Supplementary Material for "Quantum Jarzynski equality in open quantum systems from the one-time measurement scheme"

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1. BEST POSSIBLE GUESSED STATE

We introduced in the main text the concept of "guessed state". Here we show how to derive its expression following the principle of maximum entropy and the constraints imposed by the one-time measurement protocol.

Initially, the system and the bath is decoupled, and the post-measurement state of the composite system after the initial measurement is given by $|\epsilon\rangle\langle\epsilon|\otimes\tau_B$; therefore, we get a set of states after the unitary evolution $\{U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger\}_\epsilon$. These states are distributed based on the probability distribution $\{p(\epsilon)\}_\epsilon$, so that we can write the final state induced by the initial measurement as $\Theta_{SB}(t)=\sum_\epsilon p(\epsilon)U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger$. Then, we consider the following optimization problem.

Given a state $\Theta_{SB}(t)$:

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

let us consider the probability distribution $\{p(\epsilon)\}_\epsilon$ maximizing the Von-Neumann entropy $\mathcal{S}_{SB}(t)=-\mathrm{Tr}[\Theta_{SB}(t)\ln\Theta_{SB}(t)]$ under the condition that

$$\begin{aligned}&\mathrm{Tr}[\Theta_{SB}(t)]=1\\&E_S=\mathrm{Tr}[(H_S(t)\otimes\mathbb{1}_B)\Theta_{SB}(t)]\,,\end{aligned}$$

so that

$$\begin{aligned}&\delta\mathrm{Tr}[\Theta_{SB}(t)]=\sum_\epsilon\delta p(\epsilon)=0\\&\delta E_S=\delta\mathrm{Tr}[(H_S(t)\otimes\mathbb{1}_B)\Theta_{SB}(t)]=\sum_\epsilon\delta p(\epsilon)\mathrm{Tr}[(H_S(t)\otimes\mathbb{1}_B)U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger]=\sum_\epsilon\delta p(\epsilon)\mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]\,.\end{aligned}$$

Here, note we only consider $H_S(t)$ because we assume that one can only measure the energy of the system. Explicitly, $\Theta_{SB}(t)$ can be given by

$$\Theta_{SB}(t)=\sum_{\epsilon,q}p(\epsilon)\frac{1}{Z_B}e^{-\beta q}U_t|\epsilon,q\rangle\langle\epsilon,q|U_t^\dagger\,.$$

Therefore,

$$\begin{aligned}\delta\mathcal{S}_{SB}&=-\delta\mathrm{Tr}[\Theta_{SB}(t)\ln\Theta_{SB}(t)]\\&=-\sum_{\epsilon,q}\frac{e^{-\beta q}}{Z_B}\delta p(\epsilon)\Big(\ln p(\epsilon)-\ln Z_B-\beta q\Big)\\&=-\sum_\epsilon\delta p(\epsilon)\Big(\ln p(\epsilon)-\ln Z_B-\beta\mathrm{Tr}[H_B\tau_B]\Big)\,.\end{aligned}$$

By using the optimization method of Lagrange multipliers with constraints, we have:

$$\delta\Big(\mathcal{S}_{SB}-\alpha E_S-\gamma\Big)=-\sum_\epsilon\delta p(\epsilon)\Big(\ln p(\epsilon)-\beta\mathrm{Tr}[\tau_BH_B]-\ln Z_B+\alpha\mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\epsilon|)]+\gamma+1\Big)\,.$$

For any $\delta p(\epsilon)$, this has to be valid so that each term has to be independently 0. Therefore,

$$\ln p(\epsilon) - \beta \mathrm{Tr}[H_B \tau_B] - \ln Z_B + \alpha \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)] + \gamma + 1 = 0\,,$$

so that we can obtain

$$p_\alpha(\epsilon) \propto e^{-\alpha \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}\,,$$

where we put subscript α as $p_\alpha(\epsilon)$ in order to emphasize the dependence of $p(\epsilon)$ on the parameter α. Here, note that we can choose any α, and we could have infinite numbers of guessed states. As the *best* guessed state, since we do not know the final temperature, it is reasonable for us to choose $\alpha = \beta$. Since we have $\sum_\epsilon p_\beta(\epsilon) = 1$, we can write

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

where $\tilde{Z}_S(t) = \sum_\epsilon e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}$. This means that the best possible guess of the thermal state of the composite system, which rises from the one-time measurement scheme, can be given by

$$\Theta_{SB}(t) = \sum_\epsilon \frac{e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)} U_t(|\epsilon\rangle\langle\epsilon| \otimes \tau_B)U_t^\dagger\,.$$

2. GUESSED HEAT AND RELATIVE ENTROPY

We introduce the guessed heat when providing an explicit relationship between the relative entropy $D\left[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B\right]$ and the free energies, Eq. (**??**) of the main text. Here we provide an explicit proof of this result.

Proof. First, let us calculate $\mathrm{Tr}\left[\Theta_{SB}(t)\ln\Theta_{SB}(t)\right]$. Since

$$\begin{aligned}
\Theta_{SB}(t) &= \frac{1}{\tilde{Z}_S(t)} \sum_\epsilon e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]} U_t(|\epsilon\rangle\langle\epsilon| \otimes \tau_B)U_t^\dagger \\
&= \frac{1}{\tilde{Z}_S(t)} \frac{1}{Z_B} \sum_{\epsilon,q} e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]} e^{-\beta q} U_t|\epsilon,q\rangle\langle\epsilon,q|U_t^\dagger \\
&= \frac{1}{\tilde{Z}_S(t)} \frac{1}{Z_B} \sum_{\epsilon,q} e^{-\beta \mathrm{Tr}\left[(H_S(t)\otimes \mathbb{1}_B)U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger\right]} e^{-\beta q} U_t|\epsilon,q\rangle\langle\epsilon,q|U_t^\dagger\,,
\end{aligned}$$

where we use the relation

$$\mathrm{Tr}\left[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)\right] = \mathrm{Tr}\left[(H_S(t)\otimes\mathbb{1}_B)U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger\right]\,.$$

Therefore, we can obtain

$$\ln\Theta_{SB}(t) = -\ln\tilde{Z}_S(t) - \ln Z_B - \beta\sum_{\epsilon,q}\left(\mathrm{Tr}\left[(H_S(t)\otimes\mathbb{1}_B)U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger\right] + q\right)U_t|\epsilon,q\rangle\langle\epsilon,q|U_t^\dagger\,.$$

Then, we have

$$\begin{aligned}
\mathrm{Tr}\left[\Theta_{SB}(t)\ln\Theta_{SB}(t)\right] =& -\ln\tilde{Z}_S(t) - \ln Z_B \\
&- \beta\sum_{\epsilon,q}\left(\mathrm{Tr}\left[(H_S(t)\otimes\mathbb{1}_B)U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger\right] + q\right)\cdot\frac{e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)}\cdot\frac{e^{-\beta q}}{Z_B} \\
=& -\ln\tilde{Z}_S(t) - \ln Z_B \\
&- \beta\mathrm{Tr}\left[(H_S(t)\otimes\mathbb{1}_B)\frac{1}{\tilde{Z}_S(t)}\sum_\epsilon e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}U_t(|\epsilon\rangle\langle\epsilon|\otimes\tau_B)U_t^\dagger\right] - \beta\sum_q\frac{e^{-\beta q}}{Z_B}q \\
=& -\ln\tilde{Z}_S(t) - \ln Z_B - \beta\mathrm{Tr}\left[(H_S(t)\otimes\mathbb{1}_B)\Theta_{SB}(t)\right] - \beta\mathrm{Tr}\left[H_B\tau_B\right]\,.
\end{aligned}$$

Let us calculate $\mathrm{Tr}\left[\Theta_{SB}(t)\ln(\tau_S(t)\otimes\tau_B)\right]$. Since

$$\tau_S(t)\otimes\tau_B=\frac{e^{-\beta H_S(t)}}{Z_S(t)}\otimes\frac{e^{-\beta H_B}}{Z_B}=\frac{1}{Z_S(t)Z_B}e^{-\beta(H_S(t)\otimes\mathbb{1}_B+\mathbb{1}_S\otimes H_B)}\,,$$

we have

$$\mathrm{Tr}\left[\Theta_{SB}(t)\ln(\tau_S(t)\otimes\tau_B)\right]=-\ln Z_S(t)-\ln Z_B-\beta\mathrm{Tr}\left[(H_S(t)\otimes\mathbb{1}_B)\Theta_{SB}(t)\right]-\beta\mathrm{Tr}\left[(\mathbb{1}_S\otimes H_B)\Theta_{SB}(t)\right]\,.$$

Therefore, the quantum relative entropy becomes

$$\begin{aligned}D\left[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B\right]&=\mathrm{Tr}\left[\Theta_{SB}(t)\ln\Theta_{SB}(t)\right]-\mathrm{Tr}\left[\Theta_{SB}(t)\ln(\tau_S(t)\otimes\tau_B)\right]\\&=-\ln\frac{\tilde{Z}_S(t)}{Z_S(t)}-\beta\Big(\mathrm{Tr}\left[H_B\tau_B\right]-\mathrm{Tr}\left[(\mathbb{1}_S\otimes H_B)\Theta_{SB}(t)\right]\Big)\,.\end{aligned}$$

$\square$

3. RECOVERY OF THE CLOSED-SYSTEM CASE

We remark that our results are consistent with previous results obtained in the case of closed quantum system [1]. In closed quantum systems, there is no coupling to the bath, and the unitary evolution U_t can be given by $U_t=\mathcal{T}\left[e^{-i\int dtH_S(t)}\right]\otimes e^{-iH_Bt}$. Then, there is no energy loss to/from the bath, i.e., no heat, and the guessed quantum work is simply the exact quantum work, given by the energy difference, $\langle\tilde{W}\rangle=\langle W\rangle=\langle\Delta E\rangle$. The relative entropy, $D\left[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B\right]$, reduces to

$$D\left[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B\right]=D\left[\tilde{\rho}_S(t)||\tau_S(t)\right]=\frac{\tilde{Z}_S(t)}{Z_S(t)}\,,$$

where $\tilde{\rho}_S(t)=\mathrm{Tr}_B(\Theta_{SB}(t))$ can be given explicitly by

$$\tilde{\rho}_S(t)=\sum_\epsilon\frac{e^{-\beta\mathrm{Tr}\left[H_S(t)U_t^{(S)}|\epsilon\rangle\langle\epsilon|U_t^{(S)\dagger}\right]}}{\tilde{Z}_S(t)}U_t^{(S)}|\epsilon\rangle\langle\epsilon|U_t^{(S)\dagger}\,,$$

where we define $U_t^{(S)}\equiv\mathcal{T}\left[e^{-i\int dtH_S(t)}\right]$. This is the close-system best possible guessed state as in Ref. [1]. In the absence of heat, the derived quantum Jarzynski equality and the maximum work in reduce to the main results of Ref. [1]:

$$\langle e^{-\beta W}\rangle_{\tilde{P}}=e^{-\beta\Delta F_S}e^{-D[\tilde{\rho}_S(t)||\tau_S(t)]}\,,$$

and

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

4. EXAMPLES

We can further understand our main results by verifying our derived quantum Jarzynski equality:

$$\langle e^{-\beta\Delta E}\rangle_{\tilde{P}}=e^{-D[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B]-\beta\langle\tilde{Q}\rangle_B}\tag{1}$$

with two toy models with different size of baths such as two-qubit dephasing and spin-boson model with time-independent Hamiltonian.

In the following, $\boldsymbol{\sigma}_j=(\sigma_j^x,\sigma_j^y,\sigma_j^z)$ denotes the Pauli matrices for j-th spin, and a_k ($a_k^\dagger$) is the annihilation (creation) operator of the k-th bosonic mode.

The following results indicate that the system-bath interaction results in the guessed quantum work even in the composite systems characterized by the time-independent Hamiltonian.

4-1. Two-qubit dephasing model

Let us consider a single spin-1/2 system ($\mathcal{H}_S$) coupled to a single spin-1/2 bath ($\mathcal{H}_B$). For simplicity, let us consider a time-independent system Hamiltonian so that $\Delta F_S = 0$. Here, $\boldsymbol{\sigma}_j = (\sigma_j^x, \sigma_j^y, \sigma_j^z)$ ($j = S, B$) denotes the Pauli matrices for j-th spin.

Let us consider $\sigma_S^z \sigma_B^x$ coupling between system and bath. The total Hamiltonian becomes

$$H = \omega_S \sigma_S^z + \omega_B \sigma_B^z + J \sigma_S^z \sigma_B^x \,,$$

where J is the coupling strength. This simple two-qubit system models a dephasing process for the system, as populations are preserved while coherences (initially) decay, i.e. $\Phi_t(|\epsilon\rangle\langle\epsilon|) = |\epsilon\rangle\langle\epsilon|$, and in this case, the guessed state coincides with the exact state, i.e. $\Theta_{SB}(t) = U_t\,(\tau_S(0) \otimes \tau_B)\,U_t^\dagger$. The system energy is thus conserved and we have $\langle e^{-\beta\Delta E}\rangle_{\tilde{P}} = 1$. In contrast, the backaction of the system evolution onto the bath leads to a change in energy of the bath itself, and the guessed quantum heat and work can be given by

$$\langle \tilde{Q} \rangle_B = -\langle \tilde{W} \rangle = -\frac{2J^2 \omega_B \tanh(\beta\omega_B) \sin(t\sqrt{J^2 + \omega_B^2})^2}{J^2 + \omega_B^2} \,.$$

Furthermore, we can analytically obtain

$$D\left[\Theta_{SB}(t) || \tau_S \otimes \tau_B\right] = \beta \frac{2J^2 \omega_B \tanh(\beta\omega_B) \sin(t\sqrt{J^2 + \omega_B^2})^2}{J^2 + \omega_B^2} \,.$$

Then, we obtain $\beta\langle \tilde{Q}\rangle_B + D\left[\Theta_{SB}(t)||\tau_S \otimes \tau_B\right] = 0$, which verifies Eq. (1). Interestingly, this examples shows how our approach can well describe the scenario where the quantum "bath" (or environment) is small, and thus affected by a large backaction. In this case, even if there is no system energy change, we can still define heat, while the quantum relative entropy plays the role of work performed by the system onto the bath.

4-2. Spin-boson model

Let us consider the following spin-boson model with the time-independent Hamiltonian [2]

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k a_k^\dagger a_k + \sigma_z \sum_k (g_k a_k + g_k^* a_k^\dagger) \,.$$

In interaction picture, we obtain

$$H(t) = \sigma_z \sum_k (g_k a_k e^{-i\omega_k t} + g_k^* a_k^\dagger e^{+i\omega_k t}) \,,$$

and by the Magnus expansion, the propagator can be simply given by

$$U_t = \exp\left[-it(H_0 + H_1)\right] \,, \tag{2}$$

where the higher terms are vanishing, and H_0 and H_1 are, respectively, defined as

$$\begin{aligned} H_0 &\equiv \frac{1}{t}\int_0^t H(t_1)dt_1 \\ H_1 &\equiv -\frac{i}{2t}\int_0^t dt_1 \int_0^{t_1} dt_2 \left[H(t_1), H(t_2)\right] \,. \end{aligned}$$

Then, we can obtain

$$H_0 = \sigma_z \sum_k \left(G_k(t) a_k - G^*(t) a_k^\dagger\right) \,, \tag{3}$$

where

$$G_k(t) \equiv g_k \frac{\sin(\omega_k t/2)}{\omega_k t/2} e^{-i\omega_k t/2} . \tag{4}$$

Also, H_1 is given by

$$H_1 = -\sum_k \mathcal{G}_k , \tag{5}$$

where

$$\mathcal{G}_k \equiv \frac{|g_k|^2}{\omega_k} \left(1 - \frac{\sin(\omega_k t)}{\omega_k t}\right) .$$

From Eq. (3), Eq. (5) and Eq. (2), the propagator becomes

$$U_t = \exp\left[-it \sum_k \left(\sigma_z (G_k(t) a_k + G_k^*(t) a_k^\dagger) - \mathcal{G}_k\right)\right] .$$

Here, we can verify $\langle e^{-\beta \Delta E}\rangle_{\tilde{P}} = 1$. ΔE is defined as $\Delta E = \mathrm{Tr}\left[(H_S(t) \otimes \mathbb{1}_B) U_t (|\epsilon\rangle\langle\epsilon| \otimes \tau_B) U_t^\dagger\right] - \epsilon$. Due to $H_S(t) = H_S = \frac{\omega_0}{2}\sigma_z$, we can find that $[H_S, U_t] = 0$, which leads to $\Delta E = \langle\epsilon|H_S|\epsilon\rangle - \epsilon = 0$ because $|\epsilon\rangle$ is an eigenbasis of H_S corresponding to the eigenvalue ϵ. Therefore,

$$\langle e^{-\beta\Delta E}\rangle_{\tilde{P}} = 1 .$$

We can also compute the guessed quantum heat $\langle\tilde{Q}\rangle_B$, which also corresponds to the negative guessed quantum work $-\langle\tilde{W}\rangle$ in this model. The definition of the guessed heat is $\langle\tilde{Q}\rangle_B = \mathrm{Tr}\left[H_B \tau_B\right] - \mathrm{Tr}\left[H_B \Theta_{SB}(t)\right]$, where

$$\Theta_{SB}(t) = \sum_\epsilon \frac{e^{-\beta \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)} U_t (|\epsilon\rangle\langle\epsilon| \otimes \tau_B) U_t^\dagger .$$

Recall that we consider the time-independent Hamiltonian $H_S(t) = H_S$. For the dephasing process, we have $\Phi_t(|\epsilon\rangle\langle\epsilon|) = |\epsilon\rangle\langle\epsilon|$ and $\langle\epsilon|H_S|\epsilon\rangle = \epsilon$. In this case, we have $\Theta_{SB}(t) = U_t(\tau_S \otimes \tau_B) U_t^\dagger$, which is the exact state of the total system. Then, we have $\mathrm{Tr}\left[H_B \Theta_{SB}(t)\right] = \mathrm{Tr}\left[U_t^\dagger H_B U_t (\tau_S \otimes \tau_B)\right]$. From the relation $U_t^\dagger a_k U_t = a_k + itG_k(t)\sigma_z$ and $\mathrm{Tr}\left[a_k^\dagger \tau_B\right] = \mathrm{Tr}\left[a_k \tau_B\right] = 0$, we have $\langle\tilde{Q}\rangle_B = \mathrm{Tr}\left[H_B\tau_B\right] - \mathrm{Tr}\left[H_B \Theta_{SB}(t)\right] = -\sum_k \omega_k |G_k(t)|^2 t^2$, which from Eq. (4) can be explicitly given by

$$\langle\tilde{Q}\rangle_B = -\sum_k \omega_k |g_k|^2 \left(\frac{\sin(\omega_k t/2)}{\omega_k/2}\right)^2 . \tag{6}$$

The the noise spectral density is $J(\omega) = \sum_k |g_k|^2 \omega \delta(\omega - \omega_k)$; therefore

$$\langle\tilde{Q}\rangle_B = -\int_{-\infty}^{\infty} J(\omega) \left(\frac{\sin(\omega_k t/2)}{\omega_k/2}\right)^2 d\omega .$$

Since we have $\lim_{t\to\infty} \frac{\sin(\omega t/2)}{\omega/2} = \delta(\omega/2) = 2\delta(\omega)$, where we used the relation $\lim_{t\to\infty} t \cdot \frac{\sin(xt)}{xt} = \delta(x)$, we can obtain

$$\lim_{t\to\infty} \langle\tilde{Q}\rangle_B = -\int_{-\infty}^{\infty} 4J(\omega)\delta^2(\omega) d\omega = -4J(0)\delta(0) = 0 ,$$

which is consistent with our intuition that when $t \to \infty$ there will be no energy exchange between a small system and a large bath for the dephasing process.

5. BRIEF REVIEW OF QUANTUM STEIN'S LEMMA

In this section, we briefly introduce quantum Stein's lemma by following Refs. [3, 4] in our scenario. Consider that we prepare n i.i.d copies of $\Theta_{SB}(t)$ and $\tau_S(t)\otimes\tau_B$. We observe two POVM $\{O_n, \mathbb{1}-O_n\}$ at time t on unknown states. The outcome of O_n concludes that the state is $\Theta_{SB}(t)$, while the outcome of $\mathbb{1}-O_n$ indicates that the state is $\tau_S(t)\otimes\tau_B$. Here, the state $\Theta_{SB}(t)$ and $\tau_S(t)\otimes\tau_B$ are seen as the null and alternative hypothesis, respectively. Here, we define $\mathcal{A}_n(O_n)\equiv \mathrm{Tr}\left[\Theta_{SB}^{\otimes n}(t)(\mathbb{1}-O_n)\right]$ as the type-I error probability that the true state is $\Theta_{SB}^{\otimes n}(t)$ while the POVM outcome indicates $(\tau_S(t)\otimes\tau_B)^{\otimes n}$. We also define $\mathcal{B}_n(O_n)\equiv \mathrm{Tr}\left[(\tau_S(t)\otimes\tau_B)^{\otimes n}O_n\right]$ as the type-II error probability that the true state is $(\tau_S(t)\otimes\tau_B)^{\otimes n}$, while the POVM outcome indicates $\Theta_{SB}^{\otimes n}(t)$. Under the restriction that $\mathcal{A}_n(O_n)$ is upper bounded by a small quantity δ, we consider the minimum type-II error probability $\mathcal{B}_n$ defined as $\mathcal{B}_n\equiv\min_{0\le O_n\le\mathbb{1}}\{\mathcal{B}_n(O_n)|\mathcal{A}_n(O_n)\le\delta\}$. Then, quantum Stein's lemma [3, 4] states that for $0<\delta<1$ we have the following relation:

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

Therefore, the quantum relative entropy determines the scaling of the quantum hypothesis testing.

6. RELATION BETWEEN THE GUESSED QUANTUM WORK AND EXACT QUANTUM WORK

In this section, we discuss the relation between the guessed quantum work and the exact quantum work, which can be obtained by considering the conventional two-point measurement scheme on both the system and bath.

6-1. Standard Jarzynski equality from two-point measurement scheme

Let us take the same setup in the main text, and suppose that we can measure the bath. We first locally measure the system and bath, and suppose that we obtained two energy values, ϵ for the system and q for the bath, so that the post-measurement state becomes $|\epsilon, q\rangle$. Then, we evolve the total system, and locally measure the system and bath again at time t. Suppose that we obtain two energy values, ϵ' for the system and q' for the bath, so that the post-measurement state becomes $|\epsilon', q'\rangle$. Then, the quantum work is defined as the difference in the total energy of the system and bath along the trajectory $(\epsilon, q)\to(\epsilon', q')$. Here, ϵ and ϵ' are the energy eigenvalue of the time-dependent Hamiltonian of the system $H_S(0)$ and $H_S(t)$, respectively. q and q' are the energy eigenvalue of the time-independent Hamiltonian H_B of the bath. Therefore, the work can be defined as

$$W = (q'+\epsilon') - (q+\epsilon) .$$

Therefore, the Jarzynski equality from two-measurement scheme is given by

$$\langle e^{-\beta W}\rangle = \sum_{\epsilon,\epsilon' q, q'}\frac{e^{-\beta\epsilon}}{Z_S(0)}\cdot\frac{e^{-\beta q}}{Z_B}\left|\langle\epsilon', q'|U_t|\epsilon, q\rangle\right|^2 e^{-\beta\left(q'+\epsilon'-q-\epsilon\right)} = e^{-\beta\Delta F_S} , \tag{7}$$

where $\Delta F_S\equiv F_S(t)-F_S(0)$ and

$$F_S(t) = -\beta^{-1}\ln Z_S(t) = \beta^{-1}\mathrm{Tr}\left[e^{-\beta H_S(t)}\right] .$$

Also, the expectation of the work is given by

$$\langle W\rangle = \mathrm{Tr}\left[\left(H_S(t)\otimes\mathbb{1}_B + \mathbb{1}_S\otimes H_B\right)U_t\left(\tau_S(0)\otimes\tau_B\right)U_t^\dagger\right] - \left(\mathrm{Tr}\left[H_S(0)\tau_S(0)\right] + \mathrm{Tr}\left[H_B\tau_B\right]\right) , \tag{8}$$

which is the exact quantum work.

6-2. Relation between the guessed quantum work and exact quantum work

First, let us consider the relation between the expectation value of the guessed work and the exact work. The guessed quantum work is given by

$$\begin{aligned}\langle \tilde{W} \rangle =&\langle \Delta E \rangle - \langle \tilde{Q} \rangle_B \\ =&\mathrm{Tr}\left[\left(H_S(t) \otimes \mathbb{1}_B\right) U_t \left(\tau_S(0) \otimes \tau_B\right) U_t^\dagger \right] - \mathrm{Tr}\left[H_S(0)\tau_S(0)\right] - \left(\mathrm{Tr}\left[H_B \tau_B\right] - \mathrm{Tr}\left[(\mathbb{1}_S \otimes H_B)\Theta_{SB}(t)\right]\right) .\end{aligned}$$

From Eq. (8), we can obtain

$$\langle \tilde{W} \rangle = \langle W \rangle + \mathrm{Tr}\left[\left(\mathbb{1}_S \otimes H_B\right) \left(\Theta_{SB}(t) - U_t \left(\tau_S(0) \otimes \tau_B\right) U_t^\dagger \right) \right] ,$$

which shows that the guessed quantum work and the exact quantum work is different from each other by the energy difference between the reduced state of the bath of the best guessed state and the exact final state. They coincide with each other in the closed quantum systems and when the system undergoes the pure dephasing process, as we have shown in the main text and the examples in this supplemental material.

6-3. The relation between the modified and standard Jarzynski equality

From Eq. (7) and Theorem. 1, we have

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

By applying Jensen's inequality and the monotonicity of the quantum relative entropy, we can obtain

$$\langle e^{-\beta\left(W - \langle \tilde{W} \rangle\right)} \rangle \geq e^{D[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B]} \geq e^{D[\tilde{\rho}_S(t)||\tau_S(t)]} . \tag{9}$$

This means that the average of the deviation of the exact quantum work from the guessed quantum work has the lower bound characterized by the quantum relative entropy $D\left[\tilde{\rho}_S(t)||\tau_S(t)\right]$.

Furthermore, since we can also have

$$\langle e^{-\beta W} \rangle = \langle e^{-\beta \tilde{W}} \rangle_{\tilde{P}} e^{+D[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B]}$$

so that the Jensen's inequality yields the inequality for the deviation of the guessed quantum work from the exact quantum work:

$$\langle e^{-\beta\left(\tilde{W} - \langle W \rangle\right)} \rangle_{\tilde{P}} \geq e^{-D[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B]} . \tag{10}$$

Therefore, from Eq. (9) and Eq. (10), we can also obtain the following inequality with respect to these two different deviations:

$$\langle e^{-\beta\left(W - \langle \tilde{W} \rangle\right)} \rangle \langle e^{-\beta\left(\tilde{W} - \langle W \rangle\right)} \rangle_{\tilde{P}} \geq 1 .$$

7. MODIFIED JARZYNSKI EQUALITY FOR DIFFERENT INITIAL TEMPERATURES OF THE SYSTEM AND BATH

Let us consider the scenario that initially the temperatures of the system and bath are different each other. Let β_S and β_B be the initial temperature of the system and the bath, respectively, and let us define the temperature difference as

$$\Delta\beta \equiv \beta_B - \beta_S .$$

Then, we can obtain the following Theorem. 1, which can be regarded as the extension of Jarzynski-Wójcik scenario [5] from the one-time measurement scheme under the restriction that the bath is inaccessible.

Theorem 1. *When the initial temperatures of the system and bath are different from each other, The Jarzynski equality for the guessed quantum work is*

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

which also yields the following principle of maximum guessed work:

$$\langle \tilde{W} \rangle \geq \Delta F_S + \beta^{-1} D\left[\tilde{\rho}_S(t)||\tau_S(t)\right] + \frac{\Delta\beta}{\beta_S} \langle \tilde{Q} \rangle_B \,,$$

where

$$\tilde{\rho}_S(t) \equiv \mathrm{Tr}_B\left[\Theta_{SB}(t)\right] = \sum_{\epsilon} \frac{e^{-\beta_S \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)} \Phi_t\left(|\epsilon\rangle\langle\epsilon|\right) \,.$$

Proof. The proof is same to the one in Sec. 2. In this case, the initial state is given by

$$\tau_S(0) \otimes \tau_B = \frac{e^{-\beta_S H_S(0)}}{Z_S(0)} \otimes \frac{e^{-\beta_B H_B}}{Z_B} \,.$$

Then, for the internal energy difference, we can obtain

$$\langle e^{-\beta_S \Delta E} \rangle_{\tilde{P}} = e^{-\beta_S \Delta F_S} \frac{\tilde{Z}_S(t)}{Z_S(t)} \,,$$

where

$$\begin{aligned} \tilde{Z}_S(t) &= \sum_{\epsilon} e^{-\beta_S \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]} \\ Z_S(t) &= \mathrm{Tr}\left[e^{-\beta_S H_S(t)}\right] \,, \end{aligned}$$

where

$$\Phi_t\left(|\epsilon\rangle\langle\epsilon|\right) = \mathrm{Tr}_B\left[U_t\left(|\epsilon\rangle\langle\epsilon| \otimes \tau_B\right) U_t^{\dagger}\right] \,.$$

In this case, the best guessed state is given by

$$\Theta_{SB}(t) = \sum_{\epsilon} \frac{e^{-\beta_S \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)} U_t\left(|\epsilon\rangle\langle\epsilon| \otimes \tau_B\right) U_t^{\dagger} \,.$$

Then, we can obtain

$$\mathrm{Tr}\left[\Theta_{SB}(t) \ln \Theta_{SB}(t)\right] = -\ln \tilde{Z}_S(t) - \ln Z_B - \beta_S \mathrm{Tr}\left[\left(H_S(t) \otimes \mathbb{1}_B\right) \Theta_{SB}(t)\right] - \beta_B \mathrm{Tr}\left[H_B \tau_B\right] \,.$$

Also, we have

$$\mathrm{Tr}\left[\Theta_{SB}(t) \ln\left(\tau_S(t) \otimes \tau_B\right)\right] = -\ln Z_S(t) - \ln Z_B - \beta_S \mathrm{Tr}\left[\left(H_S(t) \otimes \mathbb{1}_B\right) \Theta_{SB}(t)\right] - \beta_B \mathrm{Tr}\left[\left(\mathbb{1}_S \otimes H_B\right) \Theta_{SB}(t)\right] \,.$$

Therefore, we can obtain

$$\begin{aligned} \frac{\tilde{Z}_S(t)}{Z_S(t)} &= e^{-D[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B]} e^{-\beta_B \langle \tilde{Q} \rangle_B} \\ &= e^{-D[\Theta_{SB}(t)||\tau_S(t)\otimes\tau_B]} e^{-\beta_S \langle \tilde{Q} \rangle_B} e^{-\Delta\beta \langle \tilde{Q} \rangle_B} \end{aligned}$$

where

$$\langle \tilde{Q} \rangle_B = \mathrm{Tr}\left[H_B \tau_B\right] - \mathrm{Tr}\left[(\mathbb{1}_S \otimes H_B)\Theta_{SB}(t)\right] \,, \tag{11}$$

which is the guessed quantum heat. By definition of the guessed quantum work:

$$\tilde{W} \equiv \Delta E - \langle \tilde{Q} \rangle_B \,,$$

we can obtain

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

Applying Jensen's inequality and the monotonicity of the quantum relative entropy, we can obtain

$$\langle \tilde{W} \rangle \geq \Delta F_S + \beta_S^{-1} D\left[\tilde{\rho}_S(t)||\tau_S(t)\right] + \frac{\Delta\beta}{\beta_S} \langle \tilde{Q} \rangle_B \,,$$

where

$$\tilde{\rho}_S(t) \equiv \mathrm{Tr}_B\left[\Theta_{SB}(t)\right] = \sum_\epsilon \frac{e^{-\beta_S \mathrm{Tr}[H_S(t)\Phi_t(|\epsilon\rangle\langle\epsilon|)]}}{\tilde{Z}_S(t)} \Phi_t\left(|\epsilon\rangle\langle\epsilon|\right) \,.$$

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