

Quantum Jarzynski Equality in Open Quantum Systems from the One-Time Measurement Scheme

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In open quantum systems, a clear distinction between work and heat is often challenging, and extending the quantum Jarzynski equality to systems evolving under general quantum channels beyond unitality remains an open problem in quantum thermodynamics. In this Letter, we introduce well-defined notions of *guessed quantum heat* and *guessed quantum work*, by exploiting the one-time measurement scheme, which only requires an initial energy measurement on the system alone. We derive a modified quantum Jarzynski equality and the principle of maximum work with respect to the guessed quantum work, which requires the knowledge of the system only. We further show the significance of guessed quantum heat and work by linking them to the problem of quantum hypothesis testing.

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Introduction.—Understanding the laws of thermodynamics at the most fundamental level requires clarifying the thermodynamic properties of quantum systems, and especially the contributions of coherence and correlations in the concept of work and heat are of fundamental interest [1–6]. In quantum microscopic systems, fluctuations are inevitable; therefore, the laws of thermodynamics have to be given by taking into account the effects of these quantum fluctuations. A powerful insight into fluctuations is provided by Jarzynski equality [7], one of the few equalities in thermodynamics, which relates the fluctuating work in a finite-time, nonequilibrium process with the equilibrium free energy difference:

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

Here $\beta = 1/T$ is the inverse temperature (we set the Boltzmann constant $k_B = 1$), W is the work, and ΔF_S is the equilibrium free energy difference defined by the initial, $H_S(0)$, and final Hamiltonian, $H_S(t)$. The equality is independent of process details: the final state of the process does not have to be thermal, and the temperature could change. Jarzynski equality can be also regarded as the generalization of the second law of thermodynamics, since through Jensen’s inequality it yields the principle of maximum work: $\langle W \rangle \geq \Delta F$.

The quantum version of the Jarzynski equality—the quantum Jarzynski equality—was developed by focusing on closed quantum systems in the two-time measurement scheme [8,9], which defines the work as the energy difference between the initial and final energy projection measurements in a single trajectory. Jarzynski equality has

been later extended to open quantum systems subject to dephasing process [10], unital maps [11], random projection measurements [12,13], or feedback control [14,15]; it has been verified experimentally in numerous systems, such as biomolecular systems [16], trapped ions [17,18], NV centers [19], and NMR systems [20].

Despite this progress, a general formulation of the quantum Jarzynski equality for arbitrary open quantum systems is still lacking. This stems from the fundamental challenge that work and heat are not direct observables in quantum mechanics [21]: while in closed systems work can be simply identified with energy variations, in open quantum systems a clear distinction between work and heat is not always possible [22]. While some insight can be gained by theoretically assuming knowledge of the bath state [23–27], in practice the bath cannot be measured. One solution is to assume that a particular process does not involve heat exchange. For example, by assuming heat exchange to be absent in the dephasing process because there is no population decay, one can prove that the quantum Jarzynski equality has the standard form in Eq. (1) [10,17]. Similar results [11] hold for unital maps (that is, identity-preserving maps), which describe only processes that can be microscopically reversed by monitoring the bath with feedback [28,29].

There have been several efforts to extend the quantum Jarzynski equality to nonunital maps [30–35] by using the two-time measurement scheme. However, this either requires a measurement on the bath [36], or it faces a fundamental issue [37] related to the loss of coherence in energy measurements. In open quantum system, the second

energy measurement on the system unavoidably destroys system-bath correlations, making it impossible to distinguish work and heat by energy measurements on the system alone, except for unitary or unital evolutions. In addition, the two-time measurement scheme neglects the information contribution due to the backaction of the second measurement [38]. To improve on the results obtained by the two-point measurement scheme, recent works have used dynamic Bayesian networks [39] and Maggenau-Hill quasiprobability [40], or, for closed quantum systems, avoided completely the second measurement [38,41].

In this Letter, we overcome these issues by introducing a novel definition of guessed quantum heat and work for general quantum channels, which lead to a quantum Jarzynski equality that takes into account system-bath correlations. We employ the one-time measurement scheme developed in Ref. [38] for closed quantum systems. This protocol only requires us to measure the initial energy of the system (which is initially decoupled from the thermal bath) and to evaluate the expectation value of the difference between final and initial energy of the system by introducing the concept of “best possible guess” of the final state [38]. Avoiding the final projective measurement of the energy provides a more precise description of the thermodynamic process than the traditional two-time measurement scheme, since it avoids the backaction by the second measurement and the ensuing information loss [38]. This protocol yields a modified quantum Jarzynski equality in terms of the information free energy [38,42–45], and a tighter bound on the second law of thermodynamics.

Our main result is based on a generalization of the results in Ref. [38] to general quantum channels for open quantum systems in contact with a thermal bath. Inspired by the one-time measurement scheme, we introduce well-defined notions of guessed quantum heat and guessed quantum work that only require measurements on the system. With these quantities, we can derive a modified quantum Jarzynski equality (see Theorem 1) and further update the principle of maximum work (Corollary 1). Specifically, the bound in the principle of maximum work requires knowledge of the system alone. Not only the guessed quantum heat and work provide insights into the dynamics of general open quantum systems, as we show with several examples [46], but they acquire further operational meanings from their relationship to quantum hypothesis testing.

One-time measurement scheme.—We consider a composite system comprising the target system (\mathcal{H}_S) and the bath (\mathcal{H}_B), and assume we can only measure the system. Let $H_S(t)$ be the system Hamiltonian, which is time dependent, and H_B the time-independent bath Hamiltonian. The total Hamiltonian, $H_{\text{tot}}(t) = H_S(t) \otimes \mathbb{1}_B + \mathbb{1}_S \otimes H_B + V(t)$, includes an interaction, $V(t)$, between system and bath [we assume $V(t) = 0$ for $t \leq 0$].

The initial state of the composite system is the product $\tau_S(0) \otimes \tau_B$ of thermal Gibbs states at $t = 0$ for system and

bath, $\tau_S(t) = e^{-\beta H_S(t)}/Z_S(t)$ and $\tau_B = e^{-\beta H_B}/Z_B$. Here, $Z_A(t)$ are the partition functions, $Z_A(t) = \text{Tr}[e^{-\beta H_A(t)}]$ for $A = S, B$. The composite system evolves under a unitary operator U_t as $U_t[\tau_S(0) \otimes \tau_B]U_t^\dagger$ which satisfies the usual Schrödinger’s equation $\partial_t U_t = -iH_{\text{tot}}(t)U_t$ [we set Planck constant $\hbar = 1$].

At time $t = 0$, we measure the energy of the system alone. Suppose that we obtain a value ϵ , corresponding to one of the eigenvalues of $H_S(0)$, with probability $e^{-\beta\epsilon}/Z_S(0)$. Then, the postmeasurement state of the system is the corresponding eigenstate: $|\epsilon\rangle\langle\epsilon|$. Therefore, the evolved state of the system after the measurement is

$$\Phi_t(|\epsilon\rangle\langle\epsilon|) \equiv \text{Tr}_B[U_t(|\epsilon\rangle\langle\epsilon| \otimes \tau_B)U_t^\dagger],$$

where Φ_t is a completely positive trace-preserving map in \mathcal{H}_S . This evolution includes contributions from heat exchange, because of the system coupling to the thermal bath, and from work due to the time dependence of the system Hamiltonian and to system-bath interaction, which exists even for time-independent Hamiltonians. It is however difficult to distinguish the two contributions, and, indeed, a measurement on the system alone would not be fully informative.

After the evolution, we assume that we do not perform a final measurement, but still estimate the energy difference along a certain realization trajectory, $\Delta\tilde{E}(\epsilon)$, from the expectation value of the system Hamiltonian $H_S(t)$ with respect to $\Phi_t(|\epsilon\rangle\langle\epsilon|)$:

$$\Delta\tilde{E}(\epsilon) = \text{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)] - \epsilon.$$

The probability distribution of the internal energy difference is given by

$$\tilde{P}(\Delta E) = \sum_{\epsilon} \frac{e^{-\beta\epsilon}}{Z_S(0)} \delta[\Delta E - \Delta\tilde{E}(\epsilon)].$$

This is a *good* definition because it yields the correct expectation value of the internal energy difference $\langle\Delta E\rangle$. Indeed, denoting with $\langle\cdots\rangle_{\tilde{P}}$ the average with respect to the distribution \tilde{P} , we have

$$\begin{aligned} \langle\Delta E\rangle_{\tilde{P}} &= \int \tilde{P}(\Delta E)\Delta E d(\Delta E), \\ &= \text{Tr}\{H_S(t)\Phi_t[\tau_S(0)]\} - \text{Tr}[H_S(0)\tau_S(0)], \\ &\equiv \langle\Delta E\rangle. \end{aligned} \quad (2)$$

By using $\tilde{P}(\Delta E)$, we can calculate the averaged exponentiated internal energy difference:

$$\begin{aligned} \langle e^{-\beta\Delta E}\rangle_{\tilde{P}} &= \int \tilde{P}(\Delta E)e^{-\beta\Delta E} d(\Delta E) \\ &= \frac{1}{Z_S(0)} \sum_{\epsilon} e^{-\beta\text{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}. \end{aligned}$$

We can interpret this expression by introducing a new partition function

$$\tilde{Z}_S(t) \equiv \sum_{\epsilon} e^{-\beta \text{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]},$$

yielding

$$\langle e^{-\beta\Delta E} \rangle_{\tilde{P}} = \frac{\tilde{Z}_S(t)}{Z_S(0)} = e^{-\beta\Delta\tilde{F}_S}, \quad (3)$$

where $\Delta\tilde{F}_S = \tilde{F}_S(t) - F_S(0)$ is the difference between the initial, thermal equilibrium free energy, $F_S(0) = -\beta^{-1} \ln Z_S(0)$, and the equilibrium free energy corresponding to $\tilde{Z}_S(t)$, $\tilde{F}_S(t) = -\beta^{-1} \ln \tilde{Z}_S(t)$. We note that this relation has the form of a typical Jarzynski equality, linking the energy fluctuation to the free energy; however, to give this relation a physical meaning we need to further investigate the significance of $\tilde{F}_S(t)$ by linking this quantity to an effective state.

Gessed quantum heat and gessed quantum work.—Following Ref. [38], we introduce the best possible guess for the final system state. This thermal state, $\Theta_{SB}(t)$, can be found by maximizing the system-bath Von-Neumann entropy $\mathcal{S}_{SB}(t) = -\text{Tr}[\Theta_{SB}(t) \ln \Theta_{SB}(t)]$ under the constraint of a fixed, average energy for the system alone, time-evolved after the one-time projective measurement. In other words, we apply the principle of maximum entropy [47] to find the state with minimum information content, under the given constraints. The best possible gessed state can be given by

$$\Theta_{SB}(t) = \sum_{\epsilon} p(\epsilon) U_t(|\epsilon\rangle\langle\epsilon| \otimes \tau_B) U_t^\dagger,$$

where the probabilities,

$$p(\epsilon) = \frac{e^{-\beta \text{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)},$$

are found from entropy maximization under the constraint $E_S = \text{Tr}\{[H_S(t) \otimes \mathbb{1}_B]\Theta_{SB}(t)\}$ and that the postmeasurement state of the composite system after the initial energy measurement is given by $|\epsilon\rangle\langle\epsilon| \otimes \tau_B$, before evolving under U_t (see [46]).

We note that here we assumed an isothermal process for the composite system, as expected for a closed quantum system. Then, $\Theta_{SB}(t)$ can be seen as a thermal state at the initial temperature β , even if it is *not* the thermal state of the composite system at time t , $\tau_S(t) \otimes \tau_B$. The difference can be quantified by their relative entropy $D[\Theta_{SB}(t) \|\tau_S(t) \otimes \tau_B] \equiv \text{Tr}[\Theta_{SB}(t) \ln \Theta_{SB}(t)] - \text{Tr}\{\Theta_{SB}(t) \ln[\tau_S(t) \otimes \tau_B]\}$. The relative entropy helps clarifying not only the thermodynamic contribution from the information difference of the states, but also an operational meaning of our results in terms of quantum hypothesis testing. By defining

$$\langle \tilde{Q} \rangle_B \equiv \text{Tr}[H_B \tau_B] - \text{Tr}[(\mathbb{1}_S \otimes H_B)\Theta_{SB}(t)],$$

we write D as [46]

$$D[\Theta_{SB}(t) \|\tau_S(t) \otimes \tau_B] = -\ln \frac{\tilde{Z}_S(t)}{Z_S(t)} - \beta \langle \tilde{Q} \rangle_B. \quad (4)$$

Since $\langle \tilde{Q} \rangle_B$ represents the thermal bath energy loss, we can identify it as a kind of heat [48], that we call ‘‘gessed quantum heat’’ as it arises from the definition of the best possible gessed state $\Theta_{SB}(t)$. We can similarly introduce the notion of ‘‘gessed quantum work’’ \tilde{W} , based on the first law of thermodynamics:

$$\tilde{W} \equiv \Delta E - \langle \tilde{Q} \rangle_B. \quad (5)$$

Then we can obtain the following theorem:

Theorem 1.—The quantum Jarzynski equality for the gessed quantum work is

$$\langle e^{-\beta\tilde{W}} \rangle_{\tilde{P}} = e^{-\beta\Delta F_S} e^{-D[\Theta_{SB}(t) \|\tau_S(t) \otimes \tau_B]}. \quad (6)$$

Proof.—From the definition of the equilibrium free energy, $F_S(t) = -\beta^{-1} \ln Z_S(t)$, we can write $\tilde{F}_S(t) - F_S(t) = \langle \tilde{Q} \rangle_B + \beta^{-1} D[\Theta_{SB}(t) \|\tau_S(t) \otimes \tau_B]$. Defining $\Delta F_S = F_S(t) - F_S(0)$, we have

$$\Delta\tilde{F}_S = \Delta F_S + \langle \tilde{Q} \rangle_B + \beta^{-1} D[\Theta_{SB}(t) \|\tau_S(t) \otimes \tau_B],$$

and substituting into Eq. (3), we obtain

$$\langle e^{-\beta\Delta E} \rangle_{\tilde{P}} = e^{-\beta\Delta F_S} e^{-\beta\langle \tilde{Q} \rangle_B} e^{-D[\Theta_{SB}(t) \|\tau_S(t) \otimes \tau_B]}, \quad (7)$$

which yields Eq. (6) using the definition of gessed quantum work in Eq. (5).

Note that $\tilde{F}_S(t)$ plays the role of an information free energy [38,42–45] computed with respect to the best possible gessed state $\Theta_{SB}(t)$.

We verify Eq. (7) by considering several simple models in [46]. We first discuss time-independent two-qubit interacting model, such as two-qubit dephasing. This model can be realized experimentally in two-qubit systems, such as nitrogen-vacancy (NV) centers in diamond [49], where \mathcal{H}_S and \mathcal{H}_B are the truncated electronic spin system and nuclear spin system associated with the NV center. We also consider an archetypal model of dephasing, the spin-boson model [50] without time dependence. In particular, by not assuming *a priori* that dephasing precludes heat exchange, we find that we can define gessed quantum heat for dephasing maps, and thus gessed quantum work contains not only contributions from the Hamiltonian time dependence, but also from the interaction of system and bath.

From Theorem 1, we obtain the following corollary:

Corollary.—*principle of maximum gessed quantum work.*—The average of the gessed quantum work satisfies the following inequality:

$$\langle \tilde{W} \rangle \geq \Delta F_S + \beta^{-1} D[\tilde{\rho}_S(t) \| \tau_S(t)], \quad (8)$$

where $\tilde{\rho}_S(t) \equiv \text{Tr}_B[\Theta_{SB}(t)]$.

Proof.—Applying Jensen’s inequality to Eq. (7), and using the equivalence in Eq. (2), from Eq. (5), we obtain

$$\langle \tilde{W} \rangle \geq \Delta F_S + \beta^{-1} D[\Theta_{SB}(t) \| \tau_S(t) \otimes \tau_B]. \quad (9)$$

The monotonicity of the quantum relative entropy [51] with respect to the partial trace leads to Eq. (8) via

$$D[\Theta_{SB}(t) \| \tau_S(t) \otimes \tau_B] \geq D\{\text{Tr}_B[\Theta_{SB}(t)] \| \tau_S(t)\}.$$

Discussion.—The emergence of the guessed quantum heat and work can be understood as the results of system-bath correlations deriving from their interaction. As the one-time measurement does not erase such correlations, in contrast to the two-time measurement protocol, we are able to define and distinguish heat and work (their “guessed” values), which are derived from the well-defined guessed state, even in cases such as dephasing where the two-time measurement protocol predicts no heat exchange.

Still, our results are consistent with well-known results for closed quantum systems. Since Eqs. (6) and (8) are generalizations of results in Ref. [38], we can recover the closed quantum system scenario by setting $V(t) = 0$. Then there is no energy exchange with the bath, i.e., no heat, and the guessed quantum work is simply the exact quantum work, given by the energy difference, $\langle \tilde{W} \rangle_{\bar{P}} = \langle W \rangle = \langle \Delta E \rangle$. Also, for the pure dephasing process, the guessed quantum work coincides with the exact work, as we can see from examples in [46].

In contrast, for open quantum systems Eqs. (6) and (9) introduce an additional thermodynamic contribution to the work capacity, given by the information difference between thermal and guessed state [38], as quantified by the relative entropy. More precisely, the contribution arises from the difference between the product thermal state $\tau_S(t) \otimes \tau_B$ and the system-bath correlated state $\Theta_{SB}(t)$. This implies that system-bath correlations can increase the work capacity of the system.

We indeed obtain a bound for the principle of maximum guessed quantum work that importantly only requires knowledge of the system’s state [Eq. (8)]. Avoiding measurements on the bath is essential, as this bound describes the maximum usable and extractable energy that the system can provide, which is of relevance for experiments and practical applications.

To this goal, we were able to exploit the concept of “guessed state” not only to isolate the contribution from the measurement on the system, as done previously, but also to analyze the more realistic situation where the bath is unmeasurable. In this scenario, then, $\Theta_{SB}(t)$ is a good effective state, because it can not only be estimated but it also gives a bound to the guessed quantum work, and

similarly guessed quantum heat and work assume a well-defined meaning.

Finally, we note that Eq. (6) has operational meaning associated with the scaling of the quantum hypothesis testing from the quantum Stein’s lemma [52,53]. The quantum relative entropy $D[\Theta_{SB}(t) \| \tau_S(t) \otimes \tau_B]$ quantifies the distance between the guessed state $\Theta_{SB}(t)$ and the product Gibbs’s state defined by the initial temperature and the final Hamiltonians of the system and bath $\tau_S(t) \otimes \tau_B$. This is associated with the type-II error probability that the observation indicates the state to be $\Theta_{SB}(t)$ when the real state was $\tau_S(t) \otimes \tau_B$ (see [46] for details).

Assume that we prepare n independent and identically distributed copies of $\Theta_{SB}(t)$ and $\tau_S(t) \otimes \tau_B$. Here, $\Theta_{SB}(t)$ and $\tau_S(t) \otimes \tau_B$ are seen as the null and alternative hypothesis, respectively. Let us define \mathcal{B}_n as the minimum type-II error probability in quantum Stein’s lemma that the true state is $[\tau_S(t) \otimes \tau_B]^{\otimes n}$ while the inferred state is $\Theta_{SB}^{\otimes n}(t)$. Then, in the limit of large n , we have

$$\lim_{n \rightarrow \infty} \frac{1}{n} \ln(\mathcal{B}_n) = -D[\Theta_{SB}(t) \| \tau_S(t) \otimes \tau_B]. \quad (10)$$

Relating the guessed quantum work \tilde{W} [see Eq. (6)] with the type-II probability \mathcal{B}_n ,

$$\langle e^{-\beta(\tilde{W} - \Delta F_S)} \rangle_{\bar{P}} = \lim_{n \rightarrow \infty} (\mathcal{B}_n)^{\frac{1}{n}}, \quad (11)$$

we can show that the guessed quantum work is asymptotically associated with the scaling of the quantum hypothesis testing when the true state is $\tau_S(t) \otimes \tau_B$ while the experimental result indicates $\Theta_{SB}(t)$.

In conclusion, we employ the one-time measurement scheme to derive a modified quantum Jarzynski equality and the principle of maximum quantum work in open quantum systems described by general quantum channels. We demonstrate that the one-point measurement scheme enables defining heat and work with respect to the best possible guessed state, by introducing well-defined concepts of guessed quantum heat and guessed quantum work. Our work generalizes the results obtained in Ref. [38] for closed quantum systems, where guessed quantum work coincides with the exact quantum work. The extension to open quantum systems provides novel insights to the thermodynamics of both unital and generic quantum channels, by elucidating the role of correlations between system and bath in producing work and heat exchange, as we illustrate in various examples in the Supplemental Material [46]. Finally, we also have shown the operational meaning of guessed quantum work in terms of quantum hypothesis testing. We expect that our results will contribute to a deeper understanding and further exploration of the role of work and heat in open quantum systems, as well as quantum fluctuation theorems for general open quantum systems.

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- [46] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.125.060602> for the calculations about the best possible guessed state, derivation of the relation between the guessed quantum heat and quantum relative entropy, recovery of the case for closed quantum system, examples, reviews of quantum Stein’s lemma, comparison between the guessed and exact quantum work, and the derivation of the modified Jarzynski equality for different initial temperatures of the system and bath.
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