Measurement-based Formulation of Quantum Heat Engine and Optimal Efficiency with Finite-Size Effect

Hiroyasu Tajima$^{1}$ and Masahito Hayashi$^{2,3}$

$^{1}$RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan
$^{2}$Graduate School of Mathematics, Nagoya University, Nagoya 464-0814
$^{3}$Centre for Quantum Technology, National University of Singapore, Singapore 117543

There exist two formulations for quantum heat engine. One is semi-classical scenario, and the other is full quantum scenario. The former is formulated as a unitary evolution for the internal system, and is adopted by the community of statistical mechanics. In the latter, the whole process is formulated as unitary. It was adopted by the community of quantum information. However, their formulation does not consider measurement process. In particular, the former formulation does not work when the amount of extracted work is observed. In this paper, we formulate the quantum heat engine as the measurement process because the amount of extracted work should be observed in a practical situation. Then, we clarify the contradiction of the former formulation by using a novel trade-off relation. Next, based on our formulation, we derive the optimal efficiency of quantum heat engines with the finite-size heat baths, without assuming the existence of quasi-static processes. That is, we asymptotically expand the optimal efficiency up to the third order when we extract work from the pair of hot and cold baths. The first term is shown to be Carnot efficiency. We also investigate the effect by finiteness of the resources by classifying it into two types.

I. INTRODUCTION

Thermodynamics started as a study that clarifies the upper limit of the efficiency of macroscopic heat engines [1] and has become a huge realm of science which covers from electric batteries [2] to black holes [3]. Today, with the development of experimental techniques, the studies of thermodynamics are reaching a new phase. The development of experimental techniques is realizing micro-machines in laboratories [4–6], and is clarifying the functions of bio-moleculars which are micro-machines in nature [7]. We cannot apply the standard thermodynamics to these small-size heat engines as it is, because it is a phenomenology for macroscopic systems. Therefore, we need a general theory to give the limit of the performance of these small-size heat engines, i.e., thermodynamics for small-size systems.

The thermodynamical features of small-size heat engines have been studied by the statistical-mechanical approachs, in which we formulate a heat engine as a crowd of particles, and analyze it [8–41]. The statistical rederivation of thermodynamical inequalities in macroscopic limit [8, 9, 13], thermodynamic laws for processes with measurement and feedback [14–20, 24–34] that is adopted by the community of statistical mechanics and the fully quantum scenario [12, 13, 35–41] that is adopted by the community of quantum information. In the semi-classical scenario, the heat engine and the heat baths evolves in time unitarily, under a time-dependent Hamiltonian which is controlled by the classical external system. In the fully quantum scenario, the heat engine, the heat baths and the quantum external system time evolutes unitarily such that the energy of total system conserves. Whereas it has been expected that the fully quantum scenario converges to the semi-classical scenario in a proper approximation, neither the proof nor the counterproof for the expectation has been given.

The formulation of work extraction from quantum systems The concept of the work extraction from the quantum systems is very subtle, and no consensus has been reached [43]. The previous researches on quantum systems [2, 13, 26, 33, 37–41] have been formulated in various ways, and the relationship among the formulations has not been sufficiently discussed. The formulations of the researches are roughly classified in the semi-classical scenario [2, 13, 26, 33] that was adopted by the community of statistical mechanics and the fully quantum scenario [12, 13, 35–41] that is adopted by the community of quantum information. In the semi-classical scenario, the heat engine and the heat baths evolves in time unitarily, under a time-dependent Hamiltonian which is controlled by the classical external system. In the fully quantum scenario, the heat engine, the heat baths and the quantum external system time evolutes unitarily such that the energy of total system conserves. Whereas it has been expected that the fully quantum scenario converges to the semi-classical scenario in a proper approximation, neither the proof nor the counterproof for the expectation has been given.

The quantitative understanding of thermodynamical laws in the mesoscopic scale There is no quantitative understanding of thermodynamic laws in mesoscopic systems, i.e., the systems whose number of particle is not so small but finite. Although the above experiments can be regarded as realizations of heat engine in mesoscopic systems, no theoretical study has sufficiently discussed thermodynamic laws in mesoscopic systems.

The finite-size effect of the heat baths Previous researches treat only the finiteness of working body, and do not treat the finiteness of the heat baths. For the small-size heat engines, the finiteness of the heat baths is not negligible, because the small working body might touch a small number of heat-bath particles. However, there were no quantitative understanding about the effects of finite-size heat baths on the thermodynamic laws.

In the present article, we establish a general formation of the quantum heat engines on quantum measurement theory [43, 44], and give the optimal efficiency of the heat engines with finite-size heat baths that are in mesoscopic scale by using the strong large
deviation theory \[45, 46\]. First, we formulate the work extraction from the quantum internal system as a measurement process without considering thermodynamical limit. As a minimal request for the quantum engine, we demand that there exists some equipment to assess the amount of the extracted work, and formulate an arbitrary heat engine which satisfies the requirement as a quantum measurement process. Our formulation includes the previous formulations of the full-quantum scenario as a special case, i.e., indirect measurement process. We also give a mapping from our formulation to the formulation of classical work extraction \[8, 20–25\] and show that our formulation is a natural generalization of the classical work extraction. Moreover, we derive two remarkable trade-off relations between information gain for knowing the amount of extracted work and the maintained coherence of the thermodynamic system during the work extraction process. These trade-off relations clarify that we can hardly know the amount of the extracted work when the time evolution of the internal system is close to unitary.

Second, we propose a novel method for quantitatively clarifying how the thermodynamic laws changes from the mesoscopic scale to the thermodynamical limit, with considering finite-size effect of the heat baths. As a typical topic, we extend Carnot’s theorem to the heat engines with finite-size heat baths. That is, we microscopically discuss the optimal efficiency of finite-size heat engines with hot and cold heat baths when the heat baths consist of \(n\) particles that are identical and uncorrelated. Using the information geometrical structure \[54\], we derive its upper bound, and asymptotically expand it in terms of \(q_n \approx Q_n/n\) when \(Q_n\) is the extracted heat from the hot heat bath. Then, we construct a specific work extraction as a concrete unitary transformation of the whole system. Employing the strong large deviation theory \[45, 46\], we show that the efficiency asymptotically coincides with the upper bound up to the term of the third order \(q_n^3\). The energy extracted by the optimal work extraction is extremely ordered energy, i.e., the entropy gain of the work storage is so negligibly small as compared with the energy gain of the work storage. We give the asymptotic expansion of the optimal efficiency without the assumption of the quasi-static process. Therefore, our result enables us to evaluate accuracy of the prediction of thermodynamics in the finite-particle systems from the statistical mechanic viewpoint. The prediction of thermodynamics for the optimal efficiency is accurate up to the order of \(Q_n^2/n^2\).

The remaining parts of this paper will be organized as follows. This paper mainly consists of two parts. The first part consists of Sections [11] and the second part consists of Sections [12][XIV]. The first part is devoted to the measurement-based formulation of quantum heat engine. Based on the formulation, the second part discusses the efficiency with finite-size effect. Technical lemmas and theorem are proven in Appendix. Since the structures of these parts are not so simple, we outline them in Section [11].

### II. OUTLINE

#### A. Formulation of work extraction process

There exist two well-known scenarios for the work extraction from quantum systems:

**Semi-classical scenario** \([12, 13, 35, 37–41]\): In this scenario, the classical external operation realizes the unitary time evolution

\[ U_I := T_e \exp \int -iH_I(t) dt \] on \(I\) by time-dependently controlling the control parameter of the Hamiltonian \(\hat{H}_I(t)\) of the internal system \(I\) (which usually consists of the system \(S\) and the heat bath \(B\)). During the time evolution, the loss of energy in the internal system is transmitted to the external controller through the back reaction of the control parameter. So, the energy loss is regarded as the extracted work \([9, Section 2]\). This scenario is considered as a natural quantum extension of Jarzynski’s formulation \([8]\).

**Fully quantum scenario** \([12, 13, 35, 37–41]\) This scenario considers not only the internal system \(I\) but also the external system \(E\), whose Hilbert spaces are \(\mathcal{H}_I\) and \(\mathcal{H}_E\), respectively. We perform an arbitrary unitary transformation \(U_{IE}\) on the total system \(IE\) which conserves the energy of the total system \(IE\), and regard the energy gain of \(E\) as the extracted work.

Both of the above two scenarios are persuasive. However, there exists a contradiction between them. For an arbitrary unitary transformation \(U_{IE}\) and an arbitrary fixed initial state \(\rho_E\) of the external system \(E\), the true time evolution of the internal system \(I\) is given by

\[ \Lambda_I(\rho_I) = \text{Tr}_E[U_{IE}\rho_I \otimes \rho_E U_{IE}^\dagger], \] (1)

where \(\rho_I\) is an arbitrary initial state of the internal system. According to the semi-classical scenario, the time evolution of the internal system is the unitary \(U_I\). In order that \(\Lambda_I(\rho_I) = U_I \rho_I U_I^\dagger\), the unitary \(U_{IE}\) should be written as \(U_I \otimes V_E\), where \(V_E\) is a unitary transformation on \(E\). However, such a unitary does not cause the energy transfer between \(I\) and \(E\), because \(U_I \otimes V_E\) means that \(I\) and \(E\) are detached.

The usual explanation for this contradiction is as follows: the unitary \(U_I\) is just an approximation of the true time evolution of \(I\); namely, \(U_I \rho_I U_I^\dagger \approx \Lambda_I(\rho_I)\) for an arbitrary state \(\rho_I\). If \(E\) is large enough, there might be a suitable Hilbert space \(\mathcal{H}_E\), a suitable Hamiltonian \(\hat{H}_E\) of \(E\), a suitable initial state \(\rho_E\) of \(E\), and a suitable unitary operation \(V_{IE}\) on \(IE\) such that the total energy is conserved and \(U_I \rho_I U_I^\dagger \approx \Lambda_I(\rho_I)\) is satisfied at the same time. If such a tuple \((\mathcal{H}_E, \hat{H}_E, V_{IE}, \rho_E)\) exists, we can
regard the energy loss of $I$ as the extracted work, because the energy loss of $I$ is equal to the energy gain of $E$ for an arbitrary initial state of $I$.

The above explanation sounds persuasive. However, we pose two questions for the explanation;

**Question 1:** Does such a tuple $(\mathcal{H}_E, \hat{H}_E, V_I E, \rho_E)$ really exist? 

**Question 2:** Does such a tuple $(\mathcal{H}_E, \hat{H}_E, V_I E, \rho_E)$ really satisfy the following two conditions simultaneously?

- **Approximation:** The true dynamics $\Lambda_I$ well approximates the internal unitary $U_I$.
- **Measurability:** We can know the amount of the extracted work precisely by measuring the external system $E$.

The answer to Question 1 is Yes. That is, there exists a tuple $(\mathcal{H}_E, \hat{H}_E, V_I E, \rho_E)$ satisfying energy conservation law and Approximation. However, the answer to Question 2 is No. That is, it is possible to realize a tuple $(\mathcal{H}_E, \hat{H}_E, V_I E, \rho_E)$ that satisfies only one of two conditions, Approximation and Measurability. To overcome this problem, one might consider more general framework to consider the following question instead of Question 2.

**Question 3:** Does exist a device satisfying the following two conditions simultaneously?

- **Approximation:** The true dynamics well approximates the internal unitary $U_I$.
- **Measurability:** We can know the amount of the extracted work precisely by using the device.

The difference from Question 2 is the following. In Question 2, we need to discuss the quantum system $\mathcal{H}_E$. However, in Question 3, it is enough to discuss a classical outcome that describes the amount of the extracted work. Indeed, in the real heat engine, it is hard to identify the external quantum system although it has a quantum internal part. For example, battery has the fuel part, which can be regarded as the quantum internal part. Even though it is impossible to identify the external quantum system, in the real heat engine, we can identify the amount of extracted work, which can be regarded as the measurement outcome. Hence, in this case, the heat engine can be regarded as the measurement instrument, which describes the time evolution of the internal system according to the measurement outcome $\hat{I}$. That is, to justify the semi-classical scenario, it is enough to realize a device satisfying both conditions in the sense of Question 3. So, to examine the semi-classical scenario, we need to answer Question 3. For this purpose, we give a formulation for work extraction by using the concept of instrument as Definition 1 in Section III. Since the instrument is mathematically given as a set of CP maps (completely positive maps), it is called CP-work extraction. Under this frame work, we consider several kinds of energy conservation laws (Definitions 2, 4 and 5). In Section IV, we combine the existing full quantum scenario and measurement of the Hamiltonian $\hat{H}_E$ in the external system $\mathcal{H}_E$, which is defined as FQ-work extraction in Definition 6. We discuss the relations between CP-work extraction and FQ-work extraction (Lemmas 9, 10, 11, and 12). Then, Section V addresses the above questions. Subsections VA and VB give the formulation for Approximation and Measurability, respectively. In Subsection VC to investigate Question 2, we derive trade-off relations between Approximation and Measurability in the framework of FQ-work extraction as Theorems 2 and 3. These trade-off relations show that the answer to Question 2 is No. That is, there does not exist a tuple $(\mathcal{H}_E, \hat{H}_E, V_I E, \rho_E)$ satisfying Approximation and Measurability. However, in Subsection VD we construct a tuple $(\mathcal{H}_E, \hat{H}_E, V_I E, \rho_E)$ satisfying the energy conservation law and Approximation. Further, in Subsection VE employing the relation between CP-work extraction and FQ-work extraction, we derive trade-off relations between Approximation and Measurability in the framework of CP-work extraction as Corollaries 1 and 2. These trade-off relations imply that the answer to Question 3 is also No. Even in the framework of CP-work extraction, it is impossible to satisfy Approximation and Measurability simultaneously.

These discussions seem to completely deny the semi-classical scenario. However, it is possible to partially rescue the semi-classical scenario in the following sense. In the semi-classical scenario, when the work extraction corresponds to the internal unitary $U_I$, the amount of extracted work is $\text{Tr} \rho_I \hat{H}_I - \text{Tr} U_I \rho_I U_I^\dagger \hat{H}_I$. Although there does not exist a heat engine simulating the internal unitary $U_I$ in the above sense, Subsection VB shows that there exists an FQ-work extraction, in which, the average amount of extracted work is $\text{Tr} \rho_I \hat{H}_I - \text{Tr} U_I \rho_I U_I^\dagger \hat{H}_I$. That is, Lemma 8 in Subsection VB gives a canonical one-to-one correspondence between the unitary of the total system and the internal unitary $U_I$ the above condition. Using the correspondence, we can rescue the semi-classical scenario in the above sense. However, in this case, the true dynamics is far from the internal unitary. Hence, if we discuss the coherence of the internal unitary $U_I$ under the semi-classical scenario, this type correspondence does not work.

Here, we should remark that these quantum setups cannot derive all of properties of heat engines in the thermodynamics because some of properties of heat engines in the thermodynamics root in the thermodynamic limit. That is, it is not unnatural that these quantum setups have several properties different from those of heat engines in the thermodynamics. For example, in these quantum setups, the amount of extracted work has non-zero entropy. However, we think that the entropy vanishing of extracted work should hold only with the thermodynamic limit. In fact, as mentioned in the next subsection, that entropy vanishing is shown with the thermodynamic limit.
Indeed, the validity of these quantum setups cannot be discussed only from the viewpoint of the consistency with the thermodynamics. Although the consistency with the thermodynamics is one of importance piece, this discussion requires the property of quantum theory. Our discussion is deeply based on the formulation of quantum theory.

B. Optimal efficiency with finite size system

In the second part, we discuss how can we recover thermodynamics with the thermodynamical limit. For this purpose, we discuss the optimal efficiency for the quantum heat engine when the internal system consists of hot and cold baths or it consists of hot and cold baths and a catalyst, which is often called a working body. In this case, the efficiency is defined as the ratio between the amount of extracted work and the energy loss in the hot bath, which is often called the endothermic energy. Hence, the efficiency is defined for a pair of an CP-work extraction and an initial state of the internal system. For a given initial state of the internal system, we define the optimal efficiency to be the maximum efficiency among possible CP-work extractions.

To recover the Carnot theorem, we consider \( n \)-fold tensor product states as the initial states in the hot and cold baths. Taking the limit \( n \to \infty \), i.e., the thermodynamical limit, we show that the optimal efficiency approaches the Carnot efficiency. This argument can be considered as a refinement of the Carnot theorem. We also derive higher order terms in the optimal efficiency by considering the asymptotic expansion of the optimal efficiency. These higher order terms reflect the effect of finiteness of the sizes of hot and cold baths. Their coefficients contain the energy variance and the skewness of the energy of both baths. Further, we discuss these finite-size effects by classifying them into two types.

Surprisingly, these results have a deep relation with classical model for heat engine. Indeed, these results are derived via the analysis of classical model for heat engine. Hence, to discuss these issues, we firstly prepare classical work extraction model in Subsection VII A. Then, Subsection VIII B explain the relation between classical work extractions and quantum work extractions, which is a key point for our analysis of the optimal efficiency.

Next, Subsection VII A proceeds to the optimal efficiency when the internal system consists of hot and cold baths. In this setup, the quantum setting can be reduced to the classical setting. However, this setup does not take into account the effect of a catalyst. To resolve this problem, Subsection VII B formulates the optimal efficiency when the internal system contains hot and cold baths as well as a catalyst. Under this general setup, we derive general upper bound for the optimal efficiency by using quantum information geometrical structure [54] (Theorem 5). Next, Subsection VIII A focuses on the case when the initial states in the hot and cold baths are given as \( n \)-fold tensor product states. Then, asymptotically expand the general upper bound (Theorem 6), which shows the impossibility to exceed the Carnot efficiency. To show the achievability for the bound, we recall the relation between the quantum and classical work extractions with no catalyst. We firstly show the achievability with the corresponding classical model (Theorem 7). Then, employing this relation, we show the achievability of the Carnot efficiency for the quantum setting (Theorem 8).

The first part of Subsection VIII B gives the sequence of classical work extractions that attains the optimal rate. Then, the second part of Subsection VIII B gives the sequence of FQ-work extractions that attains the optimal rate by using the preceding classical work extractions. We discuss the physical structure of the FQ-work extractions.

Finally, Section XIII address the finite-size effects by introducing two types of finiteness; One is the finiteness of the ratio between the number of particles and the amount of extracted work. The other is the finiteness of the number of particles. Although the former can be discussed in the framework of thermodynamics, the latter cannot be discussed in the framework of thermodynamics and can be only in the statistical-mechanical framework. Considering this classification, we explain the novelty of our evaluation in comparison with thermodynamics. The remaining sections are devoted to the derivation of important theorems in Subsections VII B and VIII A. Section XIV derives the general upper bound for optimal efficiency, which is valid even with a catalyst. Section XI introduces several helpful formulas for cumulant generation function, which is closely related to geometrical structure. By using the formulas given in Section XI, Section XII derives the asymptotic expansion of the upper bound under the \( n \)-fold tensor product structure.

Section XIII gives the asymptotic expansion of the efficiency of the classical work extraction given in Subsection VIII B. For this expansion, we need to calculate the relative entropy between two close distributions. Indeed, these two distribution are so close to each other that we cannot use conventional methods in information theory and quantum information theory. To resolve this problem, we employ strong large deviation by Bahadur and Rao [45, 64], which enables us to evaluate the tail probability more precisely than conventional large deviation. This method was applied in the recent papers [70, 71] in quantum information. Using this method, Section XIV gives the required expansion of the relative entropy.

III. WORK EXTRACTION AS A MEASUREMENT PROCESS

Here, we consider the heat engine, in which, the internal system is a collection of microscopic systems and the meter system is a macroscopic system, which can be regarded the output system of the heat engine. For example, fuel battery has the fuel cells as the internal system and the motor system as the meter system. Hence, as the internal system, we consider a quantum
system I, whose Hilbert spaces is $\mathcal{H}_I$. We refer to the Hamiltonian of I as $\hat{H}_I$. The internal system I usually consists of the thermodynamical system $S$ and the heat baths $\{B_m\}_{m=1}^M$, but we do not discuss such a detail structure of the internal system $I$ here. Let us formulate the work extraction from $I$. Then, we assume that the amount of the work is indicated by a meter. (Fig. 1)

In other words, we assume that we have an equipment to assess the amount of the extracted work, and that the equipment assess the work at $w_j$ with the probability $p_j$. In quantum mechanics, such a process that determines an assessed value $a_j$ with the probability $p_j$ is generally described as a measurement process. Thus, we formulate the work extraction from the quantum system as a measurement process. As the minimal requirement, we demand that the average of $w_j$ is equal to the average energy loss of $I$ during the measurement;

\begin{align}
\text{Definition 1 (CP-work extraction)} \quad & \text{Let us take an arbitrary set of a CP-instrument}\ \{\mathcal{E}_j\}_{j \in J}\ \text{and measured values}\ \{w_j\}_{j \in J}
\text{satisfying the following conditions; (1) each } \mathcal{E}_j \text{ is a completely positive (CP) map, (2) } \sum_j \mathcal{E}_j \text{ is a completely positive and trace preserving (CPTP) map, and (3) } J \text{ is the set of the outcome, which can be either a discrete set or a continuous set. When the set } \{\mathcal{E}_j, w_j\}_{j \in J} \text{ satisfy the above condition, we refer to the set } \{\mathcal{E}_j, w_j\}_{j \in J} \text{ as a CP-work extraction.}
\end{align}

Here, we note that the measurement process $\{\mathcal{E}_j\}$ is not necessarily the measurement of the Hamiltonian of the internal system. Since the heat engine need to satisfy the conservation law of energy, we consider the following energy conservation laws for a CP-work extraction $\{\mathcal{E}_j, w_j\}_{j \in J}$. Firstly, we consider the weakest condition.

\begin{align}
\text{Definition 2 (Level-1 energy conservation law)} \quad & \text{The following condition for a CP-work extraction } \{\mathcal{E}_j, w_j\}_{j \in J} \text{ is called the level-1 energy conservation law. Any state } \rho_I \text{ on } \mathcal{H}_I \text{satisfies}
\end{align}

$\text{Tr} \hat{H}_I \rho_I = \sum_j w_j \text{Tr} \mathcal{E}_j(\rho_I) + \sum_j \text{Tr} \hat{H}_I \mathcal{E}_j(\rho_I),$ (2)

where $\hat{H}_I$ is the Hamiltonian of $I$.

Since the level-1 energy conservation law is too weak, as explained latter, we introduce stronger conditions with an orthonormal basis $\{|x\rangle\}_x$ of $\mathcal{H}_I$ such that $|x\rangle$ is an eigenstate of the Hamiltonian $\hat{H}_I$ associated with the eigenvalue $h_x$. For this purpose, we introduce the spectral decomposition of $\hat{H}_I$ as $\hat{H}_I = \sum_h h P_h$, where $P_h$ is the projection to the energy eigenspace of $\hat{H}_I$ whose eigenvalue is $h$.

\begin{align}
\text{Definition 3 (Level-4 energy conservation law)} \quad & \text{A CP-work extraction } \{\mathcal{E}_j, w_j\}_{j \in J} \text{ is called a level-4 CP-work extraction when}
\end{align}

$\mathcal{E}_j(|x\rangle\langle x|) = P_{h_x - w_j} \mathcal{E}_j(|x\rangle\langle x|) P_{h_x - w_j}$ (3)

\begin{align}
\text{for any initial eigenstate } |x\rangle. \text{ The condition is called the level-4 energy conservation law.}
\end{align}

The meaning of (3) is that the resultant state $\frac{1}{\sqrt{\sum_j \mathcal{E}_j(|x\rangle\langle x|)}} \mathcal{E}_j(|x\rangle\langle x|)$ must be an energy eigenstate with energy $h_x - w_j$ because the remaining energy in the internal system is $h_x - w_j$. That is, the level-4 energy conservation law requires the conservation of energy for every possible outcome $j$. To characterize this constraint from another viewpoint, we introduce intermediate conditions between the level-1 and level-4 energy conservation laws.

\begin{align}
\text{Definition 4 (Level-2 and 3 energy conservation laws)} \quad & \text{Here, we introduce two energy conservation laws for a CP-work extraction } \{\mathcal{E}_j, w_j\}_{j \in J} \text{ when the level-1 energy conservation law holds. Let the initial state on } I \text{ to be an eigenstate } |x\rangle. \text{ After the CP-work extraction } \{\mathcal{E}_j, w_j\}_{j \in J}, \text{ we perform the measurement of } \{|y\rangle\langle y|\} \text{ to the resultant system } \mathcal{H}_I. \text{ Then, we obtain the joint distribution } P_{JY|X}(j, y|x) \text{ of the two outcomes } j \text{ and } y \text{ as follows.}
\end{align}

$P_{JY|X}(j, y|x) = \langle y| \mathcal{E}_j(|x\rangle\langle x|)|y\rangle$. (4)
Then, we introduce the random variable $K := h_x - h_y - w_j$ that describes the difference between the loss of energy and the extracted energy. So, we define the two distributions

$$P_{K|X}(k|x) := \sum_{j, y; h_y - w_j = k} P_{JY|X}(j, y|x)$$

(5)

$$P_{K|YX}(k|y, x) := \sum_{j; h_x - h_y - w_j = k} P_{J|YX}(j|y, x)$$

(6)

where

$$P_{J|YX}(j|y, x) := \frac{P_{JY|X}(j, y|x)}{\sum_j P_{JY|X}(j', y|x)}.$$  

(7)

When the distribution $P_{K|X=x}$ does not depend on the initial eigenstate $|x\rangle$, the CP-work extraction $\{\mathcal{E}_j, w_j\}_{j \in J}$ is called a level-2 CP-work extraction. Similarly, when the distribution $P_{K|Y=y, X=x}$ does not depend on the pair $(x, y)$, the CP-work extraction $\{\mathcal{E}_j, w_j\}_{j \in J}$ is called a level-3 CP-work extraction. These conditions are called the level-2 and 3 energy conservation laws.

Then, the level-4 energy conservation law can be characterized in terms of the distribution $P_{K|X}$. That is, a CP-work extraction $\{\mathcal{E}_j, w_j\}_{j \in \mathcal{J}}$ is a level-4 CP-work extraction if and only if

$$P_{K|X}(k|x) = \delta_{k, 0}$$

for any initial eigenstate $|x\rangle$. So, we find that the level-4 energy conservation law is stronger than the level-3 energy conservation law. To investigate the property of a level-4 CP-work extraction, we employ the pinching $\mathcal{P}_{\hat{H}_I}$ of the Hamiltonian $\hat{H}_I = \sum_h h H_p$ as

$$\mathcal{P}_{\hat{H}_I}(\rho) := \sum_h P_h \rho P_h.$$ 

(9)

**Lemma 1** A level-4 CP-work extraction $\{\mathcal{E}_j, w_j\}_{j \in \mathcal{J}}$ satisfies that

$$\mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\rho)) = \mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\mathcal{P}_{\hat{H}_I}(\rho))) = \mathcal{E}_j(\mathcal{P}_{\hat{H}_I}(\rho)).$$

(10)

That is, when we perform a measurement of the observable commuting the Hamiltonian $\hat{H}_I$ after any level-4 CP-work extraction, the initial state $\mathcal{P}_{\hat{H}_I}(\rho)$ has the same behavior as the original state $\rho$.

If we measure the Hamiltonian $\hat{H}_I$, we have the same result even if we apply the pinching $\mathcal{P}_{\hat{H}_I}$ before the measurement of the Hamiltonian $\hat{H}_I$. Thus, due to Lemma 1, if we measure the Hamiltonian $\hat{H}_I$ after a level-4 work extraction $\{\mathcal{E}_j, w_j\}_{j \in \mathcal{J}}$, we have the same result even if we apply the pinching $\mathcal{P}_{\hat{H}_I}$ before the level-4 work extraction $\{\mathcal{E}_j, w_j\}_{j \in \mathcal{J}}$.

**Proof:** We employ Kraus representation $\{A_{j,l}\}$ of $\mathcal{E}_j$ as

$$\mathcal{E}_j(\rho) = \sum_l A_{j,l} \rho A_{j,l}^\dagger.$$  

(11)

Then, due to the condition (3), $A_{j,l}$ has the following form

$$A_{j,l} = \sum_h A_{j,l,h},$$

(12)

where $A_{j,l,h}$ is a map from $\text{Im} P_h$ to $\text{Im} P_{h-w_j}$ and $\text{Im} P_h$ is the image of $P_h$. Thus,

$$P_h \mathcal{E}_j(\rho) P_h = \mathcal{E}_j(P_{h+w_j} \rho P_{h+w_j}) = P_h \mathcal{E}_j(P_{h+w_j} \rho P_{h+w_j}) P_h.$$  

(13)

Taking the sum for $h$, we obtain (10).

Note that an arbitrary Gibbs state of a quantum system commutes the Hamiltonian of the quantum system. Thus, when the internal system $I$ consists of the systems in Gibbs states, a level-4 CP-strong work extraction tells the energy loss of $I$ without error.

We also consider the following condition for a CP-work extraction.
Definition 5 (CP-unital work extraction) Let us take a CP-work extraction \( \{ E_j, w_j \}_{j \in J} \). When the CPTP-map \( \sum_j E_j \) is unital, namely the equation

\[
\sum_j E_j(\hat{1}_I) = \hat{1}_I
\]

holds, we refer to the CP-work extraction \( \{ E_j, w_j \}_{j \in J} \) as the CP-unital work extraction.

Because an arbitrary unital map does not decrease the von Neumann entropy \( [56] \), the CP-unital work extraction corresponds to the class of work extractions which do not decrease the entropy of \( I \). That is, an arbitrary \( \rho_I \) satisfies

\[
\Delta S_I := S\left( \sum_j E_j(\rho_I) \right) - S(\rho_I) \geq 0,
\]

where \( S(\rho) := \text{Tr}[\rho \log \rho] \).

In contrast, we have the following characterization for entropy of output random variable.

Lemma 2 Let \( \{ E_j, w_j \}_{j \in J} \) be a level-4 work extraction. We denote the random variable describing the amount of extracted work by \( W \). Then, the entropy of \( W \) is evaluated as

\[
S(W) \leq 2 \log N,
\]

where \( N \) is the number of eigenvalues of the Hamiltonian \( \hat{H}_I \) in the internal system.

Note that the evaluation (16) holds for any initial state \( \rho_I \) of the internal system.

Proof: Due to the condition for a level-4 work extraction, for a possible \( w_j \), there exist eigenstates \( x \) and \( x' \) such that \( w_j = h_x - h_{x'} \). Hence, the number of possible \( w_j \) is less than \( N^2 \). Thus, we obtain (16).

When a CP-work extraction is level-4 as well as unital, we refer to it as a standard CP-work extraction for convenience of description. We illustrate a Venn diagram of the CP-work extractions. (Fig. 2) Unfortunately, we cannot discuss the validity of these conditions for our CP-work extraction under the current setup. In the next section, to clarify the validity of these conditions, we discuss the unitary dynamics of heat engine.

IV. FULLY QUANTUM WORK EXTRACTION

A. General case

Next, we consider the unitary dynamics of the heat engine between the internal system \( I \) and the external system \( E \) which storages the extracted work from \( I \) as the existing studies \([12, 13, 35, 37, 41]\). Here, the internal system \( I \) is assumed to interact
only with \( E \), and the external system \( E \) is described by the Hilbert space \( \mathcal{H}_E \) and has the Hamiltonian \( \hat{H}_E \). In the relation with the CP-work extraction model, this type description of heat engine is given as an indirect measurement process that consists of the following two steps [44]. The first step is the unitary time evolution \( U_{IE} \) that conserves the energy of the combined system \( IE \), and the second step is the measurement of the Hamiltonian \( \hat{H}_E \). That is, the second step is given as the measurement corresponding to the spectral decomposition of the Hamiltonian \( \hat{H}_E \). This step was not discussed in the above existing studies.

**Definition 6 (Fully quantum (FQ) work extraction)** Let us consider an external system \( \mathcal{H}_E \) with the Hamiltonian \( \hat{H}_E = \sum_{j \in J} h_{E,j} P_{E,j} \). Then, a unitary transformation \( U \) on \( \mathcal{H}_I \otimes \mathcal{H}_E \) and an initial state \( \rho_E \) of the external system \( \mathcal{H}_E \) give the CP-work extraction \( \{ E_j, w_j \}_{j \in J} \) as follows.

\[
E_j(\rho) := \text{Tr}_EU(\rho_I \otimes \rho_E)U^\dagger(\hat{1}_I \otimes P_{E,j}) \quad (17)
\]

\[
w_j := h_{E,j} - \text{Tr}\hat{H}_E\rho_E \quad (18).
\]

Then, the quartet \( \mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E) \) is called a fully quantum (FQ) work extraction. The above CP-work extraction \( \{ E_j, w_j \}_{j \in J} \) is simplified to CP(\( \mathcal{F} \)). In particular, the FQ work extraction \( \mathcal{F} \) satisfying CP(\( \mathcal{F} \)) = \( \{ E_j, w_j \}_{j \in J} \) is called a realization of the CP-work extraction \( \{ E_j, w_j \}_{j \in J} \).

Here, any FQ work extraction corresponds to a CP-work extraction. Conversely, considering the indirect model for an instrument model, we can show that there exists a FQ work extraction \( \mathcal{F} \) with a pure state \( \rho_E \) for an arbitrary CP work extraction \( \{ E_j, w_j \}_{j \in J} \) such that CP(\( \mathcal{F} \)) = \( \{ E_j, w_j \}_{j \in J} \) [44][58]. Theorem 5.7].

Since the heat engine needs to satisfy the conservation law of energy, we consider the following energy conservation laws for a FQ work extraction \( (\mathcal{H}_E, \hat{H}_E, U, \rho_E) \).

**Definition 7 (FQ energy conservation law)** When a unitary \( U \) is called energy conservative under the Hamiltonian \( \hat{H}_I \) and \( \hat{H}_E \)

\[
[U, \hat{H}_I + \hat{H}_E] = 0. \quad (19)
\]

Then, an FQ work extraction \( \mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E) \) is called energy-conservative when the unitary \( U \) is energy-conservative under the Hamiltonian \( \hat{H}_I \) and \( \hat{H}_E \).

The condition (19) is called the FQ energy conservation law. Note that the above condition does not depend on the choice of the initial state \( \rho_E \) on the external system. Indeed, the condition (19) is equivalent with the condition

\[
\text{Tr}(\hat{H}_I + \hat{H}_E)U(\rho_I \otimes \rho_E)U^\dagger = \text{Tr}(\hat{H}_I + \hat{H}_E)(\rho_I \otimes \rho_E) \quad \text{for } \forall \rho_I \quad \text{and } \forall \rho_E. \quad (20)
\]

When we make some restriction for the state \( \rho_E \), the condition (20) is weaker than the condition (19). For example, when the condition (20) is given with a fixed \( \rho_E \), the CP-work extraction CP(\( \mathcal{F} \)) satisfies the level-1 energy conservation law. However, such a restriction is unnatural, because such a restricted energy conservation cannot recover the conventional energy conservation. Thus, we consider the condition (20) without any constraint for the state \( \rho_E \). Hence, we have no difference between the condition (19) and the average energy conservation law (20) in this scenario. Indeed, if we do not consider the measurement process on the external system \( E \), the model given in Definition 1 corresponds to the formulations which are used in Refs.[33][37][41].

Here, we discuss how to realize the unitary \( U \) satisfying (19). For this purpose, we prepare the following lemma.

**Lemma 3** For an arbitrary small \( \epsilon > 0 \) and a unitary \( U \) satisfying (19), there exist a Hermitian matrix \( B \) and a time \( t_0 > 0 \) such that

\[
\| B \| \leq \epsilon, \quad U = \exp(it_0(\hat{H}_I + \hat{H}_E + B)). \quad (21)
\]

**Proof:** Choose a Hermitian matrix \( C \) such that \( \| C \| \leq \pi \) and \( U = \exp(iC) \). Since \( C \) and \( \hat{H}_I + \hat{H}_E \) are commutative, we can choose a common basis \( \{ \{x\} \} \) of \( \mathcal{H}_I \otimes \mathcal{H}_E \) that diagonalizes \( C \) and \( \hat{H}_I + \hat{H}_E \) simultaneously. For any \( t \), we can choose a set of integers \( \{ n_x \} \) such that \( \| D_t \| \leq \pi \), where \( D := C - t(\hat{H}_I + \hat{H}_E) - \sum_x 2\pi n_x |x\rangle \langle x| \). Hence, the Hermitian matrix \( B := D^{\dagger}D \) satisfies both conditions in (21) with \( \epsilon = \frac{\pi}{4} t_0 \). So, choosing \( t \) enough large, we obtain the desired argument. \( \Box \)

Thanks to Lemma 3, any unitary \( U \) satisfying (19) can be realized with the sufficiently long time \( t \) by adding the small interaction Hamiltonian term \( B \). Note that the interaction \( B \) does not change in \( 0 < t < t_0 \). Thus, in order to realize the unitary \( U \), we only have to turn on the interaction \( B \) at \( t = 0 \) and to turn off it at \( t = t_0 \). From \( t = 0 \) to \( t = t_0 \), we do not have to control the total system \( IE \) time dependently. Namely, we can realize a “clockwork heat engine,” which is programmed to perform the unitary transformation \( U \) automatically.

Now, we have the following lemma.
Lemma 4 For an energy conservative FQ work extraction $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$, the CP work extraction $CP(\mathcal{F})$ satisfies the level-2 energy conservation law.

Proof: For any $j$, due to the FQ energy conservation law (19), we can choose $j'$ such that

$$\langle x | U^\dagger (\hat{I} \otimes P_{E,j}) | y \rangle = \langle x | (\hat{I} \otimes P_{E,j'}) U^\dagger | y \rangle. \quad (22)$$

Then, the FQ energy conservation law (19) implies that

$$h_x - h_y - w_j = h_x - h_y - h_{E,j} + \text{Tr} \hat{H}_E \rho_E = -h_{E,j'} + \text{Tr} \hat{H}_E \rho_E. \quad (23)$$

Hence, we can show that the distribution $P_{K|X=x}$ does not depend on $x$ as follows.

$$P_{K|X(k|x)} = \sum_{j,y:h_x-h_y-w_j=k} \text{Tr} U |x\rangle \langle y| \otimes \rho_E U^\dagger (|y\rangle \langle y| \otimes P_{E,j})$$

$$(a) = \sum_{j',y:h_{E,j'}=-k+\text{Tr} \hat{H}_E \rho_E} \text{Tr} U |x\rangle \langle y| \otimes \rho_E (\hat{I} \otimes P_{E,j'}) U^\dagger (\hat{I} \otimes \hat{I}_E)$$

$$= \sum_{j',y:h_{E,j'}=-k+\text{Tr} \hat{H}_E \rho_E} \text{Tr} U |x\rangle \langle y| \otimes \rho_E (\hat{I} \otimes P_{E,j'})$$

$$= \sum_{j',y:h_{E,j'}=-k+\text{Tr} \hat{H}_E \rho_E} \text{Tr} \rho_E P_{E,j'}, \quad (24)$$

which does not depend on $x$, where $(a)$ follows from the combination of (22) and (23).}
B. Shift-invariant case with lattice Hamiltonian

Next, we consider the case when the behavior of the heat engine does not depend on the initial state of the external system. For this purpose, we introduce a classification of Hamiltonians. A Hamiltonian $\hat{H}_I$ is called lattice when there is a real positive number $d$ such that any difference $h_i - h_j$ is an integer times of $d$ where $\{h_i\}$ is the set of eigenvalues of $\hat{H}_I$. When $\hat{H}_I$ is lattice, the maximum $d$ is called the lattice span of $\hat{H}_I$. Otherwise, it is called non-lattice. In this subsection, we assume that our Hamiltonian $\hat{H}_I$ is lattice and denote the lattice span by $h_E$. Then, we consider a non-degenerate external system $E_1$. Let $\hat{H}_{E_1}$ be the $L^2(\mathbb{Z})$ and the Hamiltonian $\hat{H}_E$ be $\sum_j h_E |j\rangle_E \langle j|$. We define the displacement operator $V_{E_1} := \sum_j |j+1\rangle_E \langle j|$.

Definition 8 (Shift-invariant unitary) A unitary $U$ on $\mathcal{H}_I \otimes \mathcal{H}_{E_1}$ is called shift-invariant when

$$UV_{E_1} = V_{E_1}U. \quad (27)$$

Indeed, there is a one-to-one correspondence between a shift-invariant unitary on $\mathcal{H}_I \otimes \mathcal{H}_{E_1}$ and a unitary on $\mathcal{H}_I$. To give the correspondence, we define an isometry $W$ from $\mathcal{H}_I$ to $\mathcal{H}_I \otimes \mathcal{H}_{E_1}$.

$$W := \sum_x |x\rangle_E \otimes |x\rangle. \quad (28)$$

Lemma 7 A shift-invariant unitary $U$ is energy-conservative if and only if $W^\dagger UW$ is unitary. Conversely, for a given unitary $U_I$ on $\mathcal{H}_I$, the operator

$$F[U_I] := \sum_j V_{E_1}^j WU_I W^\dagger V_{E_1}^{−j} \quad (29)$$

is in the non-degenerate external system $E_1$. Let us consider the situation that we perform CP-work extractions $n$ times. In these applications, the state reduction of the external system $\mathcal{H}_{E_1}$ is based on the projection postulate. Let $\rho_E^{(1)}$ be the initial state on the external system $\mathcal{H}_{E_1}$, which is assumed to be a pure state. We assume that the initial state $\rho_E^{(k)}$ on $\mathcal{H}_{E_1}$ of the $k$th CP-work extraction is the final state of the external system of the $k-1$th work extraction. Other parts of the $k$th CP-work extraction are the same as those of the first CP-work extraction. Hence, the $k$th CP-work extraction is $(\mathcal{H}_E, \hat{H}_E, \rho_E^{(k)}, U)$. Generally, the FQ work extraction $(\mathcal{H}_E, \hat{H}_E, \rho_E^{(k)}, U)$ depends on the state $\rho_E^{(k)}$. Namely, there exists a memory effect. However, when $U$ is shift-invariant, the FQ work extraction does not depend on the state $\rho_E^{(k)}$. Then the memory effect does not exist. So, we don’t have to initialize the external system after the projective measurement on the external system.

Then, the shift-invariant FQ-work extraction can simulate the semi-classical scenario in the following limited sense.
Lemma 8 Given an internal unitary $U_1$ and an state $\rho_1$ on the internal system $I$, in the shift-invariant FQ-work extraction $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, F[U_1], \rho_E)$, the average amount of extracted work is $\text{Tr} \rho_1 \hat{H}_1 - \text{Tr} U_1 \rho U_1^\dagger \hat{H}_1$.

Further, the shift-invariant FQ-work extraction yields a special class of CP-work extraction.

Lemma 9 For an energy conservative and shift-invariant FQ work extraction $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$, the CP work extraction $\text{CP}(\mathcal{F})$ satisfies the level-3 energy conservation law.

Proof: Firstly, we consider the case when $\mathcal{H}_E = \mathcal{H}_{E1}$. Similar to the proof of Lemma 4 we have

$$P_{KY|X}(k, y|x)$$

$$= \sum_{j: h_j - h_y - w_j = k} \text{Tr} U(|x⟩⟨y|) \otimes \rho_E U^\dagger(|y⟩⟨y| \otimes |j⟩⟨j|)$$

$$= \sum_{j: h_j - h_y - w_j = k} \text{Tr} U(|x⟩⟨y|) \otimes \rho_E U^\dagger(|y⟩⟨y| \otimes |j⟩⟨j|)^2$$

$$= \sum_{j: h_j - h_y - w_j = k} \text{Tr} U(|x⟩⟨y|) \otimes |j⟩⟩⟨j| |j⟩⟩⟨j| U^\dagger(|y⟩⟨y| \otimes \hat{1}_E)$$

$$= (|y⟩U_1|x⟩|^2 \sum_{j: h_j - h_y - w_j = k} \langle j| |j⟩⟩⟨j| |j⟩⟩⟨j| U^\dagger(|y⟩⟨y| \otimes \hat{1}_E)$$

where (a) can be shown by using relations similar to (22) and (23). Hence,

$$P_{KY|X}(k, y|x) = \sum_{j: h_j - h_y - w_j = k + \text{Tr} \hat{H}_EP_E} \langle j| |j⟩⟩⟨j| |j⟩⟩⟨j| U^\dagger(|y⟩⟨y| \otimes \hat{1}_E)$$

which does not depend on $x$ nor $y$.

Next, we proceed to the general case. Similarly, we can show that

$$P_{KY|X}(k, y|x)$$

$$= \sum_{j: h_j - h_y - w_j = k} \text{Tr} U(|x⟩⟨y|) \otimes \rho_E U^\dagger(|y⟩⟨y| \otimes |j⟩⟨j|)$$

$$= (\text{Tr} U_1|x⟩⟨y|) \otimes \rho_E U^\dagger(|y⟩⟨y| \otimes \hat{1}_E) \sum_{j: h_j - h_y - w_j = k + \text{Tr} \hat{H}_EP_E} \langle j| |j⟩⟩⟨j| |j⟩⟩⟨j| U^\dagger(|y⟩⟨y| \otimes \hat{1}_E)$$

Hence, we obtain (33).  

As a special case of Lemma 5 we have the following lemma.

Lemma 10 Let $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ be an energy-conservative and shift-invariant FQ work extraction. Then, the support of the initial state $\rho_E$ belongs an eigenstate of the Hamiltonian $\hat{H}_E$ if and only if the CP work extraction $\text{CP}(\mathcal{F})$ satisfies the level-4 energy conservation law.

Lemma 11 For a level-4 CP work extraction $\{\mathcal{E}_j, w_j\}_{j \in J}$, there exists an energy-conservative and shift-invariant FQ work extraction $\mathcal{F}$ such that the support of the initial state $\rho_E$ belongs an eigenstate of the Hamiltonian $\hat{H}_E$ and $\text{CP}(\mathcal{F}) = \{\mathcal{E}_j, w_j\}_{j \in J}$.

Proof: Now, we make a Stinespring extension $(\mathcal{H}_{E2}, U_{E2}, \rho_{E2})$ with a projection valued measure $\{\mathcal{E}_j\}$ on $\mathcal{H}_{E2}$ of $\{\mathcal{E}_j, w_j\}_{j \in J}$ as follows.

$$\mathcal{E}_j(\rho_1) = \text{Tr}_{E2} U_{E2} (\rho_1 \otimes \rho_{E2}) U_{E2}^\dagger (\mathcal{E}_j \otimes \rho_{E2})$$

where $\{\mathcal{E}_j\}$ is a projection valued measure on $\mathcal{H}_{E2}$ and $\rho_E$ is a pure state. This extension is often called the indirect measurement model, which was introduced by Ozawa [44]. Here, the Hamiltonian of $\mathcal{H}_{E2}$ is chosen to be 0. Next, we define the unitary $U$ on $\mathcal{H}_I \otimes \mathcal{H}_{E2} \otimes \mathcal{H}_{E1}$ as $U = F[U_{E2}]$. Here, $\mathcal{H}_{E1}$ is defined as above.

Then, we define an energy-conservative and shift-invariant FQ work extraction $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ with the above given $U$ as $\mathcal{H}_E := \mathcal{H}_{E1} \otimes \mathcal{H}_{E2}$, $\hat{H}_E := \hat{H}_{E1}$, and $\rho_E := |0⟩⟨0| \otimes \rho_{E2}$. Hence, the level-4 condition implies

$$\mathcal{E}_j(\rho) = \text{Tr} U (\rho \otimes |0⟩⟨0| \otimes \rho_{E2}) U^\dagger (\mathcal{E}_j \otimes |j⟩⟨j|)$$
It is natural to consider that the state on the additional external system $E2$ does not change due to the work extraction. Hence, we impose the following restriction for the state on the additional external system $E2$.

**Definition 10 (Stationary condition)** A shift-invariant FQ work extraction $(\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ is called to satisfy the stationary condition when the relations $\rho_E = \rho_{E1} \otimes \rho_{E2}$ and

$$\text{Tr}_{IE1}U(\rho_I \otimes \rho_E)U^\dagger = \rho_E$$  \hspace{1cm} (37)

hold for any initial state $\rho_I$ on $\mathcal{H}_I$.

Now, we have the following lemma.

**Lemma 12** Let $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ be a stationary FQ work extraction. Then, the CP work extraction $CP(\mathcal{F})$ satisfies the unital condition (14).

**Proof:** Firstly, we consider the case when $\mathcal{H}_E = \mathcal{H}_{E1}$. To show the unital condition (14), it is enough to show that

$$\text{Tr}_I|\psi_I\rangle\langle \psi_I|\text{Tr}_E(\rho_I \otimes \rho_E)U = 1$$  \hspace{1cm} (38)

for any pure state $|\psi_I\rangle$ on $\mathcal{H}_I$. In this case, $U_I := W^\dagger UW$ satisfies

$$\sum_j (y, j'|U \sum_j b_j |x, j) = b_{h_y-h_x}^+ + j'|y, j'|U |x, h_y-h_x + j').$$  \hspace{1cm} (39)

When $\rho_E = |\psi_E\rangle\langle \psi_E|$, $|\psi_E\rangle = \sum_j b_j |j\rangle$, and $|\psi_I\rangle = \sum_x a_x |x\rangle$, we have

$$\text{Tr}_I|\psi_I\rangle\langle \psi_I|\text{Tr}_E(\rho_I \otimes \rho_E)U = \sum_{x,j} |\langle \psi_I, j|U |x, \psi_E\rangle|^2 = \sum_{x,j} |\langle \psi_I, j|U |x, j\rangle|^2$$

$$= \sum_{x,j'} \sum_y a_y b_{h_y-h_x}^+ + j'|y|U |x\rangle|^2$$

$$= \sum_{y,j'} |\sum_x b_{h_y-h_x}^+ + j'|^2 \sum_x |\langle \psi_I|U |x\rangle|^2 = \|\psi_I\|^2 \|\psi_E\|^2 = 1.$$  \hspace{1cm} (40)

Hence, when $\rho_E = \sum_I \rho_I|\psi_{E,I}\rangle\langle \psi_{E,I}|$, we also have

$$\text{Tr}_I|\psi_I\rangle\langle \psi_I|\text{Tr}_E(\rho_I \otimes \rho_E)U = 1.$$  \hspace{1cm} (41)

Next, we proceed to the proof of the general case. The above discussion implies that

$$\text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \frac{1}{d_E} \otimes \rho_{E1}\right)U^\dagger = \frac{1}{d_I} \otimes \frac{1}{d_E}.$$  \hspace{1cm} (42)

Information processing inequality yields that

$$D\left(\frac{1}{d_I} \otimes \rho_{E2} \| \frac{1}{d_I} \otimes \frac{1}{d_E} \right) \geq D\left(\text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right)U^\dagger \| \text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \frac{1}{d_E} \otimes \rho_{E1}\right)U^\dagger\right)$$

$$\geq D\left(\text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right)U^\dagger \| \frac{1}{d_I} \otimes \frac{1}{d_E}\right),$$  \hspace{1cm} (43)

which implies that

$$S\left(\text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right)U^\dagger\right) \geq \log d_I + S(\rho_{E2}).$$  \hspace{1cm} (44)

Due to the condition (37), the reduced density of $\text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right)U^\dagger$ on $E2$ is $\rho_{E2}$. Under this condition, we have the inequality opposite to (44). The equality of the inequality opposite to (44) holds only when $\text{Tr}_{IE1}U\left(\frac{1}{d_I} \otimes \rho_{E2} \otimes \rho_{E1}\right)U^\dagger = \frac{1}{d_I} \otimes \rho_{E2}$, which implies the unital condition (14).
Overall, as a realizable heat engine, we impose the energy-conservative, shift-invariant, and stationary conditions to our FQ-work extractions. Also, it is natural to assume that the initial state on $E_1$ is an eigenstate of the Hamiltonian $H_{E_1}$ because it is not easy to prepare a non-eigenstate of the Hamiltonian $H_{E_1}$.

**Definition 11** When a FQ-work extraction satisfies all of these conditions, we refer to it as a standard FQ-work extraction for convenience of description.

So, for a standard FQ-work extraction $F$, the CP-work extraction $CP(F)$ is a standard CP-work extraction. In the following, we consider that the set of standard FQ-work extractions as the set of preferable work extractions. Hence, our optimization will be done among the set of standard FQ-work extractions.

However, we can consider restricted classes of standard FQ-work extractions by considering additional proper properties. For a standard FQ-work extraction $F = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$, we assume that the external system $\mathcal{H}_E$ consists only of the non-degenerate external system $\mathcal{H}_{E_1}$. In this case, the corresponding standard CP-work extraction $CP(F)$ depends only on the internal unitary $U_I = WUW^\dagger$.

**Definition 12** For the above given standard FQ-work extraction $F = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$, the standard CP-work extraction $CP(F)$ is called the standard CP-work extraction associated to the internal unitary $U_I$, and is denoted by $\hat{CP}(U_I)$.

Further, an internal unitary $U_I$ is called deterministic when $\langle x | U_I | x' \rangle$ is zero or $e^{i\theta}$ for any $x$ and $x'$. In the latter, a standard CP-work extraction associated to the deterministic internal unitary plays an important role.

Finally, We illustrate a Venn diagram of the FQ-work extractions in Figure 3 and classify the relationships among the classes of the CP-work extraction and that of the FQ-work extraction in Table I.

![Venn diagram of the FQ-work extractions](image)

**FIG. 3: A Venn diagram of the FQ-work extractions**

| $CP(F)$ | FQ-energy conservation, $\rho_E$ is not an energy eigenstate | FQ-energy conservation, $\rho_E$ is an energy eigenstate | Stationary condition | FQ-energy conservation, $\rho_E$ is not an energy eigenstate | FQ-energy conservation, $\rho_E$ is an energy eigenstate |
|---------|----------------------------------------------------------|--------------------------------------------------------|------------------------|----------------------------------------------------------|--------------------------------------------------------|
| CP-level 2 | Yes (Lemma 4) | - | - | Yes |
| CP-level 3 | - | Yes (Lemma 9) | - | Yes |
| CP-level 4 | No (Lemma 5) | - | - | Yes (Lemma 12) |
| CP-unital | - | - | Yes (Lemma 12) | - |

**C. Shift-invariant case with non-lattice Hamiltonian**

Next, we consider the non-lattice Hamiltonian $\hat{H}_I$. In this case, we cannot employ the space $L^2(\mathbb{Z})$ as the non-degenerate external system $E_1$. One idea is to replace the space $L^2(\mathbb{Z})$ by the space $L^2(\mathbb{R})$. However, in this method, to satisfy the condition with the measurement of the Hamiltonian $H_{E_1}$, we need to prepare the state whose wave function is a delta function. To avoid such a mathematical difficulty, we employ another construction of the non-degenerate external system $E_1$. 
Let \( \{ h_i \} \) be the set of eigenvalues of \( \hat{H}_I \). We choose the set \( \{ h_{E,l} \} \) satisfying the following. (1) When rational numbers \( t_1, \ldots, t_L \) satisfy \( \sum_{l=1}^L t_l h_{E,l} = 0 \), the equality \( t_l = 0 \) holds for all \( l \). (2) \( \{ h_i - h_j \}_{i,j} \subset \{ \sum_{l=1}^L n_l h_{E,l} \} \) for all \( n \in \mathbb{Z} \). Then, we choose \( \mathcal{H}_{E1} \) to be \( L^2(\mathbb{Z})^{\otimes L} \) and the Hamiltonian \( \hat{H}_{E1} \) to be \( \sum_{j_1, \ldots, j_L} h_{E1,j_1} + \ldots + h_{E1,j_L} |j_1, \ldots, j_L \rangle \langle j_1, \ldots, j_L | \).

Then, a shift-invariant unitary is defined as follows. We define \( L \) displacement operators \( V_{E1,l} := \sum_j |j + 1 \rangle_E \langle j | \) on the \( l \)-th space \( L^2(\mathbb{Z}) \).

**Definition 13 (Shift-invariant unitary)** A unitary \( U \) on \( \mathcal{H}_I \otimes \mathcal{H}_{E1} \) is called shift-invariant when
\[
UV_{E1,l} = V_{E1,l}U
\]
for \( l = 1, \ldots, L \).

Then, the definition of \( F[U] \) is changed to
\[
F[U_l] := \sum_{j_1, \ldots, j_L} (\otimes_{l=1}^L V_{E1,l}^j) W_U W_U^\dagger (\otimes_{l=1}^L V_{E1,l}^j)^\dagger.
\]
Under this replacement, we have Lemma. Other definitions and lemmas in Subsection IV B work with this replacement.

## V. APPROXIMATION TO INTERNAL UNITARY

### A. Approximation and coherence

In this section, we investigate the validity of the internal unitary formulation based on an FQ-work extraction model. Tasaki formulated the work extraction process as an unitary operator on the internal system of the heat engine. In this model, they expect that the unitary can be realized via the control of the Hamiltonian of the internal system. Since the control is realized by the external system, they consider that the work can be transferred to the external system via the control. In this scenario, they expect that the time evolution \( \Lambda \) of the internal system \( \mathcal{H}_I \) can be approximated to an ideal unitary \( U_I \). That is, when we employ an FQ-work extraction \( F = (\mathcal{H}_E, \hat{H}_E, U, \rho_E) \), the time evolution \( \Lambda \) of the internal system \( \mathcal{H}_I \) is given as
\[
\Lambda(\rho_I) = \text{Tr}_E U_I (\rho_I \otimes \rho_E) U_I^\dagger.
\]
To qualitify the approximation to the unitary \( U_I \), we need to focus on two aspects. One is the time evolution of basis states in a basis \( \{ |x \rangle \} \) diagonalizing the Hamiltonian \( \hat{H}_I \). The other is the time evolution of the superposition states under the basis. Usually, it is not difficult to realize the same evolution as that of \( U_I \) only for the former states. However, it is not easy to keep the quality of the latter time evolution, which is often called the coherence. Hence, we fix a unitary \( U_I \), and we assume that the TP-CP map \( \Lambda \) satisfies the condition
\[
\langle y | \Lambda(|x \rangle \langle x |) | y \rangle = \langle y | U_I | x \rangle \langle x | U_I^\dagger | y \rangle
\]
for any \( x, y \).

That is, we choose our time evolution among TP-CP maps satisfying the above condition. Under the condition, the quality of the approximation to the unitary \( U_I \) can be measured by the coherence of the TP-CP map \( \Lambda \). To give the measures of the coherence of \( \Lambda \), we introduce the reference system \( R \). When the initial state of the internal system is \( \rho_I \), we consider the purification \( | \Phi \rangle \) of the state \( \rho_I \), which is a pure state on \( \mathcal{H}_I \otimes \mathcal{H}_R \). Here, the state \( \rho_I \) expresses the average of the initial state on the internal system \( I \) under a given distribution of possible initial states. One of the measures of the coherence is the entanglement fidelity
\[
F_e(\Lambda, U_I, \rho_I) := \langle \Phi | U_I^\dagger \Lambda(|\Phi \rangle \langle \Phi |) U_I | \Phi \rangle.
\]
When the initial state \( | \psi_a \rangle \) is generated with the probability \( P_A(a) \), namely when \( \rho_I = \sum_a P_A(a) | \psi_{I,a} \rangle \langle \psi_{I,a} | \) holds, the entanglement fidelity \( F_e(\Lambda, U_I, \rho_I) \) characterizes any average fidelity as
\[
F_e(\Lambda, U_I, \rho_I)^2 \leq \sum_a P_A(a) | \langle \psi_a | U_I^\dagger \Lambda(| \psi_a \rangle \langle \psi_a |) U_I | \psi_a \rangle |.
\]
Since this value is zero in the ideal case, this value can be regarded as the amount of the disturbance by the time-evolution \( \Lambda \). The other measure is the entropy exchange \([67],[53, (8.51)]\)
\[
S_e(\Lambda, \rho_I) := S(\Lambda(|\Phi \rangle \langle \Phi |)).
\]
This quantity satisfies the quantum Fano inequality \([67],[53, (8.51)]\)
\[
S_e(\Lambda, \rho_I) = S_e(\Lambda U_I^\dagger \otimes \Lambda, \rho_I) \leq h(F_e(\Lambda, U_I, \rho_I)^2) + (1 - F_e(\Lambda, U_I, \rho_I)^2) \log(d_I^2 - 1),
\]
where \( \Lambda U_I^\dagger (\rho) := U_I^\dagger \rho U_I \). Since this value is also zero in the ideal case, we consider that this value is another measure of the disturbance by the time-evolution \( \Lambda \).
B. Correlation with external system

On the other hand, we need to focus on the correlation during the work extraction process due to the following reason. In order that the heat engine works properly, the amount of the extracted work needs to be reflected to the outer system that consists of the macroscopic devices because the purpose of the heat engine is to supply the work to the macroscopic devices. Hence, the amount of decreased energy in the internal system is required to be correlated with the outer system so largely that the time evolution on the joint system \( I \) and \( E \) can be regarded as a unitary \( V_{IE} \) and the state \( \rho_E \) is a pure state \( |\phi_E\rangle \). In the following, we denote the initial state \([\Phi, \phi_E]_E[\Phi, \phi_E]_E\) of the total system \( \mathcal{H}_I \otimes \mathcal{H}_R \otimes \mathcal{H}_E \) by \( \rho \).

Then, we denote the resultant state \( U[\Phi, \phi_E]_E[\Phi, \phi_E]_E[U^\dagger \rho_{IR}] \)

To decide the amount of decreased energy in the internal system, we consider the measurement of the observable \( \hat{H}_I = \sum_z z F_z \) on the joint system \( I \) and \( R \) after the time evolution \( \Lambda \). That is, by using the spectral decomposition \( \hat{H}_I = \sum_z z F_z \), we define the final state \( \rho_{Z_E}'' \) on \( H_Z \otimes H_E \) by

\[
\rho_{Z_E}'' := \sum_z |z\rangle_Z \langle z| \otimes \text{Tr}_{IR} F_z \rho_{IR}''.
\] (52)

Here, the random variable \( Z \) takes the value \( z \) with the probability \( P_Z(z) := \text{Tr}_{IR} \rho_{IR}''. \)

When the outcome \( Z = z \), the resultant state on \( E \) is \( \rho_{E|Z=z}'' := \frac{1}{P_Z(z)} \text{Tr}_{IR} \rho_{IR}''. \)

Then, the correlation between the external system \( E \) and the amount of decreased energy can be measured by the correlation on the state \( \rho_{Z_E}'' \).

Although this scenario is based on a virtual measurement, this interpretation will be justified by considering the situation without the purification in the following lemma.

**Lemma 13** We consider the case when the eigenstate \( |\psi_{I,a}\rangle \) is generated with probability \( P_A(a) \). Then, measuring the Hamiltonian \( \hat{H}_I = \sum_h h P_h \) after the time evolution \( \Lambda \), we obtain the conditional distribution \( P_{HA}(h|a) := \text{Tr}_A \Lambda (|\psi_{I,a}\rangle \langle \psi_{I,a}|) \).

Then, we chose the state \( \rho_I \) to be

\[
\rho_I = \sum_a P_A(a) |\psi_{I,a}\rangle \langle \psi_{I,a}|.
\] (53)

Under the joint distribution \( P_{HA}(h,a) := P_{HA}(h|a)P_A(a) \), the amount \( \langle \psi_{I,a}|\hat{H}_I|\psi_{I,a}\rangle - h \) of decrease energy takes values \( Z \) with the probability \( P_Z(z) \).

That is,

\[
\sum_{h,a:|\psi_{I,a}|\hat{H}_I|\psi_{I,a}\rangle - h = z} P_{HA}(h,a) = P_Z(z).
\] (54)

Since the proof of Lemma 13 is trivial, we skip its proof. Lemma 13 guarantees that the probability distribution \( P_Z(z) \) is the same as the work distribution defined in (72) under its assumption. When \( \rho_I \) is commutative with \( \hat{H}_I \), we can take the above eigenstate \( |\psi_{I,a}\rangle \) and a probability distribution \( P_A \) satisfying the above condition (53). Also, when the state \( \rho_I \) is a Gibbs state or a mixture of Gibbs states, the state \( \rho_I \) satisfies the condition in Lemma 13.

Hence, it is suitable to consider the distribution \( P_Z \) gives the distribution of the amount of the decreased energy in this case.

Here, we employ two measures of the correlation. One of the measures is the mutual information:

\[
I_{\rho_{Z_E}''}(Z;E) := D(\rho_{Z_E}''\|\rho_{Z_E}'' \otimes \rho_E')
\]

\[
= S(\rho_{E}|\rho_{Z_E}'';z) - \sum_z P_Z(z) S(\rho_{Z_E}'';z) \geq S(\rho_{E}'') = S(\Lambda(|\Phi\rangle \langle \Phi|)),
\] (55)

where \( D(\tau||\sigma) := \text{Tr}_E \log \tau - \log \sigma \). Here, the equality in the inequality (a) holds if and only if the state \( \rho_{E|Z=z}'' \) is pure for any value \( z \) with non-zero probability \( P_Z(z) \). Information processing inequality for the map \( |z\rangle \langle z| \mapsto \rho_{E|Z=z}'' \) yields that

\[
I_{\rho_{Z_E}''}(Z;E) \leq S(P_Z).
\] (56)

In particular, the equality in (56) holds in the ideal case, i.e., in the case when the states \( \{\rho_{E|Z=z}''\}_z \) are distinguishable, i.e., \( \text{Tr}_{E|Z=z}'' \rho_{E|Z=z}'' \rho_{E|Z=z'}'' = 0 \) for \( z \neq z' \) with non-zero probabilities \( P_Z(z) \) and \( P_Z(z') \). So, the imperfectness of the correlation for the decrease of the energy can be measured by the difference

\[
\Delta I_{\rho_{Z_E}''}(Z;E) := S(P_Z) - I_{\rho_{Z_E}''}(Z;E).
\] (57)
Here, we notice another expression of $I_{\rho''_{E|Z}}(Z; E)$ as
\begin{equation}
I_{\rho''_{E|Z}}(Z; E) = \min_{\sigma_E} D(\rho''_{Z|E}||\rho''_Z \otimes \sigma_E). \tag{58}
\end{equation}

Following this expression, we introduce the fidelity-type mutual information as follows
\begin{equation}
I_{F,\rho''_{E|Z}}(Z; E) := -\log \max_{\sigma_E} F(\rho''_{Z|E}, \rho''_Z \otimes \sigma_E). \tag{59}
\end{equation}

We can show the following theorem.

**Theorem 1** The relations
\begin{equation}
I_{F,\rho''_{E|Z}}(Z; E) = -\log \sum_{z,z'} P_Z(z)P_Z(z')F(\rho''_{E|Z=z}, \rho''_{E|Z=z'}) \leq S_2(P_Z) \tag{60}
\end{equation}

hold, where $S_2(P_Z) := -\log \sum_z P_Z(z)^2$. The equality holds when the states $\{\rho''_{E|Z=z}\}_z$ are distinguishable.

Theorem 1 follows from a more general argument, Lemma 28 in Appendix A.

Since the equality in (60) holds in the ideal case, we introduce another measure of the imperfectness of the correlation for the decrease of the energy as
\begin{equation}
\Delta I_{F,\rho''_{E|Z}}(Z; E) := S_2(P_Z) - I_{F,\rho''_{E|Z}}(Z; E). \tag{61}
\end{equation}

**Lemma 14** Let $\mathcal{F} = (\mathcal{H}_E, \hat{H}_E, U, \rho_E)$ be an FQ-work extraction. Assume that $\rho_1$ is commutative with $\hat{H}_I$. When the CP-work extraction $\mathcal{CP}(\mathcal{F})$ is a level-4 CP-work extraction, the states $\{\rho''_{E|Z=z}\}_z$ are distinguishable.

**Proof:** Let $w_0$ be the eigenvalue of the Hamiltonian associated with the state $\rho_E$. Then,
\begin{equation}
\text{Tr} P_{w_0 + z'} \rho''_{E|Z=z} = \delta_{z,z'}. \tag{62}
\end{equation}

Hence, the states $\{\rho''_{E|Z=z}\}_z$ are distinguishable. \qed

**Remark 1** We should remark the relation between the fidelity-type mutual information $I_{F,\rho''_{E|Z}}(Z; E)$ and an existing mutual information measure. Recently, a new type of quantum Rényi relative entropy $\tilde{D}_\alpha(\tau||\sigma)$ was introduced \cite{63,64}. When the order is $\frac{1}{2}$, it is written as
\begin{equation}
\tilde{D}_{\frac{1}{2}}(\tau||\sigma) = -2\log F(\tau, \sigma). \tag{63}
\end{equation}

Using this relation, the paper \cite{52} (I.6) introduced the quantity $\tilde{I}_{\alpha,\rho}(Z; E)$ with general order $\alpha$ by
\begin{equation}
\tilde{I}_{\alpha,\rho}(Z; E) := \min_{\sigma_E} \tilde{D}_\alpha(\rho||\rho_E \otimes \sigma_E). \tag{64}
\end{equation}

So, our fidelity-type mutual information $I_{F,\rho}(Z; E)$ is written as
\begin{equation}
2I_{F,\rho}(Z; E) = \tilde{I}_{\frac{1}{2},\rho}(Z; E). \tag{65}
\end{equation}

**C. Trade-off with imperfectness of correlation**

Many papers studied trade-off relations between the approximation of a pure state on the bipartite system and the correlation with the third party $E$. In particular, since this kind of relation plays an important role in security analysis in quantum key distribution (QKD), it has been studied mainly from several researchers in QKD and the related areas with various formulations \cite{67} Section V-C \cite{66,53} \cite{54} Theorem 1 \cite{61} Lemma 2 \cite{62} Theorem 2 \cite{60,47}.

However, these trade-off relations are not suitable for our situation. So, we derive two kinds of trade-off relations with the imperfectness of correlation, which are more suitable for our purpe.
Theorem 2 The amount of decoherence \( S_e(\Lambda, \rho_1) \) and the amount of imperfectness of correlation \( \Delta I_{\rho_{ZE}}^F(Z; E) \) satisfy the following trade-off relation:

\[
S_e(\Lambda, \rho_1) + \Delta I_{\rho_{ZE}}^F(Z; E) \geq S(P_Z).
\]

(66)

The equality holds if and only if the state \( \rho''_{E|Z=z} \) is a pure state \( |\psi_{E|Z=z} \rangle \) for any value \( z \) with non-zero probability \( P_Z(z) \). In this case, we have

\[
S_e(\Lambda, \rho_1) = I_{\rho_{ZE}}^F(Z; E) = S\left( \sum_z P_Z(z) |\psi_{E|Z=z} \rangle \langle \psi_{E|Z=z}| \right).
\]

(67)

Proof: Since (55), (50) and (57) imply that

\[
S_e(\Lambda, \rho_1) + \Delta I_{\rho_{ZE}}^F(Z; E) = S(P_Z) - I_{\rho_{ZE}}^F(Z; E) + S(\rho_{E|Z=z}^I) = S(P_Z) + \sum_z P_Z(z) S(\rho''_{E|Z=z}) \geq S(P_Z).
\]

(68)

The equality holds if and only if the state \( \rho''_{E|Z=z} \) is pure for any value \( z \) with non-zero probability \( P_Z(z) \). In this case, we have

\[
\rho''_{E|Z=z} = \sum_z P_Z(z) |\psi_{E|Z=z} \rangle \langle \psi_{E|Z=z}|,
\]

which implies (67). To give another trade-off relation, we prepare the isometry \( V_{IRZ} \) from \( \mathcal{H}_I \otimes \mathcal{H}_R \) to \( \mathcal{H}_I \otimes \mathcal{H}_R \otimes \mathcal{H}_Z \):

\[
V_{IRZ} := \sum_z |z \rangle \otimes F_z.
\]

(69)

Then, we define the distribution

\[
\tilde{P}_Z(z) := \langle \Phi | U_1^\dagger F_z U_1 | \Phi \rangle,
\]

(70)

and the pure states \( |\psi''_{IR|E=|Z=z} \rangle \) and \( |\psi''_{IR|E=|Z=z} \rangle \) by

\[
V_{IRZ} U_1 | \Phi \rangle = \sum_z \sqrt{P_Z(z)} |\tilde{\psi}_{IR|Z=z}, z \rangle,
\]

(71)

\[
V_{IRZ} U_1 | \psi_E \rangle = \sum_z \sqrt{P_Z(z)} |\psi''_{IR|E=|Z=z}, z \rangle.
\]

(72)

Theorem 3 The quality of approximation \( F_e(\Lambda, U_1, \rho_1) \) and the amount of imperfectness of correlation \( \Delta I_{F_{\rho_{ZE}}^F}(Z; E) \) satisfy the following trade-off relation:

\[
- \log F_e(\Lambda, U_1, \rho_1) + \Delta I_{F_{\rho_{ZE}}^F}(Z; E) \geq S(P_Z).
\]
D. Shift-invariant model

Next, we consider how to realize the case when the amounts of the decoherence \( S(\Lambda, \rho_I) \) and \(- \log F_c(\Lambda, U_I, \rho_I)\) are close to zero. For simplicity, we consider this problem under the shift-invariant model without an additional external system. In the shift-invariant model, once we fix the energy-conservative unitary operator \( F[U_I] \) on \( \mathcal{H}_I \otimes \mathcal{H}_E \) according to (29), the assumption of Theorem [3] holds and the distribution \( P_Z \) depends only on the initial state \( \rho_I \) on the system \( I \). That is, \( P_Z \) does not depend on the initial state \( |\psi_E\rangle \) on the external system \( E \). In this case, we have

\[
|\psi_E|_{Z=h_E} = V^j|\psi_E\rangle.
\]

(76)

In particular, when \( |\psi_E\rangle = \sum_j \sqrt{P_j(j)}|j\rangle \), the equality condition holds in both inequalities (66) and (73). Theorem[2] implies that

\[- \log F_c(\Lambda, U_I, \rho_I) = I_{F,\rho_E^E}(Z; E) = - \log \sum_{z,z'} P_Z(z)P_Z(z') \sum_j \sqrt{P_j(j)}\sqrt{P_j(j + z - z')}.
\]

(77)

For example, when

\[
P_j(j) = \begin{cases} \frac{1}{m+1} & \text{if } |j| \leq m \\ 0 & \text{otherwise.} \end{cases}
\]

(78)

\[
P_Z(h_Ej) = 0 \text{ if } |j| \geq l,
\]

(79)

we have

\[- \log F_c(\Lambda, U_I, \rho_I) = I_{F,\rho_E^E}(Z; E) \leq - \log(1 - \frac{l}{2m+1}) \leq \frac{l}{2m+1}.
\]

(80)

So, when \( m \) is sufficiently large, the quality of approximation is very small. That is, a large size of superposition enables us to keep the coherence. It gives a positive answer to Question 1 in Subsection II A.

E. Trade-off under CP-work extraction

In Subsection V C we discuss the trade-off relation between the imperfectness of correlation and the quality of approximation under a FQ-work extraction. In this subsection, we discuss the trade-off relation under a CP-work extraction \( \mathcal{G} := \{ \mathcal{E}_j, w_j \}_j \) on the internal system \( \mathcal{H}_I \) with the Hamiltonian \( \hat{H}_I \). To discuss the trade-off relation, we consider the internal unitary \( U_I \) to be approximated and the initial mixture state \( \rho_I \), which is assumed to be commutative with \( \hat{H}_I \). To qualify the approximation, we employ two measures \( S(\sum_j \mathcal{E}_j, \rho_I) \) and \( F_c(\sum_j \mathcal{E}_j, U_I, \rho_I) \). To evaluate the imperfectness of correlation, we consider the purification \( |\Phi\rangle \) of \( \rho_I \), and introduce the joint distribution \( P_{ZW} \) as

\[
P_{ZW}(z, w) := \sum_{j : w_j = w} \text{Tr}_I \mathcal{E}_j(|\Phi\rangle \langle \Phi|)^{E_z},
\]

(81)

where the projection \( E_z \) is defined in the same way as in Subsection V B. Then, we employ two measures as

\[
\Delta I_{P_{ZW}}(Z; W) = S(P_Z) - I_{P_{ZW}}(Z; W)
\]

(82)

\[
\Delta I_{F,P_{ZW}}(Z; W) = S_2(P_Z) - I_{F,P_{ZW}}(Z; W).
\]

(83)

As corollaries of Theorems[2] and[3] we have the following.

**Corollary 1** Given a CP-work extraction \( \{ \mathcal{E}_j, w_j \}_j \). The amount of decoherence \( S(\sum_j \mathcal{E}_j, \rho_I) \) and the amount of imperfectness of correlation \( \Delta I_{P_{ZW}}(Z; E) \) satisfy the following trade-off relation:

\[
S(\sum_j \mathcal{E}_j, \rho_I) + \Delta I_{P_{ZW}}(Z; W) \geq S(P_Z).
\]

(84)

**Corollary 2** Given a CP-work extraction \( \{ \mathcal{E}_j, w_j \}_j \). The quality of approximation \( F_c(\sum_j \mathcal{E}_j, U_I, \rho_I) \) and the amount of imperfectness of correlation \( \Delta I_{F,P_{ZW}}(Z; E) \) satisfy the following trade-off relation:

\[
- \log F_c(\sum_j \mathcal{E}_j, U_I, \rho_I) + \Delta I_{F,P_{ZW}}(Z; W) \geq S_2(P_Z).
\]

(85)
Proof of Corollaries 1 and 2. Notice that Theorems 2 and 3 do not assume any energy conservation law. Then, we take a Stinespring representation \((\mathcal{H}_E, U, \rho_E)\) with a pure state \(\rho_E\) of \(\{E_j, w_j\}_{j \in J}\) as follows.

\[
E_j(\rho_1) = \text{Tr}_E U_{1E} (\rho_1 \otimes \rho_E) U_{1E}^\dagger (1_I \otimes E_j),
\]

where \(\{E_j\}\) is a projection valued measure on \(\mathcal{H}_E\). Notice that \((\mathcal{H}_E, U, \rho_E)\) is an FQ-work extraction. Here, we do not care about whether the FQ-work extraction satisfies any energy conservation law. Then, we apply Theorems 2 and 3. Since information processing inequalities for the relative entropy and the fidelity yield that

\[
I_{E} \geq I_{\rho_2^{E}}(Z;E) \geq I_{\rho_1^{E}}(Z;E) \geq I_{\rho_3^{E}}(Z;E) \geq I_{\rho_4^{E}}(Z;E),
\]

the relations (66) and (73) derive (84) and (85), respectively.

Further, we have the following corollary.

Corollary 3 Assume that \(\rho_1\) is commutative with \(\hat{H}_1\). For a level-4 CP-work extraction \(\{E_j, w_j\}_{j}, \Delta I_{\rho_3^{E}}(Z;E) = \Delta I_{\rho_4^{E}}(Z;E) = 0\). So, we have

\[
S_e(\sum_j E_j, \rho_1) \geq S(P_2), \quad -\log F_e(\sum_j E_j, U_1, \rho_1) \geq S_2(P_2).
\]

This corollary says that the dynamics of a level-4 CP-work extraction is far from any internal unitary. It gives a negative answer to Question 3 in Subsection A.

VI. CLASSICAL WORK EXTRACTION

A. Formulation

So far, we treat only the work extraction from the quantum system. We can easily reduce our formulation into the work extractions from the classical systems, which is defined as follows;

Definition 14 (Classical work extraction) We consider a classical system \(\mathcal{X}\) and its Hamiltonian which is given as a real-valued function \(h_{\mathcal{X}}\) on \(\mathcal{X}\). We also consider a probabilistic dynamics \(T(x|x')\) on \(\mathcal{X}\), which is a probability transition matrix, i.e., \(\sum_x T(x|x') = 1\). We refer to the triplet \((\mathcal{X}, h_{\mathcal{X}}, T)\) as a classical work extraction.

This model includes the previous fully classical scenario\([8, 20–25]\), in which we extract work from classical systems. For example, the setup of the Jarzynski equality \([8]\) is a special case that \(T(x|x')\) is invertible and deterministic, i.e., \(T(x|x')\) is given as \(\delta_{x,f(x')}\) with an invertible function \(f\). We call such a transition matrix invertible and deterministic. In this case, the transition matrix \(T\) is simply written as \(f_s\). That is, for a distribution \(P\), we have

\[
f_s(P)(x) = P(f^{-1}(x)).
\]

Notice that the relation

\[
(g \circ f)_s(P) = g_s(f_s(P))
\]

holds. When the transition matrix \(T\) is bi-stochastic, i.e., \(\sum_x T(x|x') = 1\), there exist a set of invertible functions \(f_i\) and a distribution \(p(i)\) such that \(T = \sum_i p(i)f_i\), i.e.,

\[
T(x|x') = \sum_i p(i)\delta_{x,f_i(x')},
\]

This relation means that a bi-stochastic transition matrix \(T\) can be realized by a randomized combination of invertible and deterministic dynamics.

Under a classical work extraction \((\mathcal{X}, h_{\mathcal{X}}, T)\), because of the energy conservation, the amount of the extracted work is given as

\[
w_{x,x'} = h_{\mathcal{X}}(x) - h_{\mathcal{X}}(x')
\]
when the initial and final states are \( x \) and \( x' \). More generally, the initial state is given as a probability distribution \( P_X \) on \( \mathcal{X} \). In this case, the amount of the extracted work is \( w \) with the probability

\[
\sum_{x', x : \omega = h_X(x) - h_X(x')} P(x) T(x'|x).
\]  

(93)

For the entropy of the amount of extracted work, we can show the following lemma in the same way as Lemma 15.

**Lemma 15** We denote the random variable describing the amount of extracted work by \( W \). The entropy of \( W \) is evaluated as

\[
S(W) \leq 2 \log N,
\]  

(94)

where \( N \) is the number of elements of the set \( \{ h_X(x) \}_{x \in \mathcal{X}} \).

### B. Relation with CP-work extraction

Next, we discuss the relation between CP-work extractions and classical work extractions. A CP-work extraction can be converted to a classical work extraction under a suitable condition as follows.

**Definition 15 (classical description)** For a level-4 CP-work extraction \( \{ \mathcal{E}_j, w_j \} \), we define the probability transition matrix \( T_{\{ \mathcal{E}_j, w_j \}} \) as

\[
T_{\{ \mathcal{E}_j, w_j \}}(y|x) := \sum_j \langle y | \mathcal{E}_j (|x\rangle) |y\rangle,
\]

(95)

and the function \( h_X(x) \) is given as the eigenvalue of the Hamiltonian \( \hat{H}_I \) associated with the eigenstate \( |x\rangle \). Then, we refer to the triplet \( (\mathcal{X}, h, T_{\{ \mathcal{E}_j, w_j \}}) \) as the classical description of the level-4 CP-work extraction \( \{ \mathcal{E}_j, w_j \} \), and denote it by \( T(\{ \mathcal{E}_j, w_j \}) \).

Hence, when the support of the initial state \( \rho_I \) of a FQ-work extraction \( F = (H_E, H_E, U, \rho_E) \) belongs to an eigenspace of the Hamiltonian \( \hat{H}_E \), its classical description is given as \( T(CP(F)) \). The above classical description gives the behavior of a given level-4 CP-work extraction \( \{ \mathcal{E}_j, w_j \} \). When the initial state on the internal system \( I \) is the eigenstate \( |x\rangle \), due to the condition \( 3 \), the amount of the extracted work is \( w \) with the probability

\[
\sum_{j : w = w_j \ y : w_j = h_x - h_y} \sum_{j : w = h_x - h_y} \langle y | \mathcal{E}_j (|x\rangle) |y\rangle = \sum_{y : w = h_x - h_y} T_{\{ \mathcal{E}_j, w_j \}}(y|x).
\]

(96)

Hence, the classical description \( T(\{ \mathcal{E}_j, w_j \}) \) gives the stochastic behavior in this case. More generally, we have the following theorem.

**Theorem 4** Assume that \( \mathcal{P}_{\hat{H}_I}(\rho_I) \) is written as \( \sum_x P_X(x) \langle x | \langle x \rangle \rangle \). (For the definition of \( \mathcal{P}_{\hat{H}_I}(\rho_I) \), see \( 3 \).) When we apply a level-4 CP-work extraction \( \{ \mathcal{E}_j, w_j \} \) to the system \( I \) with the initial state \( \rho_I \), the amount of the extracted work is \( w \) with the probability

\[
\sum_{x, y : w = h_x - h_y} T_{\{ \mathcal{E}_j, w_j \}}(y|x) P_X(x).
\]

(97)

**Proof:** Due to Lemma 12, the probability of the amount of the extracted work \( w \) is

\[
\sum_{j : w = w_j} \text{Tr} \mathcal{E}_j(\rho) = \sum_{j} \text{Tr} \mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\rho)) \delta_{w, w_j} = \sum_{j} \text{Tr} \mathcal{P}_{\hat{H}_I}(\mathcal{E}_j(\rho)) \delta_{w, w_j} \]

\[
= \sum_{j} \sum_{x, y} P_X(x) \langle y | \mathcal{E}_j (|x\rangle) |y\rangle \delta_{w, w_j} \]

\[
= \sum_{j} \sum_{x, y} P_X(x) \langle y | \mathcal{E}_j (|x\rangle) |y\rangle \delta_{w, h_x - h_y} \delta_{w, h_x - h_y} \]

\[
= \sum_{j} \sum_{x, y} P_X(x) \langle y | \mathcal{E}_j (|x\rangle) |y\rangle \delta_{w, h_x - h_y} \delta_{w, h_x - h_y} \]

\[
= \sum_{x, y : w = h_x - h_y} T_{\{ \mathcal{E}_j, w_j \}}(y|x) P_X(x).
\]

(98)

where (a) and (b) follow from (3), and (c) follows from (25).
Due to this theorem, in order to discuss the amount of extracted work in the level-4 CP-work extraction, it is sufficient to handle the classical description.

**Lemma 16** Given a level-4 CP-work extraction \( \{ \mathcal{E}_j, w_j \} \), when the CP-work extraction \( \{ \mathcal{E}_j, w_j \} \) is unital, the transition matrix \( T(\mathcal{E}_j, w_j) \) is bi-stochastic.

**Proof:** Since

\[
\sum_j \langle y | \mathcal{E}_j \rangle (\frac{i}{|x|}) \langle x | y \rangle = T(\mathcal{E}_j, w_j) \langle y | x \rangle \frac{1}{|x|},
\]

when the CP-work extraction \( \{ \mathcal{E}_j, w_j \} \) is unital, the transition matrix \( T(\mathcal{E}_j, w_j) \) is bi-stochastic. \( \square \)

**Lemma 17** Given a classical work extraction \( (\mathcal{X}, h_X, T) \), the transition matrix \( T \) is bi-stochastic if and only if there exists a standard FQ-work extraction \( \mathcal{F} \) such that \( (\mathcal{X}, h_X, T) = T(\mathcal{CP}(\mathcal{F})) \).

Lemma 16 will be shown after Lemma 18. Since the set of standard FQ-work extractions is considered as the set of preferable extraction, it is sufficient to optimize the performance under the set of classical work extractions with a bi-stochastic transition matrix.

As a subclass of bi-stochastic matrices, we consider the set of uni-stochastic matrices. A bi-stochastic matrix \( T \) is called uni-stochastic when there exists a unitary matrix \( U \) such that \( T(x|x') = |U_{x,x'}|^2 \). According to the discussion in Subsections IV.B and IV.C, we can consider a FQ-work extraction \( \mathcal{F} = (\mathcal{H}_{E_1}, \hat{H}_E, F[U_1], \rho_E) \), where \( \rho_E \) is a pure eigenstate of \( \hat{H}_E \). As mentioned in the end of Subsection IV.B since the corresponding CP-work extraction \( CP(\mathcal{F}) \) depends only on the internal unitary \( U_1 \), the CP-work extraction is denoted by \( CP(U_1) \). Then, we have the following lemma.

**Lemma 18** Given a classical work extraction \( (\mathcal{X}, h_X, T) \), when the transition matrix \( T \) is a uni-stochastic matrix satisfying \( T(x|x') = |U_{1x,x'}|^2 \) with a internal unitary \( U_1 \) then

\[
(\mathcal{X}, h_X, T) = T(\mathcal{CP}(U_1)).
\]

In the corresponding FQ-work extraction \( \mathcal{F} = (\mathcal{H}_{E_1}, \hat{H}_E, F[U_1], \rho_E) \), the entropy of the final state of external system is given as

\[
S(W) \geq S(Tr_1 F[U_1] (\rho_I \otimes \rho_E) F[U_1]^\dagger)
\]

for any pure eigenstate \( \rho_E \) of \( \hat{H}_E \).

**Proof:** The relation (100) can be shown from the definition of \( CP(U_1) \). The relation (101) can be shown in the same way as (9).

**Proof of Lemma 17:** Given a bi-stochastic matrix \( T \), there exist a probability distribution \( P_A(a) \) and a unitary matrix \( U_{I,a} \) such that

\[
T(y|x) = \sum_u P_A(a) |U_{I,a; x,y}|^2.
\]

Then, we choose the fully degenerate system \( \mathcal{H}_{E_2} \) spanned by \( \{ |a\rangle_{E_2} \} \) and the initial state \( \rho_{E_2} := \sum_a P_A(a) |a\rangle_{E_2} \langle a| \). We define the unitary \( U := \sum_a F[U_{I,a}] \otimes |a\rangle_{E_2} \langle a| \). So, we have \( (\mathcal{X}, h_X, T) = T(\mathcal{H}_{E}, \hat{H}_E, U, \rho_{E_1} \otimes \rho_{E_2}) \) for any pure state \( \rho_{E_1} \) on \( \mathcal{H}_{E_1} \).

As a special case of Lemma 18 we have the following lemma.

**Lemma 19** Given a classical work extraction \( (\mathcal{X}, h_X, f_x) \) with an invertible function \( f \), the unitary

\[
U_f : |x\rangle \mapsto |f(x)\rangle
\]

satisfies \( (\mathcal{X}, h_X, T) = T(\mathcal{H}_{E_1}, \hat{H}_E, F[U_f], \rho_E) \).

Therefore, any invertible and deterministic transition matrix \( T \) can be simulated by a shift-invariant FQ-work extraction only with the non-degenerate external system.
VII. OPTIMAL EFFICIENCY FOR HEAT ENGINE

A. Optimal efficiencies without catalyst

Now, we focus on the internal system $\mathcal{H}_I$ that consists of the hot and cold heat baths $\mathcal{H}_H$ and $\mathcal{H}_L$. These baths have the Hamiltonians $\hat{H}_H$ and $\hat{H}_L$, i.e., $\hat{H}_I = \hat{H}_H + \hat{H}_L$. Given an initial state $\rho_I$ of the internal system $\mathcal{H}_I = \mathcal{H}_H \otimes \mathcal{H}_L$ and a CP-work extraction $\{\mathcal{E}_j, w_j\}$, the amount of extracted work $W(\rho_I, \{\mathcal{E}_j, w_j\})$ and the endothermic energy amount $Q_H(\rho_I, \{\mathcal{E}_j, w_j\})$ are given as

$$W(\rho_I, \{\mathcal{E}_j, w_j\}) := \sum_j w_j \text{Tr} \mathcal{E}_j(\rho_I)$$

$$Q_H(\rho_I, \{\mathcal{E}_j, w_j\}) := \text{Tr}(\rho_I - \sum_j \mathcal{E}_j(\rho_I))\hat{H}_H.$$  

So, the efficiency $\eta_Q(\rho_I, \{\mathcal{E}_j, w_j\})$ is given as

$$\eta_Q(\rho_I, \{\mathcal{E}_j, w_j\}) := \frac{W(\rho_I, \{\mathcal{E}_j, w_j\})}{Q_H(\rho_I, \{\mathcal{E}_j, w_j\})}.$$  

Then, given an initial state $\rho_I$ of the internal system $\mathcal{H}_I$ and an endothermic energy amount $Q$, the optimal efficiency $\eta_Q[\rho_I, Q]$ is given as

$$\eta_Q[\rho_I, Q] := \sup_{\{\mathcal{E}_j, w_j\}: Q_H(\rho_I, \{\mathcal{E}_j, w_j\}) = Q} \eta_Q(\rho_I, \{\mathcal{E}_j, w_j\}),$$

where CP-work extractions $\{\mathcal{E}_j, w_j\}$ are restricted to unital and level-4 CP-work extractions in the above supremum.

Next, we consider the classical counterpart. For this purpose, we focus on the internal system that consists of the hot and cold heat baths $\mathcal{X}$ and $\mathcal{Y}$. These baths have the Hamiltonians $h_X$ and $h_Y$. Given an initial distribution $P_{XY}$ on the internal system $\mathcal{X} \times \mathcal{Y}$ and a classical work extraction $(\mathcal{X} \times \mathcal{Y}, h_X + h_Y, T)$, the amount of extracted work $W(P_{XY}, T)$ and the endothermic energy amount $Q_H(P_{XY}, T)$ are given as

$$W(P_{XY}, T) := \sum_{x,y,x',y'} (h_X(x) + h_Y(y) - h_X(x') - h_Y(y'))T(x', y|x, y)P_{XY}(x, y)$$

$$Q_H(P_{XY}, T) := \sum_{x,y,x',y'} (h_X(x) - h_X(x'))T(x', y|x, y)P_{XY}(x, y).$$

So, we define the efficiency $\eta_C(P_{XY}, T)$ in the following way.

$$\eta_C(P_{XY}, T) := \frac{W(P_{XY}, T)}{Q_H(P_{XY}, T)}.$$  

Then, given an initial distribution $P_{XY}$ and an endothermic energy amount $Q$, the optimal efficiency $\eta_C[P_{XY}, Q]$ is given as

$$\eta_C[P_{XY}, Q] := \sup_{T: Q_H(P_{XY}, T) = Q} \eta_C(P_{XY}, T),$$

where transition matrices $T$ are restricted to bi-stochastic in the above supremum.

For this purpose, we fix an orthonormal basis $\{|x\rangle\}_{x \in \mathcal{X}}$ of $\mathcal{H}_H$ and an orthonormal basis $\{|y\rangle\}_{y \in \mathcal{Y}}$ of $\mathcal{H}_L$.

Lemma 20 We assume that

$$\mathcal{P}_{H_I}(\rho_I) = \sum_{x,y} P_{XY}(x, y)|x, y\rangle\langle x, y| \quad (112)$$

$$\hat{H}_H = \sum_x h_X(x)|x\rangle\langle x| \quad (113)$$

$$\hat{H}_L = \sum_y h_Y(y)|y\rangle\langle y|. \quad (114)$$

Then,

$$\eta_Q[\rho_I, Q] = \eta_C[P_{XY}, Q]. \quad (115)$$
This lemma implies that it is sufficient to treat the classical setting for calculating the optimal efficiency \( \eta_Q[\rho_I, Q] \) when the condition (112) holds.

**Proof:** For any unital level-4 CP-work extraction \( \{\mathcal{E}_j, w_j\} \), we have
\[
W(\rho_I, \{\mathcal{E}_j, w_j\}) = \sum_j w_j \text{Tr} \mathcal{E}_j(\rho_I) = \sum_j w_j \text{Tr} \mathcal{E}_j(\mathcal{P}_{\mathcal{H}_i}(\rho_I)) = \sum_j w_j \sum_{x', y'} \langle x', y' | \mathcal{E}_j(\sum_{x,y} P_{XY}(x, y)|x, y\rangle \langle x, y| x', y' \rangle
\]
\[=W(P_{XY}, T_{\{\mathcal{E}_j, w_j\}}),
\]
\[Q_H(\rho_I, \{\mathcal{E}_j, w_j\}) = \text{Tr}(\rho_I - \sum_j \mathcal{E}_j(\rho_I))\hat{H}_H
\]
\[=\text{Tr}(\mathcal{P}_{\mathcal{H}_i}(\rho_I)) - \sum_j \mathcal{E}_j(\mathcal{P}_{\mathcal{H}_i}(\rho_I))\hat{H}_H
\]
\[=\sum_{x', y'} (P_{XY}(x', y') - \sum_{x,y} \langle x', y' | \mathcal{E}_j(\sum_{x,y} P_{XY}(x, y)|x, y\rangle \langle x, y| x', y' \rangle)h_X(x')
\]
\[=Q(P_{XY}, T_{\{\mathcal{E}_j, w_j\}}).
\]

Since the transition matrix \( T_{\{\mathcal{E}_j, w_j\}} \) is bi-stochastic, we obtain (115).

\[\blacksquare\]

**B. Optimal efficiency with catalyst**

Next, we consider the improvement by the catalyst, which is described by the system \( \mathcal{H}_C \). Then, the internal system \( \mathcal{H}_I \) is given as the composite system of two baths and the catalyst system, i.e., \( \mathcal{H}_I \otimes \mathcal{H}_L \otimes \mathcal{H}_C \). For a given initial state \( \rho_B \) on the bath system \( \mathcal{H}_I \otimes \mathcal{H}_L \), our work extraction is given as a pair of a CP-work extraction \( \{\mathcal{E}_j, w_j\} \) and a state \( \rho_C \) on the catalyst system \( \mathcal{H}_C \) that satisfies the following condition.
\[
\text{Tr}_{HL} \sum_j \mathcal{E}_j(\rho_B \otimes \rho_C) = \rho_C.
\]

Note that the condition (117) depends on the initial state \( \rho_B \) on the bath system. Here, there is a possibility that the state \( \rho_C \) is not preserved when the state in the bath \( \mathcal{H}_I \) is different from \( \rho_B \). Then, the amount of extracted work \( W_C(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\}) \) and the endothermic energy amount \( Q_{HC}(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\}) \) are given as
\[
W_C(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\}) := \sum_j w_j \text{Tr} \mathcal{E}_j(\rho_B \otimes \rho_C)
\]
\[Q_{HC}(\rho_I, \rho_C, \{\mathcal{E}_j, w_j\}) := \text{Tr}(\rho_B \otimes \rho_C - \sum_j \mathcal{E}_j(\rho_B \otimes \rho_C))\hat{H}_H.
\]

So, the efficiency \( \eta_{QC}(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\}) \) is given as
\[
\eta_{QC}(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\}) := \frac{W_C(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\})}{Q_{HC}(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\})}
\]

Then, given an initial state \( \rho_B \) on the bath system and an endothermic energy amount \( Q \), the optimal efficiency \( \eta_{QC}[\rho_B, Q] \) is given as
\[
\eta_{QC}[\rho_B, Q] := \sup_{\rho_C, \{\mathcal{E}_j, w_j\}} \eta_{QC}(\rho_B, \rho_C, \{\mathcal{E}_j, w_j\}),
\]

where CP-work extractions \( \{\mathcal{E}_j, w_j\} \) are restricted to unital and level-4 CP-work extractions in the above supremum. In the above supremum, there is no restriction for the dimension of the catalyst system \( \mathcal{H}_C \).

Hence, we find the following relation.
\[
\eta_Q[\rho_B, Q] \leq \eta_{QC}[\rho_B, Q].
\]
Indeed, it is not easy to characterize $\eta_{QC}[\rho_B, Q]$ in a classical way similar to the case of $\eta_Q[\rho_I, Q]$. This is because it is hard to reduce the efficiency $\eta_{QC}(\rho_B, \rho_C; \{E_j, w_j\})$ to a classical case when the catalyst state $\rho_C$ is not commutative with the Hamiltonian $\hat{H}_C$. Instead of such a classical reduction, we can evaluate the optimal efficiency $\eta_{QC}[\rho_B, Q]$ in the following way when the states in hot and cold baths are Gibbs states.

**Theorem 5** When both heat baths $H$ and $L$ are initially in Gibbs states $\rho_{\beta_H}|\hat{h}_A\rangle := \exp(-\beta_H \hat{H}_H)/\text{Tr}[\exp(-\beta_H \hat{H}_H)]$ and $\rho_{\beta_L}|\tilde{h}_A\rangle := \exp(-\beta_L \hat{H}_L)/\text{Tr}[\exp(-\beta_L \hat{H}_L)]$, we have

$$\eta_{QC}[\rho_{\beta_H}|\hat{h}_A\rangle \otimes \rho_{\beta_L}|\tilde{h}_A\rangle, Q] \leq \left(1 - \frac{\beta_H}{\beta_L}\right)^2 \cdot \frac{D(\rho_{\beta_H}|\hat{h}_A\rangle \| \rho_{\beta_H}|\tilde{h}_A\rangle) + D(\rho_{\beta_L}|\tilde{h}_A\rangle \| \rho_{\beta_L}|\hat{h}_A\rangle)}{\beta_L Q},$$

(123)

where the real numbers $\beta_H$ and $\beta_L$ are determined by

$$\text{Tr}(\rho_{\beta_H}|\hat{h}_A\rangle - \rho_{\beta_H}|\tilde{h}_A\rangle) \hat{H}_H = Q,$$

(124)

$$S(\rho_{\beta_H}|\hat{h}_A\rangle) + S(\rho_{\beta_L}|\tilde{h}_A\rangle) = S(\rho_{\beta_H}|\hat{h}_A\rangle) + S(\rho_{\beta_L}|\tilde{h}_A\rangle).$$

(125)

**VIII. CARNOYSIS THEOREM FOR FINITE-SIZE SYSTEMS**

**A. Heat engine with $n$-particle heat baths**

Now, we consider the two heat baths $H^{\otimes n}$ and $L^{\otimes n}$ that are composed of $n$ uncorrelated identical particles. The Hamiltonian of the $n$-particle heat baths are written as $H^{(n)} := \sum_{k=1}^n \hat{H}^{(k)}$ and $\hat{H}_L^{(n)} := \sum_{k=1}^n \hat{H}_L^{(k)}$, where $\hat{H}_H^{(k)} = \hat{H}_H$ and $\hat{H}_L^{(k)} = \hat{H}_L$ are the Hamiltonians of the $k$th particle of $H$ and $L$, respectively. We assume that the dimensions of $H$ and $L$ are finite and are the same value $d$, but do not assume that the Hamiltonians $H_H$ and $H_L$ are the same. In this case, the respective Gibbs states with the inverse temperature $\beta_H$ and $\beta_L$ are the $n$-fold tensor product states $\rho_{\beta_H}|\hat{h}_A\rangle \otimes \rho_{\beta_L}|\tilde{h}_A\rangle$, respectively. Then, we discuss the optimal efficiency $\eta_{QC}[\rho_{\beta_H}^{\otimes n}|\hat{h}_A\rangle \otimes \rho_{\beta_L}^{\otimes n}|\tilde{h}_A\rangle, Q]$.  

In order to describe the asymptotic behavior of the optimal efficiency, we introduce the energy variance and the energy skewness of each particle of the heat baths:

$$\sigma_A^2(\beta) := \text{Tr}[\rho_{\beta_H}|\hat{h}_A\rangle \hat{H}_A^2] - (\text{Tr}[\rho_{\beta_H}|\hat{h}_A\rangle \hat{H}_A])^2,$$

and $\gamma_1(\beta) := \text{Tr}[\rho_{\beta_H}|\hat{h}_A\rangle (\hat{H}_A - \text{Tr}[\rho_{\beta_H}|\hat{h}_A\rangle \hat{H}_A])^3]/\sigma_A^3(\beta)$

(126)

for $A = H, L$. Then, we have the following theorem.

**Theorem 6** When a sequence of real numbers $\{Q_n\}_{n=1}^{\infty}$ satisfies $\lim_{n \to \infty} Q_n/n = 0$, the upper bound (123) has an asymptotic expansion as follows:

$$\eta_{QC}[\rho_{\beta_H}^{\otimes n}|\hat{h}_A\rangle \otimes \rho_{\beta_L}^{\otimes n}|\tilde{h}_A\rangle, Q] \leq \left(1 - \frac{\beta_H}{\beta_L}\right)^2 \cdot \sum_{k=1}^n c^{(k)}_{\beta_H, \beta_L} q_k + O(q_n^3),$$

(127)

where $q_n := Q_n/n$ and

$$c^{(1)}_{\beta_H, \beta_L} := \frac{1}{2\beta_H^2 \sigma^2(\beta_H)} + \frac{1}{2\beta_L^2 \sigma^2(\beta_L)} \cdot \frac{\beta_H^2}{\beta_L},$$

(128)

$$c^{(2)}_{\beta_H, \beta_L} := \frac{-\gamma_1(\beta_H)}{6\beta_H^2 \sigma^3(\beta_H)} + \frac{\gamma_1(\beta_L)}{6\beta_L^2 \sigma^3(\beta_L)} + \frac{1}{2\beta_L^2 \sigma^4(\beta_L)} + \frac{1}{2\beta_H^2 \beta_L^2 \sigma^2(\beta_H) \sigma^2(\beta_L)} \cdot \frac{\beta_H^3}{\beta_L^3}.$$  

(129)

Further, we define the Gibbs distribution $P_{\beta|h}$ as $P_{\beta|h}(x) := \exp(-\beta h(x))/\sum_{x'} \exp(-\beta h(x'))$.

To discuss the attainability of the upper bound (127), we consider the classical work extraction. For classical work extraction, we define $\sigma_A^2(\beta)$ and $\gamma_1(\beta)$ in the same was the quantum case. Then, we introduce a condition for a function $h$. A function $h$ is called lattice when there exists a positive number $t$ such that $\{h(x) - h(x')\}_{x, x'} \in t \mathbb{Z}$. Then, the lattice span is defined as the maximum value of the above positive value $t$. When there does not exist such a non-negative value $t$, a function $h$ is called non-lattice.
Theorem 7 Assume that the number of elements of \( \mathcal{X} \), \( \mathcal{Y} \) is less than \( d \), respectively. When a sequence of real numbers \( \{Q_n\} \) satisfies \( \lim_{n \to \infty} Q_n/n = 0 \), there exists a sequence of invertible functions \( \{f_n\} \) on \( (\mathcal{X} \times \mathcal{Y})^n \) such that

\[
\eta_C(P^n_{\beta X|h_X}P^n_{\beta Y|h_Y}, f_n) = \left(1 - \frac{\beta_X}{\beta_Y}\right) - c^{(1)}_{\beta_X, \beta_Y} q_n + O\left(\frac{1}{n}\right) + O\left(\frac{Q_n^2}{n^2}\right),
\]

(130)

\[
Q_C(P^n_{\beta X|h_X}P^n_{\beta Y|h_Y}, f_n) = nq_n + O\left(\frac{1}{n} q_n^2\right),
\]

(131)

\[
S(W) \leq 4(d - 1) \log(n + 1),
\]

(132)

where \( q_n := Q_n/n \). Further, when we assume that \( h_X \) and \( h_Y \) are non-lattice, in addition to the above conditions, the conditions (120) and (131) can be replaced by the following conditions:

\[
\eta_C(P^n_{\beta X|h_X}P^n_{\beta Y|h_Y}, f_n) = \left(1 - \frac{\beta_X}{\beta_Y}\right) - c^{(1)}_{\beta_X, \beta_Y} q_n - c^{(2)}_{\beta_X, \beta_Y} q_n^2 - d^{(1)}_{\beta_X, \beta_Y} q_n + O\left(\frac{q_n^2}{\sqrt{n}}\right) + O\left(q_n^3\right),
\]

(133)

\[
Q_C(P^n_{\beta X|h_X}P^n_{\beta Y|h_Y}, f_n) = nq_n + O\left(\frac{1}{n} q_n^3\right),
\]

(134)

where

\[
d^{(1)}_{\beta_X, \beta_Y} := \left(\frac{\gamma(\beta_X)}{2\beta_X \sigma(\beta_X)} + \frac{1}{2\beta_X \sigma^2(\beta_X)}\right)^2 + \left(\frac{\gamma(\beta_Y)}{2\beta_Y \sigma(\beta_Y)} + \frac{1}{2\beta_Y \sigma^2(\beta_Y)}\right)^2 \beta_X^2.
\]

(135)

We will give \( f_n \) concretely in the subsection VIII.B.

Combining Lemma 20 and Theorems 6 and 7, we obtain the main result of the present section:

Theorem 8 Assume (113) and (114). When \( \{Q_n\}_{n=1}^{\infty} \) satisfies \( \lim_{n \to \infty} Q_n/n = 0 \), the following equality holds:

\[
\eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] = \eta_C(P^n_{\beta H|h_H}P^n_{\beta L|h_L}, Q_n) = \eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] + o\left(\frac{Q_n}{n}\right)
\]

\[
= \left(1 - \frac{\beta_H}{\beta_L}\right) - c^{(1)}_{\beta_H, \beta_L} Q_n + O\left(\frac{1}{n}\right) + O\left(\frac{Q_n^2}{n^2}\right).
\]

(136)

Further, when we assume that \( h_X \) and \( h_Y \) are non-lattice, in addition to the above conditions, the following equality holds:

\[
\eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] = \eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] = \eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] + o\left(\frac{Q_n}{n^2}\right)
\]

\[
= \left(1 - \frac{\beta_H}{\beta_L}\right) - c^{(1)}_{\beta_H, \beta_L} Q_n - c^{(2)}_{\beta_H, \beta_L} Q_n + O\left(\frac{Q_n^2}{n^2}\right).
\]

(137)

Further, there exists a sequence of standard FQ-work extractions \( F_n = (H_{E,n}, \hat{H}_{E,n}, U_n, \rho_{E,n}) \) that attains the above bounds and satisfies

\[
S(\text{Tr}_U U_n(\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n} \otimes \rho_{E,n} U_n^\dagger)) \leq 4(d - 1) \log(n + 1).
\]

(138)

Unlike (127) and (128), the equality (137) is not just an upper bound for the optimal efficiencies \( \eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] \), \( \eta_C(P^n_{\beta H|h_H}P^n_{\beta L|h_L}, Q_n) \) and \( \eta_Q[\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n}, Q_n] \); it is an approximate equality for them. It gives us a computable approximation of the optimal efficiencies of the quantum heat engines with finite-size heat baths with the error of the order \( Q_n/n^2 \). The equality (138) gives a statistical-mechanical proof of the achievability of the Carnot efficiency at the macroscopic limit as a corollary, because the righthand-side of (137) converges into Carnot’s inequality at the limit of \( n \to \infty \). The equality (138) also evaluates the effect of the catalyst on the optimal efficiency. When the initial states of the heat baths are diagonalized by the energy eigenstates, the effect of catalyst on the optimal efficiency is at most the order of \( O(Q_n/n^2) \). Thus, when we use the heat baths which are initially in Gibbs states, the effect of catalyst on the optimal efficiency is very small in our formulation.

The relation (138) can be shown by (101) of Lemma 13 and (132) of Lemma 7. This relation shows that the entropy in the external system increases only with the order \( \log n \). That is, the regularized entropy goes to zero as

\[
\lim_{n \to \infty} \frac{1}{n} S(\text{Tr}_U U_n(\rho_{\beta H}^{\otimes n} \otimes \rho_{\beta L}^{\otimes n} \otimes \rho_{E,n} U_n^\dagger)) = 0.
\]

(139)

This fact shows us that the extracted work is extremely ordered energy. We can extract the energy and the entropy from the hot heat bath, and store only the energy in the work storage.
B. Optimal work extraction

1. Classical work extraction

Firstly, for the classical baths \( P^n_{\beta_X|X} \) and \( P^n_{\beta_Y|Y} \), we concretely give work extractions to achieve the RHS of (133) in Theorem 7. The invertible function \( f_n \) is given with the following three steps. For this purpose, we introduce the descending reordered distributions \( P^n_{\beta_X|X} \) and \( P^n_{\beta_Y|Y} \) of the distributions \( P^n_{\beta_X|X} \) and \( P^n_{\beta_Y|Y} \), respectively. First, we convert the elements \( x \) and \( y \) in \( X^n \) and \( Y^n \) to the pair of integers \((i, j)\) in the set \( \mathbb{Z}^2_{d^n} \), by using the following two functions \( g_{1nX} \) and \( g_{1nY} \) as

\[
P^n_{\beta_Y|Y} (x) = P^n_{\beta_X|X} (g_{1nX} (x)), \quad P^n_{\beta_Y|Y} (y) = P^n_{\beta_X|X} (g_{1nY} (y)),
\]

which is equivalent with \( g_{1nX,*} (P^n_{\beta_X|X}) = P^n_{\beta_Y|Y} \) and \( g_{1nY,*} (P^n_{\beta_Y|Y}) = P^n_{\beta_X|X} \). That is, we apply the function \( g_{1n} (x, y) := \langle g_{1nX}(x), g_{1nY}(y) \rangle \) to the classical system \((X \times Y)^n\).

Next, we convert the states by the function \( g_{2n} \) defined as

\[
g_{2n} : (i_A d^m + j_B, i_B d^{n-m} + j_A) \mapsto (i_A + i_B d^m, j_A + j_B d^{n-m})
\]

for \( i_A, j_B \in \mathbb{Z}_{d^n} \) and \( i_B, j_A \in \mathbb{Z}_{d^{n-m}} \), where

\[
m_n := \left\lfloor \frac{\beta_X Q_n + \beta_Y (-S_X)}{2 d} \log d \right\rfloor.
\]

Finally, we apply the inverse function \( g_{1n}^{-1} \). So, the total function \( f_n \) is given as \( g_{1n}^{-1} \circ g_{2n} \circ g_{1n} \).

2. Quantum work extraction

Next, for the quantum baths \( \rho_{\beta_X|X}^{\otimes n} \) and \( \rho_{\beta_Y|Y}^{\otimes n} \), we concretely give quantum work extractions to achieve the RHS of (133). Our optimal operation is the standard FQ-work extraction given by a classical work extraction \( f_n \) via Lemma 19 as follows. Because \( f_n \) is an invertible function, due to Lemma 19 the standard FQ-work extraction \( F := T(\mathcal{H}_E, \mathcal{H}_E, F[U_{f_n}], \rho_E) \) realizes the same performance as the classical work extraction given by \( f_n \), i.e., \((X \times Y)^n, h_{XY}, f_{1n}) = T(\mathcal{C}(\mathcal{F})) \). That is, using the unitary \( F[U_{f_n}] \) on the total system, we can attain the bound (133). For the definition of \( F[U_{f_n}] \), see Lemmas 19 and 7. The unitary \( F[U_{f_n}] \) is given as the combination of sorting the diagonal elements of the internal system \( HL \) and transferring the energy loss of \( HL \) to the external system \( E \) as follows;

\[
F[U_{f_n}] := \sum_{x,y} |f_n(x, y)\rangle_{HL} \langle HL | x, y \rangle \otimes |e + h_{XY}(x, y) - h_{XY}(f_n(x, y))\rangle_{E} E \langle e|.
\]

To consider the physical meaning of \( F[U_{f_n}] \), we divide the unitary \( F[U_{f_n}] \) into three step, which correspond to the functions \( g_{1n}, g_{2n}, \) and \( g_{1n}^{-1} \). For this purpose, we need to describe the resultant system of the unitary corresponding to \( g_{1n} \) as \( n \)-fold tensor product systems of the qudit system. This is because the ranges of the functions \( g_{1nX} \) and \( g_{1nY} \) are \( \mathbb{Z}_{d^n} \) not the \( n \)-dimensional vector space of \( \mathbb{Z}_d \). To resolve this problem, we make the following correspondence between the set \( \mathbb{Z}_{d^n} \) and the \( n \)-dimensional vector space of \( \mathbb{Z}_d \). For a vector \( x := (x_1, \ldots, x_n) \in \mathbb{Z}_{d^n} \), we define the integer \( g_{3n}(x) \in \mathbb{Z}_d \) by we make a correspondence

\[
g_{3n}(x) = \sum_{k=1}^{n} x_k d^{k-1}.
\]

Hence, we can decompose \( F[U_{f_n}] \) into the following three steps;

**Step 1** \( F[U_{g_{2n}^{-1} \circ g_{3n}}] \): By the following unitary \( F[U_{g_{2n}^{-1} \circ g_{3n}}] \), we first reorder the diagonal elements of \( \rho_{\beta_X|X}^{\otimes n} \) and \( \rho_{\beta_Y|Y}^{\otimes n} \) so that the eigenvalues are arrayed in the descending order. Then, we set the resultant state in the \( n \)-fold qudit systems with the correspondence (144).

\[
F[U_{g_{3n}^{-1} \circ g_{1n}}] := \sum_{x,y} \sum_{e} |g_{3n}^{-1}(g_{1nX}(x, y), g_{3n}^{-1}(g_{1nY}(x, y)))\rangle_{HL} \langle HL | x, y \rangle \otimes |e + h_{XY}(x, y) - h_{XY}(g_{1nX}(x, y))\rangle_{E} E \langle e|.
\]
Step 2 ($F[U_{g_{3n}}]$): By the following unitary $F[U_{g_{3n}}]$, we reorder the particles as Fig. 4:

$$F[U_{g_{3n}}] := \sum_{x,y} \sum_{e} |x_{m_{n}+1}, \ldots, x_{n}, y_{n-m_{n}+1}, \ldots, y_{n}\rangle_H H \langle x_{1}, \ldots, x_{n}| \otimes |x_{1}, \ldots, x_{m_{n}}, y_{1}, \ldots, y_{n-m_{n}}\rangle_L L \langle y_{1}, \ldots, y_{n}|$$

$$\otimes |e + h_{XY}(x,y) - h_{XY}(x_{m_{n}+1}, \ldots, x_{n}, y_{n-m_{n}+1}, \ldots, y_{n}, x_{1}, \ldots, x_{m_{n}}, y_{1}, \ldots, y_{n-m_{n}})\rangle E \langle e|.$$  

(146)

Step 3 ($F[U_{g_{3n}^{-1} o g_{1n}}]$): Finally, we perform the inverse process of the first step, i.e., we perform $F[U_{g_{3n}^{-1} o g_{1n}}]^\dagger$.

The physical meanings of the above steps are given as follows. To discuss the first step, we notice that $F_{\beta_{H}}^{n_{i}} |h_{X}(i)\rangle \approx 0$ when $i$ is large, and that $\sum_{i=1}^{n_{i} - m_{n}} P_{\beta_{H}^{n}} |h_{X}^{n_{i}}(i)\rangle \approx d^{-m_{n}}$ when $m_{n}$ is small. Under the correspondence (144), this fact can be interpreted in the following way. In the hot bath $H$, when the particle of our interest is close to the $n$-th particle, the state is almost the ground state, i.e., the particle is extremely cold. Similarly, when the particle of our interest is close to the first particle, the state is almost $1/d$, which is the Gibbs state of the infinite temperature, i.e., the particle is extremely hot. Therefore, by the operation in the first step, the energy is compressed into particles with earlier numbers. The operation in the first step does not increase the entropy in the both baths $H$ and $L$ because it is a sorting on $H$ and $L$. Hence, the resultant states have higher energy than the initial states in both baths because the initial states in both baths have the minimum energy under the same entropy. So, to realize the first step, we need to insert additional energy from the external system to both baths.

The meaning of the second step is easy. It just swaps the extremely hot particles in the hot bath and the extremely cold particles in the cold bath. When both baths have the same Hamiltonian, we need no additional energy in the second step. Finally, the third step diffuses the energy in both baths by the inverse operation of the first step. Then, the resultant states in both baths $H$ and $L$ become very close to the Gibbs states whose temperatures are $\beta_{H}^{n}$ and $\beta_{L}^{n}$. In the third step, the external system recovers a larger amount of energy than the amount of energy inserted in the first step. The amount of extracted work is the difference between the recovered and inserted energies.

We see intuitively why the operation is optimal in the physical viewpoint as follows. In order to maximize the efficiency of the heat engine, we have to transfer the entropy from the hot bath to the cold bath as efficiently as possible. Our operation exchanges the maximum entropy state and the zero entropy state between $H$ and $L$.

Finally, we point out that the optimal work extraction is an example of the heat engine which turns the disordered energy to the ordered energy. In order to illustrate this fact, we give Figure 5 as the schematic diagram. During the unitary $F[U_{f_{n}}]$, the entropy and the energy of $H$, $L$ and $E$ changes respectively. The hot bath $H$ loses the energy $Q_{n}$ and the entropy $m_{n} \log d$. The cold bath $L$ obtains the energy $(1 - \eta_{Q})Q_{n}$ and the entropy $m_{n} \log d$, and the work storage $E$ obtains the energy $\eta_{Q}Q_{n}$ and the entropy $\Delta S_{W} \leq 4(d - 1) \log n$. In order to assess the quality of the energy loss and the energy gains, let us refer to the ratio of the entropy difference to the energy difference as $A_{H}$, $A_{L}$ and $A_{E}$. Because the order of $\eta_{Q}$ is 1 and because the order of $m_{n}$ is
that Type-2 finiteness is specific to our results. In the following, we discuss Type-1 finiteness, i.e., the finiteness of framework of thermodynamics.

Both Hamiltonian are non-lattice, the difference between the optimal efficiency and the Carnot efficiency is evaluated as can be discussed in thermodynamics, however Type-2 finiteness cannot be discussed in thermodynamics. So, we can consider the energy gain of equal to the order of $Q_n$, 

$$A_H = \frac{m_n \log d}{Q_n} = O(1), \quad A_L = \frac{m_n \log d}{(1 - \eta Q_n)Q_n} = O(1), \quad A_E = \frac{\Delta S_W}{\eta Q_n} \leq \frac{4(d - 1) \log n}{\eta Q_n} = O\left(\frac{\log n}{Q_n}\right) \tag{147}$$

holds. Thus, when $Q_n = an^b$ holds with the real numbers $0 < a$ and $0 < b < 1$, the energy gain of $E$ is much better than the energy loss of $H$ in quality. Moreover, the entropy gain of $E$ is so negligibly small as compared with the energy gain $Q_n\eta Q$ in this case. Therefore, we can interpret the energy gain of $E$ as the extremely ordered energy. In order to raise the quantity of the energy gain of $E$, the cold bath $L$ is put at a disadvantage; $A_H \leq A_L$ always holds. In this meaning, we can interpret the optimal work extraction as the entropy filter; it filters out the entropy from the energy flow into $E$.

IX. DISCUSSION FOR FINITE-SIZE EFFECT

A. Two kinds of finiteness in our result

We firstly consider the situation that $Q_n = q n$ with infinitesimal small $q$. Under this situation, Theorems 6 and 7 can be converted to the following way because these theorems covers the case with an arbitrary speeds of convergence $\frac{Q_n}{n} \to 0$. When both Hamiltonian are non-lattice, the difference between the optimal efficiency and the Carnot efficiency is evaluated as

$$-\sum_{k=1}^{2} c^{(k)}_{\beta_H, \beta_L} q^k - d^{(1)}_{\beta_H, \beta_L} \frac{q}{n} + O\left(\frac{q^2}{\sqrt{n}}\right) + O(q^3) \leq \eta Q c_{\beta_H}[\rho_{n}^{\beta_H|\beta_H} \otimes \rho_{n}^{\beta_L|\beta_L}, q^n] - \left(1 - \frac{\beta_H}{\beta_L}\right) \leq -\sum_{k=1}^{2} c^{(k)}_{\beta_H, \beta_L} q^k + O(q^3). \tag{148}$$

Taking the limit $n \to \infty$, we have

$$\lim_{n \to \infty} \eta Q c_{\beta_H}[\rho_{n}^{\beta_H|\beta_H} \otimes \rho_{n}^{\beta_L|\beta_L}, q^n] = \left(1 - \frac{\beta_H}{\beta_L}\right) -\sum_{k=1}^{2} c^{(k)}_{\beta_H, \beta_L} q^k + O(q^3). \tag{149}$$

So, in this scenario, we can consider two kinds of finiteness as follows.

Type-1 finiteness: One is the finiteness of $q$. Since this type of finiteness can be regarded as the ratio between the amount of energy and the number of particle, it can be regarded as a relative finiteness. The terms $c^{(1)}_{\beta_H, \beta_L} q$ and $c^{(2)}_{\beta_H, \beta_L} q^2$ reflect Type-1 finiteness.

Type-2 finiteness: The other is the finiteness of $n$. In contrast with Type-1 finiteness, the latter can be regarded as the absolute finiteness. The term $d^{(1)}_{\beta_H, \beta_L} \frac{q}{n}$ reflects Type-2 finiteness as well as Type-1 finiteness.

We need to care about the difference of these two kinds of finiteness. As explained in the latter subsection, Type-1 finiteness can be discussed in thermodynamics, however Type-2 finiteness cannot be discussed in thermodynamics. So, we can consider that Type-2 finiteness is specific to our results. In the following, we discuss Type-1 finiteness, i.e., the finiteness of $q$ in the framework of thermodynamics.
B. Changes of the temperatures of the heat baths

Type-1 finiteness is related to the changes of the temperatures of the heat baths. This is because the temperatures are almost preserved when Type-1 finiteness is negligible. In the framework of thermodynamics, the changes of the temperatures of the heat baths cause the decrease of the efficiency. As shown in (149), even when Type-2 finiteness is negligible, the efficiency is smaller than the Carnot efficiency due to Type-1 finiteness, i.e., the finiteness of \( q \). Here, we consider how the decrease of the efficiency in (149) can be explained in terms of the changes of the temperatures of the heat baths in our framework. For this explanation, we define \( T_{ij}^n(E) \) as the inverse function of the internal energy \( E_{H}^n(1/T) := \text{Tr}[\hat{H} \hat{p}_{1/T} | H] \). Additionally, we introduce the pseudo-temperatures of the final state of the heat baths of the optimal work extraction:

\[
\begin{align*}
\tilde{T}_H &= T_{H}^{(n)}(\text{Tr}[\hat{H}^{(n)} \hat{p}_{\beta_H} | H^{(n)}]) - Q_n, \\
\tilde{T}_L &= T_{L}^{(n)}(\text{Tr}[\hat{H}^{(n)} \hat{p}_{\beta_L} | H^{(n)}]) + (1 - \eta QC)Q_n,
\end{align*}
\]

where \( \text{Tr}[\hat{H}^{(n)} \hat{p}_{\beta_H} | H^{(n)}] - Q_n \) and \( \text{Tr}[\hat{H}^{(n)} \hat{p}_{\beta_L} | H^{(n)}] + (1 - \eta QC)Q_n \) are the internal energies of the final state of the optimal work extraction.

Although the temperatures \( \tilde{T}_H \) and \( \tilde{T}_L \) are the temperatures of the states \( \rho_{1/T}^H \hat{p}_{\beta_H} | H \) and \( \rho_{1/T}^L \hat{p}_{\beta_L} | H_L \), these states are not true final states in the our optimal work extraction. Note that the final states are not necessarily Gibbs states. Hence, the temperatures \( \tilde{T}_H \) and \( \tilde{T}_L \) cannot be regarded as the temperatures of the final states. So, the temperatures \( \tilde{T}_H \) and \( \tilde{T}_L \) might be considered to be the virtual temperatures of the final states. When Type-2 finiteness is negligible, our optimal efficiency given in (149) can be expressed by using these virtual temperatures as

\[
(1 - \frac{\beta_H}{\beta_L}) \cdot c^{(1)}_{\beta_H, \beta_L} \frac{Q_n}{n} + O\left(\frac{Q_n^2}{n^2}\right) = 1 - \frac{1}{2} (\frac{\tilde{T}_H + \tilde{T}_L}{T_H + T_H})
\]

The RHS of (152) is Carnot efficiency whose temperatures are replaced by the average temperature \( (T_H + \tilde{T}_H)/2 \) and \( (T_L + \tilde{T}_L)/2 \). The equation (152) shows that the decrease of the optimal efficiency is essentially caused by the change of the temperatures of the heat baths.

\textbf{Proof of (152):} We firstly transform (152) as follows

\[
1 - \frac{1}{2} (\tilde{T}_H + \tilde{T}_L) = 1 - \frac{T_L(1 + \tilde{T}_L - T_H)}{T_H(1 + \tilde{T}_L - T_H)} = 1 - \frac{T_L}{T_H} \left(1 + \frac{\tilde{T}_L - T_L}{2T_L}\right) \left(1 - \frac{\tilde{T}_H - T_H}{2T_H}\right) + O\left(\left(\frac{\tilde{T}_H - T_H}{2T_H}\right)^2\right)
\]

\[
= 1 - \frac{T_L}{T_H} \left(\frac{T_H(\tilde{T}_H - T_H)}{2T_L}\right) + O\left(\frac{T_H(\tilde{T}_H - T_H)}{2T_H}\right) + O\left(\frac{\tilde{T}_L - T_L}{2T_L}\right) + O\left(\left(\frac{\tilde{T}_H - T_H}{2T_H}\right)^2\right)
\]

As we show below, the temperatures \( \tilde{T}_H \) and \( \tilde{T}_L \) satisfy

\[
\begin{align*}
T_H - \tilde{T}_H &= \frac{1}{\beta_H^2 \sigma_H^2(\beta_H)} \frac{Q_n}{n} + O\left(\frac{Q_n^2}{n^2}\right), \\
\tilde{T}_L - T_L &= \frac{1}{\beta_L^2 \sigma_L^2(\beta_L)} \frac{Q_n}{n} + O\left(\frac{Q_n^2}{n^2}\right).
\end{align*}
\]

Substituting (154) and (155) in (153), we obtain (152). Finally, we prove (154) and (155). Because of (150), we can rewrite (124) as follows:

\[
\tilde{T}_H = T_{H}^{(n)} \left(E_{H}^{(n)}(1/T_H) - Q_n\right) = T_{H}^{(n)} \left(E_{H}^{(n)}(1/T_H) - \frac{Q_n}{n}\right).
\]
Therefore, we obtain (154) as follows

\[ T_H^i - T_H = T_H^{(n)} \left( E_H^{(n)}(1/T_H) - Q_n \right) - T_H^{(n)} \left( E_H^{(n)}(1/T_H) \right) \]

\[ = - \frac{dE_H(E)}{dE} \bigg|_{E=E_H^{(n)}(1/T_H)} \frac{Q_n}{n} + O \left( \frac{Q_n^2}{n^2} \right) \]

\[ = \frac{1}{\beta_H^2 \sigma_H(\beta_H)} \frac{Q_n}{n} + O \left( \frac{Q_n^2}{n^2} \right). \]  \hspace{1cm} (157)

We can derive (155) in the same manner.

\[ \square \]

\section{C. Relation with thermodynamics}

As shown in the previous subsection, the decrease of the optimal efficiency is caused by the changes of the temperatures of the heat baths. This kind of effect can be treated by thermodynamics [2]. Now, when Type-2 finiteness is negligible, we derive the optimal efficiency (149) in the framework in the following way. At first, we follow Ref. [2] and give the framework of thermodynamics:

\textbf{(1) Equilibrium states and thermalization assumption:} In the present framework, we treat the three thermodynamical systems; the reservoirs \( R_H \) and \( R_L \), and the working body \( W \). The reservoirs \( R_H \) and \( R_L \) correspond to the heat baths \( H \) and \( L \) respectively, and the working body \( W \) corresponds to the catalyst \( C \). Unlike \( H \), \( L \) and \( C \), we assume that the thermodynamical systems \( R_H \), \( R_L \) and \( W \) are the macroscopic systems, i.e., they are composed of the infinitely large number of particles. We also request the thermalization assumption that the states of the isolated macroscopic system becomes the thermodynamical equilibrium after enough long time. We describe the thermodynamical equilibrium states of \( R_H \), \( R_L \) and \( W \) as \((E_{R_H}, M_{R}, X_{R_H}), (E_{R_L}, M_{R}, X_{R_L}) \) and \((E_W, M_W, X_W)\), where \( E \) is the thermodynamical temperature, \( M \) is the amount of the substance and \( X \) is the set of other extensive variables. In the present article, we consider the situation that the particle numbers of two heat baths are the same. Therefore, we set the amounts of the substance of two heat baths are the same. Note that the amount of substance \( M \) is different from the particle number \( n \) in the statistical-mechanical setup. For example, even when \( M = 1 \), the thermodynamical system consists of infinitely many particles. The amount \( M \) of substance expresses the situation that we take the particle number as \( n = M \) and take the limit of \( n \to \infty \). In this case, the thermodynamical potential is the thermodynamical entropy \( S(E, M, X) \). Note that we can obtain all of the features from the thermodynamical potential, e.g., \( \frac{1}{T(E, M, X)} = \frac{\partial S}{\partial E} \), where \( T(E, M, X) \) is the thermodynamical temperature.

\textbf{(2) Adiabatic process:} We extract work from \( R_H R_L W \), through the adiabatic operation. We request the following three assumptions for the adiabatic operation. First, we assume the first law of thermodynamics, which guarantees that the extracted work \( W_{ad} \) of the adiabatic operation from \((E_{R_H}, M_{R}, X_{R_H}) \times (E_{R_L}, M_{R}, X_{R_L}) \times (E_W, M_W, X_W)\) to \((E_{R_H}, M_{R}, X_{R_H}') \times (E_{R_L}, M_{R}, X_{R_L}') \times (E_W', M_W, X_W')\) satisfies

\[ W_{ad} = E_{R_H} + E_{R_L} + E_W - E_{R_H}' - E_{R_L}' - E_W'. \]  \hspace{1cm} (158)

Second, we assume the law of entropy increase, i.e., an adiabatic operation from \((E_{R_H}, M_{R}, X_{R_H}) \times (E_{R_L}, M_{R}, X_{R_L}) \times (E_W, M_W, X_W)\) to \((E_{R_H}', M_{R}, X_{R_H}') \times (E_{R_L}', M_{R}, X_{R_L}') \times (E_W', M_W, X_W')\) is possible only if the following inequality holds;

\[ S(E_{R_H}, M_{R}, X_{R_H}) + S(E_{R_L}, M_{R}, X_{R_L}) + S(E_W, M_W, X_W) \]

\[ \leq S(E_{R_H}', M_{R}, X_{R_H}') + S(E_{R_L}', M_{R}, X_{R_L}') + S(E_W', M_W, X_W'). \]  \hspace{1cm} (159)

Third, for arbitrary \( E < E' \) and \( X \), we assume the existence of the adiabatic operation that transforms \((E, M, X)\) to \((E', M, X)\). Combining the thermalization assumption, we can perform the adiabatic quasi-static operation, i.e., by controlling the thermodynamical variables very slowly, we can make the state of the system be in thermal equilibrium along the adiabatic process. Because the adiabatic quasi-static operation is reversible, the adiabatic quasi-static operation does not change the entropy. Then, combining the second and third assumptions and the existence of the quasi-static operation, we can prove that the inequality (159) is a necessary and sufficient condition for the existence of the adiabatic operation from \((E_{R_H}, M_{R}, X_{R_H}) \times (E_{R_L}, M_{R}, X_{R_L}) \times (E_W, M_W, X_W)\) to \((E_{R_H}', M_{R}, X_{R_H}') \times (E_{R_L}', M_{R}, X_{R_L}') \times (E_W', M_W, X_W')\) [2].

\textbf{(3) The cyclic heat engine and the optimal efficiency:} Let us define the efficiency of the cyclic adiabatic process, which transforms \((E_{R_H}, M_{R}, X_{R_H}) \times (E_{R_L}, M_{R}, X_{R_L}) \times (E_W, M_W, X_W)\) to \((E_{R_H}', M_{R}, X_{R_H}') \times (E_{R_L}', M_{R}, X_{R_L}') \times (E_W', M_W, X_W')\).
We define the endothermic energy amount \( Q_{\text{ad}} := E_{RH} - E'_{RH} \), and define the optimal efficiency

\[
\eta_{\text{ad}}[(E_{RH}, M_R, X_{RH}), (E_{RL}, M_R, X_{RL}), Q] := \sup_{E_{RH}, E'_{RH}, Q = Q_{\text{ad}}} \frac{W_{\text{ad}}}{Q_{\text{ad}}},
\]

(161)

Theorem 9

In order to compare the prediction of thermodynamics and Theorem 8, we have to assume that the thermodynamical temperature has the same form as the function of the internal energy as the statistical-mechanical temperature. Namely, we assume that

\[
T(E_{RH}, M_R, X_{RH}) = T_{H}^{(MR)}(E_{RH}), \quad T(E_{RL}, M_R, X_{RL}) = T_{H}^{(MR)}(E_{RL}), \quad T(E_W, M_W, X_W) = T_{H}^{(MR)}(E_W)
\]

where \( T_{H}(E) \) is given in the previous section. Under (162), the thermodynamical heat bath whose amount of substance is \( M_R \) has the same internal energy as the statistical heat bath whose particle number is \( M_R \), at the same temperature. Note that this is just a renormalization for parameters. The bath is characterized by the amount \( M \) of substance as a thermodynamical variable. However, we should remark that the amount \( M \) of substance does not express the number of particles in the bath, which is a statistical-mechanical variable.

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\]

(162)

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Under the above setup, as shown in Appendix A, the following theorem holds;

**Theorem 9** When \( \beta_H = 1/T(E_{RH}, M_R, X_{RH}) \) and \( \beta_L = 1/T(E_{RL}, M_R, X_{RL}) \) hold, the following expressions hold;

\[
\eta_{\text{ad}}[(E_{RH}, M_R, X_{RH}), (E_{RL}, M_R, X_{RL}), Q] = 1 - \frac{E_{RL}^{\text{quasi}} - E_{RL}}{Q},
\]

(163)

where \( E_{RL}^{\text{quasi}} \) is defined by

\[
S(E_{RH}, M_R, X_{RH}) + S(E_{RL}, M_R, X_{RL}) = S(E_{RH} - Q, M_R, X_{RH}) + S(E_{RL}^{\text{quasi}}, M_R, X_{RL}).
\]

(164)

We can asymptotically expand the equality (163) as follows;

\[
\eta_{\text{ad}}[(E_{RH}, M_R, X_{RH}), (E_{RL}, M_R, X_{RL}), Q] = 1 - \frac{\beta_H}{\beta_L} - c_{(1)}^{(1)} Q M_R - c_{(2)}^{(1)} Q^2 M_R + O \left( \frac{Q^3}{M_R} \right).
\]

(165)

Now, we can compare Theorem 8 to Theorem 9. There exists a strong resemblance between these two theorems. To compare them, we focus on two equalities (149) and (165), which are comparable forms of Theorems 8 and 9 respectively. When the ratio \( Q/M_R \) in the thermodynamics framework corresponds to \( q \) defined in Subsection IX A, the equality (149) has the same form as (165). Hence, these theorems are different only in the assumptions required in the respective theorems.

**Theorem 9** is guaranteed to hold only for the macroscopic heat baths. Although the equality (165) implies (149), it cannot imply (137). This is because (137) takes into account the finiteness of \( n \) as well as that of \( q \), but (149) takes into account only the finiteness of \( q \). In the derivation of (163), we essentially employ the law of entropy increase. That is, Theorem 9 requires the thermalization assumption. However, the thermalization assumption is not credible under Type-2 finiteness, i.e., when the particle number \( n \) is finite. Namely, thermodynamics cannot guarantees the equality (165) for the finite-particle heat baths. Therefore, we need to check whether Theorem 9 is valid even under Type-2 finiteness or not.

On the other hand, Theorem 8 does not need thermalization assumption. It can treat the finiteness \( n \) directly, i.e., Type-2 finiteness as well as Type-1 finiteness. Therefore, we can say that Theorem 8 yields (165) in Theorem 9 with a weaker assumption as follows. Theorem 8 gives the concrete form (137) of the optimal efficiency under both kinds of finiteness. Since (137) has the same form as (165) clearly, Theorem 8 guarantees (165) with the error of the order \( O(Q_n/n^2) \). That is, we can conclude that Type-2 finiteness effect has the order \( O(1/n^2) \) at most in the non-lattice case. In the lattice case, (137) guarantees that Type-2 finiteness effect has the order \( O(1/n^2) \) at most. We should remark that we do not assume the existence of the quasi-static operations because such a kind of operations have not been defined for the isolated system in the context of the statistical mechanics. This point is a big difference from the preceding papers [3, 26, 27]. We emphasize that our evaluation does not derive from thermodynamics. Theorem 8 enables us to predict how accurate thermodynamics is in the finite-size systems, by using statistical mechanics.
In the present section, we prove Theorem 5. For this purpose, we prepare the following lemma.

**Lemma 21** For an arbitrary real number $Q$, we choose $\beta_H^*$ and $\beta_L^*$ based on \[123\] and \[125\]. Then, the following equation holds:

\[
\min_{\rho_{HLC}} \left\{ D(\rho_{HLC}^{\prime} \| \rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L} \otimes \rho_C) \right\} = D(\rho_{HLC}^{\prime} \| \rho_{\beta_H^*H_R} \| \rho_{\beta_L^*H_L} \| \rho_C).
\]

(166)

Lemma 21 will be shown after the proof of Theorem 5. Now, we show Theorem 5. To derive the upper bound \[123\], we choose two states $\rho_{HLC} := \rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L} \otimes \rho_C$ and $\rho_{HLC}^{\prime} := \sum E(\rho_{HLC})$. Then, we employ the following expression of the efficiencies $\eta^{(n)}(\{E_j, w_j\})$:

\[
\eta^{QC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_C, \{E_j, w_j\}) = \left( 1 - \frac{\beta_H}{\beta_L} \right) - \frac{D(\rho_{HLC}^{\prime} \| \rho_{HLC})}{\beta_L^{QC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L} \otimes \rho_C, \{E_j, w_j\})}.
\]

(167)

We derive (167) from the relation $S(\rho_{HLC}) \leq S(\rho_{HLC}^{\prime})$ by the method in Ref. 9 as follows. Using the relation $S(\rho_{HLC}) \leq S(\rho_{HLC}^{\prime})$, we have

\[
-D(\rho_{HLC}^{\prime} \| \rho_{HLC}) \geq -\text{Tr}[\rho_{HLC} \log \rho_{HLC}]
\]

\[
= \beta_H^{\prime} \text{Tr}[\rho_{\beta_H^*H_R} \rho_{\beta_L^*H_L} \rho_C] + \beta_L \text{Tr}[\rho_{\beta_L^*H_L} \rho_{\beta_H^*H_R} \rho_C] + \beta_L \text{Tr}[\rho_{\rho_C} \rho_{\beta_L^*H_L}]
\]

\[
= (\beta_L + (\beta_H - \beta_L)) \text{Tr}[\rho_{\beta_H^*H_R} \rho_{\beta_L^*H_L} \rho_C] + \beta_L \text{Tr}[\rho_{\rho_C} \rho_{\beta_L^*H_L}]
\]

\[
= (\beta_H - \beta_L) Q_{HC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\}) + \beta_L W_{C}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\}),
\]

(168)

where $\rho_{\beta_L} := \text{Tr}_{\rho_{HLC}}[\rho_{HLC}^{\prime}]$, $\rho_{\beta_L} := \text{Tr}_{\rho_{HLC}}[\rho_{HLC}]$ and $\rho_{\rho_C} := \text{Tr}_{\rho_{HLC}}[\rho_{HLC}] = \rho_C$. Therefore, we obtain (167) as

\[
\eta^{QC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_C, \{E_j, w_j\}) = \frac{W_{C}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\})}{\rho_{\beta_H^*H_R}}
\]

\[
\leq \left( 1 - \frac{\beta_H}{\beta_L} \right) - \frac{D(\rho_{HLC}^{\prime} \| \rho_{HLC})}{\beta_L^{QC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L} \otimes \rho_C, \{E_j, w_j\})}
\]

(169)

Hence, it is sufficient to prove the inequality

\[
-D(\rho_{HLC}^{\prime} \| \rho_{HLC}) \geq D(\rho_{\beta_H^*H_R} \| \rho_{\beta_H^*H_R}) + D(\rho_{\beta_L^*H_L} \| \rho_{\beta_L^*H_L})
\]

under the constraint $Q_{HC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\}) = Q$. The endothermic energy amount $Q_{HC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\})$ is written as

\[
Q_{HC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\}) = \text{Tr}[\rho_{\beta_H^*H_R} \rho_{\beta_L^*H_L} \rho_{\rho_C}] = - \frac{1}{\beta_H} \text{Tr}[\rho_{\beta_H^*H_R} \rho_{\beta_L^*H_L} \rho_{\rho_C}] = \frac{1}{\beta_H} \left( S(\rho_{\beta_H^*H_R}) - S(\rho_{\beta_L^*H_L}) - D(\rho_{\rho_C} \rho_{\beta_L^*H_L}) \right).
\]

(171)

Thus, the constraint $Q_{HC}(\rho_{\beta_H^*H_R} \otimes \rho_{\beta_L^*H_L}, \rho_{\rho_C}, \{E_j, w_j\}) = Q$ is equivalent to $Q = \frac{1}{\beta_H} \left( S(\rho_{\beta_H^*H_R}) - S(\rho_{\beta_L^*H_L}) - D(\rho_{\rho_C} \rho_{\beta_L^*H_L}) \right)$. Because every CP-standard work extraction is unital, it preserves or increases the entropy of $HLC$. Under such entropy-increasing transformations, the relative entropy $D(\rho_{HLC}^{\prime} \rho_{HLC})$ is bounded by Lemma 21 and thus (123) holds.

To show Lemma 21, we prepare the following lemma:

**Lemma 22** For a given state $\rho$ and a real number $C > 0$,

\[
\min_{\rho': S(\rho') \geq C} -\text{Tr}[\rho' \log \rho'] = -\text{Tr} \left[ \frac{\rho^{1-x}}{\text{Tr}[\rho^{1-x}]} \log \rho \right],
\]

(172)

where $x$ is a real number satisfying that

\[
S \left( \frac{\rho^{1-x}}{\text{Tr}[\rho^{1-x}]} \right) = C
\]

(173)
Proof of Lemma 22

\[
\text{Tr} \left[ \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} \log \rho \right] - \text{Tr}[\rho' \log \rho] = \text{Tr} \left[ \left( \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} - \rho' \right) \log \rho \right] = \frac{1}{1-x} \text{Tr} \left[ \left( \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} - \rho' \right) \log \left( \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} \right) \right] \\
= \frac{1}{1-x} \left( -S\left( \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} \right) + S(\rho') + D \left( \rho' \left| \left| \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} \right| \right| \right) \right) \\
= \frac{1}{1-x} \left( S(\rho') - C + D \left( \rho' \left| \left| \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} \right| \right| \right) \right) \geq 0.
\]

(174)

The equality is valid only when \( S(\rho') = C \) and \( \rho' = \frac{\rho_{1-x}}{\text{Tr}[\rho_{1-x}]} \) hold.

Proof of Lemma 21

Firstly, we point out that the state \( \rho_{HLC}^{\text{min}} := \rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C \) satisfies the conditions

\[
S(\rho_{HLC}^{\text{min}}) \geq S(\rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C),
\]

(175)

\[
\beta_H Q = S(\rho_{\beta_H|H}) - S(\rho_{HLC}^{\text{min}}) - D(\rho_{HLC}^{\text{min}} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_C),
\]

(176)

\[
\rho_C = \rho_{C}^{\text{min}}
\]

(177)

\[
D(\rho_{HLC}^{\text{min}} \left| \left| \rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C \right| \right|) = D(\rho_{\beta_H|H} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_{C}) + D(\rho_{\beta_L|H} \left| \left| \rho_{\beta_L|H} \right| \right| \rho_{C}).
\]

(178)

Thus, we only have to prove

\[
\min_{\rho_{HLC}} \left\{ D(\rho_{HLC}^{\text{min}} \left| \left| \rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C \right| \right|) \mid S(\rho_{HLC}^{\text{min}}) \geq S(\rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C), \beta_H Q = S(\rho_{\beta_H|H}) - S(\rho_{HLC}^{\text{min}}) - D(\rho_{HLC}^{\text{min}} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_C), \rho_C = \rho_{C}^{\text{min}} \right\}
\]

\[
\leq D(\rho_{\beta_H|H} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_{C}) + D(\rho_{\beta_L|H} \left| \left| \rho_{\beta_L|H} \right| \right| \rho_{C}).
\]

(179)

Under the given constraints for \( \rho_{HLC}^{\text{min}} \), we can convert \( D(\rho_{HLC}^{\text{min}} \left| \left| \rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C \right| \right|) \) as follows;

\[
D(\rho_{HLC}^{\text{min}} \left| \left| \rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C \right| \right|) \overset{(a)}{=} -S(\rho_{HLC}^{\text{min}}) - \text{Tr}[\rho_C \log \rho_C] - \text{Tr}[\rho_H' \log \rho_{\beta_H|H}] - \text{Tr}[\rho_L' \log \rho_{\beta_L|H}]
\]

\[
\leq -S(\rho_{\beta_H|H}) - S(\rho_{\beta_L|H}) - \text{Tr}[\rho_H' \log \rho_{\beta_H|H}] - \text{Tr}[\rho_L' \log \rho_{\beta_L|H}]
\]

\[
= -S(\rho_{\beta_L|H}) - S(\rho_{\beta_L|H}) + D(\rho_{H} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_{\beta_H|H}) + S(\rho_{\beta_L|H}) - \text{Tr}[\rho_L' \log \rho_{\beta_L|H}]
\]

\[
\overset{(c)}{=} -S(\rho_{\beta_L|H}) - \beta_H Q - \text{Tr}[\rho_L' \log \rho_{\beta_L|H}]
\]

\[
\overset{(d)}{=} D(\rho_{\beta_H|H} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_{C}) + D(\rho_{\beta_L|H} \left| \left| \rho_{\beta_L|H} \right| \right| \rho_{C})
\]

\[
+ \text{Tr}[\rho_{\beta_L|H} \log \rho_{\beta_L|H}] - \text{Tr}[\rho_L' \log \rho_{\beta_L|H}]
\]

(180)

where \( (a) \) follows from the third condition \( \rho_C = \rho_{C}^{\text{min}} \), \( (b) \) follows from the first condition \( S(\rho_{HLC}^{\text{min}}) \geq S(\rho_{\beta_H|H} \otimes \rho_{\beta_L|H} \otimes \rho_C) \), \( (c) \) follows from the second condition \( \beta_H Q = S(\rho_{\beta_H|H}) - S(\rho_{\beta_L|H}) - D(\rho_{H} \left| \left| \rho_{\beta_H|H} \right| \right| \rho_{\beta_H|H}) \), and \( (d) \) follows from \( (124) \) and \( (125) \).

Thus, in order to prove Lemma 21, it is sufficient to show

\[
\text{Tr}[\rho_{\beta_L|H} \log \rho_{\beta_L|H}] \leq \text{Tr}[\rho'_L \log \rho_{\beta_L|H}]
\]

(181)

under the given constraints. As we will show below, the given constraints yield the following inequality:

\[
S(\rho'_L) \geq S \left( \frac{(\rho_{\beta_L|H})^{(1-t)}}{\text{Tr}[(\rho_{\beta_L|H})^{(1-t)}]} \right).
\]

(182)

Hence, by substituting \( \rho'_L \) and \( S \left( \frac{(\rho_{\beta_L|H})^{(1-t)}}{\text{Tr}[(\rho_{\beta_L|H})^{(1-t)}]} \right) \) for \( \rho' \) and \( C \) of Lemma 2, (182) guarantees (181).
Finally, let us prove (182). We have

\[
S(\rho_H) - S\left(\frac{(\rho_{\beta_H}|H_H)}{\text{Tr}[\rho_{\beta_H}|H_H]}\right)^{(1+s)}
\]

\[
= -\text{Tr}[\rho_H^s \log \rho_H^s] + \text{Tr}\left[\frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]} \log \frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]}\right]
\]

\[
= -\text{Tr}[\rho_H^s \log \rho_H^s] + \text{Tr}\left[\frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]} - \rho_H^s \log \frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]}\right]
\]

\[
= -D\left(\rho_H^s \left| \text{Tr}[\rho_{\beta_H}|H_H]^{(1+s)}\right.\right) + \text{Tr}\left[\frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]} - \rho_H^s \log \frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]}\right]
\]

\[
= -D\left(\rho_H^s \left| \text{Tr}[\rho_{\beta_H}|H_H]^{(1+s)}\right.\right) + (1+s)\text{Tr}\left[\frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]} - \rho_H^s \log \frac{(\rho_{\beta_H}|H_H)^{(1+s)}}{\text{Tr}[\rho_{\beta_H}|H_H]}\right]
\]

\[
= -D\left(\rho_H^s \left| \text{Tr}[\rho_{\beta_H}|H_H]^{(1+s)}\right.\right) + (1+s)(-nS(\beta_H) + \beta_H Q + S(\rho_{\beta_H}|H_H) - \beta_H Q)
\]

\[
= -D\left(\rho_H^s \left| \text{Tr}[\rho_{\beta_H}|H_H]^{(1+s)}\right.\right) \leq 0,
\]

(183)

where \(a\) follows from (124) and the relation \(S(\rho_{\beta_H}|H_H) + \text{Tr}[\rho_H^s \log \rho_H^s] = \beta_H Q\) given from (171). The subadditivity of the von Neumann entropy and the first condition \(S(\rho_{HLC}) \geq S(\rho_{\beta_H}|H_H) \otimes \rho_{\beta_L}|H_L \otimes \rho_C\) imply

\[
S(\rho_H^s) + S(\rho_L^s) = S(\rho_H^s) + S(\rho_L^s) + S(\rho_C^s) - S(\rho_C^s)
\]

\[
\geq S(\rho_{HLC}) - S(\rho_C^s) \geq S(\rho_{\beta_H}|H_H) \otimes \rho_{\beta_L}|H_L \otimes \rho_C - S(\rho_C^s)
\]

\[
S(\rho_{\beta_H}|H_H) + S(\rho_{\beta_L}|H_L).
\]

Thus, the combination of (125), (183), and (184) derives (182) as follows:

\[
S(\rho_L) \geq -S(\rho_H^s) + S(\rho_{\beta_H}|H_H) + S(\rho_{\beta_L}|H_L) \geq -S\left(\frac{(\rho_{\beta_H}|H_H)}{\text{Tr}[\rho_{\beta_H}|H_H]}\right)^{(1+s)} + S(\rho_{\beta_H}|H_H) + S(\rho_{\beta_L}|H_L)
\]

\[
= S\left(\frac{(\rho_{\beta_L}|H_L)}{\text{Tr}[\rho_{\beta_L}|H_L]}\right)^{(1-t)}
\]

(185)

where \((1+s)\beta_H = \beta_H^s\) and \((1-t)\beta_L = \beta_L^s\) by definition.

**XI. RELATION WITH CUMULANT GENERATING FUNCTION**

In the present section, we prepare several useful notations based on cumulant generating function for latter discussions. Let us introduce the cumulant generating functions \(\phi_A(1+s) := \log \text{Tr}[\rho_{\beta_A}|H_A]^{(1+s)}\) for \(A = H, L\) and \(\phi_A(1+s) := \log \sum_a P_{\beta_A} H_A(a)^{(1+s)}\) for \(A = X, Y\). Since the classical case can be discussed in the same way as the quantum case, we treat only the quantum case in this section. The corresponding notation in the classical case will be applied in Sections [XIII] and [XIV]. Then, the variance \(\sigma_A^2(\beta_A)\) and the skewness \(\gamma_A(\beta_A)\) of energy satisfy

\[
\phi_P^P(1) = \beta_A^2 \sigma_A^2(\beta_A)
\]

\[
\phi_P^S(1) = \beta_A^3 \gamma_A(\beta_A) \sigma_A^3(\beta_A).
\]

(186)

(187)

Since the Fisher information of the family \(\{\rho_{\beta_A(1+s)}|H_A\}_{s}\) is \(\phi_P^P(1+s)\) [54] and the Fisher information is closely related to the relative entropy and the entropy, these information quantities can be written by using the cumulant generating function, i.e., they are written as [54]

\[
D(\rho_{\beta_A(1+s)}|H_A) = \phi_P^P(1+s) - \phi_A(1+s)
\]

\[
S(\rho_{\beta_A(1+s)}|H_A) = -(1+s)\phi_P^S(1+s) + \phi_A(1+s) = -\phi_P^S(1+s) - D(\rho_{\beta_A(1+s)}|H_A).
\]

(188)

(189)
In the following, we focus on the entropy $S(\rho_{\beta A} | H_A)$, which is denoted by $S_A$.

In the following section, we need to discuss the above two quantities. To handle them effectively, we introduce a method to characterize them by a function with a single input variable. Since $\phi_A$ is strictly convex, we can define the inverse function of $\phi_A'$, which is denoted by $\psi_A$. The function $\psi_A$ is characterized as follows.

$$\psi_A(-S_A) = \phi_A''(1)^{-1} = \frac{1}{\beta_A^2 \sigma_A^2(\beta_A)} \tag{190}$$
$$\psi_A''(-S_A) = -\phi_A''(1)\phi_A'(1)^{-3} = -\frac{\gamma_A(\beta_A)}{\beta_A^3 \sigma_A^3(\beta_A)}. \tag{191}$$

When $s$ is close to $0$, $\phi_A'(1 + s)$ is also close to $-S_A$. Hence, using the function $\psi_A$, we can characterize the relative entropy as

$$D(\rho_{\beta A(1+s) | H_A} \| \rho_{\beta A | H_A}) = \phi_A'(1 + s) - \phi_A(1 + s) = \phi_A'(1 + s)(\psi_A(\alpha) - 1) - \phi_A(\psi_A(\alpha)) = (\psi_A(-S_A) - 1)(\alpha + S_A) + \frac{1}{2} \psi_A'(-S_A)(\alpha + S_A)^2 + \frac{1}{6} \psi_A''(-S_A)(\alpha + S_A)^3 + O((\alpha + S_A)^4) = \frac{1}{2} \psi_A'(-S_A)(\alpha + S_A)^2 + \frac{1}{6} \psi_A''(-S_A)(\alpha + S_A)^3 + O((\alpha + S_A)^4). \tag{192}$$

The entropy is characterized as

$$S(\rho_{\beta A(1+s) | H_A}) = -\frac{1}{2} \psi_A'(-S_A)(\alpha + S_A)^2 + O((\alpha + S_A)^3). \tag{193}$$

Next, we focus on the difference $\Delta_A S := S(\rho_{\beta A(1+s) | H_A}) - S_A$ from the entropy of the state $\rho_{\beta A | H_A}$. This difference is characterized as

$$\Delta_A S = -(\alpha + S_A) - \frac{1}{2} \psi_A'(-S_A)(\alpha + S_A)^2 + O((\alpha + S_A)^3), \tag{194}$$

which implies

$$-(\alpha + S_A) = \Delta_A S + \frac{1}{2} \psi_A'(-S_A)(\Delta_A S)^2 + O((\Delta_A S)^3). \tag{195}$$

Thus, the relative entropy is characterized by the difference $\Delta_A S$ as follows.

$$D(\rho_{\beta A(1+s) | H_A} \| \rho_{\beta A | H_A}) = \frac{1}{2} \psi_A'(-S_A)(\Delta_A S)^2 + (\frac{1}{2} \psi_A'(-S_A)^2 - \frac{1}{6} \psi_A''(-S_A)(\Delta_A S)^3 + O((\Delta_A S)^4)$$

$$= \frac{1}{2 \beta_A^2 \sigma_A^2(\beta_A)} (\Delta_A S)^2 + \frac{1}{2 \beta_A^3 \sigma_A^3(\beta_A)} + \frac{\gamma_A(\beta_A)}{6 \beta_A^3 \sigma_A^3(\beta_A)}(\Delta_A S)^3 + O((\Delta_A S)^4). \tag{196}$$

This relation will be used in the following sections.

### XII. ASYMPTOTIC BEHAVIOR OF GENERAL UPPER BOUND

In this section, to show Theorem 6, we analyze the asymptotic behavior of general upper bound given in Theorem 5. Since the Gibbs states are given as $\rho_{\beta H | H_H}^{\otimes n}$ and $\rho_{\beta L | H_L}^{\otimes n}$, the upper bound given in Theorem 5 is

$$\left(1 - \frac{\beta_H}{\beta_L}\right) - \frac{D(\rho_{\beta H | H_H}^{\otimes n} \| \rho_{\beta H | H_H}) + D(\rho_{\beta L | H_L}^{\otimes n} \| \rho_{\beta L | H_L})}{\beta_L Q_n} \tag{197}$$

where the real numbers $\beta_H'$ and $\beta_L'$ are determined by

$$Q_n = \text{Tr}(\rho_{\beta H | H_H}^{\otimes n} - \rho_{\beta H | H_H}^{\otimes (n)}) \tag{198}$$
$$S(\rho_{\beta H | H_H}^{\otimes n}) + S(\rho_{\beta L | H_L}^{\otimes n}) = S(\rho_{\beta L | H_L}^{\otimes n}) + S(\rho_{\beta H | H_H}^{\otimes n}). \tag{199}$$
which are equivalent with

$$\frac{Q_n}{n} = \text{Tr}(\rho_{\beta_H} | \hat{H}_H - \rho_{\beta_H} | \hat{H}_H) \hat{H}_H$$  \hspace{1cm} (200)

$$S(\rho_{\beta_H} | \hat{H}_H) + S(\rho_{\beta_L} | \hat{H}_L) = S(\rho_{\beta_H} | \hat{H}_H) + S(\rho_{\beta_L} | \hat{H}_L).$$  \hspace{1cm} (201)

Then, (200) implies that

$$-\frac{\beta_H Q_H}{n} = \Delta_H S + D(\rho_{\beta_H} | \hat{H}_H \| \rho_{\beta_H} | \hat{H}_H).$$  \hspace{1cm} (202)

Now, we employ the differences of entropies $\Delta_H S = S(\rho_{\beta_H} | \hat{H}_H) - S_H$ and $\Delta_L S = S(\rho_{\beta_L} | \hat{H}_L) - S_L$, which are introduced in Section XI. Then, (196) and (201) yield that

$$\Delta_H S + D(\rho_{\beta_H} | \hat{H}_H \| \rho_{\beta_H} | \hat{H}_H) = \Delta_H S + \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} (\Delta_H S)^2 + O((\Delta_H S)^3)$$  \hspace{1cm} (203)

$$\Delta_L S = -\Delta_H S.$$  \hspace{1cm} (204)

Thus, (202) and (203) imply

$$\Delta_H S = -\frac{\beta_H Q_H}{n} - \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} \left( \frac{\beta_H Q_H}{n} \right)^2 + O\left( \frac{\beta_H Q_H}{n} \right)^3,$$  \hspace{1cm} (205)

which yields that

$$\Delta_H S^2 = \left( \frac{\beta_H Q_H}{n} \right)^2 + \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} \left( \frac{\beta_H Q_H}{n} \right)^3 + O\left( \frac{\beta_H Q_H}{n} \right)^4$$  \hspace{1cm} (206)

$$\Delta_H S^3 = -\left( \frac{\beta_H Q_H}{n} \right)^3 + O\left( \frac{\beta_H Q_H}{n} \right)^4.$$  \hspace{1cm} (207)

Therefore,

$$nD(\rho_{\beta_H} | \hat{H}_H \| \rho_{\beta_H} | \hat{H}_H) + D(\rho_{\beta_L} | \hat{H}_L \| \rho_{\beta_L} | \hat{H}_L)) = \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} (\Delta_H S)^2 + \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} \frac{\gamma_1(\beta_H)}{6 \beta_H^2 \sigma^2(\beta_H)} (\Delta_H S)^3$$

$$+ \frac{1}{2 \beta_L^2 \sigma^2(\beta_L)} (\Delta_L S)^2 + \frac{1}{2 \beta_L^2 \sigma^2(\beta_L)} \frac{\gamma_1(\beta_L)}{6 \beta_L^2 \sigma^2(\beta_L)} (\Delta_L S)^3 + O((\Delta_H S)^4)$$

$$= \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} (\Delta_H S)^2 + \frac{1}{2 \beta_L^2 \sigma^2(\beta_L)} \left( \frac{\beta_H Q_H}{n} \right)^2$$

$$+ \frac{1}{2 \beta_H^2 \sigma^2(\beta_H)} \frac{\gamma_1(\beta_H)}{6 \beta_H^2 \sigma^2(\beta_H)} + \frac{\gamma_1(\beta_L)}{6 \beta_L^2 \sigma^2(\beta_L)} (\Delta_H S)^3 + O((\Delta_H S)^4).$$  \hspace{1cm} (208)

Therefore, substituting (208) into (197), we obtain (127).

**XIII. ASYMPTOTIC ANALYSIS FOR EFFICIENCY OF OUR OPTIMAL WORK EXTRACTION**

Although the main purpose of this section is the asymptotic analysis for the efficiency of our optimal work extraction $f_{n,x}$, we firstly show (132). In this case, we have the Hamiltonians $h_X^{(n)}(x_1, \ldots, x_n) := \sum_{i=1}^n h_X(x_i)$ and $h_Y^{(n)}(y_1, \ldots, y_n) := \sum_{i=1}^n h_Y(y_i).$ Since the number of elements of the set $\{h_X^{(n)}(x) + h_Y^{(n)}(y)\}_{(x,y) \in \mathcal{E}(X \times Y)^n}$ is less than $(n + 1)^{d-1})^2 = n!^2 = (n + 1)^{d-1} \cdot \frac{1}{d-1} \cdot \frac{1}{d-1}$, Lemma 15 guarantees (132).

To show the remaining parts of Theorem 7 we discuss the efficiency of our optimal work extraction given in Subsection VIIIB. For this purpose, we prepare the following lemma:
Lemma 23 The function $f_n$ given in Subsection VIII.B satisfies the following equation:

$$
\eta_C(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n) = \left(1 - \frac{\beta_X}{\beta_Y}\right) \frac{D(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}))}{\beta_Y Q_H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n)}.
$$

(209)

Proof: Because $f_n$ is invertible and deterministic, it preserves the entropy;

$$
S(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})) = S(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}).
$$

(210)

Thus, similarly as the derivation of (167), using the relation (210), we have

$$
-D(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) = S(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})) + \sum_{x,y} [P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (f_n^{-1}(x,y)) \log P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}(x,y)]

= S(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) + \sum_{x,y} [P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (f_n^{-1}(x,y)) \log P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}(x,y)]

= -\sum_x [(P^n_{\beta_X|h_X}(x) - \sum_y P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (f_n^{-1}(x,y)) \log P^n_{\beta_X|h_X}(x))]

-\sum_y [(P^n_{\beta_Y|h_Y}(y) - \sum_x P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (f_n^{-1}(x,y)) \log P^n_{\beta_Y|h_Y}(y))]

= \beta_X \sum_x [(P^n_{\beta_X|h_X}(x) - \sum_y P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (g_2^{-1}(x,y)))h_X(x)]

+\beta_Y \sum_y [(P^n_{\beta_Y|h_Y}(y) - \sum_x P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (g_2^{-1}(x,y)))h_Y(y)]

= (\beta_X - \beta_Y) Q_H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n) + \beta_Y W(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n).
$$

(211)

Therefore, we obtain (209).

Due to Lemma 23 in order to obtain the asymptotic expansion of $\eta_C(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n)$, it is enough to asymptotically expand the relative entropy $D(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})$ and the endothermic amount $Q_H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n)$. We do not calculate these two asymptotic expansions directly, but we calculate them with using an approximation method. To be concrete, we show the following lemma;

Lemma 24 When the sequence $\{m_n\}$ satisfies

$$
m_n < n \left(\min \left\{1 - \frac{S(P_{\beta_Y|h_Y})}{\log d}, \frac{\log \max_x P_{\beta_X|h_X}(x)}{\log d}\right\} - \epsilon\right)
$$

(212)

with a small $\epsilon > 0$, the following equalities satisfies;

$$
D(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) = D_X^n(m_n) + D_Y^n(m_n) + O(e^{-\alpha_2 m_n})
$$

(213)

$$
\beta_X Q_H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n) = m_n \log d - D_X^n(m_n) + O(e^{-\alpha_3 m_n})
$$

(214)

hold with real constants $\alpha_2 > 0$ and $\alpha_3 > 0$, where

$$
D_X^n(m_n) := \sum_{i=0}^{d^n-1} P^n_{\beta_X|h_X}(i) \log \frac{d^{m_n} P^n_{\beta_X|h_X}(i)}{P^n_{\beta_X|h_X}(i)}
$$

(215)

$$
D_Y^n(m_n) := \sum_{j=0}^{d^n-1} P^n_{\beta_Y|h_Y}(j) \log \frac{d^{m_n} P^n_{\beta_Y|h_Y}(j)}{d^{m_n} P^n_{\beta_Y|h_Y}(j)}
$$

(216)

where $[a]$ is the ceiling function of a positive number $a$.

Due to Lemma 24 in order to calculate $D(f_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})$ and $Q_H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_n)$, we only have to calculate $D_X^n(m_n)$ and $D_Y^n(m_n)$. Lemma 24 will be shown after the following Lemma 25.
Now, we simulate the distribution $g_{2n^*}(P^*_{\beta_X|h_X} P^*_{\beta_Y|h_Y})$ by a product distribution, where $g_{2n^*}$ is defined in (141). For this purpose, we introduce the two distributions $\tilde{P}_{\beta_X|h_X}^{n}$ and $\tilde{P}_{\beta_Y|h_Y}^{n}$ by

$$
\tilde{P}_{\beta_X|h_X}^{n}(i_A + i BD^{m^*}) := d^{m^*} P_{\beta_X|h_X}(i_A + i BD^{m^*}) \delta_{i_B, 0},
$$

$$
\tilde{P}_{\beta_Y|h_Y}^{n}(j_A + j BD^{m^*-m}) := d^{-m^*} P_{\beta_Y|h_Y}(j_A)
$$

for $i_A, j_B \in \mathbb{Z}_{d^{m^*}}$ and $i_B, j_A \in \mathbb{Z}_{d^{m^*-m}}$. As shown in Lemma 25, the product $\tilde{P}_{\beta_X|h_X}^{n} \tilde{P}_{\beta_Y|h_Y}^{n}$ approximates the true distribution $g_{2n^*}(P^*_{\beta_X|h_X} P^*_{\beta_Y|h_Y})$.

**Lemma 25** When a sequence $\{m_n\}$ satisfies (212) with a small $\epsilon > 0$, the relation

$$
\|g_{2n^*}(P^*_{\beta_X|h_X} P^*_{\beta_Y|h_Y}) - \tilde{P}_{\beta_X|h_X}^{n} \tilde{P}_{\beta_Y|h_Y}^{n}\|_1 = O(e^{-n\alpha})
$$

holds, where

$$
\|P - Q\|_1 := \sum_j |P(j) - Q(j)|.
$$

**Proof of Lemma 25** Due to (89) and (141), we can evaluate the LHS of (219) as

$$
\|g_{2n^*}(P^*_{\beta_X|h_X} P^*_{\beta_Y|h_Y}) - \tilde{P}_{\beta_X|h_X}^{n} \tilde{P}_{\beta_Y|h_Y}^{n}\|_1 = \sum_{i_A, i_B, j_B} |g_{2n^*}(P^*_{\beta_X|h_X} P^*_{\beta_Y|h_Y})(i_A + i BD^{m^*}, j_A + j BD^{m^*-m}) - \tilde{P}_{\beta_X|h_X}^{n}(i_A + i BD^{m^*}) \tilde{P}_{\beta_Y|h_Y}(j_A + j BD^{m^*-m})|
$$

$$
= \sum_{i_A, i_B, j_B} |P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) P^*_{\beta_Y|h_Y}(i_B BD^{m^*-m} + j_A) - \tilde{P}_{\beta_X|h_X}(i_A BD^{m^*}) \tilde{P}_{\beta_Y|h_Y}(j_A)|
$$

$$
= \sum_{i_A, i_B, j_B} \left| \sum_{i_B = 0}^{d^{m^*}-1} \sum_{j_B = 0}^{d^{m^*-m} - 1} \left( P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) - P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) \right) + \sum_{j_B = d^{m^*-m}}^{d^{m^*-m} - 1} \sum_{i_B = 0}^{d^{m^*}-1} P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) \right|
$$

$$
\leq \sum_{i_A = 0}^{d^{m^*}} \sum_{j_B = 0}^{d^{m^*-m}-1} \sum_{i_B = 0}^{d^{m^*}-1} \left( P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) - P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) \right) + \sum_{j_B = d^{m^*-m}}^{d^{m^*-m} - 1} \sum_{i_B = 0}^{d^{m^*}-1} P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B)
$$

$$
= \sum_{j_B = d^{m^*-m}}^{d^{m^*-m} - 1} \sum_{i_A = 0}^{d^{m^*-m}-1} \left( P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) - P^*_{\beta_X|h_X}(i_A BD^{m^*} + j_B) \right)
$$

$$
\leq d^{m^*-m} (n + 1)^{d-1} \max_{x} P_{\beta_X|h_X}(x)^n,
$$

which goes to zero exponentially because $m_n < -n \left( \frac{\log \max_x P_{\beta_X|h_X}(x)}{\log d} + \epsilon \right)$. Thus, when (212) holds, the equation (219) is valid.
Proof of Lemma 24. We firstly transform \( D(f_{n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \) and \( \beta X Q H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_{n*}) \) into forms that we can more easily compare with \( D_{\beta X}^n(m_{\beta X}) \) and \( D_{\beta Y}^n(m_{\beta Y}) \). Because \( g_{1n} \) is invertible and deterministic, the relative entropy \( D(f_{n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \) turns into

\[
D(f_{n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) = D(g_{1n*}(f_{n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| g_{1n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}))
\]

\[
= D(g_{2n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}).
\]

(223)

Now, we introduce the marginal distributions:

\[
P_X''(x) := \sum_y f_{n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})(x, y)
\]

(225)

\[
P_X'(i) := \sum_j g_{2n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})(i, j).
\]

(226)

Hence, we have

\[
S(P_X') = S(g_{1n*}(P_X')) = S(P_X'')
\]

(227)

\[
D(P_X'' \| P^n_{\beta_X|h_X}) = D(g_{1n*}(P_X') \| g_{1n*}(P^n_{\beta_X|h_X})) = D(P_X'' \| P^n_{\beta_X|h_X}).
\]

(228)

Because of (171), (227), and (228), the quantity \( \beta X Q H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_{n*}) \) turns into

\[
\beta X Q H(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_{n*}) = S(P^n_{\beta_X|h_X}) - S(P_X'') - D(P_X'' \| P^n_{\beta_X|h_X})
\]

(229)

Second, we define

\[
\tilde{D}_X^n(m_{\beta X}) := D(\tilde{P}^{n\downarrow}_{\beta_X|h_X} \| P^n_{\beta_X|h_X})
\]

(230)

\[
= \sum_{i=0}^{d^{n-1}} \tilde{P}^{n\downarrow}_{\beta_X|h_X}(i) \log \tilde{P}^{n\downarrow}_{\beta_X|h_X}(i)
\]

\[
= \sum_{i=0}^{d^{n-m-1}} d^{m*} P^{n\uparrow}_{\beta_X|h_X}(d^{m*} i_A) \log \frac{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(d^{m*} i_A)}{P^{n\downarrow}_{\beta_X|h_X}(i_A)}
\]

\[
= \sum_{i=0}^{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(x)} d^{m*} [d^{m*} i_A] \log \frac{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(d^{m*} [d^{m*} i_A])}{P^{n\downarrow}_{\beta_X|h_X}(i)}.
\]

Since \( \sum_{i=0}^{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(x)} \log \frac{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(d^{m*} i_A)}{P^{n\downarrow}_{\beta_X|h_X}(i)} \) is exponentially small and the difference between

\[
\log \frac{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(x)}{P^{n\downarrow}_{\beta_X|h_X}(i)} \]

and \( \log \frac{d^{m*} P^{n\uparrow}_{\beta_X|h_X}(x)}{P^{n\downarrow}_{\beta_X|h_X}(i)} \) is linear with respect to \( n \) at most, the difference \( \tilde{D}_X^n(m_{\beta X}) - D^n_{\beta X}(m_{\beta X}) \) is exponentially small. Similarly, we define

\[
\tilde{D}_Y^n(m_{\beta Y}) := D(\tilde{P}^{n\downarrow}_{\beta_Y|h_Y} \| P^n_{\beta_Y|h_Y}).
\]

(231)

Then, the difference \( \tilde{D}_Y^n(m_{\beta Y}) - D^n_{\beta Y}(m_{\beta Y}) \) is exponentially small. Hence, in order to prove (213), we only have to show that

\[
D(g_{2n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \| P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) = \tilde{D}_X^n(m_{\beta X}) + \tilde{D}_Y^n(m_{\beta Y}) + O(e^{-n\alpha}).
\]

(232)

Using Lemma 25 we show (232) as follows. Because of Fannes’s theorem [55], the equation \( S(g_{2n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y})) - S(\tilde{P}^{n\uparrow}_{\beta_X|h_X} \tilde{P}^{n\uparrow}_{\beta_Y|h_Y}) = O(ne^{-n\alpha}) \) follows from (219). The maximum \( h_{\text{max}} := \max \{ h_X(x), h_Y(y) \} \) satisfies

\[
\sum_{i,j} \left| (\tilde{P}^{n\uparrow}_{\beta_X|h_X}(i) \tilde{P}^{n\uparrow}_{\beta_Y|h_Y}(j) - P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y} (g_{2n}^{-1}(i, j))) \log P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}(i, j) \right| \leq 2n \left| \tilde{P}^{n\uparrow}_{\beta_X|h_X} \tilde{P}^{n\uparrow}_{\beta_Y|h_Y} - g_{2n*}(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}) \right| h_{\text{max}}
\]

(233)

= O(ne^{-n\alpha}).
Thus, we obtain (232) as follows:
\[
D(n^2, \beta_{\hat{X}|X} P_{\hat{X}|X}^n P_{\hat{Y}|X}^n, P_{\hat{X}|X}^n P_{\hat{Y}|X}^n) - D_X(n) - D_X^*(n)
= -S(n^2, \beta_{\hat{X}|X} P_{\hat{X}|X}^n P_{\hat{Y}|X}^n) + S(\hat{P}_{\hat{X}|X}^n P_{\hat{Y}|X}^n)
- \sum_{i,j} |(\hat{P}_{\hat{X}|X}^n P_{\hat{Y}|X}^n(i) \hat{P}_{\hat{Y}|X}^n(j)) - P_{\hat{X}|X}^n P_{\hat{Y}|X}^n(g_{X}^{-1}(i, j)))| \log P_{\hat{X}|X}^n P_{\hat{Y}|X}^n(i, j))
= O(n e^{-n\alpha_1}).
\] (234)

Thus, we have shown (232), which implies (213).

Next, we will show (214). Using (171), we deform $\beta_X Q_H(P_{\hat{X}|X}^n P_{\hat{Y}|X}^n, f_{n*}) - m_n \log d + D_X^*(n)$ as follows:
\[
\beta_X Q_H(P_{\hat{X}|X}^n P_{\hat{Y}|X}^n, f_{n*}) - m_n \log d + D_X^*(n)
= S(P_X) - S(\hat{P}_{\hat{X}|X}^n P_{\hat{Y}|X}^n) + \sum_i \left[\left(\sum_j \hat{P}_{\hat{X}|X}^n P_{\hat{Y}|X}^n(g_{X}^{-1}(i, j)) - \hat{P}_{\hat{X}|X}^n P_{\hat{Y}|X}^n(i)\right) \log P_{\hat{X}|X}^n P_{\hat{Y}|X}^n(i)\right].
\] (235)

Therefore, similar to (232), we find that $\beta_X Q_H(n - m_n \log d - D_X^*(n)$ is exponentially small. Since the difference $D_X(n) - D_X^*(n)$ is also exponentially small, we obtain (214).

As shown in the next section, we have the following lemma.

**Lemma 26** When $m_n = o(n)$,
\[
D_X(n) = (m_n \log d)^2 n^{-1} \frac{\psi_X(-S_X)}{2} + O((m_n \log d)n^{-1} + O((m_n \log d)^3 n^{-2}).
\] (236)
\[
D_Y^*(n) = (m_n \log d)^2 n^{-1} \frac{\psi_Y(-S_Y)}{2} + O((m_n \log d)n^{-1} + O((m_n \log d)^3 n^{-2})
\] (237)

Furthermore, when $h_X$ and $h_Y$ are non-lattice,
\[
D_X(n) = (m_n \log d)^2 n^{-1} \frac{\psi_X(-S_X)}{2} + (m_n \log d)^3 n^{-2} \left(\frac{\psi_X(-S_X)}{6} - \frac{\psi_X(-S_X)^2}{2}\right)
+ (m_n \log d)^2 n^{-2} \left(\frac{\psi_X(-S_X)}{2\psi_X(-S_X)} - \psi_X(-S_X)^2\right) + O(m_n \log d)^5 n^{-2} + O(m_n \log d)^3 n^{-3}.
\] (238)
\[
D_Y^*(n) = (m_n \log d)^2 n^{-1} \frac{\psi_Y(-S_Y)}{2} + (m_n \log d)^3 n^{-2} \left(\frac{\psi_Y(-S_Y)}{6} + \frac{\psi_Y(-S_Y)^2}{2}\right)
+ (m_n \log d)^2 n^{-2} \left(\frac{\psi_Y(-S_Y)}{2\psi_Y(-S_Y)} - \psi_Y(-S_Y)^2\right) + O(m_n \log d)^5 n^{-2} + O(m_n \log d)^3 n^{-3}
\] (239)

We can obtain Theorem 6 by combining Lemma 23, Lemma 24, and Lemma 26 as follows:

**Proof of Theorem 6** Now, we show Theorem 6 when $P_X$ and $P_Y$ are non-lattice. We choose
\[
m_n = \left[\frac{\beta X Q_n + \psi_X(-S_X)}{2n} \beta_X^2 Q_n^2\right].
\] (240)

Then, we obtain (134) as follows:
\[
Q_n(P_{\hat{X}|X}^n P_{\hat{Y}|X}^n, f_{n*}) \overset{(a)}{=} \frac{m_n \log d}{\beta_X} - \frac{D_X(n)}{\beta_X} + O(e^{-n\alpha_3})
\overset{(b)}{=} \frac{m_n \log d}{\beta_X} - (m_n \log d)^2 n^{-1} \frac{\psi_X(-S_X)}{2\beta_X} + O(m_n \log d)^3 n^{-2} + O(m_n \log d)^3 n^{-3}
\overset{(c)}{=} Q_n + \frac{\beta X Q_n^2 \psi_X(-S_X)}{2n} - \frac{\beta X Q_n^2 \psi_X(-S_X)}{2n} + O(Q_n^3) + o(1) = Q_n + O(Q_n^3) + o(1),
\] (241)

where (a), (b), and (c) follow from (214), (238), and (240), respectively.
Substituting the relation (240) into (233) and (239), we have

\[
D^n_X(m_n) = (\beta_X Q_n)^2 n^{-1} \left( \frac{\psi_X'(-S_X)}{2} + (m_n \log d)^2 n^{-2} \left( \frac{\psi_X'(-S_X)}{2} - \psi_X'(-S_X) \right)^2 \right) + O(Q_n^3 n^{-5/2}) + O(Q_n^4 n^{-3}),
\]

\[
D^n_Y(m_n) = (\beta_X Q_n)^2 n^{-1} \left( \frac{\psi_Y'(-S_Y)}{2} + (m_n \log d)^2 n^{-2} \left( \frac{\psi_Y'(-S_Y)}{2} - \psi_Y'(-S_Y) \right)^2 \right) + (\beta_X Q_n)^2 n^{-2} \left( \frac{\psi_Y'(-S_Y)}{2} - \psi_Y'(-S_Y) \right)^2 + O(Q_n^3 n^{-5/2}) + O(Q_n^4 n^{-3}).
\]

(242)

(243)

Therefore, (190) and (191) imply that

\[
D^n_X(m_n) + D^n_Y(m_n) = c^{(1)}_{\beta_X, \beta_Y} (\beta_X Q_n)^2 n^{-1} + c^{(2)}_{\beta_X, \beta_Y} (\beta_X Q_n)^3 n^{-2} + d^{(1)}_{\beta_X, \beta_Y} (\beta_X Q_n)^2 n^{-2} + O(Q_n^3 n^{-5/2}) + O(Q_n^4 n^{-3}).
\]

(244)

Combining (209), (213) and (244), we obtain the following expansion

\[
\eta_c(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_{n*}) = \left( 1 - \frac{\beta_X}{\beta_Y} \right) - c^{(1)}_{\beta_X, \beta_Y} q_n - c^{(2)}_{\beta_X, \beta_Y} q_n^2 - d^{(1)}_{\beta_X, \beta_Y} q_n + O\left( \frac{q_n^3}{\sqrt{n}} \right) + O\left( \frac{q_n^4}{n^2} \right),
\]

which is the same as (133).

Now, we consider the case when \( P_X \) or \( P_Y \) is lattice. Using (236) and (237) instead of (238) and (239), we obtain

\[
\eta_c(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_{n*}) = \left( 1 - \frac{\beta_X}{\beta_Y} \right) - c^{(1)}_{\beta_X, \beta_Y} q_n + O\left( \frac{1}{n} \right) + O\left( \frac{Q_n^2}{n^2} \right),
\]

which is the same as (133). Also, we obtain (131) as follows;

\[
Q_n(P^n_{\beta_X|h_X} P^n_{\beta_Y|h_Y}, f_{n*}) \overset{(a)}{=} \frac{m_n \log d}{\beta_X} - \frac{D^n_X(m_n)}{\beta_X} + O(e^{-n\alpha_3})
\]

\[
\overset{(b)}{=} \frac{m_n \log d}{\beta_X} - (m_n \log d)^2 n^{-1} \frac{\psi_X'(-S_X)}{2\beta_X} + O((m_n \log d)n^{-1}) + O((m_n \log d)^3 n^{-2})
\]

\[
\overset{(c)}{=} Q_n + \frac{\beta_X Q_n^2 \psi_X'(-S_X)}{2n} - \frac{\beta_X Q_n^2 \psi_X'(-S_X)}{2n} + O(Q_n n) + O\left( \frac{Q_n^2}{n^2} \right) = Q_n + O\left( \frac{Q_n}{n} \right) + O\left( \frac{Q_n^3}{n^2} \right),
\]

(245)

where (a), (b), and (c) follow from (244), (236), and (240), respectively.

**XIV. RELATIVE ENTROPY BETWEEN TWO DISTRIBUTIONS WITH SUBTLE DIFFERENCE**

**A. Preparation**

To show Lemma (226), we need to asymptotically expand the relative entropy \( D^n_X(m_n) \) between the two distributions \( P^n_{\beta_X|h_X} \) and \( \hat{P}^{n,\perp}_{\beta_X|h_X} \), which are very close to each other. However, these two distributions have the same information spectrum in the sense Han’s book [63] up to the second order. That is, any real number \( R \) satisfies that

\[
\lim_{n \to \infty} P^n_{\beta_X|h_X} \left\{ j \mid - \log P^n_{\beta_X|h_X}(j) \leq n S_X + \sqrt{n} R \right\} = \lim_{n \to \infty} \hat{P}^{n,\perp}_{\beta_X|h_X} \left\{ j \mid - \log \hat{P}^{n,\perp}_{\beta_X|h_X}(j) \leq n S_X + \sqrt{n} R \right\}.
\]

(246)

Hence, the conventional approaches for information theory and quantum information theory do not work well. To resolve this problem, we employ strong large deviation by Bahadur-Rao and Blackwell-Hodges [43, 64] that brings us a more detailed evaluation for the tail probability. In particular, since the RHSs of (238) and (239) are related to higher order moments of the sample mean, we prepare several formulas for them. After these preparations, we show Lemma (226).

We focus on the logarithmic likelihood of \( P^n_{\beta_A|h_A} (A = X, Y) \), which can be regarded as the logarithmic likelihood ratio between the distribution \( P^n_{\beta_A|h_A} \) and the counting measure \( P_C \). Now, we define the random variable \( Z_A := (\log P^n_{\beta_A|h_A}(j) + \cdots) \).
Then, when \( j = P_C \{ Z_A \geq a \} \), \( j \) is the maximum integer satisfying \( \log P_{\beta_A|h_A}^{n,\upharpoonright}(j) \geq -nS_A + \sqrt{n}a \). We have the relations

\[
\begin{align*}
E[Z_A] &= 0 \\
E[Z_A^2] &= \phi''_A(1) = \frac{1}{\psi_A(-S_A)} \\
E[Z_A^3] &= \phi'''_A(1) = -\frac{\psi''_A(-S_A)}{\psi_A(-S_A)^3 \sqrt{n}} \\
E[Z_A^4] &= 3\phi''_A(1)^2 + \frac{\phi''_A(1)}{n} = -\frac{3}{\psi_A(-S_A)^2} + \frac{3\psi''_A(-S_A)}{\psi_A(-S_A)^3} \frac{1}{n},
\end{align*}
\]

where \( E \) is the expectation under the distribution \( P_{\beta_A|h_A}^{n,\upharpoonright} \).

Next, we focus on the Legendre transform of \( \phi_A \), which is written as

\[
\max_s sR - \phi_A(s) = \psi_A(R)R - \phi_A(\psi_A(R)).
\]

Then, we have the following proposition, which is the special case of strong large deviation by Bahadur-Rao and Blackwell-Hodges. Indeed, the strong large deviation gives the limiting behavior of the tail probability for independent and identical distribution of an arbitrary probability distribution. The following is the special case when the probability distribution is the counting measure.

**Proposition 1** Assume that \( \log P_{\beta_A|h_A} \) is a non-lattice function. When we choose suitable smooth functions \( f_{A,k}(R) \), the following relations hold [43, 46].

\[
\begin{align*}
\log P_C \{ \log P_{\beta_A|h_A}^{n,\upharpoonright}(j) \geq nR \} &= -n(\psi_A(R)R - \phi_A(\psi_A(R))) - \log \sqrt{2\pi n\phi''_A(\psi_A(R))\psi_A(R)} \\
&\quad + \frac{1}{n\psi''_A(\psi_A(R))} \left[ \frac{5\phi''_A(\psi_A(R))}{24\phi''_A(\psi_A(R)^2)} + \frac{\phi'''_A(\psi_A(R))}{8\phi''_A(\psi_A(R))} \right] - \frac{\phi''_A(\psi_A(R))}{2\psi_A(R)\phi''_A(\psi_A(R))} - \frac{1}{\psi_A(R)^2} \\
&\quad + \sum_{k=3}^l f_{A,k}(R)n^{1-k} + o(\frac{1}{n^{l-1}}),
\end{align*}
\]

The lattice case is given as follows. Let \( d \) be the lattice span of \( \log P_{\beta_A|h_A} \). When we choose suitable smooth functions \( f_{A,k}(R) \), the following relations hold [54, 55, Theorem 3.7.4].

\[
\begin{align*}
\log P_C \{ \log P_{\beta_A|h_A}^{n,\upharpoonright}(j) \geq nR \} &= -n(\psi_A(R)R - \phi_A(\psi_A(R))) - \log \sqrt{2\pi n\phi''_A(\psi_A(R))(1 - e^{-d\psi_A(R)})} \\
&\quad + \sum_{k=2}^l f_{A,k}(R)n^{1-k} + o(\frac{1}{n^{l-1}}),
\end{align*}
\]

In the following, for a unified treatment, in the non-lattice case, the functions \( -(\psi_A(R)R - \phi_A(\psi_A(R))) \), \(-\log \sqrt{2\pi} - \log \psi_A(R) + \frac{1}{2} \log \psi_A'(R) \), and \( \frac{1}{8\psi_A(R)^2} + \frac{1}{6\psi_A(R)^3} + \frac{1}{2\psi_A(R)\psi_A'(R)} - \frac{\psi_A''(R)}{\psi_A'(R)^2} \) are written as \( f_{A,0}(R) \), \( f_{A,1}(R) \), and \( f_{A,2}(R) \). So, (252) is simplified as \( \log P_C \{ \log P_{\beta_A|h_A}^{n,\upharpoonright}(j) \geq nR \} = \sum_{k=0}^l f_{A,k}(R)n^{1-k} - \frac{1}{2} \log n + o(\frac{1}{n^{l-1}}) \). In the lattice case, \( f_{A,0}(R) \) is defined as the same way, and \( f_{A,1}(R) \) is defined to be \(-\log \sqrt{2\pi n\phi''_A(\psi_A(R))(1 - e^{-d\psi_A(R)})} \).
B. First step

Now, we start to prove Lemma 26 based on the above preparation. Although we show (236) and (237) with the general case and (238) and (239) with the non-lattice case, the first step for our proof works commonly for both cases.

From the above proposition, we have

$$\log F_A(Z_A) := \log P_C\{\log P_{\beta_A|h_A}(j) \geq -nS_A + \sqrt{n}Z_A\}$$

$$= \sum_{k=0}^{l} \sum_{t=0}^{2l-k} \frac{f^{(t)}_{A,k}(-S_A)n^{1-k-\frac{t}{2}}}{t!} Z_A^t - \frac{1}{2} \log n + o\left(\frac{1}{n^{l-1}}\right).$$

(254)

Now, we introduce the random variables $\Delta X Z_X$ and $\Delta Y Z_Y$ as

$$F_X(Z_X + \Delta X Z_X)d^{m_n} = F_X(Z_X),$$

$$F_Y(Z_Y)d^{m_n} = F_Y(Z_Y - \Delta Y(Z_Y)).$$

(255)

(256)

These two conditions are equivalent with

$$m_n \log d = \log F_X(Z_X) - \log F_X(Z_X + \Delta X Z_X)$$

$$m_n \log d = \log F_Y(Z_Y - \Delta Y Z_Y) - \log F_Y(Z_Y).$$

(257)

(258)

Hence, $\Delta X Z_X$ and $\Delta Y Z_Y$ satisfy the equations

$$m_n \log d = \sum_{i=1}^{2l} \alpha_{X,i}(Z_X)\left(\Delta X Z_X\right)^i + o(n^{1-l})$$

$$m_n \log d = -\sum_{i=1}^{2l} \alpha_{Y,i}(Z_Y)\left(-\Delta Y Z_Y\right)^i + o(n^{1-l}),$$

(259)

(260)

where $\alpha_{A,i}(Z_A) := -\sum_{k=0}^{l} \frac{f^{(i)}_{A,k}(S_A)n^{1-k-\frac{i}{2}}}{i!} Z_A^i$, where $f^{(i)}_{A,k}$ is the $i$-th derivative of $f_{A,k}$ for $A = X, Y$.

Due to the definition (255), we have

$$D^n_X(m_n) = \sum_{j=0}^{d^{m_n}} \frac{P^{n,i}_{\beta_X|h_X}(j)(m_n \log d) + \log P^{n,i}_{\beta_X|h_X}(j) - \log P^{n,i}_{\beta_X|h_X}(\lfloor d^{m_n} j \rfloor)}{n}$$

$$= \mathbb{E}[\log(m_n \log d) + \log P^{n,i}_{\beta_X|h_X}(j) - \log P^{n,i}_{\beta_X|h_X}(\lfloor d^{m_n} j \rfloor)]$$

$$= \mathbb{E}[\log(m_n \log d) + (-nS_X + \sqrt{n}Z_X) - (-nS_X + \sqrt{n}(Z_X + \Delta X Z_X))] = \mathbb{E}[(m_n \log d) - \sqrt{n}\Delta X Z_X].$$

(261)

Hence, it is needed to solve the equation (259) with respect to $\Delta X Z_X$. Notice that $\alpha_{A,i}(Z_A) = O(n^{1-\frac{i}{2}})$. We apply Lemma 30 to the equation (259) with $x = \frac{\Delta X Z_X}{n^{\frac{1}{2}}}$, $a_i = \alpha_{A,i}(Z_A)n^{\frac{1}{2}}$, and $\epsilon = \frac{m_n \log d}{n^{\frac{1}{2}}}$. Then, we obtain

$$\frac{\Delta X Z_X}{\sqrt{n}} = \frac{m_n \log d}{\sqrt{n}\alpha_{X,1}(Z_X)} - \frac{\alpha_{X,2}(Z_X)(m_n \log d)^2}{\sqrt{n}\alpha_{X,1}^3(Z_X)} + \frac{\alpha_{X,3}(Z_X)(m_n \log d)^3}{\sqrt{n}\alpha_{X,1}^4(Z_X)} + O(m_n^4n^{-4}).$$

(262)

That is, we obtain

$$\Delta X Z_X = \frac{m_n \log d}{\alpha_{X,1}(Z_X)} - \frac{\alpha_{X,2}(Z_X)(m_n \log d)^2}{\alpha_{X,1}^2(Z_X)} + \frac{\alpha_{X,3}(Z_X)(m_n \log d)^3}{\alpha_{X,1}^3(Z_X)} + O(m_n^4n^{-4}).$$

(263)

C. Second step for general case

From now, our discussion becomes specialized to the proofs of (236) and (237). That is, we discuss the general case. After these proofs, we give a more detail discussion for the proofs of (238) and (239).
Since $S_X = -\phi_X'(1)$, using the relations (190) and (191), we have

$$f'_{X,0}(R) = -\psi_X(R), \quad f''_{X,0}(R) = -\psi'_X(R). \quad (264)$$

Thus,

$$\alpha_{X,1}(Z_X) = \sqrt{n} + \psi_X'(-S_X)Z_X + O\left(\frac{1}{\sqrt{n}}\right) \quad (265)$$

$$\alpha_{X,2}(Z_X) = \frac{\psi_X'(-S_X)}{2} + \frac{\psi'_X(-S_X)}{2\sqrt{n}}Z_X + O\left(\frac{1}{n}\right) \quad (266)$$

$$\alpha_{X,3}(Z_X) = \frac{1}{\sqrt{n}} \frac{\psi''_X(-S_X)}{6} + O(n^{-1}). \quad (267)$$

We have

$$m_n \log d = m_n \log d \left[n^{-1/2} - n^{-1}\psi'_X(-S_X)Z_X + O(n^{-3/2})\right] \quad (268)$$

and

$$\frac{\alpha_{X,2}(Z_X)(m_n \log d)^2}{\alpha_{X,1}(Z_X)} = \left(m_n \log d\right)^2 \left[n^{-3/2}\frac{\psi'_X(-S_X)}{2} + O(n^{-2})\right]$$

$$\frac{2\alpha_{X,2}(Z_X)^2(m_n \log d)^3}{\alpha_{X,1}(Z_X)} = \left(m_n \log d\right)^3 n^{-5/2} \frac{\psi'_X(-S_X)^2}{2} + O(m^3 d^3 n^{-3})$$

$$\frac{\alpha_{X,3}(Z_X)(m_n \log d)^3}{\alpha_{X,1}(Z_X)} = \left(m_n \log d\right)^3 n^{-5/2} \frac{\psi''_X(-S_X)}{6} + O(m^3 d^3 n^{-3}). \quad (269)$$

Therefore,

$$m_n \log d - \sqrt{n} \Delta X$$

$$= m_n \log d \left[n^{-1/2}\psi'_X(-S_X)Z_X + O(n^{-1})\right]$$

$$+ \left(m_n \log d\right)^2 \left[n^{-1}\frac{\psi'_X(-S_X)}{2} + O(n^{-3/2})\right] + O((m_n \log d)^3 n^{-2}). \quad (270)$$

Now, we take the expectation of $m_n \log d - \sqrt{n} \Delta X$ with use of (247), (248), (249), and (250). We have

$$\mathbb{E}[m_n \log d - \sqrt{n} \Delta X] = (m_n \log d)^2 n^{-1} \frac{\psi'_X(-S_X)}{2} + O(m^3 d^3 n^{-2}) + O(m_n n^{-1}). \quad (271)$$

Hence, using (261), we obtain (236).

Similar to (261), due to the definition (256), we have

$$D_Y^\psi(m_n) = \mathbb{E}[-(m_n \log d) + \sqrt{n} \Delta_Y Z_Y]. \quad (272)$$

Following the same way as (236), we obtain (237) by solving (260).
D. Second step for non-lattice case

Now, we proceed to the proofs of (238) and (239) for the non-lattice case. The following discussion continues (263). Since $S_X = -\phi_X'(1)$, using the relations (190) and (191), we have

$$f_{X,0}^{(j)}(R) = -\psi_X^{(j-1)}(R)$$

(273)

$$f_{X,1}^{(j)}(R) = -\frac{\psi_X'(R)}{\psi_X(R)} + \frac{\psi_X''(R)}{2\psi_X'(R)}$$

(274)

$$f_{X,1}^{(2)}(R) = -\frac{\psi_X'(R)\psi_X(R) - \psi_X''(R)}{\psi_X(R)} + \frac{\psi_X''(R)\psi_X(R) - \psi_X''(R)}{2\psi_X'(R)}$$

(275)

$$f_{X,1}^{(3)}(R) = -\frac{\psi_X(R)\psi_X'(R) - 3\psi_X'(R)\psi_X''(R) + 2\psi_X''(R)}{\psi_X(R)^3} + \frac{\psi_X(R)^2\psi_X''(R) - 3\psi_X'(R)\psi_X''(R) + 2\psi_X''(R)^3}{2\psi_X'(R)^3}$$

(276)

$$f_{X,2}^{(1)}(R) = -\frac{1}{8} \frac{\psi_X'(R)\psi_X''(R) - 2\psi_X''(R)^2}{\psi_X'(R)^3} + \frac{1}{6} \frac{2\psi_X'(R)\psi_X''(R)\psi_X''(R) - 3\psi_X''(R)^3}{\psi_X'(R)^4}$$

(277)

Thus,

$$\alpha_{X,1}(Z_X) = \sqrt{n} + \psi_X'(0)\psi_X''(0) + \frac{1}{\sqrt{n}} (\psi_X'(0)\psi_X''(0) - \frac{\psi_X''(0)}{6}) + \frac{1}{n^3/2}(\psi_X''(-S) - \frac{1}{\psi_X'(0)\psi_X''(0) - \frac{\psi_X''(0)}{6}}) + \frac{1}{n^3/2} \frac{D_{X,1}Z_X}{D_{X,3}} + O(n^{-2})$$

(278)

$$\alpha_{X,2}(Z_X) = \frac{\psi_X''(-S) - \frac{1}{\psi_X'(0)\psi_X''(0) - \frac{\psi_X''(0)}{6}}}{2} + \frac{2}{\sqrt{n}} (\psi_X''(-S) - \frac{1}{\psi_X'(0)\psi_X''(0) - \frac{\psi_X''(0)}{6}}) + \frac{D_{X,1}}{D_{X,3}} + O(n^{-3/2})$$

(279)

$$\alpha_{X,3}(Z_X) = \frac{1}{\sqrt{n}} (\psi_X''(-S) - \frac{1}{\psi_X'(0)\psi_X''(0) - \frac{\psi_X''(0)}{6}}) + O(n^{-1})$$

(280)

where

$$D_{X,1} := -\psi_X''(-S) + \psi_X'(0)\psi_X''(0) + \frac{1}{2} \frac{\psi_X''(0)^2}{\psi_X'(0)\psi_X''(0) - \frac{\psi_X''(0)}{6}}$$

(281)

$$D_{X,2} := -\psi''(-S) + \frac{3}{2} \psi'(-S)\psi''(-S) - 2\psi'(-S)^3$$

(282)

$$D_{X,3} := \frac{1}{8} \frac{\psi''(-S)}{\psi'(S)} + \frac{1}{6} \frac{2\psi'(-S)\psi''(-S) - 3\psi''(-S)^3}{\psi'(-S)^3}$$

(283)

We have

$$m_n \log \frac{d}{\alpha_{X,1}(Z_X)} = m_n \log d \left[ n^{-1/2} - n^{-1/2} \psi_X''(0)Z_X + n^{-3/2} \left( \frac{\psi_X''(0)^2}{2} - \psi_X'(0)^2 \right) - \frac{1}{\psi_X'(0)} + n^{-2} \left( \psi_X''(-S) - \psi_X'(0)^2 + \psi_X'(0)\psi_X''(-S) \right) \right] + O(m_n n^{-3})$$

(284)
and

\[
\frac{\alpha_{X,2}(Z_X)(m_n \log d)^2}{\alpha_{X,1}(Z_X)} = (m_n \log d)^2 \left[ n^{-3/2} \psi_x'(S_X) + n^{-2} \left( -\frac{3 \psi_x'(S_X)^2}{2} + \psi_x''(S_X) \right) Z_X \\
+ n^{-1/2} \frac{\psi_x''(S_X)}{2} - \frac{9}{4} \psi_x'(S_X) \psi_x''(S_X) + 3 \psi_x'(S_X)^3 Z_X^2 \right] \\
- D_{X,1} - \frac{3}{2} \psi_x'(S_X)^2 + \frac{3}{4} \psi_x''(S_X) + O(m_n^2 n^{-3})
\]

\[
\frac{2 \alpha_{X,2}(Z_X)^2 (m_n \log d)^3}{\alpha_{X,1}(Z_X)^3} = (m_n \log d)^3 n^{-5/2} \left( \psi_x'(S_X)^2 \right)^2 + O(m_n^3 n^{-3})
\]

\[
\frac{\alpha_{X,3}(Z_X)(m_n \log d)^3}{\alpha_{X,1}(Z_X)^3} = (m_n \log d)^3 n^{-5/2} \left( \psi_x'(S_X)^2 \right)^2 + O(m_n^3 n^{-3}).
\]  

Therefore,

\[
m_n \log d - \sqrt{n} \Delta Z_X
= m_n \log d \left[ n^{-1/2} \psi_x'(S_X) Z_X - n^{-1} \left( -\frac{\psi_x''(S_X)}{2} + \psi_x'(S_X)^2 \right) (Z_X - \frac{1}{\psi_x'(S_X)}) \\
- n^{-3/2} \psi_x'(S_X) + \psi_x''(S_X)^3 + \psi_x'(S_X) \psi_x'(S_X) Z_X^2 \\
- n^{-3/2} (D_{X,1} + 2 \psi_x'(S_X)^2 - \psi_x''(S_X)) Z_X \\
- n^{-2} \left( (\psi_x'(S_X)^4 - \frac{3}{2} \psi_x''(S_X)^2 \psi_x''(S_X) + \frac{1}{4} \psi_x''(S_X)^2 + \frac{1}{3} \psi_x'(S_X) \psi_x''(S_X) \psi_x''(S_X) - \frac{1}{24} \psi_x''''(S_X) \right) Z_X^4 \\
+ (-3 \psi_x'(S_X)^3 + \frac{5}{2} \psi_x'(S_X) \psi_x''(S_X) - \frac{1}{2} \psi_x'(S_X) \psi_x''(S_X)^2 - 2 \psi_x'(S_X) D_{X,1} + \frac{D_{X,2}}{2}) Z_X^2 \\
+ (\psi_x'(S_X) - \frac{\psi_x''(S_X)}{2} \psi_x'(S_X)^2 + D_{X,3}) \right] \\
+ (m_n \log d)^2 \left[ n^{-1} \psi_x'(S_X) \right] + n^{-3/2} \left( -\frac{3 \psi_x'(S_X)^2}{2} + \psi_x''(S_X) \right) Z_X \\
+ n^{-2} \left( \psi_x''(S_X) + \frac{9}{4} \psi_x'(S_X) \psi_x'(S_X) + 3 \psi_x'(S_X)^3 Z_X^2 - \frac{D_{X,1}}{2} \right) - \frac{3}{2} \psi_x'(S_X)^2 + \frac{3}{4} \psi_x''(S_X) \right] \\
+ (m_n \log d)^3 n^{-2} \left( \psi_x''(S_X) \right) + O(m_n^3 n^{-5/2}) + O(m_n^3 n^{-3}).
\]  

(286)

Now, we take the expectation of \( m_n \log d - \sqrt{n} \Delta Z_X \) with use of (2.47), (2.48), (2.49), and (2.50). Then, the coefficient of the term \((m_n \log d)^{-2}\) equals

\[
(-\frac{\psi_x''(S_X)}{6} - \psi_x'(S_X)^3 + \psi_x'(S_X) \psi_x'(S_X) \psi_x''(S_X)) \frac{\psi_x''(S_X)}{\psi_x'(S_X)^3} \\
- \frac{3}{2} \frac{1}{\psi_x'(S_X)} (\psi_x'(S_X)^4 - \frac{3}{2} \psi_x'(S_X)^2 \psi_x''(S_X) + \frac{1}{4} \psi_x''(S_X)^2 + \frac{1}{3} \psi_x'(S_X) \psi_x''(S_X) \psi_x''(S_X) - \frac{1}{24} \psi_x''''(S_X)) \\
- \frac{1}{\psi_x'(S_X)} (-3 \psi_x'(S_X)^3 + \frac{5}{2} \psi_x'(S_X) \psi_x''(S_X) - \frac{1}{2} \psi_x'(S_X) \psi_x''(S_X)^2 - 2 \psi_x'(S_X) D_{X,1} + \frac{D_{X,2}}{2}) \\
- (\psi_x'(S_X) - \frac{\psi_x''(S_X)}{2} \psi_x'(S_X)^2 - D_{X,3}) \right] = 0.
\]  

(287)
Therefore, we have

\[ E[m_n \log d - \sqrt{n} \Delta Z X] = (m_n \log d)^2 n^{-1} \frac{\psi_X'(-S X)}{2} \left( \frac{\psi''_X'(-S X)}{6} - \frac{\psi'_X(-S X)^2}{2} \right) \\
+ (m_n \log d)^2 n^{-2} \left[ \frac{\psi''_X'(-S X)}{4 \psi'_X(-S X)} - \frac{9}{4} \psi'_X(-S X) + 3 \psi'_X(-S X)^2 - \frac{D X,1}{2} - \frac{3}{2} \psi'_X(-S X)^2 + \frac{3}{4} \psi''_X(-S X) \right] \\
+ O(m_n^3 n^{-5/2}) + O(m_n^4 n^{-4}) \]

\[ = (m_n \log d)^2 n^{-1} \frac{\psi_X'(-S X)}{2} \left( \frac{\psi''_X'(-S X)}{6} - \frac{\psi'_X(-S X)^2}{2} \right) \\
+ (m_n \log d)^2 n^{-2} \left( \frac{\psi''_X'(-S X)}{2 \psi'_X(-S X)} - \psi'_X(-S X) \right)^2 \\
+ O(m_n^3 n^{-5/2}) + O(m_n^4 n^{-4}). \] (288)

Hence, we obtain (238).

Similar to (261), due to the definition (256), we have

\[ D_Y^n(m_n) = E[-(m_n \log d) + \sqrt{n} \Delta_Z Y]. \] (289)

Following the same way as (238), we obtain (239) by solving (260).

**XV. CONCLUSION**

In the present article, we have given two results. First, we have established the formulation for quantum heat engines on the quantum measurement theory. We have formulated the work extraction as the CP-instrument. Our formulation is so general as to include any work extraction that has an equipment to assess the amount of the extracted work. We also have clarified the relationships among the fully quantum work extraction, the CP-work extraction and the classical work extraction. Moreover, we have given a trade-off relation in order to show the problem in the semi-classical scenario. The trade-off relation means that we have to demolish the coherence of the thermodynamic system in order to know the amount of the extracted energy. Therefore, when the time evolution of the internal system is close to unitary, we cannot know the amount of the extracted work.

Second, we have extended Carnot’s theorem to the efficiency of heat engines with finite-particle heat baths. We have microscopically derived a general upper bound for the optimal efficiency, and have given a concrete optimal work extraction that attains the upper bound up to the order of $Q^n_2/n^2$. In order to calculate the optimal efficiency, we needed to asymptotically expand the relative entropy between the two distributions which are very close to each other. Since these distributions have the same information spectrum up to the second order in the sense of Han [63], the conventional approaches for information theory and quantum information theory do not work well. To resolve this problem, we have employed the strong large deviation theory, and have established a novel method to calculate the optimal efficiency approximately. We also have shown that the energy extracted by the optimal work extraction is extremely ordered, i.e., in the work storage, the entropy gain is much smaller than the energy gain for the optimal work extraction. Our result also enables us to evaluate accuracy of the prediction of thermodynamics in the finite-particle systems from the statistical mechanic viewpoint. Thus, we have found that the prediction of thermodynamics for the optimal efficiency is accurate within the error of the order $O(Q^n_2/n^2)$.

Finally, we discuss the future work of our results. We can expect our formulation and method to have many applications. For example, the following four themes can be considered:

**Refinement of the principle of maximum work** It is natural to expect that there exists the refined version not only for Carnot’s Theorem, but also other expressions of the second law.

**Variance of the extracted work** In the present article, we use the entropy gain of the work storage to evaluate how the extracted work is ordered. However, there is another way to evaluate it; we can use the variance of the extracted work. We expect that we can evaluate the variance by applying our calculation method.

**Higher order expansion of the optimal efficiency** The thermodynamical prediction for the optimal efficiency is accurate up to the order of $Q^n_2/n^2$. However, there is no guarantee that it is accurate in the orders higher than $Q^n_2/n^2$. If we derive the higher order expansion of the optimal efficiency, we can evaluate the limit of the size of the isolated system in that thermodynamics is accurate.

**Effect of catalyst under the constraints on the total unitary** In the present article, we request only three conditions on the unitary time evolution of the total system; the energy conservation condition, the shift-invariant condition and the stationary condition. When we request other restrictions on the realizability unitary time evolutions, the effect of the catalyst might
become larger than Theorem 8. For example, when we request the following realistic restrictions, the effect of the catalyst might become larger than the order of $O(Q_n/n^2)$.

1. We forbid the direct interaction between each bath and the external system, and permit only the direct interactions between the catalyst and each heat bath and the catalyst and the external system.
2. We impose the request that the total unitary time evolution finishes within a finite time $\tau$.

They are beyond the range of the present paper, and thus we remain them for future works.

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**Appendix A: Relations among fidelities on tripartite system**

In this appendix, we derive several useful relations among fidelities on a tripartite system $\mathcal{H}_A, \mathcal{H}_B, \mathcal{H}_C$. We consider the state $|\Psi\rangle := \sum_a \sqrt{P_A(a)}|a, \psi_{B|a}\rangle$ on $\mathcal{H}_A \otimes \mathcal{H}_B$, and the state $|\Phi\rangle := P_A(a)|a, \phi_{BC|a}\rangle$ on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, Then, we denote $\rho := |\Psi\rangle\langle\Psi|$. We also define $|\phi_{C|a}\rangle := \langle\psi_{BC|a}|\phi_{BC|a}\rangle$.

In this case, we have the following lemma.

**Lemma 27**

\[ F(|\Psi\rangle\langle\Psi|, \rho_{AB}) = \sum_{a,a'} \sqrt{P_A(a)P_A(a')} \sqrt{P_A(a')P_A(a)} \langle \phi_{C|a'}|\phi_{C|a}\rangle \]  

**Proof:**

\[
F(|\Psi\rangle\langle\Psi|, \rho_{AB}) \\
= \max_{|\psi_C\rangle} F(|\Psi\rangle\langle\psi_C|, |\psi_C\rangle\langle\Phi|)^2 \\
= \max_{|\psi_C\rangle} \left| \sum_z \sqrt{P_A(a)P_A(a)} \langle \psi_{B|a}, \psi_C|\phi_{BC|a}\rangle \right| \\
= \max_{|\psi_C\rangle} \left| \sum_z \sqrt{P_A(a)P_A(a)} |\phi_{C|a}\rangle \right| \\
= \sum_{a,a'} \sqrt{P_A(a)P_A(a')} \sqrt{P_A(a')}P_A(a) \langle \phi_{C|a'}|\phi_{C|a}\rangle
\]

**Lemma 28** When $\rho_{AC}$ is written as $\sum_a P_A(a)\langle a| \otimes \rho_{C|a}$, we have

\[ \max_{\sigma_C} F(\rho_{AC}, \rho_A \otimes \sigma_C) = \sum_{a,a'} P_A(a)P_A(a') F(\rho_{C|a}, \rho_{C|a'}). \]  

**Proof:** We firstly show the case when the state $\rho_{C|a}$ is a pure state $|\phi_{C|a}\rangle$. We choose the purification $|\Phi(\{e^{i\theta_a}\})\rangle := \sum_a e^{i\theta_a} \sqrt{P_A(a)}|a, \phi_{C|a}\rangle$ of $\rho_{AC}$ on $\mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$, and the purification $|\Psi(\{e^{i\theta_a}\})\rangle := \sum_a e^{i\theta_a} \sqrt{P_A(a)}|a, a\rangle$ of $\rho_A$ on
\( \mathcal{H}_A \otimes \mathcal{H}_B \). Applying Lemma \( \ref{lem:27} \) we have

\[
\max_{\sigma_C} F(\rho_{AC}, \rho_A \otimes \sigma_C) \\
= \max_{\sigma_C} \max_{\{e^{i\theta_a}\}, \{e^{i\theta_a'}\}} F(\langle \Psi(\{e^{i\theta_a}\})|\langle \Psi(\{e^{i\theta_a'}\})\rangle \otimes \sigma_C, |\Phi(\{e^{i\theta_a}\})\rangle) \\
= \max_{\{e^{i\theta_a}\}, \{e^{i\theta_a'}\}} \max_{\sigma_C} F(\langle \Psi(\{e^{i\theta_a}\})|\langle \Psi(\{e^{i\theta_a'}\})\rangle \otimes \sigma_C, |\Phi(\{e^{i\theta_a}\})\rangle) \\
= \max_{\{e^{i\theta_a}\}, \{e^{i\theta_a'}\}} F(\langle \Psi(\{e^{i\theta_a}\})|\langle \Psi(\{e^{i\theta_a'}\})\rangle, Tr_C |\Phi(\{e^{i\theta_a}\})\rangle) \\
= \max_{\{e^{i\theta_a}\}, \{e^{i\theta_a'}\}} \sum_{a, a'} e^{i(\theta_a - \theta_a') - i(\theta_a - \theta_a')} P_A(a) P_A(a') \langle \phi_{C|a'}|\phi_{C|a}\rangle \\
= \sum_{a, a'} e^{i(\theta_a - \theta_a') - i(\theta_a - \theta_a')} P_A(a) P_A(a') \langle \phi_{C|a'}|\phi_{C|a}\rangle, \tag{A4}
\]

which implies \( \text{(A3)} \).

Now, we going to the general case. We fix a purification \( |\phi_{C|a}| \) of \( \rho_{C|a} \) on \( \mathcal{H}_C \otimes \mathcal{H}_D \) so that \( F(\rho_{C|a}, \rho_{C|a'}) = |\langle \phi_{C|a'}|\phi_{C|a}\rangle| \).

We choose the purification \( |\Phi(\{e^{i\theta_a}\})\rangle := \sum_a e^{i\theta_a} \sqrt{P_A(a)} |a, \phi_{C|a}| \) of \( \rho_{AC} \) on \( \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C \otimes \mathcal{H}_D \), and the purification \( |\Psi(\{e^{i\theta_a'}\})\rangle := \sum_a e^{i\theta_a'} \sqrt{P_A(a)} |a, \phi_{C|a}| \) of \( \rho_A \) on \( \mathcal{H}_A \otimes \mathcal{H}_B \). Similarly, we have

\[
\max_{\sigma_C} F(\rho_{AC}, \rho_A \otimes \sigma_C) \\
= \max_{\sigma_{CD}} \max_{\{e^{i\theta_a}\}, \{e^{i\theta_a'}\}} F(\langle \Psi(\{e^{i\theta_a}\})|\langle \Psi(\{e^{i\theta_a'}\})\rangle \otimes \sigma_{CD}, |\Phi(\{e^{i\theta_a}\})\rangle) \\
= \max_{\{e^{i\theta_a}\}, \{e^{i\theta_a'}\}} \max_{\sigma_{CD}} F(\langle \Psi(\{e^{i\theta_a}\})|\langle \Psi(\{e^{i\theta_a'}\})\rangle \otimes \sigma_{CD}, |\Phi(\{e^{i\theta_a}\})\rangle) \\
= \sum_{a, a'} e^{i(\theta_a - \theta_a') - i(\theta_a - \theta_a')} P_A(a) P_A(a') \langle \phi_{C|a'}|\phi_{C|a}\rangle \\
= \sum_{a, a'} e^{i(\theta_a - \theta_a') - i(\theta_a - \theta_a')} P_A(a) P_A(a') F(\rho_{C|a}, \rho_{C|a'}) \tag{A5},
\]

which implies \( \text{(A3)} \).

\textbf{Lemma 29} When \( P_A = \tilde{P}_A \),

\[
F(|\Phi\rangle \langle \Phi|, \rho_{AB}) \leq \max_{\sigma_C} F(\rho_{AC}, \rho_A \otimes \sigma_C). \tag{A6}
\]

The equality hold if and only if \( \langle \phi_{C|a'}|\phi_{C|a}\rangle \geq 0 \) and \( \langle \phi_{C|a'}|\phi_{C|a}\rangle = 1 \).

\textbf{Proof:} We use the notations in Lemmas \( \ref{lem:27} \) and \( \ref{lem:28} \) Then, we have

\[
\langle \phi_{C|a'}|\phi_{C|a}\rangle + \langle \phi_{C|a'}|\phi_{C|a}\rangle \leq 2F(\rho_{C|a}, \rho_{C|a'}). \tag{A7}
\]

Combining Lemmas \( \ref{lem:27} \) and \( \ref{lem:28} \) we have

\[
F(|\Phi\rangle \langle \Phi|, \rho_{AB}) \\
= \sum_{a, a'} \sqrt{P_A(a)} P_A(a') \langle \phi_{C|a'}|\phi_{C|a}\rangle \\
\leq \sum_{a, a'} P_A(a) P_A(a') F(\rho_{C|a}, \rho_{C|a'}) \tag{A8}
\]

Hence, we obtain \( \text{(A6)} \). The equality in \( \text{(A6)} \) holds if and only if that in \( \text{(A7)} \) holds. So, we obtain the desired equivalence. \hfill \blacksquare
Lemma 30 Consider the equation
\[ \epsilon = \sum_{i=1}^{l} a_i x^i. \]  
(B1)

When \( \epsilon \) is sufficiently small, the solution \( x \) is approximated as
\[ x = \sum_{i=1}^{l} \epsilon^i x_i + O(\epsilon^{l+1}). \]  
(B2)

where \( x_1 \) is given as \( \frac{1}{a_1} \) and \( x_1 \) with \( l \geq 2 \) is inductively given as
\[ \frac{1}{a_1} \sum_{i_1, i_2, \ldots, i_{l-1} : \sum_{k=1}^{l-1} i_k = l} a_{\sum_{k=1}^{l-1} i_k} \frac{(\sum_{k=1}^{l-1} i_k)!}{i_1! \cdots i_{l-1}!} \prod_{k=1}^{l-1} x_k^{i_k}. \]

Specially, \( x_2 \) and \( x_3 \) are given as
\[ x_2 = -\frac{1}{a_1} x_1^2 = -\frac{1}{a_1^2} \]  
(B3)
\[ x_3 = -\frac{1}{a_1} (x_1^3 + 2x_1x_2) = -\frac{1}{a_1^2} + \frac{2}{a_1^3}. \]  
(B4)

This lemma can be shown as follows. First, we substitute \( \{B2\} \) into \( \{B1\} \). Then, compare the coefficients with the order \( \epsilon^l \). Hence, we obtain \( x_1 = -\frac{1}{a_1} \sum_{i_1, i_2, \ldots, i_{l-1} : \sum_{k=1}^{l-1} i_k = l} a_{\sum_{k=1}^{l-1} i_k} \frac{(\sum_{k=1}^{l-1} i_k)!}{i_1! \cdots i_{l-1}!} \prod_{k=1}^{l-1} x_k^{i_k}. \)

Appendix C: Proof of Theorem[9]

Because of \( \{160\} \),
\[ S(E_W, M_W, X_W) + S(E_{RH}, M_R, X_{RH}) + S(E_{RL}, M_R, X_{RL}) \]
\[ \leq S(E_W, M_W, X_W) + S(E_{RH} - Q, M_R, X_{RH}) + S(E_{RL} + Q - W_{ad}, M_R, X_{RL}) \]  
(C1)
holds. Because of \( \{164\} \), the inequality \( \{C1\} \) turns into
\[ S(E_{RL}^{\text{quasi}}, M_R, X_{RL}) \leq S(E_{RL} + Q - W_{ad}, M_R, X_{RL}) \]  
(C2)

Because the thermodynamic entropy is an increasing function of the internal energy \( \{2\} \), we obtain
\[ W_{\text{ext}} \leq Q + E_{RL} - E_{RL}^{\text{quasi}} \]  
(C3)
where \( E_{RL}^{\text{quasi}} \) is defined by \( \{164\} \). Thus, we obtain
\[ \eta_{ad}[(E_{RH}, M_R, X_{RH}), (E_{RL}, M_R, X_{RL}), Q] \leq 1 - \frac{E_{RL}^{\text{quasi}} - E_{RL}}{Q}. \]  
(C4)

The equality of \( \{C4\} \) is achieved when the equality of \( \{C1\} \) holds. In the framework of thermodynamics, we assume the thermalization assumption, and thus we can perform the adiabatic quasi-static process which achieves the equality of \( \{C1\} \). Hence, we obtain \( \{163\} \).

Finally, we derive \( \{165\} \). We firstly change the variable of \( \{163\} \) from the internal energy to the entropy. We define the internal energy as a function \( E(S, M, X) \) of \( S, M, \) and \( X \) such that
\[ S(E(S, M, X), M, X) = S. \]  
(C5)

Because the thermodynamical entropy \( S(E, M, X) \) is a strictly increasing function of the internal energy \( E \), we define \( E(S, MX) \) uniquely as above. We also define \( S_H := S(E_{RH}, M_R, X_{RH}) \), \( S_L := S(E_{RL}, M_R, X_{RL}) \), \( \Delta S := \).
$S(E_{R_h}, M_R, X_{R_h}) - S(E_{R_h} - Q, M_R, X_{R_h})$. By using them, we obtain

$$E_{R_L}^{\text{quasi}} - E_{R_L} = \int_{S_L}^{S_L + \Delta S} T(S, M_R, X_{R_L})dS, \quad (C6)$$

$$Q = \int_{S_H - \Delta S}^{S_H} T(S, M_H, X_{R_h})dS, \quad (C7)$$

$$T(S, M, X) := \frac{\partial E(S, M, X)}{\partial S}. \quad (C8)$$

Therefore, the RHS of (163) can be rewritten as follows;

$$1 - \frac{\int_{S_L}^{S_L + \Delta S} T(S, M_R, X_{R_L})dS}{\int_{S_H - \Delta S}^{S_H} T(S, M_H, X_{R_h})dS} \quad (C9)$$

We can obtain (165) by performing Taylor expansion about $\Delta S$ on (C7) and (C9) and putting them in order. We expand (C7)

$$Q = \sum_{i=1}^{3!} \frac{\partial^i Q}{\partial S^i} (\Delta S)^i. \quad (C10)$$

We substitute $Q$ for $\epsilon$ and $1 - \frac{\partial^i Q}{\partial S^i} (\Delta S)^i$ into $a_i$ and $\Delta S$ into $x$ in Lemma 30. Then, (B1) of Lemma 30 becomes (C10). Therefore, with using (B2) and (B3), we obtain

$$\Delta S = \frac{1}{T(S_H, M_R, X_{R_h})} Q - \frac{1}{(\frac{\partial Q}{\partial S})^2} Q^2 + O(Q^3). \quad (C11)$$

We also expand (C9)

$$1 - \frac{\int_{S_L}^{S_L + \Delta S} T(S, M_R, X_{R_L})dS}{\int_{S_H - \Delta S}^{S_H} T(S, M_H, X_{R_h})dS}$$

$$= 1 - \frac{T(S_L, M_R, X_{R_L}) + \frac{1}{2} \frac{\partial T(S_L, M_R, X_{R_L})}{\partial S} \Delta S + \frac{1}{3!} \frac{\partial^2 T(S_L, M_R, X_{R_L})}{\partial S^2} (\Delta S)^2 + \frac{1}{3!} \frac{\partial^3 T(S_L, M_R, X_{R_L})}{\partial S^3} (\Delta S)^3}{T(S_H, M_R, X_{R_h})} + O((\Delta S)^3)$$

$$= 1 - \frac{1}{T(S_H, M_R, X_{R_h})} \left( 1 + \left( \frac{\partial T(S_L, M_R, X_{R_L})}{\partial S} + \frac{1}{2} \frac{\partial^2 T(S_L, M_R, X_{R_L})}{\partial S^2} + \frac{1}{3} \frac{\partial^3 T(S_L, M_R, X_{R_L})}{\partial S^3} \right) \frac{1}{T(S_H, M_R, X_{R_h})} (\Delta S)^2 \right) + O((\Delta S)^3) \quad (C12)$$

Because $E(S, X)$ is defined uniquely, the equalities $\beta_H = 1/T(S_H, M_R, X_{R_h})$ and $\beta_L = 1/T(S_L, M_R, X_{R_L})$ hold. Therefore, by substituting $\beta_H = 1/T(S_H, M_R, X_{R_h})$, $\beta_L = 1/T(S_L, M_R, X_{R_L})$ and (C11) into (C12), we obtain

$$1 - \frac{\int_{S_L}^{S_L + \Delta S} T(S, M_R, X_{R_L})dS}{\int_{S_H - \Delta S}^{S_H} T(S, M_H, X_{R_h})dS}$$

$$= 1 - \beta_H \frac{\partial^3 T(S_L, M_R, X_{R_L})}{\partial S^3} - \beta_H \frac{\partial^2 T(S_L, M_R, X_{R_L})}{\partial S^2} + \frac{\beta_H^2}{2} \frac{\partial T(S_L, M_R, X_{R_L})}{\partial S} Q + O(Q^3) \quad (C13)$$

Let us prove that the coefficients of (C13) are equal to those of (165). In order to prove that, we define the reverse function of $S_H(\beta)$ as $\beta_H(S)$. Because the von Neumann entropy $S_H(\beta) := -\text{Tr}[\rho_H \log \rho_H]$ is a strictly decreasing function of $\beta$, we
can define $\beta_R(S)$ uniquely. Because the relationships among thermodynamic functions which are defined in thermodynamics are the same as that of statistical mechanics, the following relationships follows from (162):

$$T(S, M_R, X_{R_H}) = \frac{1}{\beta_{H(M_R)}(S)} , \quad T(S, M_R, X_{R_L}) = \frac{1}{\beta_{H(M_R)}(S)} .$$

(C14)

With using these relations, we can obtain the following equalities by straightforward algebra:

$$\beta_L \frac{\partial T(S_L, M_R, X_{R_L})}{\partial S} = \beta_L \frac{\partial}{\partial S} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_L} = \beta_L \frac{\partial}{\partial S} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_L} = \frac{1}{\beta_L^2} \sigma^2(\beta_L) \frac{1}{M_R}$$

(C15)

$$\beta_H \frac{\partial T(S_H, M_R, X_{R_H})}{\partial S} = \beta_H \frac{\partial}{\partial S} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_H} = \beta_H \frac{\partial}{\partial S} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_H} = \frac{1}{\beta_H^2} \sigma^2(\beta_H) \frac{1}{M_R}$$

(C16)

$$\beta_L \frac{\partial^2 T(S_L, M_R, X_{R_L})}{\partial S^2} = \beta_L \frac{\partial^2}{\partial S^2} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_L} = \beta_L \frac{\partial^2}{\partial S^2} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_L} = \frac{1}{\beta_L^2} \sigma^3(\beta_L) \frac{1}{M_R^2}$$

(C17)

$$\beta_H \frac{\partial^2 T(S_H, M_R, X_{R_H})}{\partial S^2} = \beta_H \frac{\partial^2}{\partial S^2} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_H} = \beta_H \frac{\partial^2}{\partial S^2} \frac{1}{\beta_{H(M_R)}(S)} \bigg|_{S=S_H} = \frac{1}{\beta_H^2} \sigma^3(\beta_H) \frac{1}{M_R^2}$$

(C18)

Therefore, we obtain (165).

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