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Quantum signatures in the work fluctuation-dissipation relation protocol

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Contents

Abstract

Quantum thermodynamics deals with the behavior of thermal machines that operate in the quantum regime, where coherences and entanglement can have a significant impact. However, detecting such quantum effects in thermal machines can be challenging, as they are primarily manifested as fluctuations. This thesis theoretically studies the protocol for the work fluctuation-dissipation relation (FDR) from stochastic thermodynamics. We find Quantum signatures including coherence and entanglement in the FDR. When there is coherence or entanglement, corrections are introduced into the FDR. To study the effect of entanglement, a generalized protocol is proposed.

Acknowledgements

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I would also like to thank Xufan Zhao for accompanying me throughout the completion of this project and providing helpful suggestions on my writing.

List of Abbreviations

FDR Fluctuation-dissipation Relation

TPM Two-point Measurement Scheme

DUT Discrete Unitary Transformation

DTT Discrete Thermalising Transformation

DUQ Discrete Unitary Quench

1 Introduction

Classical thermodynamics is a successful theory to describe complex physics systems using several quantities including heat, work, and energy. One natural idea is to extend classical thermodynamics to the quantum regime. In that case, quantum effects including coherence and entanglement play roles [4, 18]. However, it is not easy to experimentally observe genuine quantum effects from microscopic thermal machines.

Stochastic thermodynamics is a framework to study the thermodynamics of small systems where fluctuations play a crucial role. The work fluctuation-dissipation relation from stochastic thermodynamics:

$$\frac{\beta}{2}\mathrm{Var}(W) = \langle W \rangle - \Delta F \tag{1}$$

gives us a chance to detect the quantumness of the system. In the relation, W is the work, β is the inverse temperature and F is the free energy. $\mathrm{Var}(W)$ is the variance of work: $\langle W^2 \rangle - \langle W \rangle^2$. It has been both theoretically and experimentally verified that the relation can be violated when there is coherence in the system [8, 9, 13]. This is a genuine quantum signature from the effect of coherence. This result reveals how quantum coherence influences the work extraction protocol. Since entanglement is also a quantum effect, it is natural to ask whether entanglement will also bring violations to the fluctuation-dissipation relation. In this work, our goal is to extend this result to the case when there is entanglement. To reach the goal, we study a two-qubit system since in such a system the entanglement of a mixed quantum state can be easily found [11].

In the series of studies on coherence, a quantum process with discrete quenches on the Hamiltonian and thermalization is considered [8, 9, 13]. We first generalize the discrete thermodynamical protocol proposed by Scandi et al (2020) when studying the coherence system [13]. We argue that a generalization of the protocol within the framework of the discrete quantum process is needed to study the effect of the entanglement. Specifically, one extra unitary global evolution is applied to the thermal state. We proved that all two-qubit unitary operators can be divided into two subsets. Operators in one set are able to generate entanglement while operators in the other set can not. When entanglement operators are applied, there is a larger violation of the work fluctuation-dissipation relation. This can be understood as a quantum signature from entanglement.

The thesis is organized as follows: necessary theory and concepts are introduced first. Basic concepts that will be used including density matrices, the definition of quantum work, the fluctuation-dissipation relation, discrete thermodynamical quantum processes, coherence, and entanglement will all be introduced. After that, we will first introduce the fluctuation protocol and calculate the experimentally verified single-qubit case as an example. This example, as discussed before, shows the quantum effect of coherence on the fluctuation-dissipation relation. After that, we will generalize the protocol and explain the necessity of the generalization. Then a simple case is calculated as an example. Finally, we divide all two-qubit unitary operations into parts and show that the part that brings entanglement to the systems will introduce a larger correction to the fluctuation-dissipation relation. This final result shows the effect of entanglement on the relation as a quantum signature.

2 Theory and concepts

2.1 Density matrices

Suppose that a probability mixture of quantum state s is prepared [6]:

$$s = \{p_i; |\psi_i\rangle\}_{i=1}^{n} \tag{2}$$

Then we can write the quantum state as a Hermitian, positive semi-definite matrix ρ with $Tr(\rho) = 1$:

$$\rho = \sum_{i=1}^{n} p_i \, |\psi_i\rangle \, \langle\psi_i| \tag{3}$$

Suppose that a collection of generalized measurement operators $\{M_m\}$ is given, then the probability of getting m from the measurement is:

$$p(m|\rho) = Tr(M_m^\dagger M_m \rho) \tag{4}$$

Density operators are an alternative description of the quantum state in comparison to normalized vectors in the Hilbert space. It is used to describe an ensemble of pure quantum states.
Now we give an example of measurement operators. Consider a Hamiltonian $H = \sum_i E_i |E_i\rangle\langle E_i|$, the probability of getting eigenenergy E_i is $Tr((|E_i\rangle\langle E_i|)^\dagger (|E_i\rangle\langle E_i|)\rho)$ and one should notice that $Tr((|E_i\rangle\langle E_i|)^\dagger (|E_i\rangle\langle E_i|)\rho) = Tr(|E_i\rangle\langle E_i|\rho^{th}) = \langle E_i|\rho|E_i\rangle$. In that case $|E_i\rangle\langle E_i|$ is the measurement operator. This is called projective measurement.

2.1.1 Gibbs state

Suppose that the Hamiltonian of a system is H. The Gibbs state or thermal state is:

$$\rho^{th} = \frac{1}{Z} e^{-\beta H} \tag{5}$$

where Z is a partition function, β is the inverse temperature. The thermal state ρ^{th} is the state with the largest entropy in a system with constant average energy.

2.2 Two-point measurement (TPM) scheme

In quantum thermodynamics, work has to be carefully defined [16]. In the following, the two projective measurement scheme (TPM) will be used. In the TPM scheme, two projective measurements of energy are performed at the end and the beginning of the process, and the work is defined as the difference between the two measurement outcomes [17]. Detailed discussion will be shown later. Classically the energy can be determined by the Hamiltonian of the system. We can write the Hamiltonian as $H(z, \lambda)$ where z is the point of the phase space and λ is the parameter of the protocol. The protocol λ alters the energy and hence work will be applied to or taken from the system. One convenient way to define work is to choose the inclusive definition of work. That is, the work is given by the energy difference at the end and the beginning of the force protocol. The TPM scheme is an adaptation of this definition to quantum systems. Further discussion can be seen in [16]. We will use this inclusive definition of work.

2.3 Work Fluctuation-Dissipation-Relation (FDR)

In a small system, we have to consider thermal and quantum fluctuations. One important method to describe the thermodynamics of a small system is to use stochastic thermodynamics[14]. In the framework of stochastic thermodynamics, physical quantity such as work is described by a random variable with a probability distribution. One important result from the field of stochastic thermodynamics is the work Fluctuation-Dissipation-Relation (FDR):

$$\frac{\beta}{2}\mathrm{Var}(W) = \langle W \rangle - \Delta F \tag{6}$$

where W is the work, F is the free energy and β denotes the inverse temperature. This relation is valid for isothermal processes that are close to equilibrium[4, 8, 15]. The topic of our project is to explore possible violations of this relation for systems with quantum fluctuations.

2.4 Thermodynamics of discrete quantum processes

The discrete quantum process is a key concept in the project. It has been shown that a continuous quantum thermal process can be approximated using a combination of discrete quantum processes[1]. There are two kinds of discrete transformations, the process that is close to equilibrium considered in this article is built up by these two discrete transformations.

2.4.1 Discrete Unitary Transformations (DUTs)

Suppose that the quantum system we are interested in is described by the quantum state ρ and Hamiltonian H, we then write the configuration of the system to be (ρ, H). The discrete unitary transformation is defined to be:

$$(\rho_i, H_i) \xrightarrow{DUT} (\rho_f, H_f) \tag{7}$$

Here (ρ_i, H_i) denotes the initial configuration and (ρ_f, H_f) denotes the final configuration. Notice that the change of the Hamiltonian is rather arbitrary and it is not necessarily in the same form as the unitary evolution of the state. For example, it can be a non-unitary quench [13].

2.4.2 Discrete Unitary Quenches (DUQs)

Discrete Unitary Quenches are a special case of DUTs. The quench is a process to change the Hamiltonian. The change is so fast that the system density matrix does not change. That is:

$$(\rho_i, H_i) \xrightarrow{DUQ} (\rho_i, H_f) \tag{8}$$

2.4.3 Discrete Thermalising Transformations (DTTs)

Thermalization is a transformation of the quantum state:

$$(\rho_i, H_i) \xrightarrow{DTT} (\rho^{th}, H_f) \tag{9}$$

Here $\rho^{th} = \frac{1}{Z}e^{-\beta H}$ as defined in eq.5.

2.5 Coherence and entanglement

Coherence and entanglement are quantum properties to study in this project. In this section, we briefly introduce these concepts.

2.5.1 Coherence

A classical state ρ has no off-diagonal terms, it just represents a classical probability mixture. However, a quantum state ρ can have off-diagonal terms. We expand a pure state as:

$$|\psi_k\rangle = \sum_{i=1}^{n} c_i^{(k)} |i\rangle \tag{10}$$

Then probability mixture of pure states is:

$$\rho = \sum_{l=1}^{l} p_k \left|\psi_k\right\rangle \left\langle\psi_k\right| \tag{11}$$

Then the off-diagonal term $\rho_i j$ is:

$$\begin{aligned} \rho_{ij} = \langle i|\rho|j\rangle &= \sum_{k=1}^{l} p_k \langle i|\psi_k\rangle\langle\psi_k|j\rangle = \sum_{k=1}^{l} p_k \sum_{l,m=1}^{n} c_l^{(k)} c_m^{(k)\star} \langle i|l\rangle\langle m|j\rangle \\ &= \sum_{k=1}^{l} p_k c_i^{(k)} c_j^{(k)\star}. \end{aligned} \tag{12}$$

From the equation above, we can find that off-diagonal terms of the density matrix come from the superposition of quantum states, which is a quantum effect.

2.5.2 Entanglement

Given a quantum state ρ, if $Tr(\rho^2) < 1$, the state is called a mixed state, otherwise it is a pure state. The quantum entanglement of pure states is simpler to analyze than mixed states. We will mainly deal with the mixed-state case. Suppose that there is a bipartite system $H_A \otimes H_B$, if a density operator ρ^{AB} of the total system can be written as:

$$\rho^{AB} = \sum_i p_i \rho_i^A \otimes \rho_i^B \tag{13}$$

where p_i is a positive probability, then ρ^{AB} is called separable, otherwise it is an entangled state. It is a difficult problem to say whether a state is entangled or not. However, in 2×2 dimensional systems, this has been solved [11].

2.5.3 Negativity and partial transpose

In this section two important concepts are introduced: negativity and partial transpose. Given a bipartite system $H_A \otimes H_B$, a basis of the system can be written as $|ij\rangle = |i\rangle_A \otimes |j\rangle_B$ where $|i\rangle_A$ and $|i\rangle_B$ are orthonormal basis vector of H_A and H_B respectively. Then the

operation of taking partial transpose can be written as:

$$\rho_{ij,kl} \to \rho_{il,kj} \tag{14}$$

where $\rho_{ij,kl} = \langle ij|\rho|kl\rangle$. Given a density operator ρ, we write ρ^{pt} as its partial transpose The negativity of a quantum state is defined as:

$$\mathcal{N}(\rho) = \frac{\sum_i (|\lambda_i| - \lambda_i)}{2} \tag{15}$$

where λ_i is a eigenvalue of ρ^{pt}. The negativity is an entanglement monotone, meaning it will not be changed under local operations.

2.5.4 Peres–Horodecki criterion

Given a 2×2 quantum system, it has been shown that $N(\rho) > 0$ is a necessary and sufficient condition for the existence of entanglement [11]. This is called the Peres–Horodecki criterion.

2.5.5 Two-qubit entanglers

It is known that any two-qubit unitary operator $O \in \mathrm{SU}(4)$ can be written as [12]:

$$\hat{O} = \left(\hat{A}_1 \otimes \hat{B}_1\right) e^{-i(c_1\hat{\sigma}_1\otimes\hat{\sigma}_1 + c_2\hat{\sigma}_2\otimes\hat{\sigma}_2 + c_3\hat{\sigma}_3\otimes\hat{\sigma}_3)} \left(\hat{A}_2 \otimes \hat{B}_2\right) \tag{16}$$

where σ_i's are Pauli matrices and A_i, B_i are single qubit operations. Notice that A_i and B_i are just local single-qubit unitary operations and they can not change the entanglement, thus we can define a new operator:

$$\mathcal{O} = e^{-i(c_1\hat{\sigma}_1\otimes\hat{\sigma}_1 + c_2\hat{\sigma}_2\otimes\hat{\sigma}_2 + c_3\hat{\sigma}_3\otimes\hat{\sigma}_3)} \tag{17}$$

Other operators O are just local equivalents of this operator. In the computational basis, we can write the matrix form of $\mathcal{O}$ and A_i, B_i as [12, 7]:

$$\mathcal{O} = \begin{pmatrix} e^{-\mathrm{i}}c_3c^- & & & -\mathrm{i}e^{-\mathrm{i}c_3}s^- \\ & e^{\mathrm{i}c_3}c^+ & -\mathrm{i}e^{\mathrm{i}c_3}s^+ & \\ & -\mathrm{i}e^{\mathrm{i}}c_3s^+ & e^{\mathrm{i}}c_3c^+ & \\ -\mathrm{i}e^{-\mathrm{i}}c_3s^- & & & e^{-\mathrm{i}}c_3c^- \end{pmatrix} \tag{18}$$

where $c^\pm = \cos(c_1 \pm c_2)$, $s^\pm = \sin(c_1 \pm c_2)$.

$$\hat{A}_i = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & -e^{\mathrm{i}}\lambda\sin\left(\frac{\theta}{2}\right) \\ e^{\mathrm{i}}\phi\sin\left(\frac{\theta}{2}\right) & e^{\mathrm{i}}(\phi+\lambda)\cos\left(\frac{\theta}{2}\right) \end{pmatrix} \tag{19}$$

where θ, λ, ϕ are parameters of A_i. B_i can be parametrized in the same way.

3 Systems

The goal of our project is to find the possible correction of the work fluctuation-dissipation-relation. We want to explore the effects of quantum fluctuation on this relation. To see this, we define a new function:

$$Q = \frac{\beta}{2}\mathrm{Var}(W) - (\langle W\rangle - \Delta F) \tag{20}$$

This is just the correction function of Eq. (6). We want to explore what will this function be like when there is entanglement and/or coherence. Our goal is to find a clear relationship between Q and entanglement and coherence. If there is a larger correction function Q when there is quantum entanglement or coherence, it can be concluded that there is a genuine quantum signature. To study this, it is needed to carefully choose a thermodynamical protocol and a quantum system. In the protocol, coherence, and entanglement should be generated. For the coherence case, there are already theoretical and experimental results[9, 13]. In the first part of this section, we will briefly review the work-fluctuation protocol proposed by Scandi et al. (2020)[13]. We will also calculate Q in the single-qubit case of the protocol which has been experimentally verified [9]. In the second section, we will propose a generalized work-fluctuation protocol to study the correction of FDR caused by entanglement. Then we will calculate the Q in a two-qubit case to show the quantum signature of entanglement.

3.1 Coherence and work fluctuation protocol

In this section, we reproduce the main result from the article [9] theoretically. The coherence work fluctuation protocol consists of N steps and there are two procedures in each steps [13]:
1. Quench on the Hamiltonian (DUQs and also DUTs): The process is so fast that the Hamiltonian H is changed while the quantum state is unchanged.
The quench, as discussed before, is an instantaneous change of the Hamiltonian that leaves the quantum state unchanged. The quench can have a different form for example:

$$H_i \longrightarrow \hat{U}_i^\dagger H_i \hat{U}_i = H_{i+1} \tag{21}$$

This is the case we will consider. There can also be a classical quench, which will just change the energy. There is an example:

$$H_i = \frac{1+i\Delta}{4}\hat{\sigma}_z \longrightarrow H_{i+1} = \frac{1+(i+1)\Delta}{4}\hat{\sigma}_z \tag{22}$$

Notice that this is not in the form of Eq. (21) and can not give us any correction to the FDR since we can not generate coherence from this [13]. We will not consider this kind of quench.
2. The thermalization procedure (DTTs): The quantum state is thermalized to the Gibbs state:

$$\rho^{th} = \frac{1}{Z}e^{-\beta H} \tag{23}$$

The work is defined by the TPM scheme as before. There is a projective measurement after the thermalization and before the quench. Then the second measurement happens

after the quench. Notice that our measurement is always a projective measurement of the Hamiltonian and the Hamiltonian H_i at the beginning and H_{i+1} at the end are different. Then the two measurement operators are different. Suppose that at the beginning of the i-th step $H_i = \sum_j E_j^i |E_j^i\rangle\langle E_j^i|$. We can easily find that:

$$H_{i+1} = \sum_j E_j^{i+1} |E_j^{i+1}\rangle\langle E_j^{i+1}| = \sum_j E_j^i \hat{U}_i^\dagger |E_j^i\rangle\langle E_j^i|\hat{U}_i = \hat{U}_i^\dagger H_i \hat{U}_i \tag{24}$$

One important observation from the equation above is that the projective measurement operator of H_{i+1} can be written in the form:

$$\hat{P}_j^{i+1} = \hat{U}_i^\dagger |E_j^i\rangle\langle E_j^i|\hat{U}_i \tag{25}$$

We can also explicitly write the probability of getting the work ω in the i-th step for an arbitrary kind of quench: (At the beginning we have a Gibbs state ρ_i^{th})

$$P_i(\omega) = \sum_{E_l^{i+1} - E_k^i = \omega} \langle E_k^i|\rho_i^{th}|E_k^i\rangle |\langle E_k^i|E_l^{i+1}\rangle|^2 \tag{26}$$

Notice that since $|E_l^{i+1}\rangle$ is a eigenbasis of H_{i+1}, we can write $|\langle E_k^i|E_l^{i+1}\rangle|^2 = |\langle E_k^i|U_i^\dagger|E_l^i\rangle|^2$ from eq. (25). Now we can rewrite Eq. (26) as:

$$P_i(\omega) = \sum_{E_l^{i+1} - E_k^i = \omega} \langle E_k^i|\rho_i^{th}|E_k^i\rangle |\langle E_k^i|\hat{U}_i^\dagger|E_l^i\rangle|^2 \tag{27}$$

In the experimental work of Onishchenko et al. (2022) [9], a single qubit case is considered. In that case, the energy can be 0 or 1. The operator of the quench is:

$$\hat{U}_i^\dagger = \exp\left(-i(\Delta\theta/2)\hat{\sigma}_x\right) = \begin{pmatrix} \cos\frac{\Delta\theta}{2} & -\mathrm{i}\sin\frac{\Delta\theta}{2} \\ -\mathrm{i}\sin\frac{\Delta\theta}{2} & \cos\frac{\Delta\theta}{2} \end{pmatrix} \tag{28}$$

We can regard the quench as an operation to change the basis. After each step i, we can set the new basis of the Hilbert space as $|E_k^{i+1}\rangle = U_i^\dagger |E_k^i\rangle$. From this, all steps are identical and can be understood as a quantum circuit which is shown in Fig. 1 [9].
Thus the protocol can be regarded as repeating the circuit N steps with the thermal state:

$$\rho^{th} = \frac{1}{Z}\begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta} \end{pmatrix} \tag{29}$$

where $Z = \frac{1}{1+e^{-\beta}}$. Notice that the average work of each step is:

$$\langle W_i\rangle = \sum_w \omega P_i(\omega) \tag{30}$$

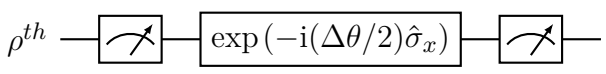

Figure 1: The equivalent quantum circuit corresponding to one step

And it is obvious that:

$$\langle W_i^2 \rangle = \sum_w \omega^2 P_i(\omega) \tag{31}$$

Since each step is identical, we can write the total work as:

$$\langle W \rangle = N \langle W_i \rangle \tag{32}$$

where N is the number of steps.

3.1.1 Results

Notice that the free energy change $\Delta F = 0$ since the quench is just a rotation of the basis [9]. From all discussion above we can get the correction function Q under the given quench operator $\exp(-i(\Delta\theta/2)\hat{\sigma}_x)$ with the initial Hamiltonian $H_0 = |1\rangle\langle 1|$:

$$Q = N \sin^2\left(\frac{\Delta\theta}{2}\right)\left[\frac{\beta}{2}\left(1 - \sin^2\left(\frac{\Delta\theta}{2}\right)(1-2p)^2\right) - (1-2p)\right] \tag{33}$$

where p is given by:

$$1 - 2p = \tanh(\beta/2) \tag{34}$$

Suppose that there are N steps and the Hamiltonian changes from $H_0(0)$ to $H_f(\theta)$, where H_f is the final Hamiltonian after all steps. Then $\Delta\theta = \frac{\theta}{N}$. If the process is slow and close to equilibrium, then N is large, and $\Delta\theta$ is small. From this, we can use the small angle approximation $sin(\Delta\theta) \sim \Delta\theta$. Then we can rewrite the correction function as:

$$Q = N\frac{(\Delta\theta)^2}{4}\left[\frac{\beta}{2} - \tanh(\beta/2)\right] + O((\Delta\theta)^2) = N\frac{(\Delta\theta)^2}{4} f(\beta) + O((\Delta\theta)^2) \tag{35}$$

where $f(\beta) = \frac{\beta}{2} - \tanh(\beta/2)$. This is the same as what Onishchenko et al. (2022)[9] get.

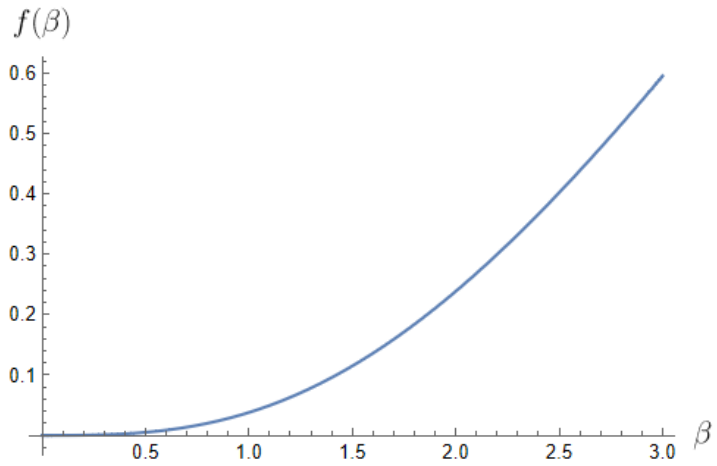

Figure 2: Plot of $f(\beta)$. β is the inverse temperature. Given a final θ parameter and a number of steps N, the correction Q is determined by $f(\beta)$.

3.2 Entanglement protocol

In this section, we first generalize the protocol used before. After that, we set up a two-qubit system to study the correction function Q when there is entanglement and compare the new result with the result found in the last section.

3.2.1 An explanation of the protocol

Here we briefly explain the reason why a new protocol is needed to consider the effect of entanglement. To consider entanglement, there should be at least two systems S_A and S_B. Initially, the Hamiltonian of each system is H_A and H_B respectively. Suppose that $|E_A\rangle$ and $|E_B\rangle$ are eigenbasis of H_A and H_B, then $|E_A\rangle \otimes |E_B\rangle$ is the eigenbasis of the total Hamiltonian $H_{AB} = H_A \otimes I + I \otimes H_B$. If there is a global quench operator $\hat{U}$, as before: $H_{AB} \longrightarrow \hat{U}^\dagger H_{AB} \hat{U} = H'$. In that case, the new eigenbasis is: $\hat{U}^\dagger(|E_A\rangle \otimes |E_B\rangle)$. If $\hat{U}$ is an entangler that transforms $|E_A\rangle \otimes |E_B\rangle$ into a entangled state, then the measurement operator $\hat{P} = U^\dagger(|E_A\rangle \otimes |E_B\rangle)(\langle E_A| \otimes \langle E_B|)\hat{U}$ of the second measurement in TPM becomes inseparable. And the system becomes completely inseparable, we can not write the total Hamiltonian as $H_{AB} = H_A \otimes I + I \otimes H_B$ anymore. There is only a total system S_{AB}. In that case, if we run the protocol for N times, there is not any difference between this process and the process we have calculated before except that the dimension of the new system is larger. The new equivalent quantum circuit is the same as in Figure.1. Thus to introduce entanglement to the protocol, there should be two conditions:
1. The protocol should make the total system a bipartite system. That is, the measurement operator $\hat{P}_{AB}$ should be in the form of $\hat{P}_{AB} = \hat{P}_A \otimes \hat{P}_B$. Otherwise, there is still only a single larger system and it is meaningless to consider the "entanglement" of a single closed system.
2. The protocol should be able to generate entanglement. Given an initial separable thermal state ρ^{th}_{AB}, there should be an operation that makes ρ^{th}_{AB} becomes an entangled state.
All these two conditions are to guarantee that there is entanglement in the system because our goal is to explore the entanglement signature of the FDR relation in the system. It has to be guaranteed that there is entanglement and the entanglement case should be compared with the separable case. Also, we want to consider the problem only under the TPM scheme. That is, the two measurements should be the projective measurement of the system Hamiltonian. Under all conditions above, we slightly generalized the protocol as:
1. The thermalization procedure (DTTs): this step is the same as before.
2. A unitary evolution of the state (DUTs): The quantum state evolute and becomes an entangled state. This is a new procedure to generate entanglement. Suppose that the Hamiltonian of systems S_A and S_B are H_A and H_B respectively. Then the total Hamiltonian is $H_A \otimes I + I \otimes H_B + H_{int}$. There is a small interaction term H_{int} and in this procedure that makes the thermal state ρ^{th} evolute to an entangled state.
3. Local quenches (DUQs and also DUTs): locally everything is the same as before: $H_A \longrightarrow \hat{U}^\dagger H_A \hat{U} = H'_A$ and $H_B \longrightarrow \hat{U}^\dagger H_B \hat{U} = H'_B$
Comparing the new protocol with the one before, there is one new step added. Obviously, the new protocol satisfies our two conditions and is still under the scheme of thermodynamics of discrete quantum processes[1]. This protocol is nothing but a generalization of the prior protocol proposed by Scandi et al (2020) [13]. With this protocol, it is possible to include entanglement in the process.

3.2.2 Detailed system set up

To simplify the calculation, we assume that the Hamiltonian of the two subsystems $H_A = H_B = H$ where H is the same Hamiltonian as the single qubit case of the coherence protocol and the same quench happens locally. That is, in the quench step:

$$\begin{aligned} H_A &\longrightarrow \hat{U}^\dagger H_A \hat{U} = H'_A \\ H_B &\longrightarrow \hat{U}^\dagger H_B \hat{U} = H'_B \end{aligned} \tag{36}$$

Here the operator of the unitary quench is:

$$\hat{U}^\dagger = \exp\left(-i(\Delta\theta/2)\hat{\sigma}_x\right) = \begin{pmatrix} \cos\frac{\Delta\theta}{2} & -\mathrm{i}\sin\frac{\Delta\theta}{2} \\ -\mathrm{i}\sin\frac{\Delta\theta}{2} & \cos\frac{\Delta\theta}{2} \end{pmatrix} \tag{37}$$

as before. The evolution operator in the second procedure is:

$$\hat{R} = \hat{R}_{xx}(\Delta t) = \exp\left(-\mathrm{i}(\Delta t/2)\hat{\sigma}_x \otimes \hat{\sigma}_x\right) \tag{38}$$

The operator has a new parameter Δt. This is to describe the evolution in the second procedure. We can write the matrix form of the operator as:

$$\hat{R}_{xx}(\Delta t) = \begin{pmatrix} \cos\left(\frac{\Delta t}{2}\right) & 0 & 0 & -\mathrm{i}\sin\left(\frac{\Delta t}{2}\right) \\ 0 & \cos\left(\frac{\Delta t}{2}\right) & -\mathrm{i}\sin\left(\frac{\Delta t}{2}\right) & 0 \\ 0 & -\mathrm{i}\sin\left(\frac{\Delta t}{2}\right) & \cos\left(\frac{\Delta t}{2}\right) & 0 \\ -\mathrm{i}\sin\left(\frac{\Delta t}{2}\right) & 0 & 0 & \cos\left(\frac{\Delta t}{2}\right) \end{pmatrix} \tag{39}$$

Again as before, the quench can be understood as a change of the basis. From this, each step is the same and can be understood as a circuit shown in Fig. 3. In the circuit model, ρ_A^{th} and ρ_B^{th} are just local thermal states and their matrix form are shown in Eq. (40).

$$\rho_A^{th} = \rho_B^{th} = e^{-\beta H} = \frac{1}{Z}\begin{pmatrix} 1 & 0 \\ 0 & e^{-\beta} \end{pmatrix} \tag{40}$$

In the new protocol, the probability of getting work ω in each step is:

$$P(\omega) = \sum_{E'_l - E^i_k = \omega} \langle E_k|\rho_i^{th}|E_k\rangle |\langle E_k|\hat{R}(\hat{U}^\dagger \otimes \hat{U}^\dagger)|E_l\rangle|^2 \tag{41}$$

In the two-qubit system, the set of eigenstates $\{|E_l\rangle\} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ with eigenenergies $0, 1, 1, 2$ respectively. R and $U^\dagger$ are already given before. With the probability

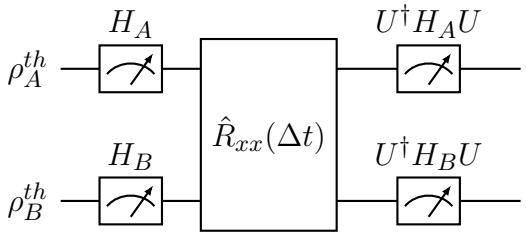

Figure 3: The equivalent quantum circuit corresponding to one step: the entanglement case.

distribution $P(\omega)$ we can again calculate the correction function Q as before.

3.2.3 Results

Before showing the result, we have to show that there is indeed entanglement generated. That is, we have to show that the negativity $\mathcal{N}(R(\rho_A^{th}\otimes\rho_B^{th})R^\dagger)>0$. The negativity is:

$$\mathcal{N}(R(\rho_A^{th}\otimes\rho_B^{th})R^\dagger)=\frac{|4e^b-2\sqrt{\left(e^{2b}-1\right)^2\sin^2(\Delta t)}|-4e^b+2\sqrt{\left(e^{2b}-1\right)^2\sin^2(\Delta t)}}{8\left(e^b+1\right)^2} \tag{42}$$

We can find that there is entanglement when the temperature is not too high. If $\Delta t=0$, there is no entanglement.
Then we can calculate the correction function Q_{AB}. Notice that the correction function $Q=\frac{\beta}{2}\mathrm{Var}(W)-(\langle W\rangle-\Delta F)$ can be decomposed as:

$$Q=\frac{\beta}{2}(\langle W^2\rangle-\langle W\rangle^2)-\langle W\rangle \tag{43}$$

since $\Delta F=0$ as discussed before. We have already written the distribution of work in Eq. (41), then we can write $\langle W^2\rangle=N\sum\omega^2P(\omega)$ and $\langle W\rangle=N\sum\omega P(\omega)$ since each step is identical.
To simplify the expression we use the small angle approximation and neglect the high-order term:

$$Q_{AB}=N\left\{\frac{(\Delta\theta)^2}{2}\left[\frac{\beta}{2}-\tanh(\beta/2)\right]+\frac{(\Delta t)^2}{2}\left[\beta\frac{1+e^{-2\beta}}{1+2e^{-\beta}+e^{-2\beta}}-\tanh(\beta/2)\right]\right\} \tag{44}$$

If we define a function $g(\beta)=\beta\frac{1+e^{-2\beta}}{1+2e^{-\beta}+e^{-2\beta}}-\tanh(\beta/2)$ and use the function $f(\beta)$ as

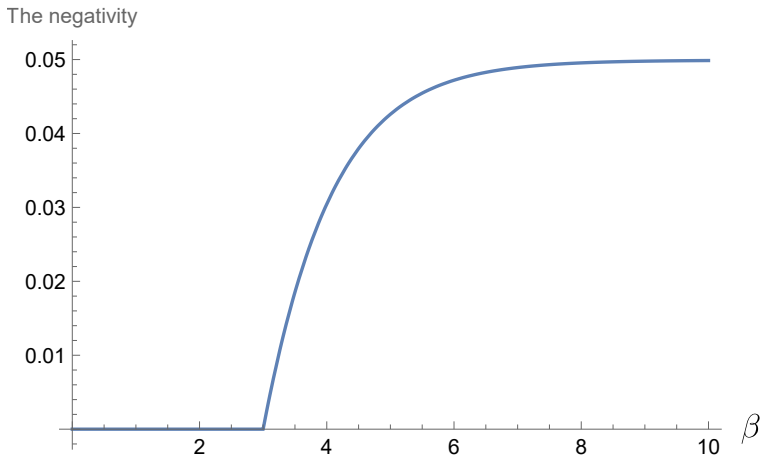

Figure 4: Plot of the negativity. β is the inverse temperature. Δt is setted to be 0.1. When the negativity is larger than 0 there is entanglement. There is a transition of negativity. One possible reason is, at very high temperatures (low β), the mixedness of the state is too high to generate entanglement [2].

before we can rewrite Q_{AB} as:

$$Q_{AB} = N\left[\frac{(\Delta\theta)^2}{2}f(\beta) + \frac{(\Delta t)^2}{2}g(\beta)\right] \tag{45}$$

Notice that when $\Delta t = 0$, we have:

$$Q_{AB} = 2Q = N\frac{(\Delta\theta)^2}{2}f(\beta) \tag{46}$$

where Q is the single qubit correction we get before. We can now easily find that when there is an entanglement operation R, there is an extra term $g(\beta)$ with parameter Δt in the correction function Q_{AB}.

3.3 FDR with Generalized two-qubit entangler

Our goal is to find the relation between entanglement and the correction Q of the FDR. In the last section, a unitary operator R_{xx} is chosen and we have found that R_{xx} is able to generate entanglement from the initial state $\rho_A^{th} \otimes \rho_B^{th}$. At the same time, if there is a unitary evolution R_{xx}, the correction Q_{AB} becomes larger. However, till now there is no direct connection found between the entanglement and the larger correction. In this section, we will try to reveal the connection. The approach is as follows: given an initial thermal state $\rho_A^{th} \otimes \rho_B^{th}$, we try to find all two-qubit unitary operators that transform the state into an entangled state. Then we can classify the set of all two-qubit unitary operators into two subsets, one can generate entanglement while the other can not. We choose different operators from these two subsets in the FDR protocol and compare the correction Q_{AB}. If it is found that operators from the entanglement subset are able to introduce more correction in the FDR protocol, a connection between entanglement and the FDR is discovered. Finally, we can conclude that there is a quantum signature caused by entanglement.

Theorem 1. The negativity $\mathcal{N}(\mathcal{O}(\rho_A^{th} \otimes \rho_B^{th})\mathcal{O}^\dagger) = 0$ if $c_1 - c_2 = 0$ where $\mathcal{O}$ is defined in Eq. (17) and ρ_A^{th}, ρ_B^{th} are defined in Eq. (40).

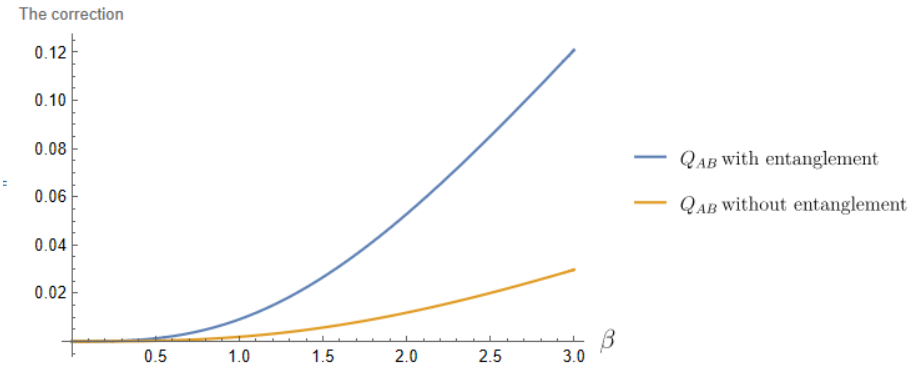

Figure 5: The plot of the correction function Q_{AB} when $N = 10$, $\Delta\theta = 0.1$. The parameter Δt is setted to be $\Delta t = 0.1$ or $\Delta t = 0$ for entangled and non-entangled case.

Proof. The negativity $\mathcal{N}(\mathcal{O}(\rho_A^{th} \otimes \rho_B^{th})\mathcal{O}^\dagger)$ is:

$$\max\left\{0, \frac{-2e^b + \sqrt{\left(e^{2b}-1\right)^2 \sin^2(2c_1 - 2c_2)}}{2\left(e^b+1\right)^2}\right\} \tag{47}$$

Obviously, the negativity is zero when $c_1 = c_2$ □

From the theorem above, we find two subsets of the two-qubit operators set $\mathbb{A}$, $\mathbb{B}$, and $\mathbb{C}$. $\mathbb{B}$ is the subset of all two-qubit unitary operators that satisfies $c_1, c_2, c_3 \neq 0$ when decomposing the operator into the form in Eq. (16). $\mathbb{C}$ is the subset of operators satisfies $c_1 = c_2$. Obviously, $\mathbb{C} \in \mathbb{B} \in \mathbb{A}$.

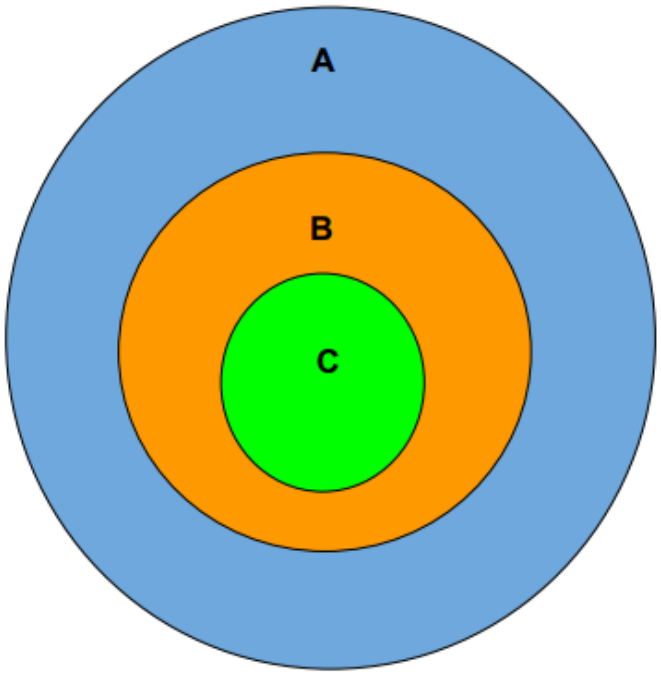

Figure 6: This graph shows the relationship between different two-qubit unitary operators. Region A represents all two-qubit unitary operators, B represents all ono-local two-qubit operators ($c_1, c_2, c_3 \neq 0$). Region C represents operators that can generate entanglement from $\rho_A^{th} \otimes \rho_B^{th}$ ($c_1 \neq c_2$), which is the starting thermal state in the protocol.

Now we replace the R_{xx} gate in the original entanglement protocol with a general two-qubit unitary operator and then observe if the unitary operators in subset $\mathbb{A}$ compared to those outside of $\mathbb{A}$ will have different effects on the correction function Q_{AB}. If operators that are able to bring entanglement to the system produce more correction to the FDR, we can conclude that we find a relation between entanglement and the correction of Q_{AB}. This is a quantum signature from entanglement.

3.3.1 Results

Due to the complexity of general two-qubit operators, we give a simplified analytical result here.
To simplify the problem, we only consider $\mathcal{O} = e^{-i(c_1\sigma_1\otimes\sigma_1+c_2\sigma_2\otimes\sigma_2+c_3\sigma_3\otimes\sigma_3)}$ here since other two-qubit operators are just its local equivalents. Again we use Eq. (41) where R is replaced by $\mathcal{O}$ here. Under the small angle approximation, we get:

$$Q_{AB} = N\left[\frac{(\Delta\theta)^2}{2}f(\beta) + 2(c_1 - c_2)^2 g(\beta)\right] \tag{48}$$

This can be derived simply the same way as the derivation of Eq. (44). The only difference is that we replace $\hat{R}$ in the Eq. (41) by $\mathcal{O} = e^{-\mathrm{i}(c_1\sigma_1\otimes\sigma_1+c_2\sigma_2\otimes\sigma_2+c_3\sigma_3\otimes\sigma_3)}$.
Obviously when $c_1 \neq c_2$, there is entanglement and there is an extra term in the correction function Q_{AB}. Numerical results comparing the $c_1 = c_2$ operators with the $c_1 \neq c_2$ operator are also shown.

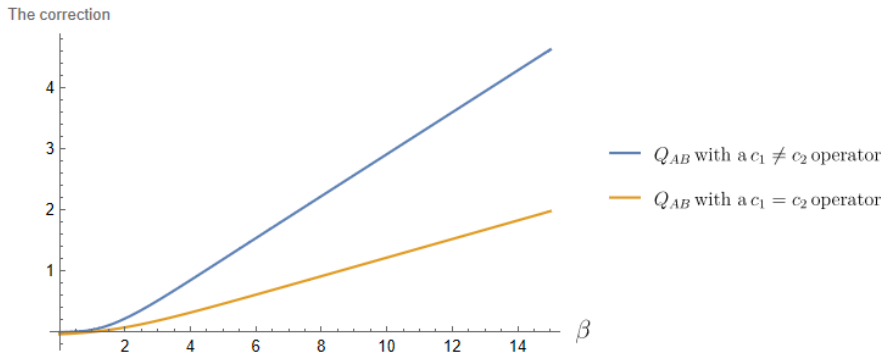

Figure 7: The plot of the correction function Q_{AB} when $N = 10$. To describe general two-qubit unitary operators, 15 parameters are needed. All parameters are set to be 0.1 except c_1. In the separable $c_1 = c_2$ case, c_1 is also set to be 0.1. In the entanglement $c_1 \neq c_2$ case, $c_1 = 0.2$. It can be found that the correction function Q_{AB} is larger in the entanglement case.

4 Conclusions

4.1 Discussion

Our results which are shown in Eq. (48) and Fig. 7 reveal the relation between entanglement and the correction of the FDR. As discussed before, when the entanglement operator is applied, an extra term appears in the correction function Q_{AB}. As a result, the correction Q_{AB} is larger when there is entanglement. From this, theoretically entanglement as a quantum signature is observed in the fluctuation-dissipation relation. It is interesting to discuss Eq. (48). This equation is the analytical result to show the correction function Q_{AB} in a two-qubit case. One should notice that when deriving the equation, we assume that the unitary evolution is $\mathcal{O} = e^{-\mathrm{i}(c_1\sigma_1\otimes\sigma_1+c_2\sigma_2\otimes\sigma_2+c_3\sigma_3\otimes\sigma_3)}$ However, this is not the most general two-qubit unitary operator. The most general two-qubit operator is:

$$\hat{O} = \left(\hat{A}_1 \otimes \hat{B}_1\right) e^{-\mathrm{i}(c_1\sigma_1\otimes\sigma_1+c_2\sigma_2\otimes\sigma_2+c_3\sigma_3\otimes\sigma_3)} \left(\hat{A}_2 \otimes \hat{B}_2\right)$$

This special choice is to simplify the expression of Q_{AB}. A general level of generality has been maintained in the choice since the interaction unitary operator $\mathcal{O} = e^{-\mathrm{i}(c_1\sigma_1\otimes\sigma_1+c_2\sigma_2\otimes\sigma_2+c_3\sigma_3\otimes\sigma_3)}$ describe all interaction content of a two-qubit unitary operator and two-qubit unitary operators are locally equivalent when they have the same parameters c_1, c_2, c_3 as proposed in [5]. Our goal is to study the effect of entanglement in the FDR. Thus we are only interested in the interaction of the two subsystems. That is an argument to discuss the validity of only choosing $\mathcal{O}$ to calculate the analytical result of Q_{AB}.
There is also a further discussion on the analytical result of Q_{AB}. One can easily find that when there is no entanglement ($c_1 = c_2$), the correction function Q_{AB} is:

$$Q_{AB} = N\left[\frac{(\Delta\theta)^2}{2} f(\beta)\right] \tag{49}$$

This is just two times the single-qubit correction of the FDR in the coherence protocol as shown in Eq. (35). Also one should notice that if we delete the interaction evolution of the two subsystems, the system is just two copies of the single-qubit coherence system. In conclusion, if there is no entanglement, we can not find any detail of the interaction of the two subsystems from the fluctuation-dissipation relation. This observation emphasizes our conclusion that the quantum signature of entanglement is observed from the FDR. Suppose that we apply a non-entanglement interaction unitary operator: $\mathcal{O} = e^{-\mathrm{i}(c(\sigma_1\otimes\sigma_1+\sigma_2\otimes\sigma_2)+c_3\sigma_3\otimes\sigma_3)}$ where c is an real number. In that case, we can not observe any extra correction of the FDR. The reason is that this interaction operation is not an entanglement operation. This kind of operation will not violate the FDR.
To reach the final result, we have developed a general method to study entanglement in the work FDR. First, we generalize the protocol to include a unitary evolution. This is to entangle the quantum state. Then to compare with the separable system we prove that in our case, all two-qubit unitary evolution can be divided into two sets: entanglement evolution and non-entanglement evolution. Then we find that there is an extra correction of the FDR only if an entanglement evolution is applied.

4.2 Outlook

In this work, we have only studied a two-qubit system. However, as discussed above, the method developed in the thesis can be used to analyze arbitrary systems. However, due to the limitation of our knowledge of mixed-state entanglement, it is not easy to generalize our results to arbitrary bipartite quantum systems. First, to generalize the result, we need a criterion to determine whether a mixed quantum state is separable or not. However, the Peres–Horodecki criterion we have used is only valid for 2×2 or 2×3 systems. Also, it is not easy to find the decomposition of the unitary operator as proposed in Eq.(16) in larger systems. Generally, it is still an open question to find entanglers in larger systems [3].

Throughout the discussion, we are always under the scheme of the two-point measurement scheme as discussed in [17]. This measurement scheme could also be changed to study the fluctuation of work [10].

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