrt{2\pi}\Delta^2} \ \varrho(x), \tag{12}
\]

where \(\Delta := \sqrt{m/\beta}\) is a “thermal momentum uncertainty” (which also is an indirect measure of temperature), \(\beta\) is an inverse temperature, and
\( \rho(x) \) is a generic probability distribution\(^4\). By its turn, the agent is given the Gaussian distribution \( \mathcal{G}_{x,\sigma_x}(x, p) = \mathcal{G}_{\bar{x},\sigma_x}(x) \mathcal{G}_{\bar{p},\sigma}(p) \), with \( \bar{r} = (\bar{x}, \bar{p}) \), \( \sigma_x = \hbar/(2\sigma) \), and
\[
\mathcal{G}_{\bar{u},\sigma_u}(u) := \exp\left[\frac{-(u-\bar{u})^2}{2\sigma_u^2}\right],
\]
where \( \bar{u} \) and \( \sigma_u \) respectively denote the center and the width of the Gaussian distribution. With distribution (11), the averaging prescribed by (10) for the function \( f(W(\Gamma_0)) = e^{-\beta_W(\Gamma_0)} \) results in
\[
\langle e^{-\beta_1 W} \rangle_{\text{GTC}} = \frac{m_1 + m_2}{|m_1 - m_2|}. \tag{14}
\]
In comparison with the BK formula (2), the differences are clear and insightful, specially with respect to the finite inertia of the agent. Notably, the BK formula is recovered as \( m_2 \to 0 \), limit in which \( x_2' \to x_2'' = x_0'' + p_0'' t/m_2 \). This is the precise regime for which the BK equality was deduced, viz. the one presuming that the agent acts as a deterministic classical driven whose dynamics (not necessarily uniform) can in no way be disturbed by the receiver. Therefore, the dependence of the result (14) on the masses is a direct consequence of the autonomous character of the dynamics under scrutiny. Also noticeable is the fact that (14) does not depend on the details of the preparation, such as \( r_2, \sigma_2, \) and \( \Delta_1 = \sqrt{m_1/\beta_1} \). This may be a consequence of the quadratic structure of the model and eventual peculiarities underlying the time interval chosen. In any case, this reveals that, as long as the condition \( m_2 > m_1 \) is satisfied, the BK equality holds even in the regime of a highly fluctuating agent distribution, for which the notion of a deterministic classical control can no longer be sustained.

We now conduct our second case study, wherein both receiver and agent are initially given thermal states with respective inverse temperatures \( \beta_1 \) and \( \beta_2 \). The composite thermal-thermal (TT) distribution reads
\[
\rho_{\text{TT}}(\Gamma_0) = \mathcal{T}_{\Delta_1}(x_1^0, p_1^0) \mathcal{T}_{\Delta_2}(x_2^0, p_2^0), \tag{15}
\]
where \( \Delta_i = \sqrt{m_i/\beta_i} \) with \( i \in \{1, 2\} \). The calculations show that the result is identical to previous one, that is, \( \langle e^{-\beta_1 W} \rangle_{\text{TT}} = \langle e^{-\beta_1 W} \rangle_{\text{GTC}} \). Again,

\(^4\)In some thermodynamic instances, \( \rho(x) \) has been chosen to characterize a particle confined in a box [9, 61].

the inertial aspects are seen to prevail over any other elements of the preparation, even the arbitrary temperatures \( \beta_{1,2} \).

The situation gets more interesting when we come to our third case study. Here we let not only thermal ingredients be present but also correlations. The initial distribution is chosen to be
\[
\rho_c(\Gamma_0) = \mathcal{T}_{\Delta_1}(x_1^0, p_1^0) \rho_c(x_2^0) \delta_0(p_2^0 - c p_1^0), \tag{16}
\]
where \( \delta_0 \) is the Dirac delta function, \( c \in \mathbb{R}_{>0} \) is a dimensionless parameter whose role is discussed below, and again \( \rho_c(x_2^0) \) is a generic probability distribution. It is not difficult to check that both marginals are thermal distributions, that is,
\[
\rho_c(x_1^0, p_1^0) = \int dx_2^0 dp_2^0 \rho_c(\Gamma_0) = \mathcal{T}_{\Delta_2}(x_1^0, p_1^0), \tag{17}
\]
with \( i, j \in \{1, 2\} \) and \( j \neq i \). An interesting aspect is the appearance of the local inverse temperature \( \beta_2(c) \equiv \frac{\beta_2 m_2}{mc} \) deriving from the connection \( \Delta_2 = c \Delta_1 \). We see, therefore, that \( c \) is a direct estimate of both the correlations between the particles and the agent’s thermal momentum uncertainty. Through the procedure established previously, we arrive at
\[
\langle e^{-\beta_1 W} \rangle_{\rho_c} = \frac{m_1 + m_2}{|m_1 - m_2 + 2mc|}. \tag{18}
\]
In direct comparison with (14), the above result demonstrates that classical correlations can influence work FTs in a relevant way. In particular, for \( m_1 = m_2 \), one has \( \langle e^{-\beta_1 W} \rangle_{\rho_c} = \frac{1}{4} = \sqrt{\beta_2/\beta_1} \), which makes explicit the strong dependence of the result also on the local temperatures. From a broader perspective, result (18) reveals an interesting generalization of the BK formula: by getting apart from the typical thermodynamics setting wherein the agent is a deterministic driver, we find that work FTs can strongly depend on both inertia and, via correlations, agent’s effective temperature, \( T_2 = [k_B \beta_2(c)]^{-1} \).

With the aim of getting more insight about our results, it is opportune to make some digression on energetics. Direct application of Jensen’s inequality, \( \langle g(X) \rangle \geq g(\langle X \rangle) \), with \( g \) a convex function and \( X \) a random variable, allows us to express the Jarzynski equality (1) in the form \( \langle W_{\text{inc}}(t, 0) \rangle \geq \Delta F \), where \( F_t = -\beta^{-1} \ln \mathcal{Z}_t \) denotes the equilibrium free energy at instant \( t \) and \( \Delta F = F_t - F_0 \). This inequality bounds the mean inclusive work with quantities directly associated with the thermodynamic equilibrium and
allows one to make inferences, through the sign of $\Delta F$, about the spontaneity of a physical process. On the other hand, no symptom of thermodynamic equilibrium shows up straightforwardly in the BK equality (2). Still, the derivation of this formula presumes important thermodynamic elements, namely, the preparation of a thermal state for the receiver and an external classical control. These aspects are crucial for a deeper understanding of the relation $(\mathcal{W}_{\text{exc}}(t,0)) \geq 0$ bounding the mean exclusive work. Basically, this inequality states that the agent can only deliver energy to the receiver. This can be explained via the following rationale. One, the thermal state imposes to the receiver a scenario of energetic minimization constrained to a certain temperature. Two, the agent has no need to consume energy from its interaction with the receiver because the agent’s dynamics is deterministically pumped by an external control. Thus, the average result of such interactions cannot be other than an increase of the receiver’s internal energy. To make contact with the scenarios are different, since in BK’s regime evaporates. Interestingly, we see by means of the operator transformation that, even in the regime of mechanical equilibrium $(22)$, one of the particles approximately remains in uniform motion (mechanical equilibrium). Although the BK formula is retrieved in this regime, the scenarios are still different, since in BK’s approach the agent’s motion, being dictated by $\lambda_1$, does not need to be uniform. On the other hand, whenever $(e^{-\beta_1 W})_g \gg 1$, the work FTs largely deviate form the BK formula, and the lower bound in (19) can become significantly negative, meaning that the agent is now allowed to draw energy from the receiver. This regime is favored when $m_1 \simeq m_2$, an instance in which energy exchange between agent and receiver is expected to be ubiquitous throughout the dynamics and, hence, the concept of mechanical equilibrium evaporates. Interestingly, we see by (18) that, even in the regime of mechanical equilibrium $(m_2 \gg m_1)$, an amount $c = \frac{(m_2 - m_1)}{2m_2}$ of classical correlations is able to significantly disturb the directionally of the energetic flow typical of the BK scenario. Given the above, it is fair to conclude that the work FTs we have thus far obtained make important connections with elements of mechanical (instead of thermodynamic) equilibrium.

### 3 Quantum autonomous scenario

In full analogy with the classical model studied in the previous section, we now consider particles of masses $m_1$ and $m_2$ evolving autonomously under the unitary dynamics implied by the Hamiltonian operator

$$H = \frac{P_1^2}{2m_1} + \frac{P_2^2}{2m_2} + \frac{k}{2}(X_2 - X_1)^2,$$

(20)

where $X_i$ $(P_i)$ is the position (momentum) operator of the $i$-th particle. The quantum preparation $\rho$ and $H$ act on the joint Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$. As before, particle 1 (2) will play the role of the receiver (agent).

Since we are interested in exploring FTs under a mechanical perspective, we employ the definition of work proposed in [59]. Accordingly, we use the Heisenberg picture, wherein the operators evolve in time according to the relation $O(t) = U_t^\dagger O U_t$, where $O^\dagger$ is the correspond- Schrödinger operator and $U_t = \exp(-iHt/\hbar)$ is the time evolution operator. In this framework, the velocity and the acceleration of the receiver can be respectively expressed as $\tilde{X}_1 = [X_1, H]/i\hbar$ and $\tilde{X}_1^2 = [\tilde{X}_1, H]/i\hbar$. The quantum mechanical work done by the agent on the receiver within a time interval $[t_1, t_2]$ is then defined as [59]

$$W(t_2, t_1) := \int_{t_1}^{t_2} dt m \frac{\langle X_1, \tilde{X}_1 \rangle}{2} = \Delta K,$$

(21)

where $\Delta K = K_1(t_2) - K_1(t_1)$, with $K_1(t) = \frac{m_1 X_1^2(t)}{2}$ being the kinetic energy of particle 1 (receiver’s internal energy). Definition (21) can be seen as the quantum analog of (4), i.e., the Heisenberg statement of the energy-work theorem, which, as shown in [59], is just a specialization of a more general formulation for quantum systems.

We now proceed to obtain explicit expressions for $W(t_2, t_1)$. Again, we decouple the Hamiltonian operator as $H = P_{cm}^2/2M + P_2^2/2\mu + kX_r^2/2$, by means of the operator transformation

$$X_{cm} = \frac{(m_1 X_1 + m_2 X_2)}{M},$$
$$X_r = X_2 - X_1,$$
$$P_{cm} = P_1 + P_2,$$
$$P_r = \mu (P_2/m_2 - P_1/m_1).$$

(22)
As in the classical model, the analytical solutions are very simple and allow us to write [59]

\[ P_1(t) = a(t) P_1^p + b(t) P_2^p + c(t) (X_2^f - X_1^f), \]

with the same functions \( a(t), b(t), \) and \( c(t) \) defined in (8). Restricting again our analysis to the time interval \([t_1, t_2] = [0, v\tau]\), with \( \tau = \pi/\omega \) and \( v \) an odd integer, and introducing the compact notation \( W = W(v\tau, 0) \), we find

\[ W = \frac{2}{M^2} (m_1 P_2^p - m_2 P_1^p) (P_1^s + P_2^s) \]

for the operator work done by the agent in the process defined by the time interval \([0, v\tau]\). It is clear that \( W \) is diagonal in the composite basis \( \{|p_1, p_2\}\}, \) with eigenvalues \( w_{p_1,p_2} = \frac{1}{M}(m_1 p_2 - m_2 p_1)(p_1 + p_2) \) giving a direct conceptual connection with the classical work (9). This tells us that by jointly measuring \( P_1^s, P_2^s \), one prepares an amount \( w_{p_1,p_2} \) of work in the interval \([0, v\tau]\). It is worth noticing that one does not really “measure” work by measuring the momenta. As discussed in [59] and readily seen from the computations above, a work measurement cannot be performed (not even within the classical paradigm) simply because a two-time observable is not definable at a single time. Instead, we “prepare” work for the interval \([0, v\tau]\) through the establishment of \( \rho \) at \( t = 0 \).

Having computed the work observable (24), we can raise the statistics associated with any well-behaved function \( f(W) \) for an initial state \( \rho \) acting on the joint space \( \mathcal{H} \) via

\[ \langle f(W) \rangle_\rho = \int dp_1 dp_2 f(w_{p_1,p_2}) \rho(p_1, p_2), \]

where \( \rho(p_1, p_2) = \langle p_1, p_2 | \rho | p_1, p_2 \rangle. \) In what follows, we analyze the expectation value of the operator \( f(W) = e^{-\beta_1 W} \) in instances analogous to those considered in the classical context, but also, and most importantly, in fundamentally quantum scenarios. For the sake of notational compactness and analytical convenience, we introduce the parameters

\[ \epsilon \equiv \frac{\sigma_1}{\Delta_1} \quad \text{and} \quad \gamma \equiv \frac{\sigma_1 \sigma_2}{\Delta_1 \Delta_1}, \]

in terms of which most of the discussion that follows will be conduct. The interpretations of \( \sigma_{1,2} \) and \( \Delta_1 \) are the same ones employed in the classical scenarios of Section 2.

### 3.1 Thermal-Gaussian state

Let us start with the case involving a thermal-Gaussian state given by

\[ \rho_{\text{TG}} = T_{\Delta_1}(\sigma_1) \otimes G_{\bar{r}_2, \sigma_2}, \]

where \( G_{\bar{r}_2, \sigma_2} = |\bar{r}_2 \rangle \langle \bar{r}_2| \) denotes a pure Gaussian state, meaning that

\[ \langle x_2 | \bar{r}_2 \rangle = \left( \frac{2\sigma_2^2}{\pi\hbar} \right)^{1/4} e^{-\frac{x_2^2}{2\sigma_2^2}}, \]

\[ \langle p_2 | \bar{r}_2 \rangle = \frac{1}{(2\pi\sigma_2^2)^{1/4}} e^{-\frac{p_2^2}{2\sigma_2^2}}, \]

where \( \bar{r}_2 = (\bar{x}_2, \bar{p}_2) \) is the centroid and \( \sigma_2 \) is the agent’s momentum uncertainty. For the receiver, we have the effective thermal state

\[ T_{\Delta_1}(\sigma_1) = \int dp \frac{e^{-\frac{p^2}{\Delta_1^2}}}{\sqrt{2\pi\Delta_1^2}} G_{(0,p),\sigma_1}, \]

where we recall that \( \Delta_1 = \sqrt{m_1/\beta_1} \). Able to avoid the singularities and normalization problems typical of continuum bases and being very convenient for analytical computations, this state actually is an approximation to a genuine thermal state with inverse temperature \( \beta_1 \). This can be checked from the matrix elements

\[ \langle p_1 | T_{\Delta_1}(\sigma_1) | p_1 \rangle = \exp \left[ -\frac{\rho_1^2}{4\Delta_1^2(1+\epsilon^2)} - \frac{(\rho_1-\rho)^2}{8\Delta_1^2(1+\epsilon^2)} \right], \]

which renders, as \( \epsilon \to 0 \), vanishing coherences and the populations \( \langle p_1 | T_{\Delta_1}(\sigma_1) | p_1 \rangle \propto e^{-\beta_1 K_1} \) with \( K_1 = p_1^2/2m_1 \). That is, when the momentum fluctuation \( \sigma_1 \) of the Gaussian state \( G_{(0,p),\sigma_1} \) is much smaller than the thermal fluctuation \( \Delta_1 \), then \( T_{\Delta_1}(\sigma_1) \) approaches a fully incoherent mixture (in the kinetic energy basis) with thermal populations. Consequently, whenever \( \epsilon \ll 1 \), \( \rho_{\text{TG}} \) as defined by (27) is a reasonable quantum analog of \( \rho_{\text{CG}} \) as given by (11). Following the prescription indicated by (25), with \( f(W) = e^{-\beta_1 W} \), we arrive at

\[ \langle e^{-\beta_1 W} \rangle_{\rho_{\text{TG}}} = \frac{(m_1 + m_2)}{2M} \exp \left( \frac{2m_1^2 \epsilon^2 p_2^2}{2M^2 \Delta_1^2} \right), \]

where

\[ M \equiv \sqrt{(m_1 - m_2)^2 - 4m_1 (\epsilon^2 + m_2^2)}. \]
The above FT, which has been derived under the convergence condition $\mathfrak{M}^2 > 0$ for generic values of $\sigma_{1,2}$ and $\Delta_1$, clearly depends on the equilibrium temperature, through $\Delta_1$, but also on the momentum uncertainties $\sigma_{1,2}$ and the masses $m_{1,2}$, whose values regulate the connection with mechanical equilibrium. Now, series expansion to first order in $\epsilon$, for arbitrary $\sigma_2$, yields

$$\langle e^{-\beta_1 W} \rangle_{\text{PTG}} \approx \frac{m_1 + m_2}{|m_2 - m_1|} \bar{\Gamma},$$

(32)

where $\bar{\Gamma} \equiv \left[ 1 - \left( \frac{2m_1 \gamma}{m_1 - m_2} \right)^2 \right]^{-\frac{1}{2}}$. Note that the instance of a localized agent ($\sigma_2 \gg \Delta_1$) is allowed as long as the convergence condition is preserved. On the other hand, when the agent looses spatial localization, so that $\epsilon \ll \gamma \ll 1$, then we retrieve the classical result (14), that is, $\langle e^{-\beta_1 W} \rangle_{\text{PTG}} \approx \langle e^{-\beta_1 W} \rangle_{\text{PTG}}$ and no dependence on the temperature $\Delta_1$ remains. Again, inertia is seen to play a role in the FT and BK's formula for the nonautonomous scenario is readily retrieved for $m_2 \gg m_1$. It is worth emphasizing that the BK context is conceptually approached only when, in addition to $m_2 \gg m_1$, we consider a dispersion-free state for the agent. However, this does not guarantee a prescription $\lambda_t$ for the agent’s motion, so that, strictly speaking, BK’s regime is still not attained.

### 3.2 Thermal-thermal state

In analogy with the classical distribution (15), our next case study focus on the effective thermal-thermal state

$$\rho_{\text{TT}} = T_{\Delta_1}(\sigma_1) \otimes T_{\Delta_2}(\sigma_2),$$

(33)

where $T_{\Delta_i}(\sigma_i)$ has the same structure as (29). As shown before, when $\sigma_i \ll \Delta_i$ these reduced states become thermal, with respective inverse temperatures $\beta_i$. Direct calculations for generic values of parameters give the exact result

$$\langle e^{-\beta_1 W} \rangle_{\text{TT}} = \frac{(m_1 + m_2)}{\sqrt{\mathfrak{M}^2 + \epsilon^2 m_1^2 (\Delta_2/\Delta_1)^2}},$$

(34)

provided that $\mathfrak{M}^2 + \epsilon^2 m_1^2 (\Delta_2/\Delta_1)^2 > 0$. In the regime where $\epsilon \ll \gamma \ll 1$, we obtain the same approximated results of the previous case, so that $\langle e^{-\beta_1 W} \rangle_{\text{PTG}} \approx \langle e^{-\beta_1 W} \rangle_{\text{PTG}}$. However, it is clear that the ratio of temperatures plays a significant role in general.

### 3.3 Momentum-momentum correlation state

Consider the classically correlated quantum state

$$\rho_c = \int dp \frac{e^{-\frac{p^2}{2m_1}}}{\sqrt{2\pi m_1^2}} G(0,p,\sigma) \otimes G(0,cp,\sigma),$$

(35)

where $c \in \mathbb{R}_{\geq 0}$ a parameter that correlates the momenta of the particles, in analogy with the scenario defined by (16). Notice that we considered $\sigma_2 = \sigma_1 = \sigma$ in this case. Again, directly from (25) for generic parameters, we deduce

$$\langle e^{-\beta_1 W} \rangle_{\rho_c} = \frac{m_1 + m_2}{\sqrt{(m_1 - m_2 + 2m_1 c)^2 - \bar{\mathfrak{F}}}},$$

(36)

under the convergence condition $\bar{\mathfrak{F}} \leq (m_1 - m_2 + 2m_1 c)^2$, where

$$\bar{\mathfrak{F}} = 4m_1^2 \left[ c^2 + c^2 \left( \frac{m_2}{m_1} \right) \right].$$

(37)

Whenever the momentum fluctuations of the Gaussian states are small enough ($\sigma_{1,2} = \sigma \ll \Delta_1$), so that $\epsilon \ll 1$, then the reduced states $\rho_1 = \text{Tr}_{\text{2}} \rho_c$ and $\rho_2 = \text{Tr}_{\text{1}} \rho_c$ can be locally identified as thermal, with inverse temperatures $\beta_1$ and $\beta_2 = \frac{\beta_1 m_2}{m_1}$, respectively. In this regime, we find $\bar{\mathfrak{F}} \equiv 0$ and

$$\langle e^{-\beta_1 W} \rangle_{\rho_c} \approx \frac{m_1 + m_2}{m_1 - m_2 + 2m_1 c},$$

(38)

which agrees with the classical expression (18). Maybe not so surprisingly, in the regime where $\epsilon \ll 1$ we have thus far found a complete match between classical and quantum predictions with regard to work FTs within a mechanical perspective. Next we analyze scenarios without classical counterparts.

### 3.4 Agent in quantum superposition

Let us consider now the preparation

$$\rho_{\text{TS}} = T_{\Delta_1}(\sigma_1) \otimes \left( \frac{\xi + \chi}{N} \right),$$

(39)

where

$$\xi = |\mathbf{\bar{r}}_2\rangle \langle \mathbf{\bar{r}}_2| + |\mathbf{\bar{r}}_2'\rangle \langle \mathbf{\bar{r}}_2'|,$$

$$\chi = |\mathbf{\bar{r}}_2\rangle \langle \mathbf{\bar{r}}_2' + \mathbf{\bar{r}}_2|,$$

(40)

with $|\mathbf{\bar{r}}_2\rangle$ and $|\mathbf{\bar{r}}_2'\rangle$ Gaussian states with center at $\mathbf{\bar{r}}_2 = (\bar{x}_2, \bar{p}_2)$ and $\mathbf{\bar{r}}_2' = \mathbf{\bar{r}}_2 + (\delta_x, 0)$, respectively, and momentum uncertainty $\sigma_2$. $\delta_x$ is a generic spatial displacement and the normalization factor
is given \( N = \text{Tr}(\chi + \xi) = 2 \left[ 1 + \exp(-\eta^2/8) \right] \), where \( \eta \equiv 2\sigma_2 \delta_x / \hbar \). In this case, we arrive at

\[
\langle e^{-\beta_1 W} \rangle_{\rho_{TS}} = \langle e^{-\beta_1 W} \rangle_{\rho_{TC}} \left( \frac{1 + e^{-\Omega \eta^2}}{1 + e^{-\frac{1}{2} \eta^2}} \right) \cos \Theta,
\]

where

\[
\Omega \equiv 1 + \left( \frac{2m_1 \gamma}{2M} \right)^2, \quad \Theta \equiv \frac{\hbar p_2}{\delta_x \Delta_1} \left( \frac{m_1 + m_2}{m_1 - m_2} \right)^2,
\]

again with the convergence condition \( 2M^2 > 0 \). Interestingly enough, we see that the “Gaussian influence” of the agent’s initial state factorizes from the other terms, those which encode via \( \eta \) the superposition elements.

Different scenarios can emerge from the above result. First, when the local state of the receiver is nearly thermal (\( \epsilon \ll 1 \)) and no restriction is imposed on the agent initial state, we have \( \langle e^{-\beta_1 W} \rangle_{\rho_{TS}} \approx \frac{m_1 + m_2}{m_1 - m_2} \), which is no different from the results found when the agent starts in a Gaussian or thermal state. On the other hand, if we consider in addition that \( \sigma_2 \gg \Delta_1 \), so that \( |\vec{r}_2\rangle \) and \( |\vec{r}_2'\rangle \) turn out to be extremely sharp Gaussian states, then we get

\[
\langle e^{-\beta_1 W} \rangle_{\rho_{TS}} \approx \frac{(m_1 + m_2)}{m_1 - m_2} \Gamma \Xi,
\]

where \( \Xi \equiv \frac{1 + \exp(-\eta^2 \Gamma^2/8)}{1 + \exp(-\eta^2/8)} \). In this case, the role of interference can be analyzed through \( \eta \) and \( \Xi \).

Note that \( \eta = 2\sigma_2 \delta_x / \hbar \) dictates whether a spatial interference pattern is detectable for the preparation: if \( \eta \gg 1 \), meaning that the distance \( \delta_x \) between the wave packets is much greater than their width \( \frac{\hbar}{2\sigma_2} \), then no interference pattern is visible via position measurements, although the agent’s initial state is a coherent superposition. In this case, one has \( \Xi \approx 1 \), and the expression (43) reduces to (32), which can be shown to be the FT also when the agent state is prepared in the mixture \( \xi/2 \). On the other hand, if \( \eta \) is not too big, so that interference is observable for the agent’s initial state, then \( \Xi \) becomes smaller than unit and the FT is significantly influenced by the agent’s spatial coherence. It can readily be seen from the plot of \( \Xi \) as a function of \( \eta \) and \( m_1/m_2 \) (Figure 1) how interference and inertia effects can be combined to maximally influence the work FT. Interference becomes most important when, to begin with, it meets the conditions to manifest itself through position measurements on the preparation (which means \( \eta \) small) and when the ratio of masses comes closer to its upper bound \((1 + 2\gamma)^{-1}\), regime which is maximally far apart from the scenario of a heavy agent.

![Figure 1: Attenuation factor \( \Xi \) as a function of the interference parameter \( \eta \) and \( m_1/m_2 \), in the regime \( \sigma_1 \ll \Delta_1 \ll \sigma_2 \) (which is equivalent to \( \epsilon \ll \gamma \ll 1 \)), for \( \gamma = 0.25 \). The combined effects of inertia and interference are seen to be mostly significant in the upper half plane.](image)

### 3.5 Agent entangled with receiver

At last, we consider an entangled initial state, \( \rho_e = |\psi_e\rangle \langle \psi_e| \), where

\[
|\psi_e\rangle = \int dp \frac{e^{-\frac{p^2}{4\kappa^2}}}{\sqrt{4\pi \kappa \Delta_1^2}} |0,p\rangle \otimes |(p,0)\rangle,
\]

\( \kappa \equiv \sqrt{1 + \epsilon^2 + \delta_x^2/2} \). \(|0,p\rangle\) is a receiver’s Gaussian state with center at the mean phase space point \( \vec{r}_1 = (0,p) \) and momentum uncertainty \( \sigma_1 \), and \(|(p,0)\rangle\) is an agent’s Gaussian state with center at \( \vec{r}_2 = (p,0) \) and momentum uncertainty \( \sigma_2 \). The parameter \( \epsilon \in \mathbb{R}_{\geq 0} \) regulates the correlation of the receiver’s momentum with the agent’s position. In the limits \( \sigma_1 \to 0 \) and \( \sigma_2 \to \infty \), the Gaussian states \(|0,p\rangle\) and \(|(p,0)\rangle\) approach momentum and position eigenstates, respectively, with \(|\psi_e\rangle\) thus representing a highly entangled
state. Moreover, it can be shown that in these limits (as long as $(\sigma_1 \sigma_2)^{-1}$ remains bounded) the reduced matrices $\langle p_1^2 | \rho_1 \rangle_1$ and $\langle x_2^2 | \rho_2 \rangle_2$ are nearly diagonal with respective thermal populations $\exp[-p_1^2/(2\Delta_1^2)]$ and $\exp[-x_2^2/(2\Delta_1^2)]$. That is, not only $\rho_1$ is effectively thermal but also $\rho_2$ approximates a mixture of position eigenstates with Gaussian weights of mean value 0 and dispersion $\epsilon \Delta_1$.

To make the discussion about quantum correlations quantitative, we compute the amount of entanglement $E(\rho_1) = 1 - \text{Tr} \rho_2^2$ encoded in $\rho_1$ by measuring how far the purity $\text{Tr} \rho_2^2$ of the subsystem $s \in \{1, 2\}$ is from unit (the maximum purity). Direct calculations lead to

$$E(\rho_1) = 1 - \frac{e^2 (1 + e^2 + \vartheta e^{-2})}{(1 + e^2) (e^2 + \vartheta e^{-2})},$$

(45)

where $\vartheta \equiv h/(2\epsilon \sigma_1 \sigma_2)$. It is straightforward to check that $dE/\text{d}x \geq 0$, with equality holding for $\epsilon = 0$. This shows that entanglement is a monotonic function of $\epsilon$, so that, modulo its dimensional unit, this parameter is itself an estimate of entanglement\(^3\). It is also interesting to note that here the momentum of particle 1 is classically correlated with the position (instead of the momentum) of particle 2 through the parameter $\epsilon \in \mathbb{R} \geq 0$. Just as for $\rho_1$, when $\sigma_1 \to 0$ and $\sigma_2 \to \infty$ with $(\sigma_1 \sigma_2)^{-1}$ remaining bounded, the reduced states become nearly thermal. The exact FT, for arbitrary parameters, turns out to be simply $(e^{-\beta_1 W})_{\rho_1} = (m_1 + m_2)/2\mathcal{H}$. When $\epsilon \ll 1$ this result can be written as

$$(e^{-\beta_1 W})_{\rho_1} \approx \frac{m_1 + m_2}{\sqrt{(m_1 - m_2)^2 - \frac{h^2 \beta_1^2}{\epsilon^2 \sigma_1^2}}},$$

(49)

where $\beta_1 \equiv \hbar/(2\epsilon \sigma_1 \sigma_2)$. The formal comparison with result (47) is now immediate. In particular, we see that the scenarios are comparable when $\vartheta, \epsilon \gg 1$. Also noteworthy is the fact that the relation $h\beta_1/(\varsigma \vartheta \epsilon) = 2\beta_1 \sigma_1 \sigma_2$ shows that (49) is $\hbar$-independent and, therefore, can be claimed to be a fundamentally classical result. In any case, though, it is clear that quantum and purely classical correlations, in combination with thermal and inertial aspects, generally have different impacts in the work FT. This difference disappears as $\hbar \beta_1/m_2$ is sufficiently small, for in this regime both (47) and (49) coalesce to the form typically found throughout this article, namely, $(m_1 + m_2)/|m_1 - m_2|$. Moreover, BK’s formula is retrieved as $m_1 \ll m_2$.

Before closing this section, two remarks are in order. First, with regard to energetics, application of Jensen’s inequality allows us to write, as in the classical context, $(W)_{\rho} \geq -\beta_1^{-1} \ln (e^{-\beta_1 W})_{\rho}$. The state of affairs is then such that, while the BK equality (2) imposes that the average work can never be negative in any time interval, here we have shown that there exist processes wherein the lower bound for the average mechanical work can assume negative values. This means that, within the present perspective in which work is a Hermitian operator and the system is autonomous, a finite-mass agent can also draw energy from the receiver. Such result reveals significant deviations from the mechanical equilibrium emerging when $m_2 \gg m_1$.

Second, work FTs are commonly tested by usage of two-point measurement (TPM) protocols and incoherent states in the energy basis [1,5,30], so it is relevant to examine if and how such methods would deal with the present proposal. Usually, TPM protocols are employed to raise
work statistics under the premise that work is a stochastic energy change induced by an external driving parameter $\lambda_t$ \cite{1,5,30}. It has enabled the experimental validation of important quantum FTs (see, for instance, Refs. \cite{1,5,16} and references therein) and it gives a relatively simple and fairly general way of accounting for work statistics in the quantum thermodynamics domain. It is often applied to a system $S$ described by a time-dependent Hamiltonian $H^s(t) = H^s(\lambda_t)$. After being prepared at $t = 0$ in a generic state $\rho_S$, the system is submitted to a projective measurement of energy at $t_1$, thus jumping to an $H^s(t_1)$ eigenstate $|e_n\rangle$ with probability $p_n = \langle e_n|\rho_S|e_n\rangle$. The system then evolves unitarily (via $\mathcal{U}_\Delta t$, with $\Delta t = t_2 - t_1$) until the instant $t_2$, when a second measurement is performed and a random eigenvalue $\varepsilon_m$ of $H^s(t_2)$ is obtained with probability $p_{mn} = |\langle \varepsilon_m|\mathcal{U}_\Delta t|e_n\rangle|^2$. In this run of the experiment, work is computed as $w_{mn} = \varepsilon_m - \varepsilon_n$. After many runs, the work probability density $\varphi_w = \sum_{mn} p_{mn|n} p_n \delta(w - w_{mn})$ is built, where $\int dw \varphi_w = 1$. It follows that the $k$-th moment of work can be evaluated as $\langle w^k \rangle = \int dw w^k \varphi_w = \sum_{mn} p_{mn|n} p_n w_{mn}^k$. We now examine an adaptation of this protocol to our mechanical perspective. First, it is worth noticing from Eq. (23) that the kinetic energy operator $K_1$ of particle 1 at times 0 and $\nu \tau$ are such that $[K_1(\nu \tau), K_1(0)] = 0$. Therefore, it might be expected \cite{30} that the statistics underlying the work observable $W = K_1(\nu \tau) - K_1(0)$ would coincide with TPM predictions. It turns out, however, that this does not materialize for the entangled state $\rho_c$, since the first measurement of a TPM protocol cancels out the quantum correlation term. To prove that, we compute the probability density $\varphi_{p_1} = \langle |p_1\rangle \langle p_1| \otimes 1_2 \rangle \rho_c\rangle$ of finding a momentum $p_1$, and a corresponding kinetic energy $p_1^2/2m_1$, in the first measurement. We find

$$\varphi_{p_1} = \frac{\exp \left[ \frac{-p_1^2}{2(\Delta_1^2 + \sigma_1^2)} \right]}{\sqrt{2\pi(\Delta_1^2 + \sigma_1^2)}},$$

As soon as the first measurement is concluded, the state of the system is approximately represented by $G_{(0,p),\sigma_1} \otimes G_{(p,0),\sigma_2}$, with $\sigma_1$ sufficiently small. Now, considering the same procedure for the classically correlated state $\rho_c$, we find the same probability density for the first measurement, that is, $\text{Tr} \left[ (|p_1\rangle \langle p_1| \otimes 1_2) \rho_c \right] = \varphi_{p_1}$. Also, via state reduction, the same state $G_{(0,p),\sigma_1} \otimes G_{(p,0),\sigma_2}$ emerges after the measurement. Therefore, the probability densities related to the first measurement on $\rho_c$ and $\rho_t$ are the same and the states right after it also coincide, so that the TPM statistics resulting for $\rho_c$ and $\rho_t$ cannot be distinct. Therefore, a relation like (46) cannot be experimentally verified through a TPM protocol, even when the internal energies in the beginning and at the end commute.

4 Concluding remarks

Crucial to the assessment of physical systems’ responses to applied perturbations, FTs allow us to analyze averages of fluctuating quantities in terms of physical aspects imposed by thermodynamic equilibrium. Studies in these lines have typically been conducted under classical-like assumptions. Nevertheless, searching for eventual effects of relaxing such constraints is vital for one to build a better comprehension of nonequilibrium thermodynamics, specially in quantum regime.

In this article, we avoided classicalities in several ways: we considered (i) an exclusive work observable, (ii) a finite-mass agent, (iii) an autonomous agent-receiver dynamics, and (iv) fundamentally quantum global states which are thermal only locally. Then, we computed work FTs for specific processes and proved, by explicit examples, that the BK formula (2) cannot be extended to such regimes. Interestingly, we have been able to show that quantum agent’s features such as inertia, effective temperature, quantum coherence, and quantum correlations with the receiver directly influence the work FTs. In any case, the BK formula is retrieved for very massive agents, a regime in which energy can only be delivered to the receiver and the dynamics reaches mechanical equilibrium, with the agent in uniform motion. Apart from this very particular regime, our FTs show how inertia and quantum resources lead to the breakdown in the mechanical equilibrium. Finally, we showed that the usually adopted TPM protocol is unable to capture the influence of entanglement on work FTs.

It would be interesting to further explore the work observable formalism of \cite{59} in other autonomous processes and, hopefully, finding a universal bound. As shown here, the notion of work
observable allows us to dig deeper into the extension of FTs to regimes closer to the quantum domain, specially within a fundamentally mechanical perspective. Moreover, we believe that some of the predictions made here can be experimentally tested in near future in the promising trapped ion platforms [62,63].

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