LA-UR- 08-8069

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Intended for:	Physical Review E

Los Alamos
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EST. 1943

Form 836 (7/06)

Quantum Crooks fluctuation theorem and quantum Jarzynski equality in the presence of a reservoir

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We consider the quantum mechanical generalization of Crooks Fluctuation and Jarzynski Equality Theorem for an open quantum system. The explicit expression for microscopic work for an arbitrary prescribed protocol is obtained, and the relation between quantum Crooks Fluctuation Theorem, quantum Jarzynski Equality and their classical counterparts are clarified. Numerical simulations based on a two-level toy model are used to demonstrate the validity of the quantum version of the two theorems beyond linear response theory regime.

PACS numbers: 05.70.Ln, 05.40.-a

I. INTRODUCTION:

Nonequilibrium thermodynamics has been an intriguing research subject for more than one hundred years [1]. Yet our understanding about nonequilibrium thermodynamic phenomena, especially about those far-from-equilibrium regime (beyond the linear response regime), remains very limited. In the past fifteen years, there are several significant breakthroughs in this field, such as Evans-Searls Fluctuation Theorem [2], Jarzynski Equality (JE) [3], and Crooks Fluctuation Theorem (Crooks FT) [4]. These new theorems not only have important applications in nanotechnology and biophysics, such as extracting equilibrium information from nonequilibrium measurements, but also shed new light on some fundamental problems, such as improving our understanding of how the thermodynamic reversibility arise from the underlying time reversible dynamics.

Since the seminal work by Jarzynski and Crooks a dozen of years ago, the studies of nonequilibrium thermodynamics in small system attract numerous attention [5], and the validity and universality of these two theorems in classical systems has been extensively studied not only by numerical studies [6], but also by experimental exploration [7] in single RNA molecules, and for both deterministic and stochastic processes. For quantum systems, possible quantum extension of Crooks FT and JE have also been reported [8]. Nevertheless, we notice that almost all of these reports about quantum extension of Crooks FT focus on isolated quantum systems [9], and the explicit expression of microscopic work, and their distributions in the presence of a heat bath are not extensively studied. In addition, the relationship between classical and quantum Crooks FT is not addressed adequately so far. As a result, the experimental studies of quantum Crooks FT and JE are not explored (an exception is the experimental scheme of quantum JE of isolated system based on trapped ions [10]).

In this paper, we will give a detailed proof of the validity of quantum Crooks FT and quantum JE for an open quantum system based on the explicit expression of microscopic work and their corresponding probability distributions for an arbitrary prescribed controlling protocol. We also clarify the relation between quantum Crooks FT, quantum JE and their classical counterparts. In the last part of the paper, the studies based on a two-level system is given as an illustration to demonstrate our central idea.

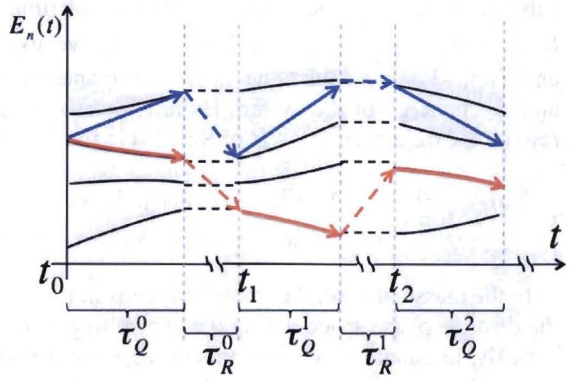

FIG. 1: Trajectories of a quantum system in a nonequilibrium process. Similar to Ref. [4] every step (from t_n to t_{n+1}) is divided into two substeps: the controlling substep of time τ_Q^n, in which the energy spectrum (black solid line) of the system change with time, and the relaxation substep of time τ_R^n in which the energy spectrum (black dashed line) remains unchanged. In the controlling substep (solid line) work is done, but there is no heat exchange; While in the relaxation substep, there is heat exchange between the system and the heat bath, but there is no work done. Blue trajectory corresponds to fast controlling protocol, during which there are usually interstate excitations in the controlling substep. Red trajectory corresponds to slow (quantum adiabatic) controlling protocol, and the system remains in its instantaneous eigenstate in the controlling substep. Red trajectory is the counterpart of classical case.

II. NOTATIONS AND ASSUMPTIONS:

Crooks FT [4] is first derived in classical systems in a microscopically reversible Markovian stochastic process. In the proof of a classical Crooks FT, a key technique is to separate work steps from heat steps. In the following discussion of quantum extension of Crooks FT and JE, we will employ the same technique as that used in Ref. [4] to separate the controlling process into two substeps: controlling substep and relaxation substep (see Fig. 1). The controlling substep proceeds so quickly in comparison with the thermalization process of the system that we can ignore the influence of the heat bath during the controlling substep. So there is only work done in

the controlling substep. In the relaxation substep, on the other hand, there is only heat exchange.

Having clarified the main strategy (separating work substep from heat substep), let us come to the details of the notations and assumptions. We employ the same notations and assumptions as that in Ref. [4] to prove the quantum Crooks FT. In Ref. [4] the author assumes discrete time and discrete phase space. Here, the discrete energy spectrum in a quantum system in place of the discrete phase space of a classical system arise naturally. We also assume discrete time t_0, t_1, t_2, t_3, $\cdots$, t_N for the quantum system (see Fig. 1). The parameter $\lambda(t)$ is controlled according to an arbitrary prescribed protocol $\lambda(t_0) = \lambda_A$, $\lambda(t_1) = \lambda_1$, $\lambda(t_2) = \lambda_2$, $\cdots$, $\lambda(t_N) = \lambda_B$, where A and B depict the initial and final point of the process. Every step $t_n \rightarrow t_{n+1}$ is separated into controlling substep of time τ_Q^i and relaxation substep of time time τ_R^i, $t_{i+1} = t_i + \tau_Q^i + \tau_R^i$ (see Fig. 1). If we use $|i_n, \lambda_m\rangle$ and $E(i_n, \lambda_m)$ to depict the i_n-th instantaneous eigenstate and eigenenergy of the system Hamiltonian $H(\lambda_m)$, we can rewrite the trajectory $A \rightarrow B$ of Ref. [4] in the following way

$$\begin{aligned} &|i_0, \lambda_0\rangle \rightarrow |i_0, \lambda_1\rangle \rightarrow |i_1, \lambda_1\rangle \rightarrow |i_1, \lambda_2\rangle \rightarrow |i_2, \lambda_2\rangle \\ &\quad \rightarrow \cdots \rightarrow |i_{N-1}, \lambda_N\rangle \rightarrow |i_{N-1}, \lambda_N\rangle \rightarrow |i_N, \lambda_N\rangle \end{aligned} \tag{1}$$

In the classical case, the system remains in its i_n-th state of the discrete phase space during the controlling substep. Analogously, in quantum systems, this process corresponds to the quantum adiabatic regime, i.e., the system remains in its i_n-th eigenstate of the instantaneous Hamiltonian when we control the parameter $\lambda(t)$ of the Hamiltonian $H[\lambda(t)]$ so slowly that the quantum adiabatic conditions are satisfied, and the above trajectories (1) can be achieved (red trajectory of Fig. 1). However, if we control the parameter of the Hamiltonian very quickly in the controlling substep, and then the quantum adiabatic conditions are not satisfied, the trajectory $A \rightarrow B$ in general should be written as (see blue trajectory of Fig. 1)

$$\begin{aligned} &|i_0, \lambda_0\rangle \rightarrow |i_0', \lambda_1\rangle \rightarrow |i_1, \lambda_1\rangle \rightarrow |i_1', \lambda_2\rangle \rightarrow |i_2, \lambda_2\rangle \\ &\quad \rightarrow \cdots \rightarrow |i_{N-1}, \lambda_N\rangle \rightarrow |i_{N-1}', \lambda_N\rangle \rightarrow |i_N, \lambda_N\rangle \end{aligned} \tag{2}$$

The main difference of the above two kinds of trajectories (1) and (2) is that after the controlling substep the system may not be in the same eigenstate as that before the controlling, i.e., $i_n \neq i_n'$. The internal excitation $|i_n, \lambda_n\rangle \rightarrow |i_n', \lambda_{n+1}\rangle$ is due to the quantum randomness and has no classical counterpart. Actually this difference of (1) and (2) highlights the main difference between the quantum and classical Crooks FT. For a quantum system, the microscopic work done in every controlling substep is equal to the difference of the energy before and after the controlling substep: $W_n = E(i_n', \lambda_{n+1}) - E(i_n, \lambda_n)$, and the heat exchanged with the heat bath is equal to the difference of the energy of the system before and after the relaxation substep $Q_n = E(i_n, \lambda_n - E(i_{n-1}', \lambda_n)$. For the trajectory (2) as a whole, we must make $2N$ times quantum measurements to confirm the microscopic work done and heat exchanged with the heat bath. Similar to the classical case, the total work W performed on the system, the total heat Q exchanged with the heat bath are given by the summation of work and heat in every step, $W = \sum_{n=0}^{N-1} \left[E(i_n', \lambda_{n+1}) - E(i_n, \lambda_n)\right], Q = \sum_{n=0}^{N} \left[E(i_n, \lambda_n) - E(i_{n-1}', \lambda_n)\right]$, and the total change in energy is $\Delta E = Q + W = E(i_N, \lambda_N) - E(i_0, \lambda_0)$. Note that the work and heat depend on the trajectory, but the energy change depends only on the initial and final energy, and does not depend on the trajectory.

Similar to the classical case [4] we assume the trajectories (2) to be Markovian, and the forward process starts from the thermal equilibrium distribution $P(|i_0, \lambda_0\rangle) = \frac{e^{-\beta E(i_0, \lambda_0)}}{\sum_i e^{-\beta E(i, \lambda_0)}}$. The joint probability for a given trajectory (2) can be expressed as

$$\begin{aligned} P_F(A \rightarrow B) =& P(|i_0, \lambda_0\rangle) \prod_{n=0}^{N-1} P_F(|i_n, \lambda_n\rangle \rightarrow |i_n', \lambda_{n+1}\rangle) \\ &\times P_F(|i_n', \lambda_{n+1}\rangle \rightarrow |i_{n+1}, \lambda_{n+1}\rangle) \end{aligned} \tag{3}$$

It can be seen that the above probability (3) of a trajectory for a quantum case is different from the classical case [4] by the extra term $P(|i_n, \lambda_n\rangle \rightarrow |i_n', \lambda_{n+1}\rangle)$ arising from quantum randomness. When the quantum adiabatic conditions are satisfied, $P(|i_n, \lambda_n\rangle \rightarrow |i_n', \lambda_{n+1}\rangle) = \delta_{i_n, i_n'}$, we regain the probability of a trajectory in classical systems [4]. We will see later that the quantum Crooks FT and quantum JE in the quantum adiabatic regime are the counterpart of classical Crooks FT and classical JE.

To prove the quantum Crooks FT, we also need to consider the time-reversed trajectory [11] of the original trajectory (2). The time-reversed trajectory corresponding to the forward time trajectory $A \leftarrow B$ in Eq. (2) can be written as

$$\begin{aligned} &\Theta\,|i_0, \lambda_0\rangle \leftarrow \Theta\,|i_0', \lambda_1\rangle \leftarrow \Theta\,|i_1, \lambda_1\rangle \leftarrow \Theta\,|i_1', \lambda_2\rangle \leftarrow \\ &\cdots \leftarrow \Theta\,|i_{N-1}, \lambda_N\rangle \leftarrow \Theta\,|i_{N-1}', \lambda_N\rangle \leftarrow \Theta\,|i_N, \lambda_N\rangle \end{aligned} \tag{4}$$

where $\Theta\,|i_n, \lambda_n\rangle = |i_n, \lambda_n\rangle^*$ is the microscopic state in the time-reversed trajectory [12]. The sequence in which states are visited is reversed, as is the order in which λ is changed. The work done W, the heat exchange Q with the heat bath, the change of the internal energy ΔE, and the change of free energy ΔF for the reversed time direction are the negative value of that of the forward time trajectory. The joint probability for time reversed trajectory $A \leftarrow B$ can be expressed as

$$\begin{aligned} P_R(A \leftarrow B) = &\prod_{n=0}^{N-1} P_R(\Theta\,|i_n, \lambda_n\rangle \leftarrow \Theta\,|i_n', \lambda_{n+1}\rangle) \\ &\times P_R(\Theta\,|i_n', \lambda_{n+1}\rangle \leftarrow \Theta\,|i_{n+1}, \lambda_{n+1}\rangle) \\ &\times P(\Theta\,|i_N, \lambda_N\rangle) \end{aligned} \tag{5}$$

where $P(\Theta\,|i_N, \lambda_N\rangle) = \frac{e^{-\beta E(i_N, \lambda_N)}}{\sum_i e^{-\beta E(i, \lambda_N)}}$ is the initial thermal distribution for the time-reversed trajectory. Also there is en extra term $P_R(\Theta\,|i_n, \lambda_n\rangle \leftarrow \Theta\,|i_n', \lambda_{n+1}\rangle)$ arising due to the quantum randomness in comparison with the classical case.

III. PROOF OF QUANTUM CROOKS FT AND QUANTUM JE

As we have mentioned before, in a trajectory every step consists of two substeps, the controlling substep (not necessarily to be quantum adiabatic) and the relaxation substep. The relaxation substeps are assumed to be microscopically reversible, and therefore obey the detailed balance [4, 13] for all fixed value of the external control parameter λ

$$\frac{P_F(|i'_{n-1},\lambda_n\rangle \to |i_n,\lambda_n\rangle)}{P_R(\Theta|i'_{n-1},\lambda_n\rangle \leftarrow \Theta|i_n,\lambda_n\rangle)} = \frac{e^{-\beta E(i_n,\lambda_n)}}{e^{-\beta E(i'_{n-1},\lambda_n)}}. \quad (6)$$

To compare the ratio of the probabilities of forward (3) and time-reversed (5) trajectories, we also need to know the ratio of the probabilities in the controlling substep. In the following we will focus on the study of controlling substep and its time reversal. As we mentioned before, during the controlling substep, the system can be regarded as an isolated quantum system and the evolution is completely determined by a time-dependent Hamiltonian $H[\lambda(t)]$. For example, when the controlling parameter λ is changed from λ_n to λ_{n+1}, the probability of the excitation from a microscopic state $|i_n,\lambda_n\rangle$ to another microscopic state $|i'_n,\lambda_{n+1}\rangle$ can be expressed as

$$P_F(|i_n,\lambda_n\rangle \to i'_n,\lambda_{n+1}) = |\langle i'_n,\lambda_{n+1}|U|i_n,\lambda_n\rangle|^2 \quad (7)$$

where $U = \mathrm{T}e^{-\imath\int_{t_0}^{t_1} H[\lambda(t)]dt}$ is the unitary matrix describing the evolution of the isolated quantum system in the controlling substep, and T is the time-ordered operator. Similarly, in the time-reversed trajectory the excitation probability from the microscopic state $\Theta|i'_n,\lambda_{n+1}\rangle$ to another microscopic state $\Theta|i_n,\lambda_n\rangle$ in the time reversed trajectory can be expressed as [14]

$$\begin{aligned} &P_R(\Theta|i_n,\lambda_n\rangle \leftarrow \Theta|i'_n,\lambda_{n+1}\rangle) \\ &= |\left(\langle i_n,\lambda_n|\overleftarrow{\Theta}\right)\Theta U\overleftarrow{\Theta}\left(\Theta|i'_n,\lambda_{n+1}\rangle\right)|^2, \end{aligned} \quad (8)$$

where $\Theta U\overleftarrow{\Theta} = \mathrm{T}e^{-\imath\int_{t_0}^{t_1} H[\lambda(t_0+t_1-t)]dt} = (U^\dagger)^* = U^T$ is the time-reversed unitary matrix. Because of the properties of the time-reversed transformation $\Theta|i_n,\lambda_n\rangle = |i_n,\lambda_n\rangle^*$, and the property of the Hermitian conjugate matrix,

$$(\langle i_n,\lambda_n|)^* U^T (|i'_n,\lambda_{n+1}\rangle)^* \equiv \langle i'_n,\lambda_{n+1}|U|i_n,\lambda_n\rangle \quad (9)$$

it is not difficult to prove that

$$\frac{P_F(|i_n,\lambda_n\rangle \to |i'_n,\lambda_{n+1}\rangle)}{P_R(\Theta|i_n,\lambda_n\rangle \leftarrow \Theta|i'_n,\lambda_{n+1}\rangle)} \equiv 1. \quad (10)$$

Based on the above two results (6), (10) and Eqs. (3) and (5), we reproduce the Crooks FT for a quantum mechanical system

$$\frac{P_F(A\to B)}{P_R(A\leftarrow B)} = e^{\beta(W-\Delta F)}. \quad (11)$$

From Eq. (11) we group all those trajectories with the same amount of microscopic work, and obtain

$$\frac{P_F(W|_a)}{P_R(-W|_{-a})} = e^{\beta(a-\Delta F)}. \quad (12)$$

Eq. (12) is the Crooks FT. Similar to the derivation in Ref. [4], we obtain the JE for a quantum open system straightforwardly $\langle e^{-\beta W}\rangle = e^{-\beta\Delta F}$. Here, we would like to emphasize that though quantum generalization of Crooks FT and JE have been reported in some previous work, the explicit consideration of the influence of the heat bath, i.e., the explicit expression of microscopic work in the presence of a heat bath has not been reported before. Also the relation between quantum and classical trajectories are not addressed clearly. Hence our quantum mechanical extensions of Crooks FT and JE are highly nontrivial.

IV. ILLUSTRATION OF QUANTUM CROOKS FT AND QUANTUM JE IN A TWO-LEVEL SYSTEM

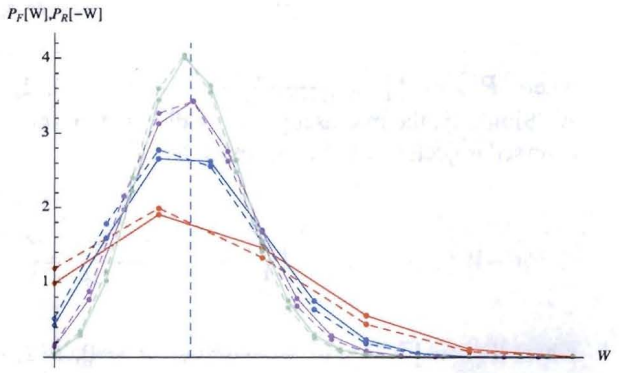

FIG. 2: Microscopic work distribution $P_F(W)$ of forward trajectories (solid lines), and the negative reverse work distribution $P_R(-W)$ of their corresponding time-reversed trajectories (dashed lines). The probabilities have been normalized. Here we fix $\Delta(t_0)$ and $\Delta(t_N)$. Different distributions represent different controlling time (the more steps, the longer control time). The controlling time are chosen to be $N = 5$ (red), $N = 10$ (blue), $N = 15$ (purple), and $N = 20$ (green). It can be seen that the work distributions for both forward and reversed trajectories are not Gaussian. Moreover, the decrease of the controlling speed, the fluctuation of the distributions decreases, and the difference between the work distribution of the forward and time-reversed trajectories becomes less obvious. The corresponding forward and negative reverse work distribution cross at $W = \Delta F$, and this is a direct consequence of the quantum Crooks FT.

Having generalized the Crooks FT and JE to quantum systems in the presence of a heat bath. In the following, we use the studies based on a two-level system [15] as an illustration to demonstrate our main idea. The Hamiltonian of the two-level system is $H = \frac{1}{2}\Delta(t)(\sigma_z + 1)$, where $\Delta(t)$ is the parameter of the Hamiltonian, and σ_z is Pauli matrix. The initial and final value of the parameter are $\Delta_A = \Delta(t_0)$ and $\Delta_B = \Delta(t_N)$ respectively. The controlling scheme is the same as that in Ref. [15]: We divide the whole process into N even steps. Hence the parameter in the nth step is $\Delta(t_n) = \Delta(t_0) + n\Delta$, where $\Delta = \frac{\Delta_B - \Delta_A}{N}$ is the change of the parameter in every step. Every step consists of two substeps: the controlling substep, in which we

change the parameter from $\Delta(t_n)$ to $\Delta_{n+1} = \Delta(t_n) + \Delta$, and the relaxation substep. For simplicity, we consider the case where the system reaches thermal equilibrium with the heat bath in every relaxation substep. Hence, the probability for the forward and reverse relaxation substep can be expressed as $P_F(|i'_{n-1}, \lambda_n\rangle \to |i_n, \lambda_n\rangle) = \frac{e^{-\beta E(i_n,\lambda_n)}}{\sum_i e^{-\beta E(i,\lambda_n)}}$, and $P_R(\Theta|i'_{n-1}, \lambda_n\rangle \leftarrow \Theta|i_n, \lambda_n\rangle) = \frac{e^{-\beta E(i'_{n-1},\lambda_n)}}{\sum_i e^{-\beta E(i,\lambda_n)}}$. Also we assume the quantum adiabatic conditions are satisfied in every controlling substep. That is $P_F(|i_n, \lambda_n\rangle \to |i'_n, \lambda_{n+1}\rangle) = \delta_{i_n,i'_n}$, and $P_R(\Theta|i_n, \lambda_n\rangle \leftarrow \Theta|i'_n, \lambda_{n+1}\rangle) = \delta_{i_n,i'_n}$. Based on these assumptions, the microscopic work distribution for the forward trajectories can be obtained [15]

$$P_F(W|_{k\Delta}) = P_e^F \prod_{l=0}^{N-k-1} \frac{e^{\beta\Delta_B} - e^{\beta(\Delta_A+l\Delta)}}{e^{\beta(l+1)\Delta} - 1}, \qquad (13)$$

where $P_e^F = \prod_{j=1}^{N} \frac{e^{-\beta[\Delta_A+(j-1)\Delta]}}{1+e^{-\beta[\Delta_A+(j-1)\Delta]}}$, $k = 0, 1, 2, \cdots, N$. Similarly, the microscopic work distribution for the time-reversed trajectory can be expressed as

$$P_R(-W|_{-k\Delta}) = P_e^R \prod_{l=0}^{N-k-1} \frac{e^{\beta\Delta}[e^{\beta\Delta_B} - e^{\beta(\Delta_A+l\Delta)}]}{e^{\beta(l+1)\Delta} - 1}, \qquad (14)$$

where $P_e^R = \prod_{j=1}^{N} \frac{e^{-\beta[\Delta_B-(j-1)\Delta]}}{1+e^{-\beta[\Delta_B-(j-1)\Delta]}}$, $k = 0, 1, 2, \cdots, N$. We plot the above distributions (13) and (14) of microscopic work in Fig. 2. Here the probability distribution in the excited state are $P_e(\Delta_A) = \frac{e^{-\beta\Delta_A}}{1+e^{-\beta\Delta_A}} = \frac{1}{3}$, and $P_e(\Delta_B) = \frac{e^{-\beta\Delta_B}}{1+e^{-\beta\Delta_B}} = \frac{1}{5}$. The free energy difference is $\Delta F_{AB} = \left[\ln(1+\frac{1}{2}) - \ln(1+\frac{1}{4})\right] k_B T \approx 0.263(\ln 4 - \ln 2) k_B T$. It can be seen (see Fig. 2) that the corresponding forward and negative reverse work distributions cross at $W = \Delta F$, no matter what the controlling protocol is, and this result is a direct consequence of Crooks FT. It should be pointed out that the work distributions (13) and (14) are non-Gaussian [15]. Hence, the processes discussed here are beyond the linear response regime. Yet we will see both Crooks FT and JE holds. We also Plot the logarithm of the ratio of the forward and negative reverse work distribution (See Fig. 3A). It can be seen that all data collapse onto the same straight line. In addition, the slope of the line is equal to unit, and the line cross the horizontal axis at $W = 0.263(\ln 4 - \ln 2) k_B T = \Delta F_{AB}$. Thus our numerical simulation confirms the validity of quantum Crooks FT when the process is beyond the linear response regime. We also plot the logarithm of the exponent averaged work $\ln\langle e^{-\beta W}\rangle$ and averaged work $\langle W\rangle$ of the forward process (see Fig. 3B) to test the validity of quantum JE. It can be seen that the averaged work is greater than the free energy difference $\langle W\rangle \geqslant \Delta F$, while the logarithm of the exponent averaged work is identical to the difference of the free energy $\ln\langle e^{-\beta W}\rangle \equiv \Delta F = \ln\frac{1+1/2}{1+1/4} \approx 0.1823 k_B T$ no matter what the controlling protocol is. Hence, Fig. 3B verifies quantum JE when the process is beyond the linear response regime.

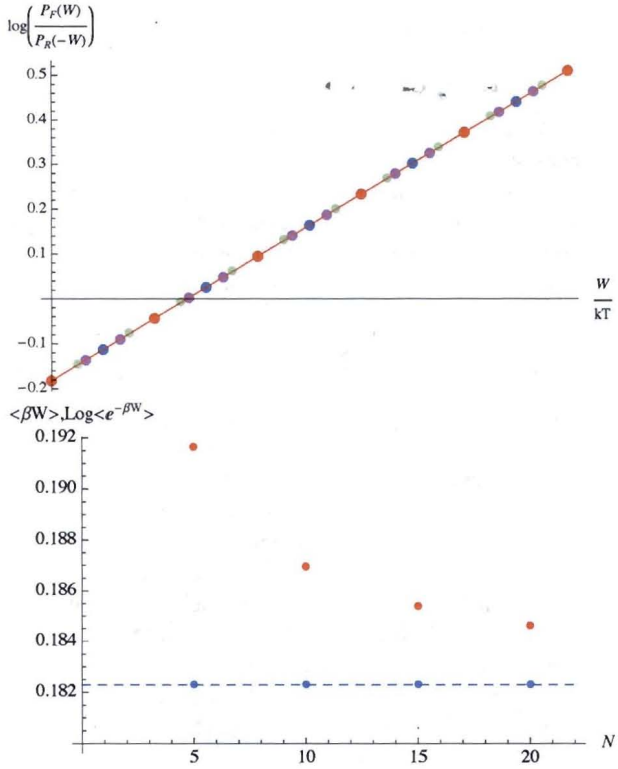

FIG. 3: Above: The logarithm of the probabilities of forward and time-reversed trajectories as a function of work. It can be seen that all data of different work and different control protocols ($N = 5$ (red), $N = 10$ (blue), $N = 15$ (purple), $N = 20$ (green)) collapse onto the same straight line. The slop of the line is equal to unity, and the line cross the horizontal axes at $W = \Delta F$. Thus the numerical result verifies the quantum Crooks FT $\ln\frac{P_F(W|_a)}{P_R(-W|_{-a})} = \beta(a - \Delta F)$. Below: The averaged work VS. the logarithm of averaged exponent work for different control protocols. It can be seen that the averaged work $\langle W\rangle$ is always greater than the difference of free energy ΔF_{AB} and differ from one control protocol to another, while the logarithm of the exponentially averaged work $\ln\langle e^{-\beta W}\rangle$ is always equivalent to the difference of free energy irrespective of the control protocols. Thus the numerical result verifies the JE $\ln\langle e^{-\beta W}\rangle \equiv \Delta F$

V. CONCLUSION AND REMARKS

In this paper, we explicitly consider the quantum Crooks FT and quantum JE in the presence of an external heat bath. Our proof includes the proof of classical Crooks FT as a special case. When the quantum adiabatic conditions are satisfied, we reproduce the result of Crooks FT and JE for classical systems. Our work indicates that in quantum systems, the probabilities (Eqs. (3) and (5)) comes from both the quantum randomness and statistical mechanical randomness, while in classical system, the randomness only comes from the later case. We use the two-level system as an illustration to demonstrate the validity of quantum Crooks FT and quantum JE beyond the linear response regime.

Before concluding the paper, we would like to mention the following points. First, though the quantum randomness is

introduced into the controlling substep, this substep is time reversal symmetric. I. e., all the time asymmetry is due the relaxation substep (statistical mechanical randomness), rather than the controlling substep (quantum randomness). This is the same as the classical case. Second, when we change the Hamiltonian slowly, we reproduce the proof of Crooks for classical systems. In this sense, we say that our proof includes the classical Crooks FT and classical JE as a special case. Third, for classical system, the Crooks FT and JE have been experimentally verified [7]. However, for a quantum mechanical system, the experimental exploration on Crooks FT and JE has not been reported (an exception is [10]). This perhaps is mainly due to the fact that microscopic work in a quantum mechanical system is not a well defined observable [18]. There is no well defined pressure or force for a quantum system [17]. Hence, we cannot follow the way that we do in classical system to measure the force and make the integral of the force by the extension. On the contrary, we will have to introduce quantum measurement processes to confirm the initial and final energy of the system and then calculate the microscopic work done from the difference of the initial and final energy difference [16]. Fourth, though the numerical simulations consider only the special cases: 1) the system reach thermal equilibrium with the heat bath in every relaxation substep, and 2) the quantum adiabatic conditions are satisfied in every controlling substep, the quantum Crooks FT and quantum JE are not constrained in these special cases. Finally, our numerical simulations based on a two-level system can possibly be testified by employing Josephson Junction charge qubit [19]. Discussion about employing Josephson Junction qubit to test the quantum Crooks FT and quantum JE will be given later.

VI. ACKNOWLEDGMENTS

HTQ thanks Wojciech H. Zurek, G. Crooks and Rishi Sharma for stimulating discussions and gratefully acknowledges the support of the U.S. Department of Energy through the LANL/LDRD Program for this work.

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