No-Go Theorem for the Characterization of Work Fluctuations in Coherent Quantum Systems

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An open question of fundamental importance in thermodynamics is how to describe the fluctuations of work for quantum coherent processes. In the standard approach, based on a projective energy measurement both at the beginning and at the end of the process, the first measurement destroys any initial coherence in the energy basis. Here we seek extensions of this approach which can possibly account for initially coherent states. We consider all measurement schemes to estimate work and require that (i) the difference of average energy corresponds to average work for closed quantum systems and that (ii) the work statistics agree with the standard two-measurement scheme for states with no coherence in the energy basis. We first show that such a scheme cannot exist. Next, we consider the possibility of performing collective measurements on several copies of the state and prove that it is still impossible to simultaneously satisfy requirements (i) and (ii). Nevertheless, improvements do appear, and in particular, we develop a measurement scheme that acts simultaneously on two copies of the state and allows us to describe a whole class of coherent transformations.

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The second law of thermodynamics, as a statement about average work and average heat, remains correct even when one goes down to the microscopic scale. Nevertheless, unlike the macroscopic case, fluctuations of work and heat become significant for small systems and are not negligible anymore. As a consequence, and starting with the seminal papers [1,2], fluctuations of work have become a topic of central interest to statistical thermodynamics (see, e.g., Refs. [3–6]).

At the same time, small scales bring quantum effects along with them, and the very notion of a work variable becomes challenging to define [7–25]. Indeed, it is no surprise that although quantum mechanics is very definitive when it comes to averages (hence, average work is a well-defined quantity), it abolishes the notion of phase-space trajectories, thereby making it impossible to define the work variable by directly applying the classical intuition. This problem is generic to quantum mechanics, and is captured by the so-called full counting statistics [26,27]. In fact, the latter can be used in the problem of defining a work variable [12,28,29].

In this article, the scenario under consideration consists of a system described by a quantum state ρ and Hamiltonian H. The system undergoes an externally controlled Hamiltonian evolution, described by a unitary transformation U, and ends up in a new quantum state, $\rho \xrightarrow{\text{evol}} U\rho U^\dagger$, with a new Hamiltonian H'. Given this process, there are several approaches to obtaining the statistics of work, namely, the set of outcomes $\{W\}$ and their probability distribution P_W [9,11,16]. This diversity comes from the fact that, unlike in classical mechanics, in order to build P_W in quantum physics, one has to specify the measurement scheme through which such knowledge is obtained. Furthermore, measurements are invasive, so the observation itself can modify the original process, $\rho \xrightarrow{\text{evol}} U\rho U^\dagger$, and hence the energetics.

In order to design a scheme that is minimally invasive, and at the same time physically well motivated, we demand two requirements on the corresponding P_W.

(i) In a closed quantum system, the difference of average internal energy corresponds to work. This imposition goes back to the very definition of work and heat in phenomenological thermodynamics in which, for closed systems, every change of energy comes in the form of work. For the considered process, this is equivalent to demanding

$$\sum_W W P_W = \mathrm{tr}(U\rho U^\dagger H') - \mathrm{tr}(\rho H). \tag{1}$$

This should remain valid for all ρ's and U's.

(ii) For states with no quantum coherence, the results of classical stochastic thermodynamics should be recovered. Classical stochastic thermodynamics, in particular, fluctuation theorems, have been extended in the quantum regime by the two-projective-energy-measurements scheme [4,8,30,31], referred to as the TPM scheme here. In this Letter, we demand strict agreement with this scheme for classical diagonal states. By using this requirement, we ensure that our definition of fluctuating work has a proper classical limit [16,20].

While these two requirements appear reasonable, it is straightforward to see that the existing definitions of work do not satisfy both of them. For example, the TPM scheme trivially satisfies (ii) but fails to satisfy (i) whenever the state has quantum coherence, as the first measurement becomes invasive and destroys all the coherences in the state [32]. The incompatibility also remains for Gaussian energy measurements [16,33]. On the other hand, the operator of work [10] satisfies (i) but not (ii). Other recent definitions of work [11–13], in which both requirements are satisfied, suffer from negative probabilities, which cannot be understood as a quantum measurement [34].

The main result of this Letter is to rigorously prove that this incompatibility is not just a shortcoming of particular approaches but rather a fundamental limitation imposed by quantum mechanics. Namely, we show that there exists no measurement of work that simultaneously satisfies the two requirements imposed above for all processes and states. This shows that observing the microstatistics inherently changes the global (average) work when dealing with quantum systems. This result represents a no-go result in the definition of work as a fluctuating quantity in quantum mechanics and sheds light on different definitions of work in the literature [8,11–16,25].

Besides this no-go result, we also construct new schemes for estimating fluctuating work which can approximately describe coherent transformations. More concretely, we construct a scheme that satisfies (ii) exactly, and (i) to a certain level of approximation. The main idea behind the scheme is to use global measurements, where a number of copies of the state independently undergoing the same process can be measured simultaneously. As such, the backaction of the measurement can be reduced, and hence we can work more closely with the original process $\rho \xrightarrow{\text{evol}} U\rho U^\dagger$. This represents a first step towards the measurement of fluctuating work in quantum coherent evolutions.

Fluctuations of work, generalized quantum measurements, and convexity.—In this Letter, we assume that fluctuations of work can be characterized by a real random variable W, to which a probability distribution P_W can be assigned [35]. We also follow the standard approach, adopted in most of the previous attempts, and assume that work fluctuations can be observed. In quantum physics, this means that they can be estimated through a measurement process, which in turn can always be described by a generalized quantum measurement, defined by a positive-operator-valued measure (POVM) [36]. A POVM is a set of non-negative Hermitian operators $\{M^{(W)}\}$, which satisfy $\sum_{\{W\}} M^{(W)} = \mathbb{I}$. Each possible value of work W is associated with an operator $M^{(W)}$, so the probability to obtain W can be computed through the generalized Born rule:

$$P_W = \mathrm{tr}(\rho M^{(W)}). \tag{2}$$

We consider measurement operators $M^{(W)}$ that can depend on the process, $\Pi = (H, H', U)$, but are independent of the initial state ρ:

$$M^{(W)} = M^{(W)}(\Pi). \tag{3}$$

Indeed, one would like to have a *universal* scheme to estimate work so that there is no need for adjusting the measurement apparatus to the initial state.

One may question why quantum work fluctuations should correspond to an observable quantity and thus be defined through a measurement. Interestingly, it is possible to arrive at expressions (2) and (3) using an alternative, slightly more formal approach. The starting point is the same; namely, work fluctuations should be described by a random variable, where to each outcome W, a probability P_W is assigned. In general, this assignment can depend both on the process and the state: $P_W = P_W(\Pi, \rho)$. Now, it is natural to assume that if one picks the initial state ρ_1 with probability p_1 and state ρ_2 with probability p_2 ($p_1 + p_2 = 1$), then the resulting work distribution is the mixture of the individual work distributions, $\{P_W(\Pi, \rho_1)\}$ with probability p_1 and $\{P_W(\Pi, \rho_2)\}$ with probability p_2. In other words,

$$P_W(\Pi, p_1\rho_1 + p_2\rho_2) = p_1 P_W(\Pi, \rho_1) + p_2 P_W(\Pi, \rho_2) \tag{4}$$

for all W's. Imposing this requirement, a Gleason-type argument (see Sec. I of Ref. [37]) guarantees that for each W there exists a non-negative Hermitian operator $M^{(W)}$ independent of ρ, such that $P_W(\Pi,\rho) = \mathrm{tr}(M^{(W)}\rho)$. Thereby, this shows that invoking POVMs and imposing (2) and (3) can interchangeably be replaced with the single linearity condition (4). Put differently, Eqs. (2) and (3) not only imply linearity of P_W with respect to convex combinations of density matrices but are also equivalent to it.

Minimal requirements for the statistics of work.—Given the previous definitions, we can now express the requirements presented in the introduction in detail. Regarding requirement (i), the average work of a certain process is given by $\sum_W \mathrm{tr}(M^{(W)}\rho)W$. By introducing the operator

$$X = \sum_W W M^{(W)}, \tag{5}$$

it can be rewritten as $\langle W \rangle_\rho = \mathrm{tr}(X\rho)$ [40]. From expression (1), one then obtains $\mathrm{tr}(X\rho) = \mathrm{tr}\big((H - U^\dagger H' U)\rho\big)$. Since this must hold for any ρ, requirement (i) is equivalent to

$$X = H - U^\dagger H' U. \tag{6}$$

Note that this does not fix the measurement scheme—there can be many combinations of non-negative $M^{(W)}$'s summing up to $\mathbb{I}$ and yielding the same X.

In order to describe requirement (ii), let us briefly recall the TPM scheme. Expand the Hamiltonians as $H = \sum_i E_i |i\rangle\langle i|$ and $H' = \sum_i E'_i |i'\rangle\langle i'|$ [41]. Now, the first step of the scheme consists of a projective energy measurement of ρ, which yields E_i with probability $\langle i|\rho|i\rangle$. Only after this measurement is the process implemented, and the state $|i\rangle$ evolves under U. Finally, a projective energy measurement with respect to the final Hamiltonian is performed, yielding $|j'\rangle$ with conditional probability $|\langle j'|U|i\rangle|^2$. To this realization, a work value $W^{(ij)} = E_i - E'_j$ is assigned, with the corresponding probability of occurrence $p^{(ij)} = \rho_{ii} p_{i,j}$, where $p_{i,j} = |\langle j'|U|i\rangle|^2$. The resulting probability distribution for work can be written as $P_{\mathrm{TPM}}(W) = \sum_{ij} \delta(W - W^{(ij)}) p^{(ij)}$, where δ is the Dirac delta function. As noted in Ref. [42], the whole scheme can be expressed by the following POVM: $M^{(W)}_{\mathrm{TPM}} = \sum_{ij} \delta(W - (E_i - E'_j)) p_{i,j} |i\rangle\langle i|$. Formally, requirement (ii) then simply states that

$$\mathrm{tr}(\rho M^{(W)}) = \mathrm{tr}(\rho M^{(W)}_{\mathrm{TPM}}), \quad \forall\ W, \quad \forall\ \rho = D_H(\rho), \tag{7}$$

where D_H is the operation removing all coherence between eigenspaces of H.

Before proving our main result—the incompatibility of these two requirements—let us study condition (7) in more detail. Generally speaking, realizations of work (W in $M^{(W)}$) can take any real value. However, by considering $\rho = |k\rangle\langle k| \forall k$ in Eq. (7), and setting $W \neq E_i - E'_j$, we obtain

$$\langle k|M^{(W)}|k\rangle = 0 \quad \forall\ k \quad \text{if } W \neq E_i - E'_j. \tag{8}$$

Since $M^{(W)}$ is a non-negative operator, this means that $M^{(W)} = 0$, whenever $W \neq E_i - E'_j$. Hence, the only values of W that can be observed, i.e., those for which $M^{(W)} \neq 0$, are the energy differences.

Next, we focus on the case where the possible values of work, $E_i - E'_j$, are nondegenerate. We introduce the operators $M^{(ij)} \equiv M^{(E_i - E'_j)}$ and write the POVM of the TPM scheme as

$$M^{(ij)}_{\mathrm{TPM}} = p_{i,j} |i\rangle\langle i|. \tag{9}$$

Consequently, Eq. (7) will acquire the following form:

$$\mathrm{tr}(\rho M^{(ij)}) = \rho_{ii} p_{i,j} \quad \forall\ \rho = D_H(\rho) \quad \text{and} \quad \forall i, j. \tag{10}$$

By again considering $\rho = |k\rangle\langle k| \forall k$, we obtain from Eq. (10) that $\langle k|M^{(ij)}|k\rangle = \delta_{ik} p_{i,j}$. Now, since there is only one nonzero diagonal element, the non-negativity of $M^{(ij)}$ implies that all off-diagonal elements are zero. Therefore, the conditions (8) and (10) unambiguously fix the measurement operators $M^{(ij)}$ to be identical to the ones in Eq. (9).

No-go result for the characterization of work fluctuations in coherent processes.—We are now ready to prove that the two requirements cannot be jointly satisfied for all processes and states. For that, note that it is enough to construct a counterexample. Consider a two-level system with initial state ρ. It starts with Hamiltonian $H = \epsilon|1\rangle\langle 1|$ and ends with $H' = \epsilon'|1\rangle\langle 1|$, and the process is such that the unitary evolution operator is given by $U = |0\rangle\langle +| + |1\rangle\langle -|$, with $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$. As we showed above, requirement (ii) fixes the POVM matrices to be $M^{(ij)} = p_{i,j}|i\rangle\langle i|$, which, through Eq. (5), give us an expression for X: $X = -\epsilon'|0\rangle\langle 0|/2 + (2\epsilon - \epsilon')|1\rangle\langle 1|/2$. On the other hand, requirement (i) demands, through Eq. (6), that X equals $H - U^\dagger H' U = \epsilon|1\rangle\langle 1| - \epsilon'|-\rangle\langle -|$. For any nonzero ϵ', the two expressions for X do not coincide. Hence, this provides the counterexample.

This no-go result shows that any apparatus for measuring work that gives correct classical outputs for classical states necessarily disturbs the process so much that it changes the average work. The implications of this result for existing methods to describe the fluctuations of work in externally driven quantum systems are discussed in Table I.

Extension to global measurements.—In order to reduce the backaction of the measurements, we now extend our considerations to global measurements, where N copies of the state independently undergoing the same process can be globally processed. In this case, expression (2) is replaced by

$$P_W = \mathrm{tr}(\rho^{\otimes N} M^{(W)}). \tag{11}$$

Examples of global measurements include sequential measurements, in which a different measurement is implemented in each copy,

$$M^{(W)} = M^{(W)}_1 \otimes M^{(W)}_2 \otimes \ldots \otimes M^{(W)}_N, \tag{12}$$

feedback measurements, in which $M^{(W)}_j$ can depend on the previous outcomes, and finally, entangling measurements, which cannot be written as a convex combination of measurements like Eq. (12). Clearly, global measurements can provide an advantage here, and the intuition behind this is twofold: On the one hand, one can measure some copies at the beginning and some others at the end of the process, thereby minimizing the disturbance induced by the measurement apparatus. On the other hand, in the many-copy case, the relative weight of energy-basis coherences becomes less significant [43]. It is also important to note that by assuming the form (11), we break the convexity (4) of P_W, thereby increasing the class of allowed functions.

When considering N copies of the state, $\rho^{\otimes N}$, there are two natural ways to generalize our previous considerations: Either one considers the total work extracted in the process $\rho^{\otimes N} \longrightarrow (U\rho U^\dagger)^{\otimes N}$, or one coarse-grains the measurements to estimate the work extracted from a single copy. In the latter case, the other $N - 1$ copies are used to obtain a

TABLE I. Comparison between three different approaches to characterize the fluctuations of work in externally driven quantum systems: the TPM scheme [8], the operator of work [10], and approaches based on quasiprobabilities [11–13]. Each approach fails to satisfy a different requirement, as expected from the no-go result.

	Measurable	Fluctuation theorems	Coherent processes
TPM scheme	✓	✓	✗
Operator of work	✓	✗	✓
Quasiprobabilities	✗	✓	✓

more refined description of the evolution. In either case, we show that no measurement scheme exists that can simultaneously satisfy (i) and (ii) exactly, and we thereby extend our previous result to collective measurements. For clarity of the discussion, here we focus on the individual work and leave the details of the total work for Sec. II A of Ref. [37].

For global measurements on N copies of the state, the operators $M_N^{(W)}$ act on $\rho^{\otimes N}$ instead of ρ. Then, requirement (ii) can be expressed as $\mathrm{tr}(\rho^{\otimes N} M^{(W)}) = \mathrm{tr}(\rho M_{\mathrm{TPM}}^{(W)})$ $\forall \rho = D_H(\rho)$. Requirement (i) reads as $\mathrm{tr}(\rho^{\otimes N} X) = \mathrm{tr}(\rho H) - \mathrm{tr}(U\rho U^\dagger H')$, $\forall \rho$, where $X = \sum_W W M^{(W)}$. Notice that essentially the same restrictions are imposed on the measurement operators $M^{(W)}$, which now act on a Hilbert space of dimension d^N instead of d, the dimension of ρ. This gives an enormous freedom that was not present before.

Nevertheless, despite the freedom to choose the $M^{(W)}$, we construct a process where both requirements cannot be simultaneously satisfied (see Sec. II B of Ref. [37]). The counterexample is based on taking unitaries of the form $U(\varepsilon) = \sqrt{1-\varepsilon^2}\mathbb{I} + \varepsilon i \sigma_y$, to then show that, if ε decreases fast enough with the increase of N, the fluctuations arising from $U(\varepsilon)$ can never be completely characterized. Hence, we show the incompatibility between preserving the average work and recovering the classical limit for the most general conceivable measurements.

A new measurement scheme to evaluate the quantum fluctuations of work.—Based on the idea of collective measurements, here we construct a new measurement scheme to approximately describe the fluctuations of work in coherent processes. For that, let us first introduce

$$T_j \equiv U^\dagger |j'\rangle\langle j'| U, \tag{13}$$

where we recall that $H' = \sum_j E_j' |j'\rangle\langle j'|$. Consider now the expansion, $T_j = T_j^{(\mathrm{diag})} + T_j^{(\mathrm{off\text{-}diag})}$, with $T_j^{(\mathrm{diag})} = \sum_k |\langle j'|U|k\rangle|^2 |k\rangle\langle k|$ and $T_j^{(\mathrm{off\text{-}diag})} = \sum_{l\neq s} \langle l|U|j'\rangle \langle j'|U|s\rangle |l\rangle\langle s|$. Clearly, $T_j^{(\mathrm{off\text{-}diag})}$ acts on the off-diagonal elements of ρ, and, since $\mathrm{tr}(U\rho U^\dagger H') = \sum_j E_j' \mathrm{tr}(\rho T_j)$, it brings the coherent part of work.

Now, the measurement scheme acts on two copies of ρ, $\rho^{\otimes 2}$, and is given by the following POVM elements (see Sec. III of Ref. [37] for a detailed derivation),

$$M_\lambda^{(ij)} = |i\rangle\langle i| \otimes \left(\langle i|T_j^{(\mathrm{diag})}|i\rangle \mathbb{I} + \lambda T_j^{(\mathrm{off\text{-}diag})} \right), \tag{14}$$

where the parameter λ is chosen such that

$$\lambda = \max_\alpha (\alpha\colon\ M_\alpha^{(ij)} \geq 0 \quad \forall\ i,j). \tag{15}$$

The probability $\mathrm{tr}(\rho^{\otimes 2} M_\lambda^{(ij)})$ is then associated with the value of work $E_i - E_j'$.

The measurement scheme (14) is a combination of two measurements: a projective energy measurement on the first copy of ρ at the beginning of the process, and a (in general) nonprojective measurement on the second copy after being evolved through U. The parameter λ given by Eq. (15) is introduced to ensure the positivity of the POVM elements so that this measurement scheme is operationally well defined and can be experimentally implemented. Furthermore, notice that

$$M_\lambda^{(ij)} = M_{\mathrm{TPM}}^{(ij)} \otimes \mathbb{I} + \lambda |i\rangle\langle i| \otimes T_j^{\mathrm{off-diag}}. \tag{16}$$

Hence the scheme can be seen as an extension of the standard TPM scheme: It acts in the same way on the diagonal part of ρ and additionally brings information about the coherent work through the second term in Eq. (16). More precisely, the enhancement with respect to the TPM scheme is quantified by λ: For $\lambda = 1$, the average work remains unchanged, whereas for $\lambda = 0$, one obtains the same results of the TPM scheme. In Sec. V of Ref. [37], we determine λ for generic qubit evolutions.

In order to show the power of this scheme, we focus on a particular family of evolutions, namely, maximally coherent processes, which are unitary operations of the form

$$W = \frac{1}{\sqrt{d}} \sum_{j,k}^{d-1} e^{-\frac{2\pi i}{d} jk} |j\rangle\langle k|, \tag{17}$$

where d is the Hilbert space dimension. Unitary operations of the form (17) map basis states to maximally coherent states and vice versa, and hence are of great importance here. For such processes, the maximization (15) yields $\lambda = 1$; see Sec. IV of Ref. [37]. Furthermore, the POVM elements take the simple form

$$M_{\lambda=1}^{(ij)} = |i\rangle\langle i| \otimes W^\dagger |j\rangle\langle j| W, \tag{18}$$

which simply corresponds to a projective energy measurement on the first copy, followed by a projective energy measurement on the second copy after the evolution.

Let us now look at the probabilities generated by Eq. (18) for the simplest instance of the evolution (17) with $d = 2$ acting on a fully coherent state, i.e.,

$$|+\rangle \xrightarrow{W} |0\rangle, \tag{19}$$

with $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. By applying Eq. (18) on $|+\rangle^{\otimes 2}$, and using $W|0\rangle = W^\dagger|0\rangle = |+\rangle$, one obtains $p^{(00)} = p^{(10)} = 1/2$ and $p^{(01)} = p^{(11)} = 0$. This predicts that the probability of ending in the ground state, $p^{(10)} + p^{(00)}$, is 1. These results are in contrast with those predicted with the TPM scheme, given by $p^{(00)} = p^{(01)} = p^{(10)} = p^{(11)} = 1/4$, which bear little resemblance to the factual evolution.

Conclusions.—Our results show that two physically necessary properties of quantum work, namely, respecting the classical limit and obeying the first law of thermodynamics, cannot be simultaneously measured. As a consequence, while the observation of work fluctuations does not change the work output for macroscopic processes, this is no longer true in quantum systems with coherence. This result sheds light on the crucial role of measurements [25,44–49] and coherence [50–55] in quantum thermodynamics, and seems to imply that there will probably never be an equivalently universal notion of a work variable that is independent of the context in quantum mechanics.

The basic reason behind this incompatibility is the presence of quantum coherence, together with the backaction induced by quantum measurements. In order to decrease the backaction, we explored the possibility of using collective measurements. Although we showed that the no-go result remains valid for such global measurements, the set of describable coherent transformations increases. In particular, using a measurement on two copies of the state, we provided a new scheme that can approximately describe the fluctuations in quantum coherent processes.

Future work also includes a comparison between the methods developed here for describing the fluctuations of work in coherent processes and other approaches in the literature [11–16,25–29,56,57]. Also particularly interesting are the results on fluctuations of work obtained in the context of the resource theory of thermodynamics, where the fluctuations of work are directly mapped upon the state of an external work-exchange agent—the "weight" [56,57]. As a final remark, we note that the scheme (14) can be used to approximately characterize the fluctuations of work in work extraction processes from entangled states [58].

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[32] On the other hand, the TPM scheme satisfies (1) with ρ substituted by its decohered version. In other words, the TPM scheme satisfies the energy balance, but for the process it generates. However, the latter is generally different from the original one.
[33] In Ref. [16], for Gaussian energy measurements in the von Neumann measurement model, it is observed that, when the pointer is weakly coupled to the system, the average work is given by (1); for strong coupling, one recovers the TPM results. This motivates the authors to name the quantity (1) untouched work, as it refers to the average work in the absence of any backaction from the measurement apparatus.
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